



## Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 07:48 am GMT

PDB ID : 7NEP  
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 : 6KN8, 3I5G, 5JLH

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

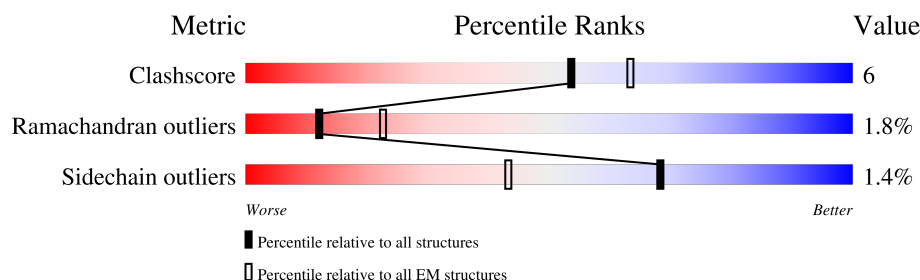
# 1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>50%</div> <div>86%13% .</div> </div>
1	B	374	<div> <div>50%</div> <div>87%11% .</div> </div>
1	C	374	<div> <div>48%</div> <div>85%14% .</div> </div>
1	D	374	<div> <div>48%</div> <div>86%13% .</div> </div>
1	E	374	<div> <div>42%</div> <div>85%14% .</div> </div>
1	F	374	<div> <div>45%</div> <div>83%16% .</div> </div>
1	G	374	<div> <div>47%</div> <div>88%11% .</div> </div>
1	H	374	<div> <div>56%</div> <div>87%12% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	374	
1	J	374	
1	K	374	
2	P	251	
2	Q	251	
2	T	251	
2	U	251	
3	L	813	
3	M	813	
4	N	148	
4	O	148	
5	R	144	
5	S	144	

## 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.

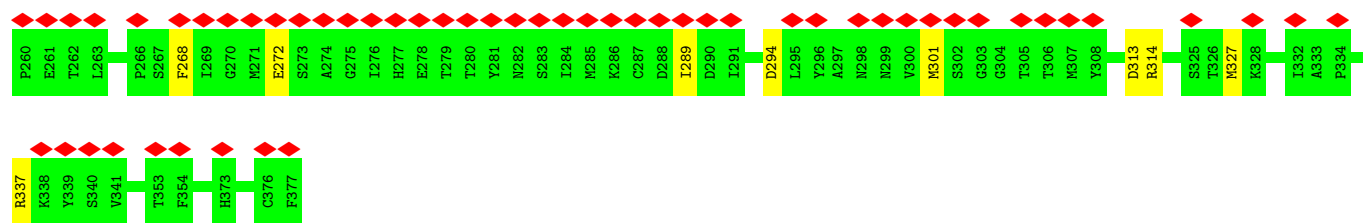
Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	144	Total	C	N	O	S	0	0
			1144	724	185	227	8		
5	S	144	Total	C	N	O	S	0	0
			1144	724	185	227	8		

### 3 Residue-property plots [i](#)

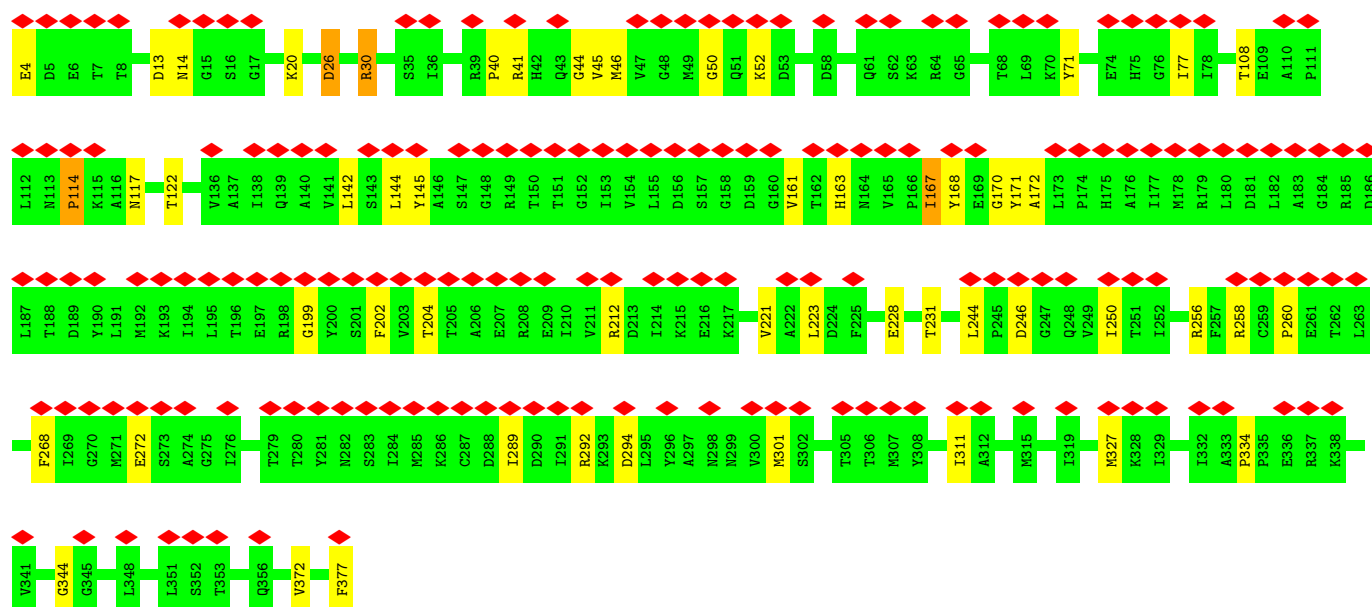
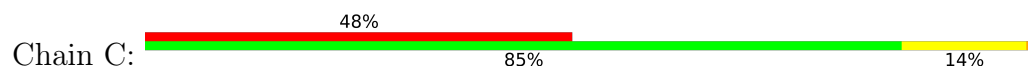
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Actin, alpha skeletal muscle

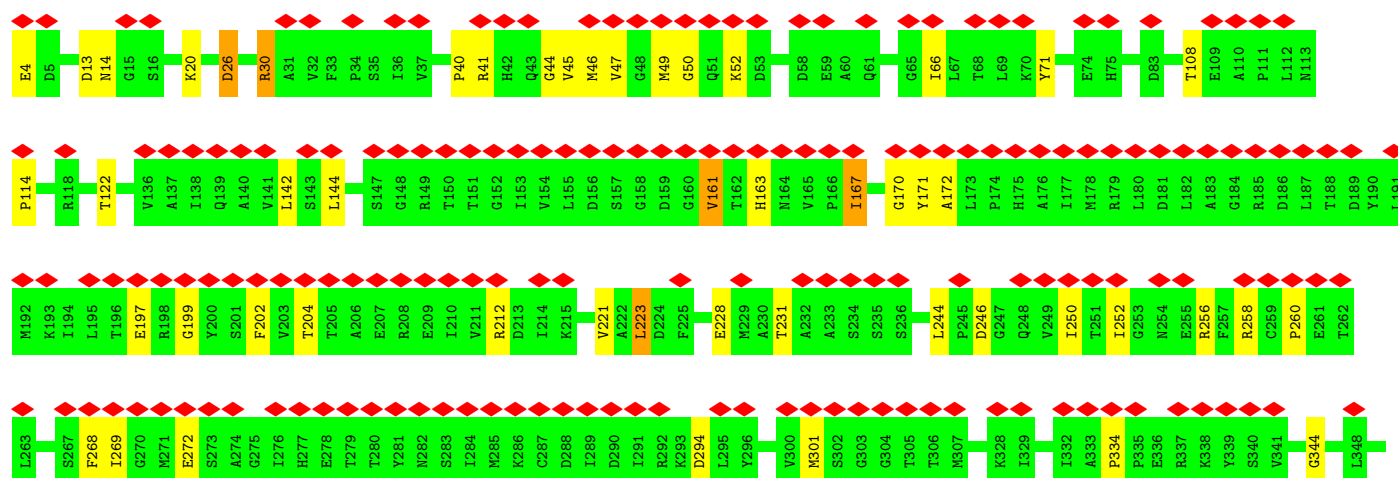
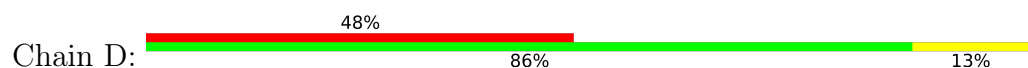




- Molecule 1: Actin, alpha skeletal muscle

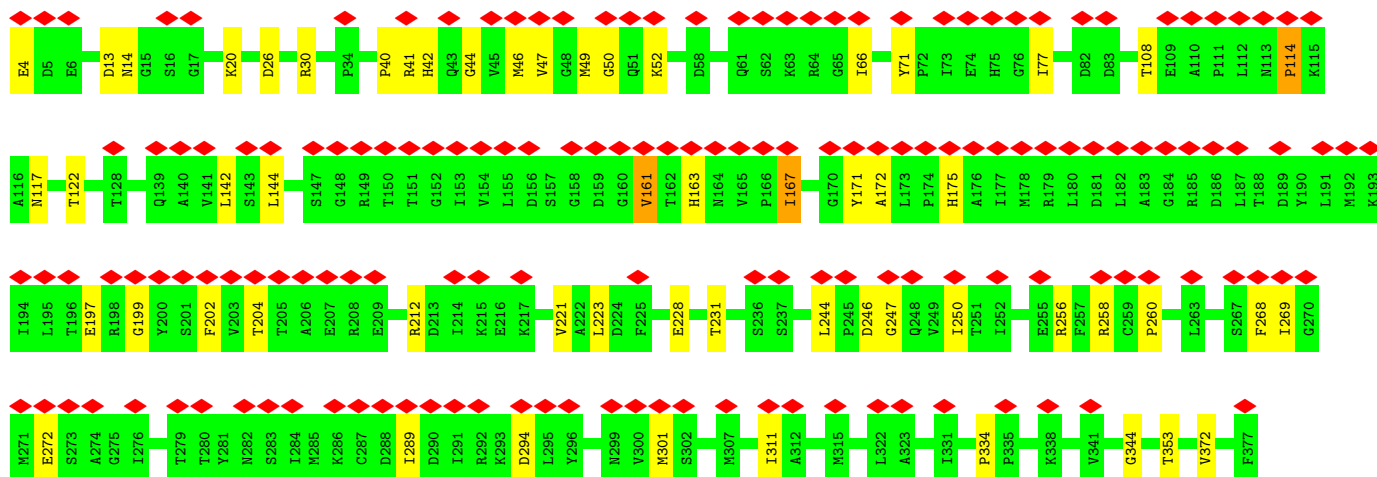
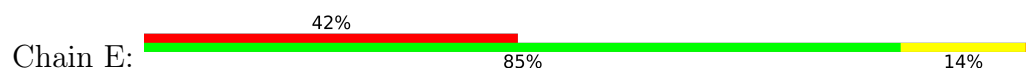


- Molecule 1: Actin, alpha skeletal muscle

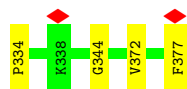
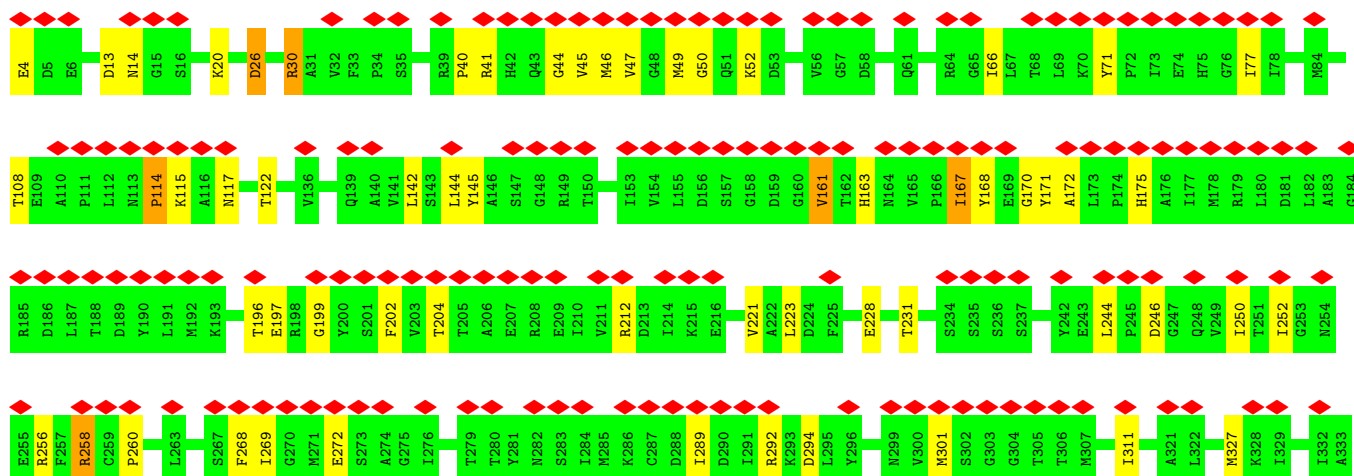
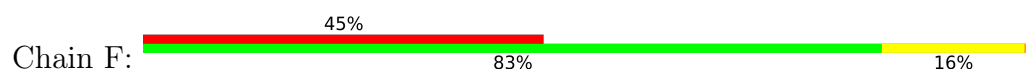




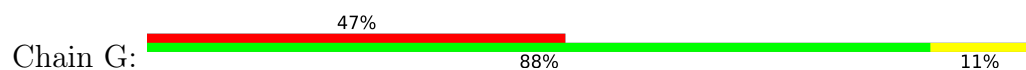
- Molecule 1: Actin, alpha skeletal muscle



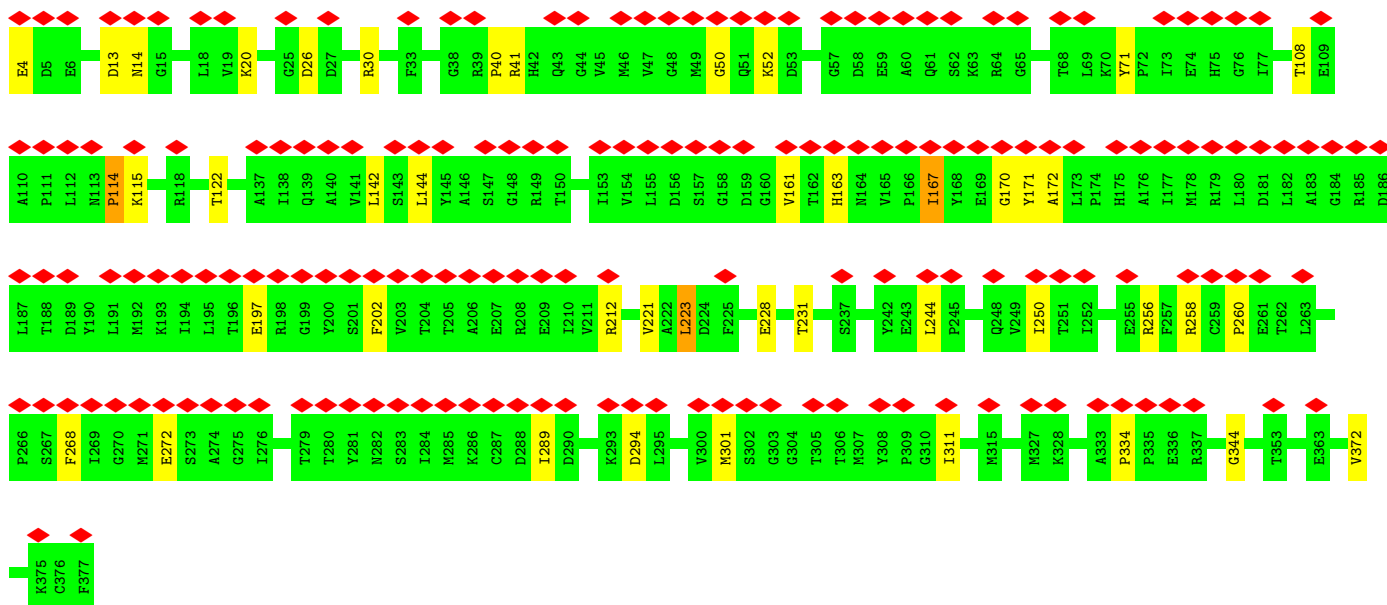
- Molecule 1: Actin, alpha skeletal muscle



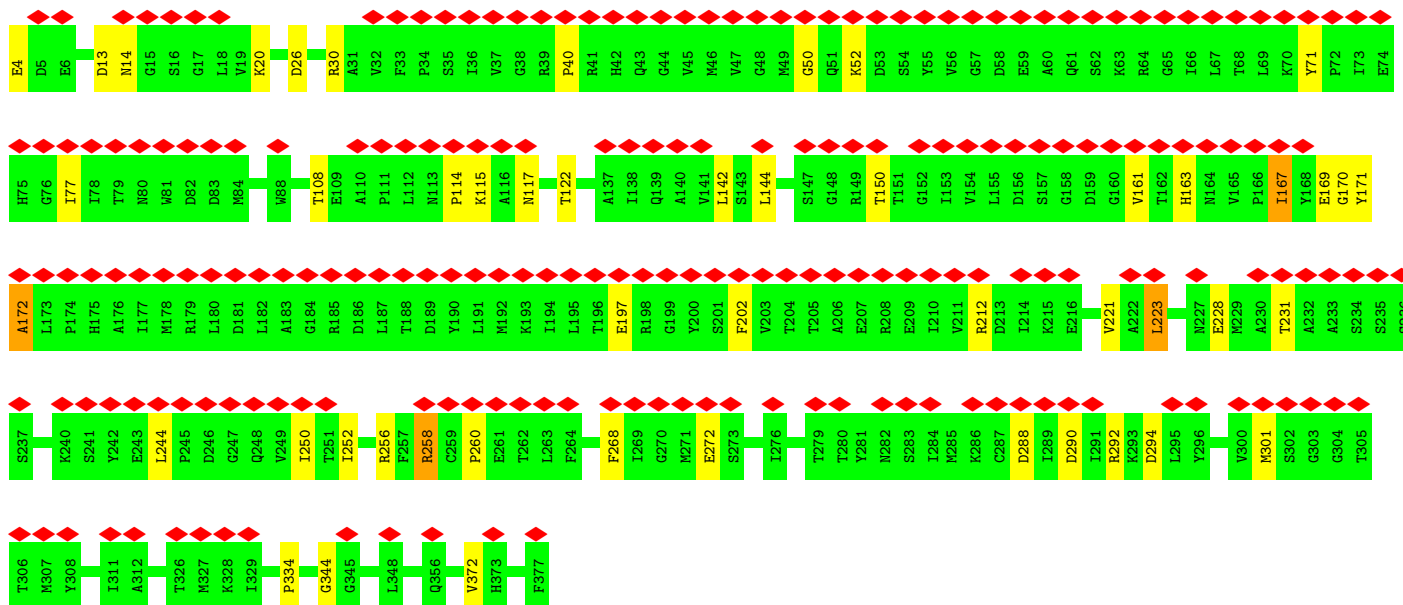
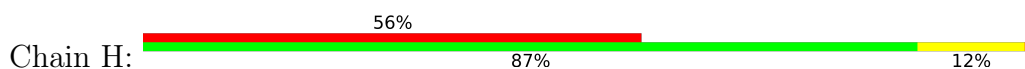
- Molecule 1: Actin, alpha skeletal muscle



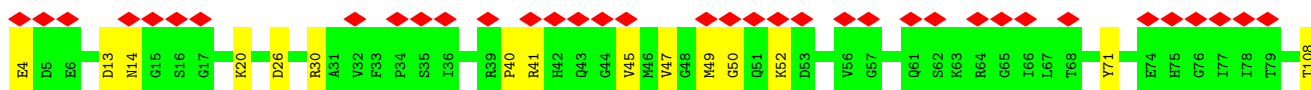
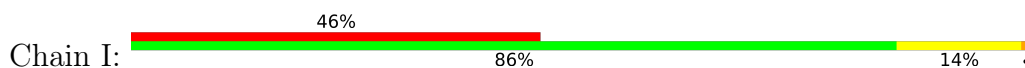


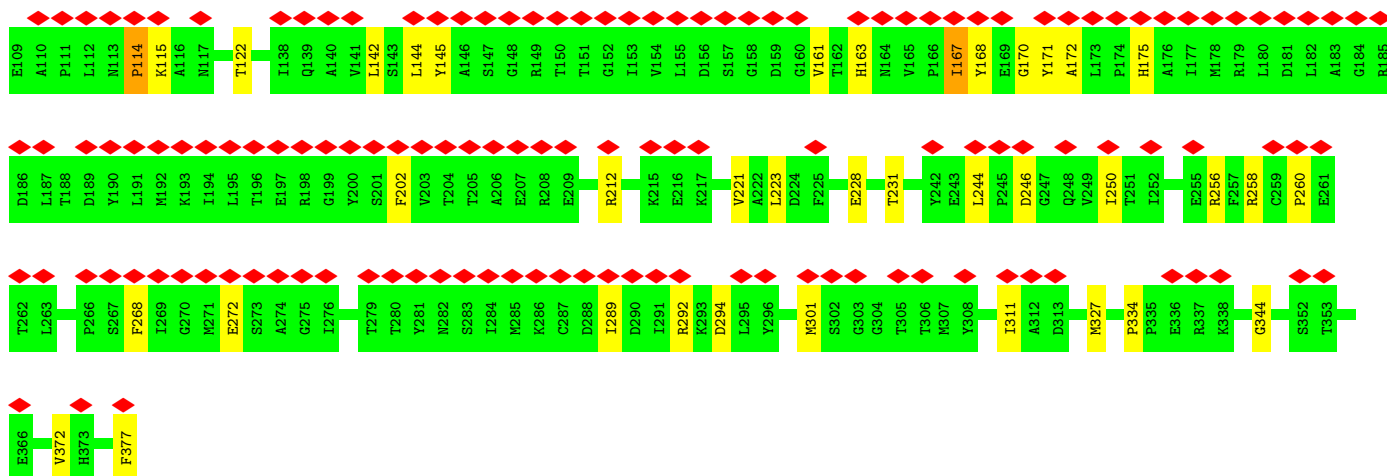


- Molecule 1: Actin, alpha skeletal muscle

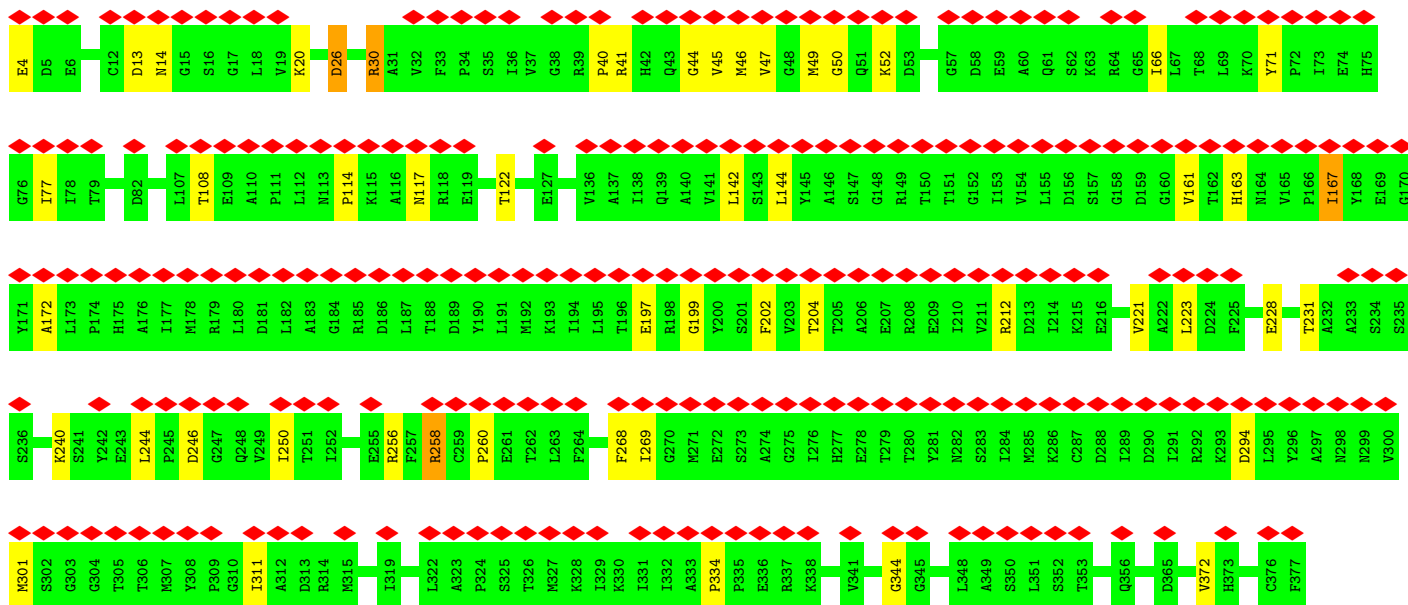
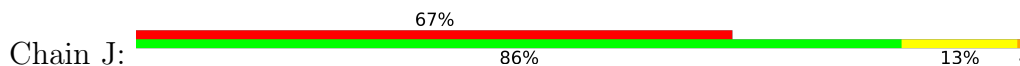


- Molecule 1: Actin, alpha skeletal muscle

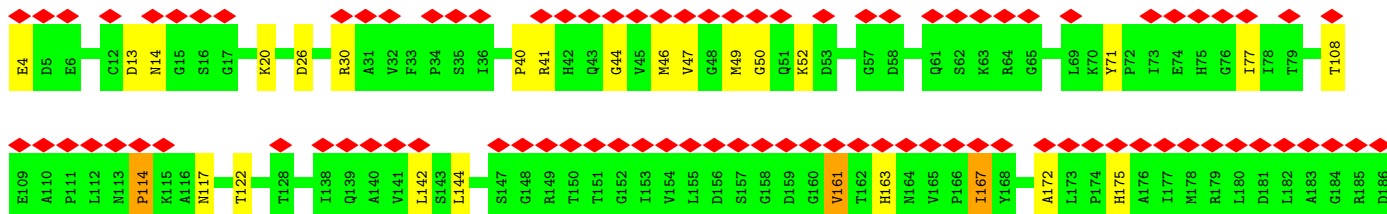
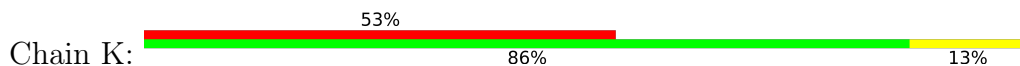


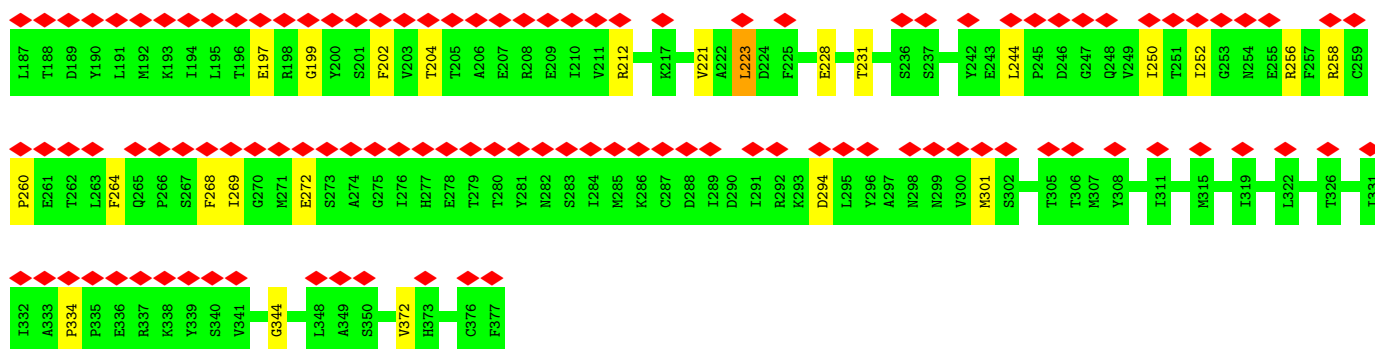


- Molecule 1: Actin, alpha skeletal muscle

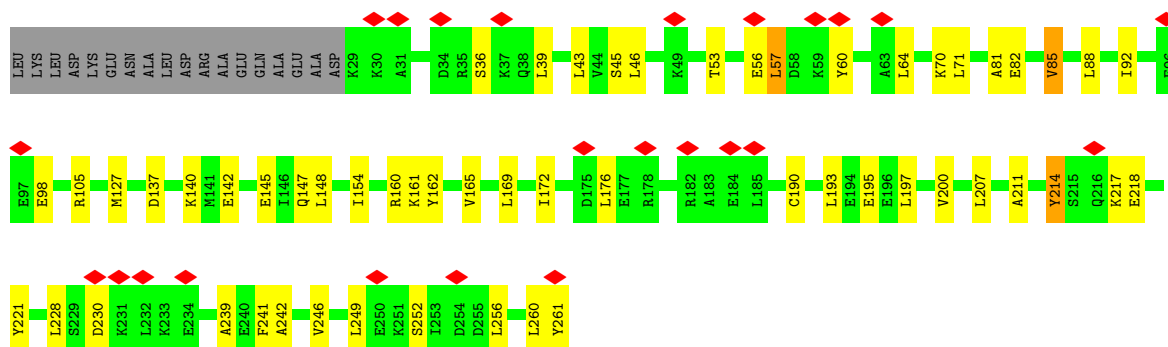


- Molecule 1: Actin, alpha skeletal muscle

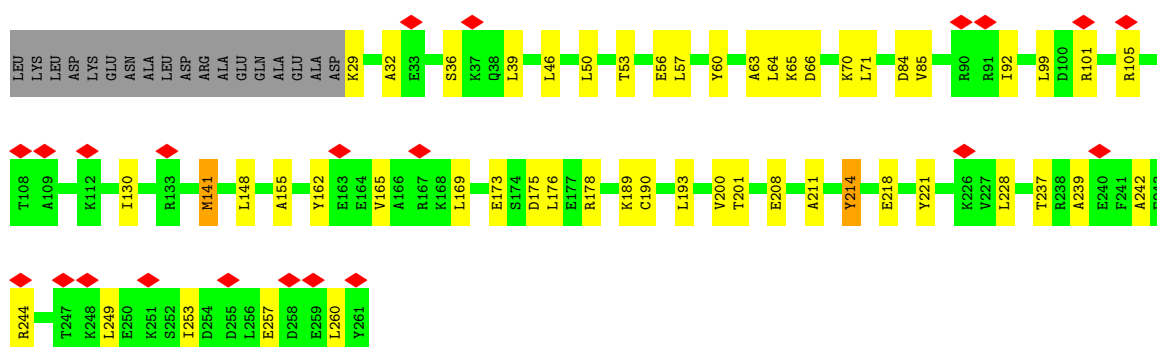




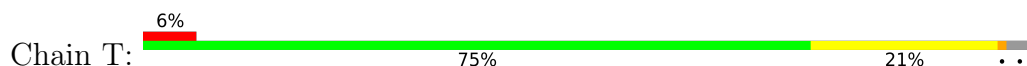
• Molecule 2: Tropomyosin alpha-1 chain

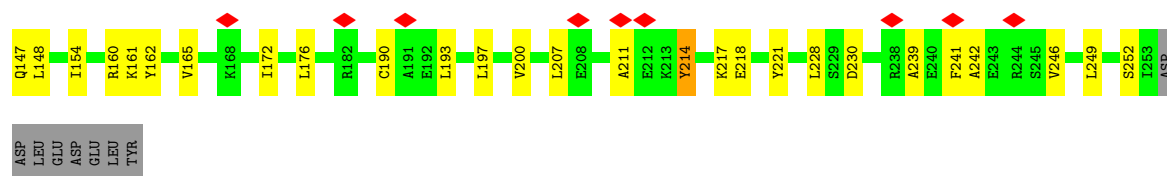


• Molecule 2: Tropomyosin alpha-1 chain

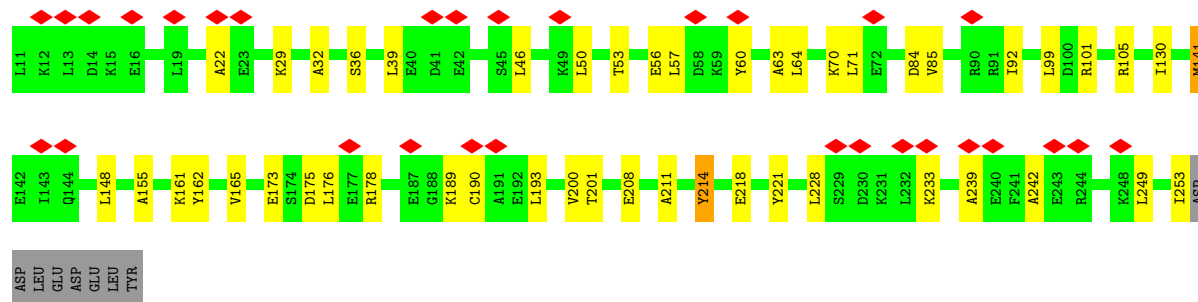
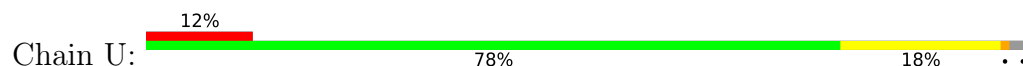


• Molecule 2: Tropomyosin alpha-1 chain

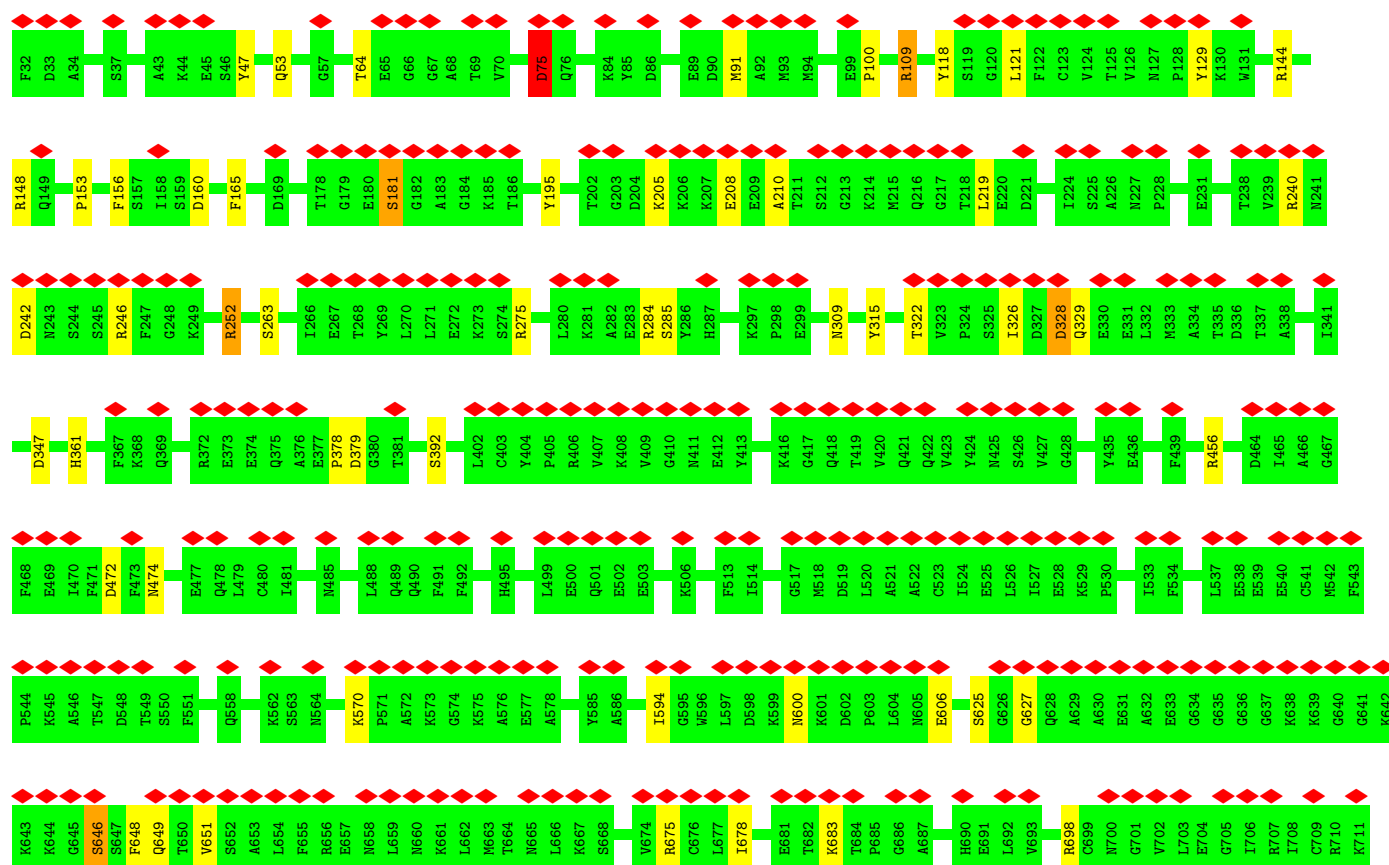
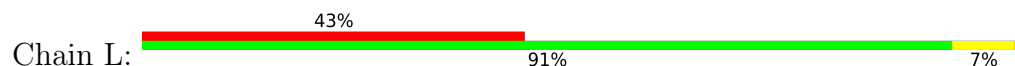


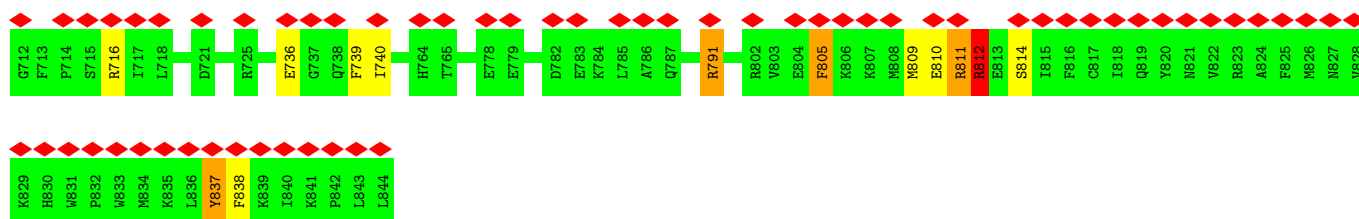


• Molecule 2: Tropomyosin alpha-1 chain

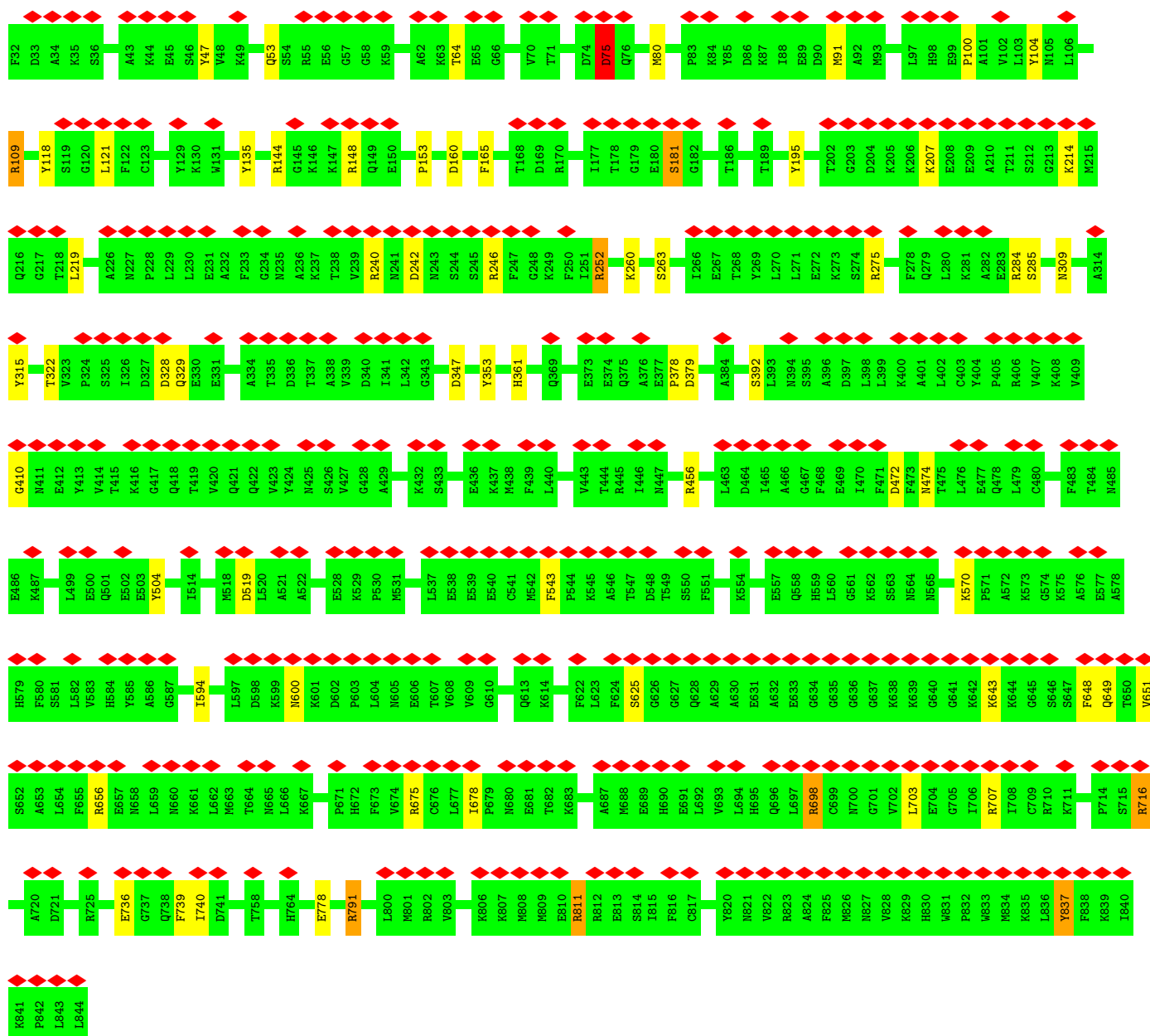
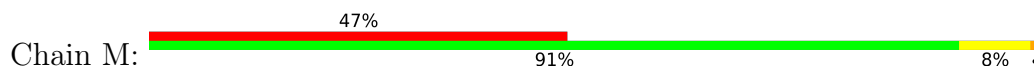


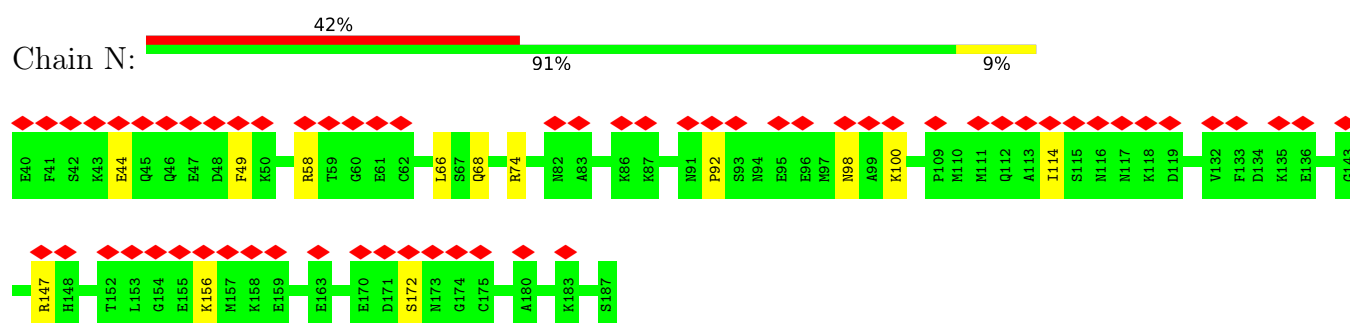
• Molecule 3: Myosin-4



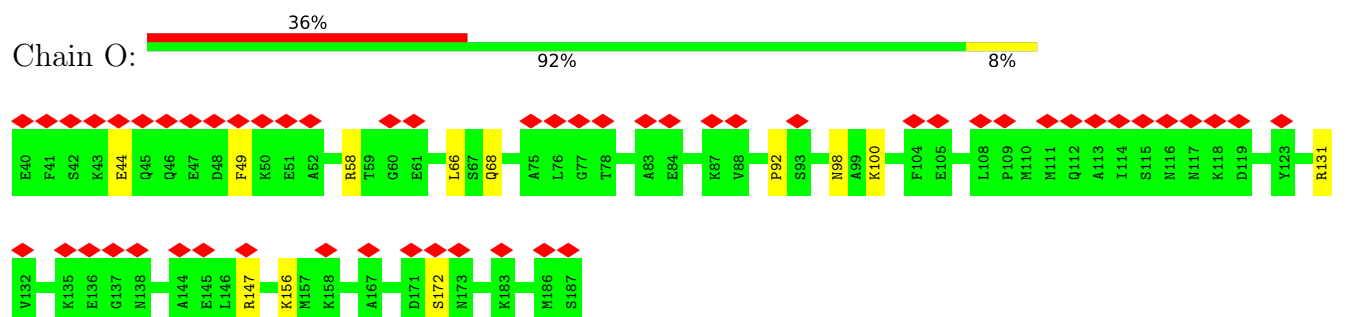


• Molecule 3: Myosin-4

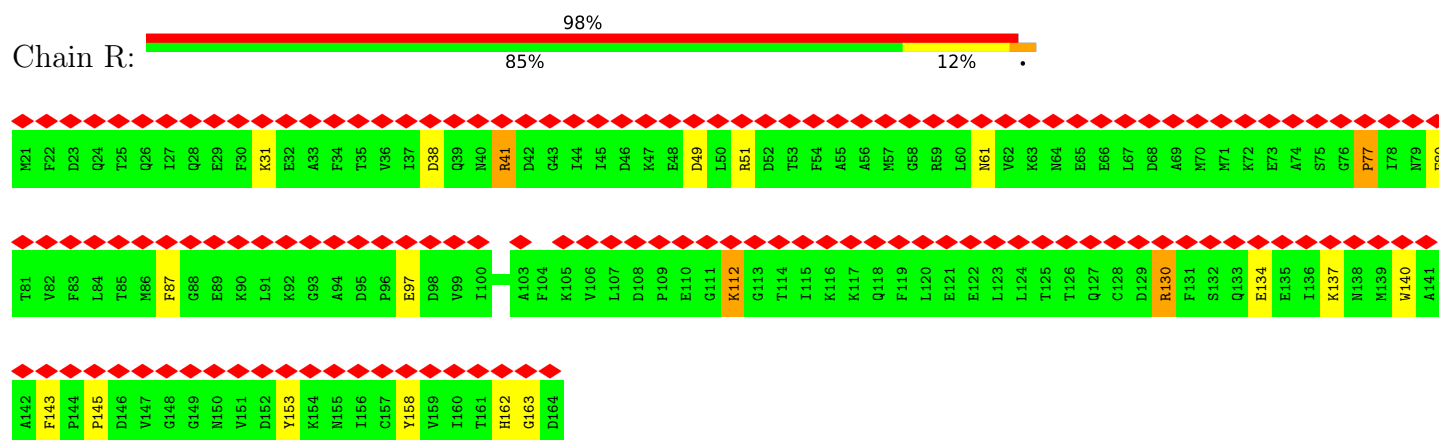




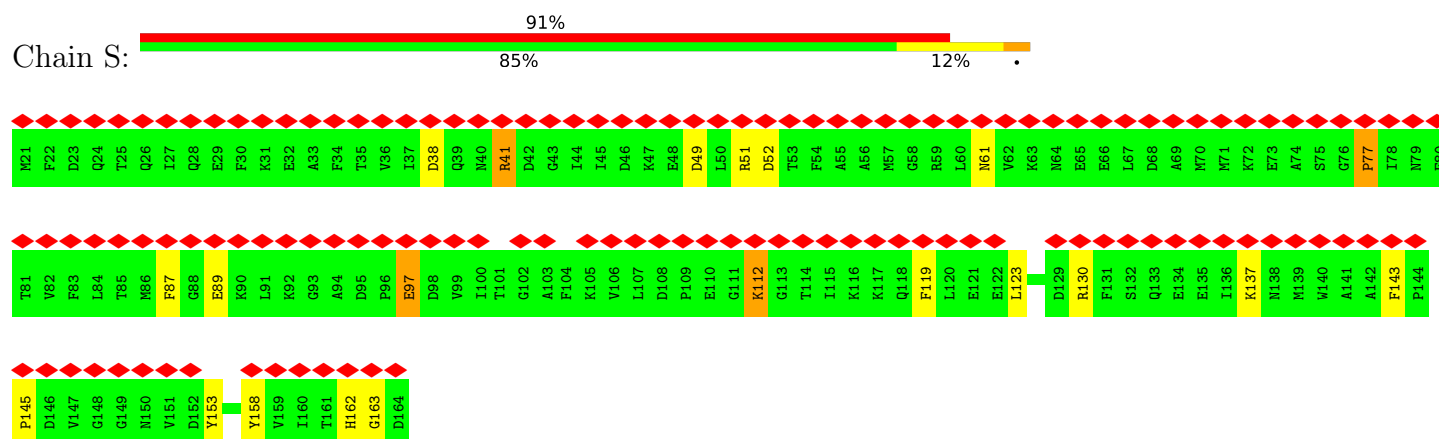
- Molecule 4: Myosin light chain 1/3, skeletal muscle isoform



- 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	0.71	0/2988	1.15	18/4047 (0.4%)
1	B	0.71	0/2988	1.15	16/4047 (0.4%)
1	C	0.77	0/2988	1.20	9/4047 (0.2%)
1	D	0.77	0/2988	1.20	9/4047 (0.2%)
1	E	0.77	0/2988	1.20	9/4047 (0.2%)
1	F	0.77	0/2988	1.20	9/4047 (0.2%)
1	G	0.77	0/2988	1.20	9/4047 (0.2%)
1	H	0.77	0/2988	1.20	9/4047 (0.2%)
1	I	0.77	0/2988	1.20	9/4047 (0.2%)
1	J	0.77	0/2988	1.20	9/4047 (0.2%)
1	K	0.77	0/2988	1.20	10/4047 (0.2%)
2	P	0.81	0/1887	1.19	7/2515 (0.3%)
2	Q	0.82	0/1887	1.23	5/2515 (0.2%)
2	T	0.81	0/1957	1.19	7/2607 (0.3%)
2	U	0.81	0/1957	1.23	5/2607 (0.2%)
3	L	0.72	0/6643	1.10	28/8946 (0.3%)
3	M	0.72	0/6643	1.09	28/8946 (0.3%)
4	N	0.73	0/1174	1.09	4/1571 (0.3%)
4	O	0.73	0/1174	1.08	4/1571 (0.3%)
5	R	0.75	1/1164 (0.1%)	1.21	9/1565 (0.6%)
5	S	0.70	0/1164	1.20	8/1565 (0.5%)
All	All	0.76	1/58518 (0.0%)	1.17	221/78925 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	140	TRP	CD2-CE3	-5.26	1.32	1.40

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	791	ARG	NE-CZ-NH2	10.78	125.69	120.30
3	M	240	ARG	NE-CZ-NH2	10.37	125.48	120.30
3	L	791	ARG	NE-CZ-NH2	10.36	125.48	120.30
3	L	240	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	A	212	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	B	212	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	212	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	B	212	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	A	149	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	H	212	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	K	212	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	212	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	G	212	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	E	212	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	F	212	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	D	212	ARG	NE-CZ-NH1	7.95	124.28	120.30
5	S	143	PHE	CB-CG-CD1	7.94	126.36	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	212	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	K	30	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	F	30	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	I	212	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	J	30	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	D	30	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	P	214	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	E	30	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	H	30	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	185	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	30	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	T	214	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	G	30	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	I	30	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	T	214	TYR	CB-CG-CD1	7.73	125.64	121.00
5	R	41	ARG	NE-CZ-NH1	7.63	124.11	120.30
2	P	214	TYR	CB-CG-CD1	7.60	125.56	121.00
5	S	143	PHE	CB-CG-CD2	-7.54	115.53	120.80
5	S	41	ARG	NE-CZ-NH1	7.41	124.00	120.30
3	L	805	PHE	CB-CG-CD1	7.39	125.98	120.80
2	Q	141	MET	CG-SD-CE	-7.38	88.40	100.20
2	U	141	MET	CG-SD-CE	-7.35	88.44	100.20
1	H	301	MET	CG-SD-CE	-7.30	88.52	100.20
1	C	301	MET	CG-SD-CE	-7.29	88.53	100.20
1	F	301	MET	CG-SD-CE	-7.29	88.54	100.20
1	D	301	MET	CG-SD-CE	-7.27	88.56	100.20
1	G	301	MET	CG-SD-CE	-7.27	88.57	100.20
1	E	301	MET	CG-SD-CE	-7.27	88.57	100.20
1	J	301	MET	CG-SD-CE	-7.27	88.57	100.20
1	K	301	MET	CG-SD-CE	-7.25	88.59	100.20
1	I	301	MET	CG-SD-CE	-7.25	88.60	100.20
3	L	315	TYR	CB-CG-CD2	-7.24	116.66	121.00
5	R	143	PHE	CB-CG-CD1	7.22	125.86	120.80
3	M	315	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	B	8	THR	N-CA-CB	7.15	123.89	110.30
1	B	185	ARG	NE-CZ-NH2	-7.11	116.75	120.30
3	M	811	ARG	NE-CZ-NH1	-7.11	116.75	120.30
2	U	105	ARG	NE-CZ-NH1	7.11	123.85	120.30
2	Q	105	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	M	275	ARG	NE-CZ-NH2	-7.05	116.78	120.30
3	M	240	ARG	NE-CZ-NH1	-7.03	116.79	120.30
5	R	143	PHE	CB-CG-CD2	-7.00	115.90	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	105	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	337	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	L	252	ARG	NE-CZ-NH2	-6.85	116.88	120.30
3	L	805	PHE	CB-CG-CD2	-6.79	116.05	120.80
2	T	105	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	337	ARG	NE-CZ-NH1	6.76	123.68	120.30
3	L	181	SER	C-N-CA	6.67	136.31	122.30
1	A	255	GLU	N-CA-CB	-6.63	98.66	110.60
1	B	198	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	M	181	SER	C-N-CA	6.56	136.08	122.30
3	L	646	SER	N-CA-CB	6.54	120.32	110.50
3	M	252	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	L	315	TYR	CB-CG-CD1	6.53	124.92	121.00
1	A	149	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	118	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	255	GLU	N-CA-CB	-6.45	98.99	110.60
3	L	109	ARG	NE-CZ-NH1	6.44	123.52	120.30
3	L	275	ARG	NE-CZ-NH2	-6.44	117.08	120.30
3	M	109	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	198	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	118	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	268	PHE	CB-CG-CD1	6.36	125.25	120.80
1	A	185	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	268	PHE	CB-CG-CD1	6.32	125.22	120.80
1	B	185	ARG	NE-CZ-NH1	6.31	123.46	120.30
3	M	315	TYR	CB-CG-CD1	6.30	124.78	121.00
3	L	165	PHE	CB-CG-CD1	6.29	125.20	120.80
5	S	158	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	268	PHE	CB-CG-CD2	-6.26	116.42	120.80
3	M	181	SER	CB-CA-C	6.24	121.95	110.10
3	L	165	PHE	CB-CG-CD2	-6.24	116.43	120.80
1	B	39	ARG	NE-CZ-NH2	-6.22	117.19	120.30
5	R	87	PHE	CB-CG-CD1	6.21	125.15	120.80
3	M	275	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	202	PHE	CB-CG-CD1	6.15	125.10	120.80
5	S	158	TYR	CB-CG-CD1	6.14	124.69	121.00
1	E	202	PHE	CB-CG-CD1	6.14	125.10	120.80
1	G	202	PHE	CB-CG-CD1	6.13	125.09	120.80
5	S	87	PHE	CB-CG-CD1	6.11	125.08	120.80
2	Q	178	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	268	PHE	CB-CG-CD1	6.10	125.07	120.80
1	A	268	PHE	CB-CG-CD2	-6.09	116.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	268	PHE	CB-CG-CD1	6.08	125.05	120.80
1	D	202	PHE	CB-CG-CD1	6.07	125.05	120.80
3	L	275	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	H	202	PHE	CB-CG-CD1	6.06	125.04	120.80
1	J	202	PHE	CB-CG-CD1	6.06	125.04	120.80
1	K	202	PHE	CB-CG-CD1	6.06	125.04	120.80
1	H	268	PHE	CB-CG-CD1	6.05	125.03	120.80
2	U	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	Q	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	202	PHE	CB-CG-CD1	6.04	125.03	120.80
1	I	268	PHE	CB-CG-CD1	6.04	125.03	120.80
1	K	268	PHE	CB-CG-CD1	6.04	125.03	120.80
3	L	181	SER	CB-CA-C	6.03	121.55	110.10
1	G	268	PHE	CB-CG-CD1	6.02	125.01	120.80
1	I	202	PHE	CB-CG-CD1	6.01	125.01	120.80
2	U	178	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	F	268	PHE	CB-CG-CD1	5.99	125.00	120.80
1	J	268	PHE	CB-CG-CD1	5.99	124.99	120.80
3	L	698	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	E	268	PHE	CB-CG-CD1	5.97	124.98	120.80
3	M	165	PHE	CB-CG-CD1	5.97	124.98	120.80
3	L	240	ARG	NE-CZ-NH1	-5.97	117.32	120.30
3	M	75	ASP	N-CA-CB	-5.92	99.95	110.60
3	L	91	MET	CG-SD-CE	-5.88	90.79	100.20
3	M	698	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	301	MET	CG-SD-CE	-5.84	90.85	100.20
3	M	181	SER	CA-C-N	5.81	127.83	116.20
3	M	165	PHE	CB-CG-CD2	-5.81	116.74	120.80
3	M	716	ARG	NE-CZ-NH1	5.78	123.19	120.30
4	O	49	PHE	CB-CG-CD1	5.74	124.82	120.80
1	A	301	MET	CG-SD-CE	-5.73	91.03	100.20
5	R	158	TYR	CB-CG-CD2	-5.71	117.57	121.00
3	L	181	SER	CA-C-N	5.71	127.62	116.20
3	M	91	MET	CG-SD-CE	-5.69	91.10	100.20
3	L	811	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	G	268	PHE	CB-CG-CD2	-5.60	116.88	120.80
4	N	74	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	I	268	PHE	CB-CG-CD2	-5.60	116.88	120.80
3	L	144	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	H	26	ASP	CB-CG-OD1	5.59	123.33	118.30
2	P	160	ARG	NE-CZ-NH1	5.59	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	44	GLU	N-CA-CB	-5.58	100.56	110.60
1	C	268	PHE	CB-CG-CD2	-5.58	116.90	120.80
1	C	26	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	268	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	K	268	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	H	268	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	B	30	ARG	NE-CZ-NH1	5.56	123.08	120.30
5	R	87	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	J	26	ASP	CB-CG-OD1	5.55	123.29	118.30
1	I	26	ASP	CB-CG-OD1	5.54	123.28	118.30
1	K	26	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	26	ASP	CB-CG-OD1	5.53	123.27	118.30
1	G	26	ASP	CB-CG-OD1	5.53	123.27	118.30
1	F	26	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	26	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	268	PHE	CB-CG-CD2	-5.49	116.95	120.80
2	T	160	ARG	NE-CZ-NH1	5.49	123.04	120.30
5	R	158	TYR	CB-CG-CD1	5.49	124.29	121.00
1	J	268	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	E	268	PHE	CB-CG-CD2	-5.47	116.97	120.80
3	L	75	ASP	N-CA-CB	-5.45	100.80	110.60
4	O	147	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	55	TYR	CB-CG-CD2	-5.43	117.74	121.00
3	L	812	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	55	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	C	258	ARG	NE-CZ-NH2	5.41	123.00	120.30
3	L	838	PHE	CB-CG-CD2	-5.38	117.03	120.80
3	M	118	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	39	ARG	NE-CZ-NH2	-5.37	117.61	120.30
5	S	87	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	G	258	ARG	NE-CZ-NH2	5.36	122.98	120.30
4	N	147	ARG	NE-CZ-NH1	5.36	122.98	120.30
4	N	49	PHE	CB-CG-CD1	5.34	124.54	120.80
3	M	811	ARG	NE-CZ-NH2	5.32	122.96	120.30
5	S	119	PHE	CB-CG-CD2	-5.32	117.08	120.80
2	P	57	LEU	CB-CA-C	-5.29	100.14	110.20
3	L	118	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	T	57	LEU	CB-CA-C	-5.26	100.20	110.20
1	A	242	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	F	258	ARG	NE-CZ-NH2	5.25	122.92	120.30
5	R	130	ARG	NE-CZ-NH1	-5.25	117.68	120.30
3	L	181	SER	O-C-N	-5.22	114.33	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	258	ARG	NE-CZ-NH2	5.21	122.91	120.30
2	T	230	ASP	CB-CG-OD1	5.21	122.99	118.30
3	M	181	SER	O-C-N	-5.20	114.36	123.20
1	I	258	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	U	214	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	H	294	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	E	258	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	D	294	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	G	294	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	258	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	P	230	ASP	CB-CG-OD1	5.17	122.95	118.30
3	M	656	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	I	294	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	K	294	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	J	294	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	F	294	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	E	294	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	Q	214	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	H	258	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	C	294	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	J	258	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	200	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	P	45	SER	N-CA-CB	5.08	118.12	110.50
4	O	131	ARG	NE-CZ-NH2	5.08	122.84	120.30
5	R	51	ARG	NE-CZ-NH2	5.08	122.84	120.30
3	L	284	ARG	NE-CZ-NH2	5.08	122.84	120.30
3	M	707	ARG	NE-CZ-NH1	5.08	122.84	120.30
4	O	44	GLU	N-CA-CB	-5.07	101.47	110.60
2	T	45	SER	N-CA-CB	5.06	118.09	110.50
3	M	144	ARG	NE-CZ-NH1	5.05	122.82	120.30
3	L	156	PHE	CB-CG-CD1	5.03	124.32	120.80
3	M	284	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	A	256	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	K	264	PHE	CB-CG-CD1	-5.01	117.29	120.80
3	M	80	MET	CG-SD-CE	-5.01	92.18	100.20
3	M	353	TYR	CB-CG-CD2	-5.00	118.00	121.00

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
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

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Mol	Chain	Res	Type	Group
1	I	223	LEU	Peptide
1	I	256	ARG	Sidechain
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

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Mol	Chain	Res	Type	Group
5	S	112	LYS	Peptide
5	S	163	GLY	Peptide
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	78	0
1	B	2925	0	2887	104	0
1	C	2925	0	2886	69	0
1	D	2925	0	2887	65	0
1	E	2925	0	2887	60	0
1	F	2925	0	2887	70	0
1	G	2925	0	2887	51	0
1	H	2925	0	2887	72	0
1	I	2925	0	2885	43	0
1	J	2925	0	2887	38	0
1	K	2925	0	2887	62	0
2	P	1881	0	1879	90	0
2	Q	1881	0	1879	105	0
2	T	1952	0	1960	90	0
2	U	1952	0	1960	87	0
3	L	6503	0	6511	8	0
3	M	6503	0	6511	6	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	14	0
All	All	57453	0	56922	629	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 (629) 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
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:B:46:MET:HE2	1:H:150:THR:O	1.54	1.07
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:D:170:GLY:HA3	1:K:46:MET:HE2	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HG2	1:C:41:ARG:HD2	1.44	0.99
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:VAL:H	1:H:171:TYR:C	1.82	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: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: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:44:GLY:C	1:H:171:TYR:HA	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:223:LEU:HD22	2:Q:66:ASP:CG	2.10	0.72
1:B:45:VAL:C	1:H:171:TYR:O	2.28	0.71
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
1:B:49:MET:HE1	1:H:171:TYR:CD1	2.25	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:A:246:ASP:O	1:B:327:MET:HE1	1.90	0.71
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
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
1:C:145:TYR:HH	1:F:47:VAL:H	1.41	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
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:47:VAL:H	1:F:145:TYR:HH	1.40	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:D:170:GLY:CA	1:K:46:MET:HE1	2.24	0.67
2:P:56:GLU:C	2:Q:57:LEU:HD21	2.15	0.67
1:B:41:ARG:HH11	1:G:272:GLU:CG	2.07	0.66
5:R:80:PHE:CD2	5:S:51:ARG:CD	2.58	0.66
1:A:327:MET:HE1	1:E:246:ASP:O	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:246:ASP:CG	1:G:289:ILE:HG23	2.16	0.65
2:T:56:GLU:C	2:U:57:LEU:HD21	2.15	0.65
1:A:246:ASP:OD1	1:B:289:ILE:HG23	1.95	0.65
1:G:197:GLU:HB2	1:H:115:LYS:HD2	1.79	0.65
1:A:327:MET:HE1	1:E:246:ASP:C	2.16	0.64
1:A:41:ARG:CD	1:C:272:GLU:HG2	2.25	0.64
1:B:46:MET:CE	1:H:150:THR:O	2.39	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: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: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:A:246:ASP:O	1:B:327:MET:CE	2.47	0.62
1:B:41:ARG:CD	1:G:272:GLU:HG2	2.27	0.62
1:D:47:VAL:N	1:F:145:TYR:HH	1.95	0.61
1:C:145:TYR:HH	1:F:47:VAL:N	1.95	0.61
1:D:46:MET:HG3	1:F:170:GLY:HA2	1.82	0.61
2:P:56:GLU:C	2:Q:57:LEU:CD2	2.69	0.61
1:A:327:MET:CE	1:E:246:ASP:O	2.48	0.61
1:D:170:GLY:HA2	1:K:46:MET:HE1	1.81	0.61
2:T:56:GLU:C	2:U:57:LEU:CD2	2.69	0.61
1:A:173:LEU:CD2	1:E:42:HIS:CD2	2.83	0.61
1:D:171:TYR:HE1	1:K:44:GLY:CA	2.13	0.60
1:B:46:MET:CE	1:H:170:GLY:H	2.14	0.60
1:E:289:ILE:CG2	1:I:246:ASP:CG	2.70	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)
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: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:I:175:HIS:HB3	1:K:269:ILE:O	2.03	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: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
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
1:E:171:TYR:OH	1:I:49:MET:SD	2.64	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:A:246:ASP:CG	1:B:289:ILE:HG23	2.26	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
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:327:MET:HE3	1:E:247:GLY:HA3	1.90	0.54
1:A:44:GLY:N	1:B:171:TYR:CD1	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:170:GLY:C	1:K:46:MET:SD	2.86	0.54
1:B:45:VAL:N	1:H:171:TYR:C	2.58	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:292:ARG:HD2	1:E:246:ASP:CG	2.26	0.53
1:B:44:GLY:C	1:H:171:TYR:CD1	2.75	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:J:204:THR:HG23	1:K:272:GLU:CD	2.29	0.53
1:D:246:ASP:O	1:F:327:MET:HE1	2.09	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
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
1:D:197:GLU:O	1:E:114:PRO:HA	2.10	0.52
2:T:98:GLU:C	2:U:99:LEU:HD13	2.29	0.52
2:P:98:GLU:C	2:Q:99:LEU:HD13	2.29	0.52
3:M:109:ARG:HH22	3:M:153:PRO:HG2	1.75	0.52
1:D:204:THR:HG23	1:E:272:GLU:CD	2.29	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
2:T:64:LEU:HD13	2:U:64:LEU:N	2.26	0.51
1:B:46:MET:HE3	1:H:170:GLY:N	2.25	0.51
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:246:ASP:C	1:F:327:MET:HE1	2.32	0.50
1:D:66:ILE:HD11	1:F:168:TYR:HB3	1.93	0.50
1:A:327:MET:HE3	1:E:247:GLY:CA	2.42	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: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: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
1:B:46:MET:HE2	1:H:170:GLY:H	1.78	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
2:P:64:LEU:HD13	2:Q:63:ALA:C	2.33	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
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
2:P:46:LEU:HD13	2:Q:50:LEU:HD13	1.95	0.49
2:T:64:LEU:HD13	2:U:63:ALA:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:327:MET:HE1	1:J:246:ASP:O	2.12	0.48
2:T:88:LEU:O	2:U:92:ILE:CD1	2.58	0.48
1:E:289:ILE:HG23	1:I:246:ASP:CG	2.34	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:G:228:GLU:OE2	2:Q:65:LYS:NZ	2.46	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
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
2:P:70:LYS:C	2:Q:71:LEU:HD23	2.35	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
1:I:327:MET:HE1	1:J:246:ASP:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:T:70:LYS:C	2:U:71:LEU:HD23	2.35	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:B:49:MET:HE3	1:H:171:TYR:CZ	2.50	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:71:LEU:HD13	2:U:70:LYS:C	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:LEU:HD13	2:Q:70:LYS:C	2.36	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
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
1:C:292:ARG:HH11	1:F:246:ASP:CG	2.19	0.45
2:T:57:LEU:CA	2:U:57:LEU:HD23	2.44	0.45
1:B:46:MET:HE3	1:H:170:GLY:H	1.82	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:252:SER:HB3	2:U:253:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH1	1:C:272:GLU:CG	2.75	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: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
5:R:134:GLU:CD	5:R:134:GLU:H	2.21	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
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: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
2:T:137:ASP:HA	2:U:141:MET:SD	2.58	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
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
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:A:272:GLU:CD	1:F:204:THR:HG23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:I:272:GLU:CD	1:K:204:THR:HG23	2.40	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
2:P:56:GLU:CB	2:Q:57:LEU:HD21	2.49	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:A:4:GLU:N	1:A:4:GLU:CD	2.73	0.42
1:C:144:LEU:HD22	1:C:167:ILE:HG21	2.01	0.42
1:D:171:TYR:H	1:K:46:MET:CG	2.33	0.42
1:E:204:THR:HG23	1:F:272:GLU:CD	2.40	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:B:46:MET:HE1	1:H:144:LEU:HD21	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:145:TYR:HH	1:E:47:VAL:H	1.61	0.41
1:B:49:MET:HE3	1:H:171:TYR:CE1	2.54	0.41
1:E:197:GLU:O	1:F:114:PRO:HA	2.20	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
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: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: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:B:49:MET:HE1	1:H:171:TYR:CG	2.53	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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:A:327:MET:CE	1:E:246:ASP:C	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	14	52
1	B	372/374 (100%)	345 (93%)	22 (6%)	5 (1%)	12	48
1	C	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	D	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	E	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	F	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	G	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	H	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	I	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
1	J	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	372/374 (100%)	354 (95%)	13 (4%)	5 (1%)	12	48
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%)	4	26
3	M	811/813 (100%)	725 (89%)	61 (8%)	25 (3%)	4	27
4	N	146/148 (99%)	136 (93%)	4 (3%)	6 (4%)	3	23
4	O	146/148 (99%)	137 (94%)	4 (3%)	5 (3%)	3	26
5	R	142/144 (99%)	121 (85%)	13 (9%)	8 (6%)	2	19
5	S	142/144 (99%)	121 (85%)	13 (9%)	8 (6%)	2	19
All	All	7234/7328 (99%)	6786 (94%)	316 (4%)	132 (2%)	12	40

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	43	65
1	B	317/317 (100%)	307 (97%)	10 (3%)	39	61
1	C	317/317 (100%)	315 (99%)	2 (1%)	86	92
1	D	317/317 (100%)	314 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	317/317 (100%)	314 (99%)	3 (1%)	78	87
1	F	317/317 (100%)	314 (99%)	3 (1%)	78	87
1	G	317/317 (100%)	315 (99%)	2 (1%)	86	92
1	H	317/317 (100%)	315 (99%)	2 (1%)	86	92
1	I	317/317 (100%)	315 (99%)	2 (1%)	86	92
1	J	317/317 (100%)	315 (99%)	2 (1%)	86	92
1	K	317/317 (100%)	314 (99%)	3 (1%)	78	87
2	P	202/216 (94%)	201 (100%)	1 (0%)	88	93
2	Q	202/216 (94%)	201 (100%)	1 (0%)	88	93
2	T	208/216 (96%)	206 (99%)	2 (1%)	76	86
2	U	208/216 (96%)	207 (100%)	1 (0%)	88	93
3	L	699/699 (100%)	687 (98%)	12 (2%)	60	78
3	M	699/699 (100%)	685 (98%)	14 (2%)	55	74
4	N	125/125 (100%)	124 (99%)	1 (1%)	81	89
4	O	125/125 (100%)	124 (99%)	1 (1%)	81	89
5	R	124/124 (100%)	119 (96%)	5 (4%)	31	55
5	S	124/124 (100%)	116 (94%)	8 (6%)	17	42
All	All	6203/6247 (99%)	6116 (99%)	87 (1%)	68	80

All (87) 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	159	ASP
1	A	161	VAL
1	A	167	ILE
1	A	205	THR
1	A	294	ASP
1	A	313	ASP
1	B	4	GLU
1	B	27	ASP
1	B	53	ASP
1	B	82	ASP
1	B	108	THR

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Mol	Chain	Res	Type
1	B	159	ASP
1	B	161	VAL
1	B	167	ILE
1	B	294	ASP
1	B	313	ASP
1	C	108	THR
1	C	167	ILE
1	D	108	THR
1	D	161	VAL
1	D	167	ILE
1	E	108	THR
1	E	161	VAL
1	E	167	ILE
1	F	108	THR
1	F	161	VAL
1	F	167	ILE
1	G	108	THR
1	G	167	ILE
1	H	108	THR
1	H	167	ILE
1	I	108	THR
1	I	167	ILE
1	J	108	THR
1	J	167	ILE
1	K	108	THR
1	K	161	VAL
1	K	167	ILE
2	P	85	VAL
2	Q	29	LYS
2	T	15	LYS
2	T	85	VAL
2	U	29	LYS
3	L	75	ASP
3	L	121	LEU
3	L	160	ASP
3	L	242	ASP
3	L	322	THR
3	L	347	ASP
3	L	361	HIS
3	L	379	ASP
3	L	472	ASP
3	L	606	GLU

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Mol	Chain	Res	Type
3	L	739	PHE
3	L	837	TYR
4	N	68	GLN
5	R	49	ASP
5	R	61	ASN
5	R	77	PRO
5	R	137	LYS
5	R	153	TYR
3	M	75	ASP
3	M	121	LEU
3	M	160	ASP
3	M	242	ASP
3	M	260	LYS
3	M	322	THR
3	M	347	ASP
3	M	361	HIS
3	M	379	ASP
3	M	472	ASP
3	M	519	ASP
3	M	739	PHE
3	M	778	GLU
3	M	837	TYR
4	O	68	GLN
5	S	49	ASP
5	S	61	ASN
5	S	77	PRO
5	S	89	GLU
5	S	97	GLU
5	S	123	LEU
5	S	137	LYS
5	S	153	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	103	HIS
1	A	163	HIS
1	B	103	HIS
1	B	163	HIS
1	B	373	HIS
1	C	61	GLN

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Mol	Chain	Res	Type
1	E	61	GLN
1	F	61	GLN
1	G	61	GLN
1	H	61	GLN
1	I	61	GLN
1	J	61	GLN
1	K	61	GLN
3	L	98	HIS
3	L	670	HIS
3	L	730	ASN
3	M	98	HIS
3	M	235	ASN
3	M	670	HIS
3	M	730	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 monosaccharides 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.

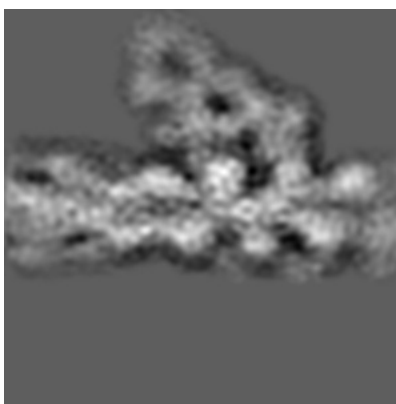
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

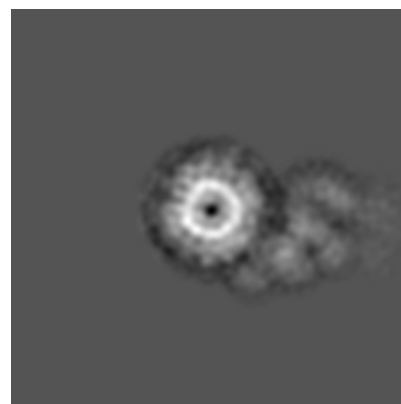
#### 6.1.1 Primary map



X

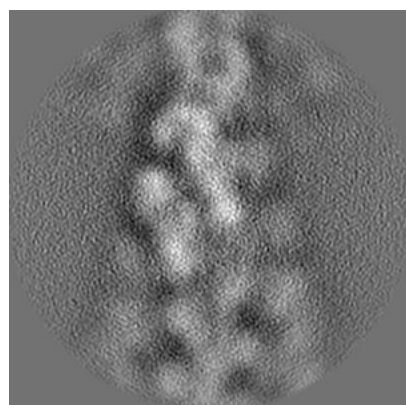


Y

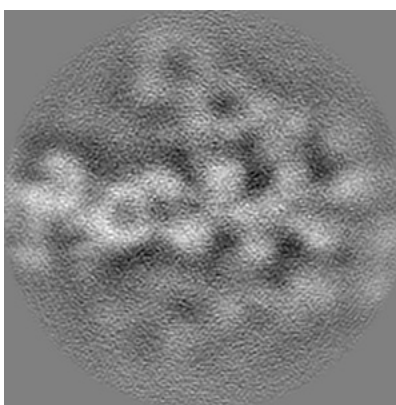


Z

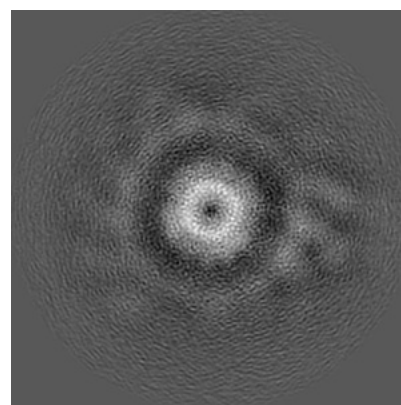
#### 6.1.2 Raw map



X



Y



Z

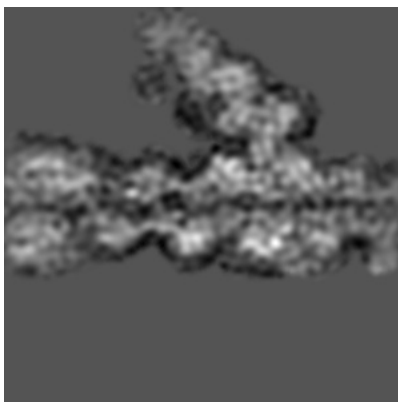
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

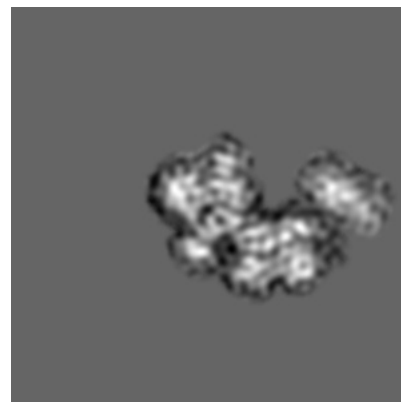
### 6.2.1 Primary map



X Index: 100

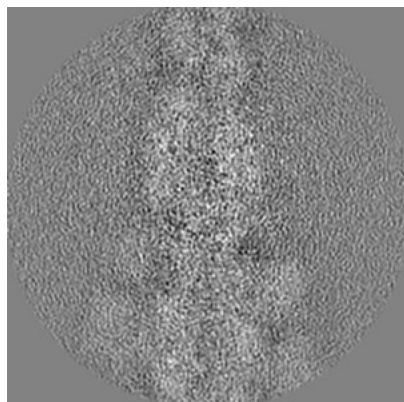


Y Index: 100

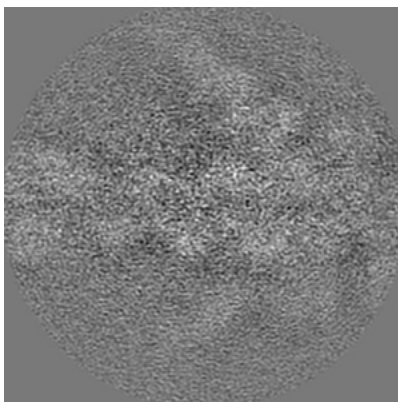


Z Index: 100

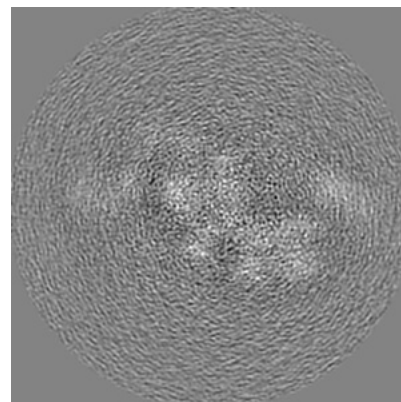
### 6.2.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

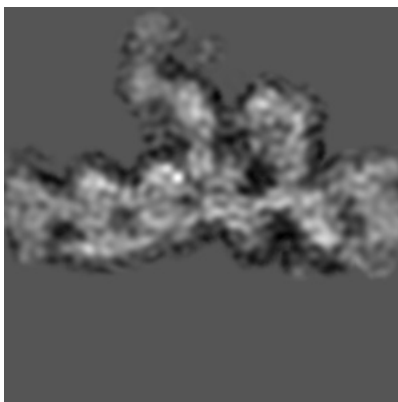
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

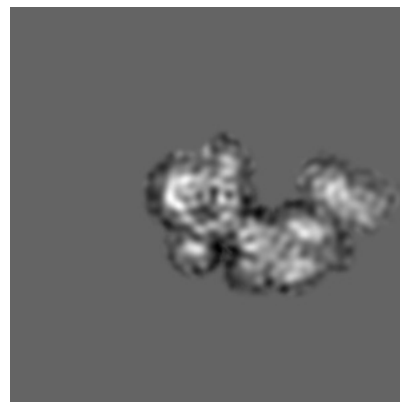
### 6.3.1 Primary map



X Index: 113

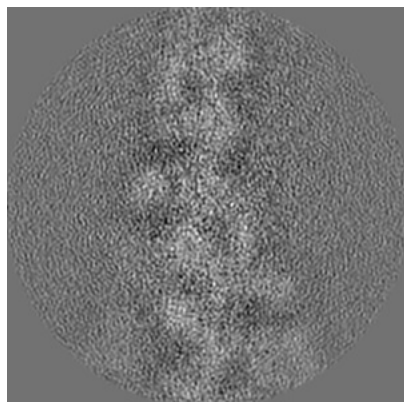


Y Index: 87

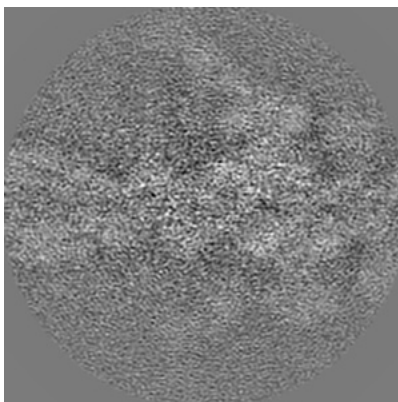


Z Index: 96

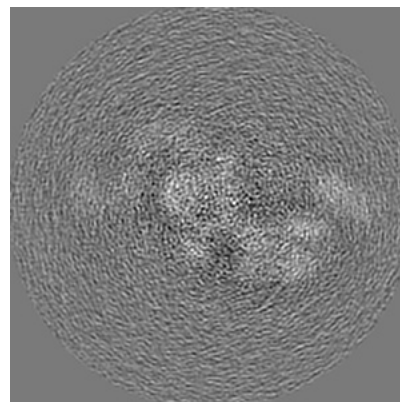
### 6.3.2 Raw map



X Index: 112



Y Index: 97



Z Index: 97

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

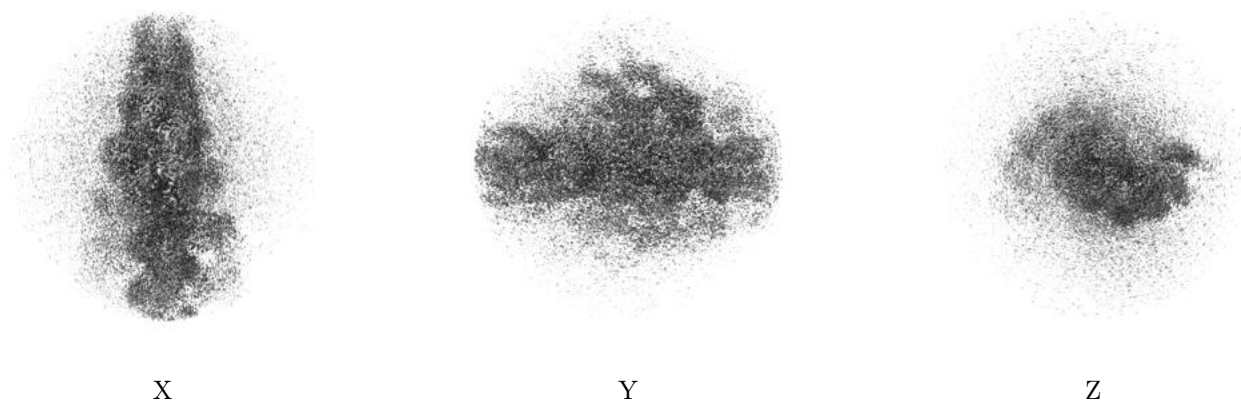
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

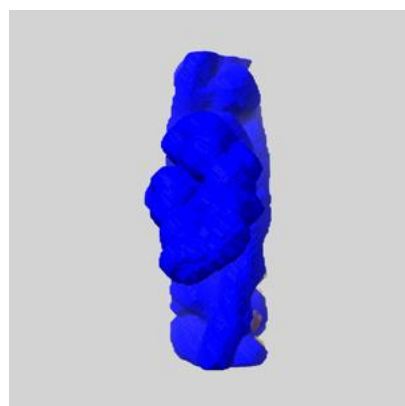
## 6.5 Mask visualisation [i](#)

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

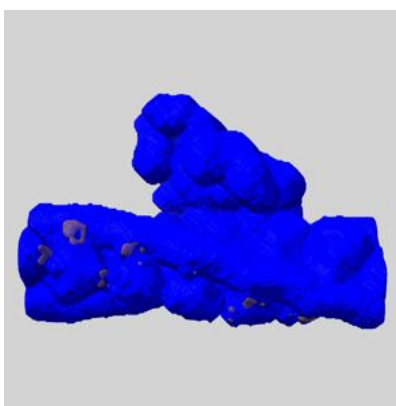
A mask typically either:

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

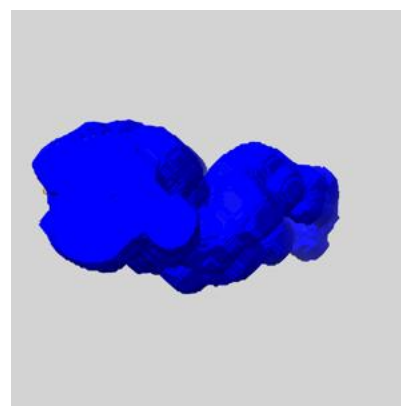
### 6.5.1 emd\_12289\_msk\_1.map [i](#)



X



Y

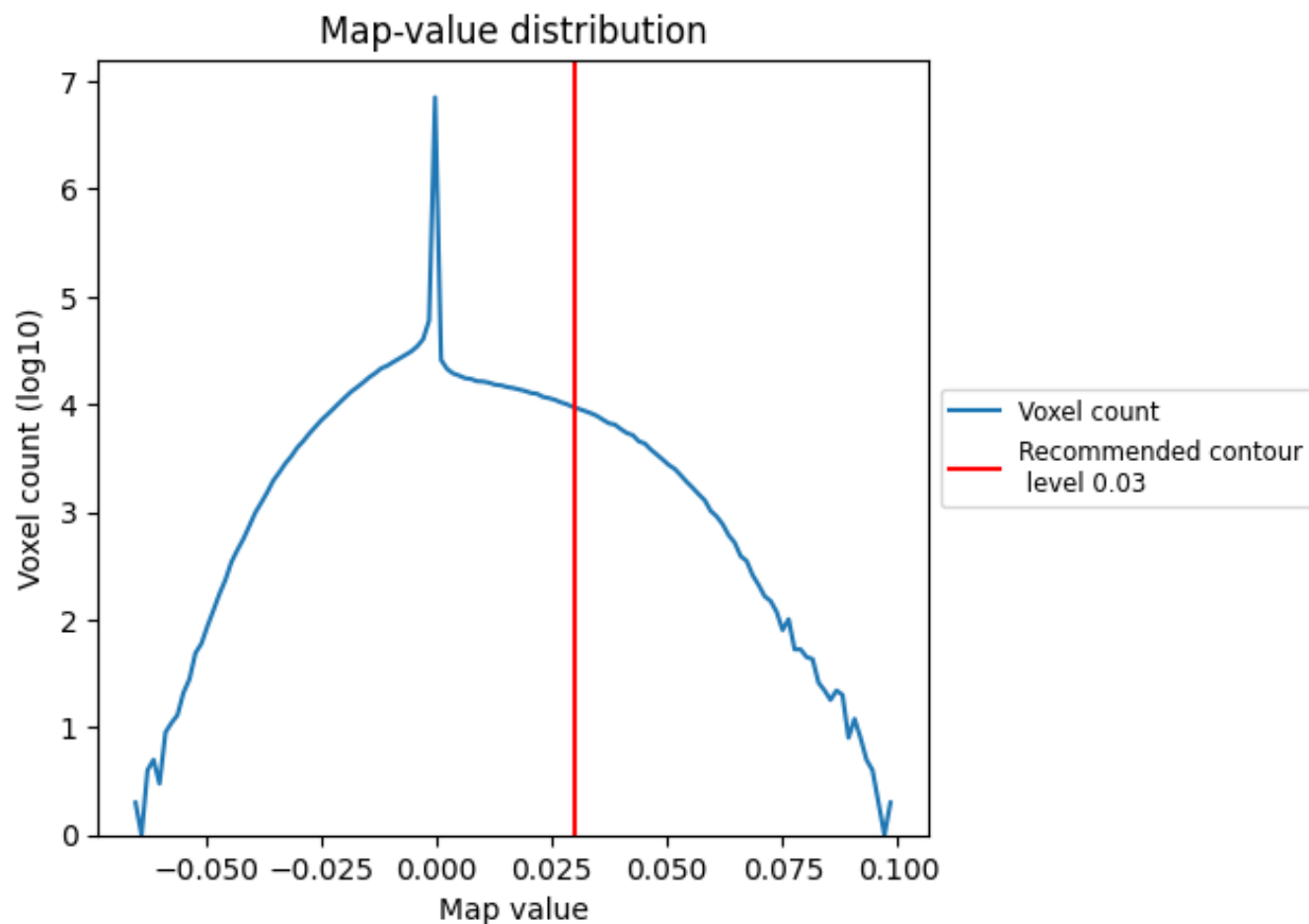


Z

## 7 Map analysis [i](#)

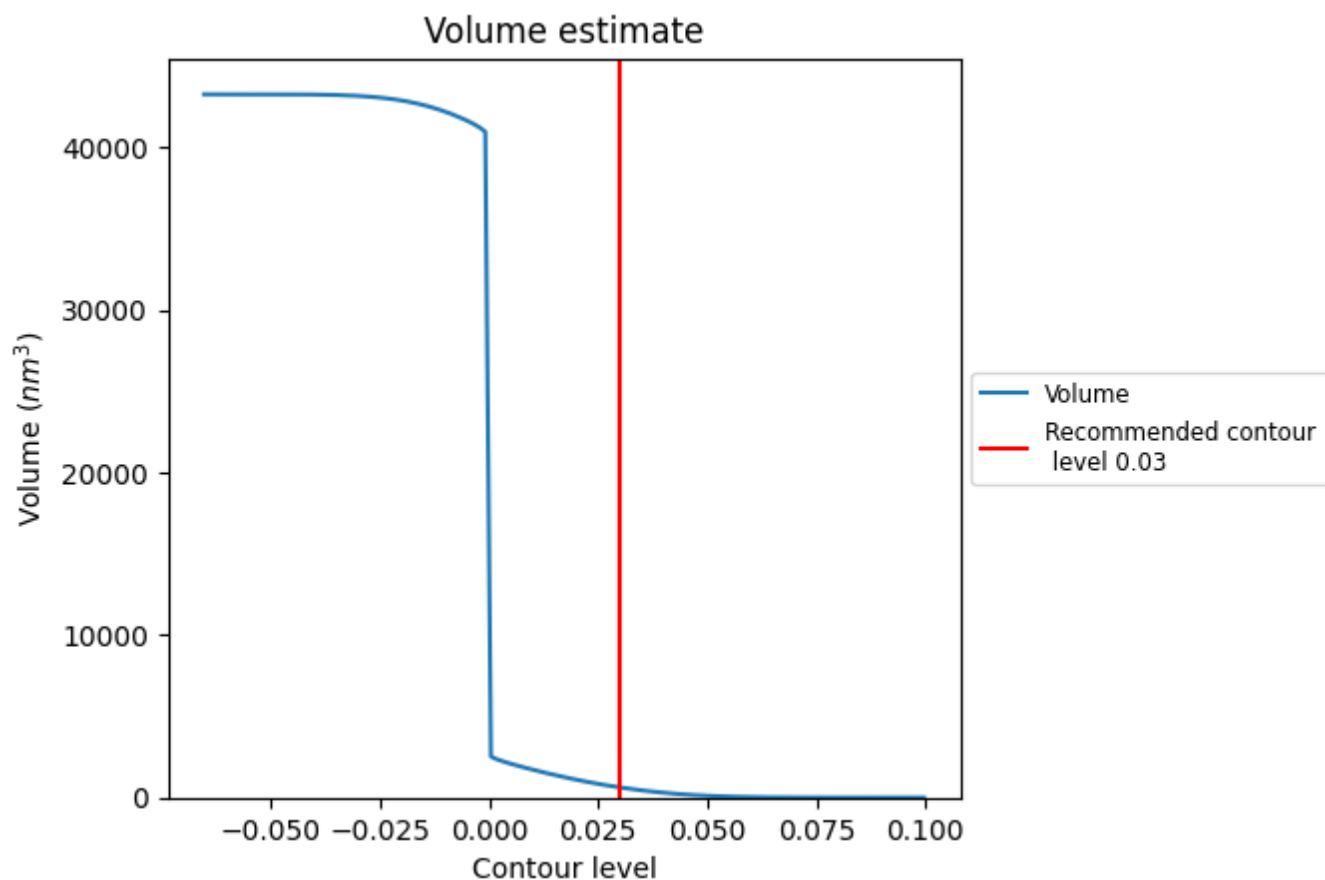
This section contains the results of statistical analysis of the map.

### 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](#)

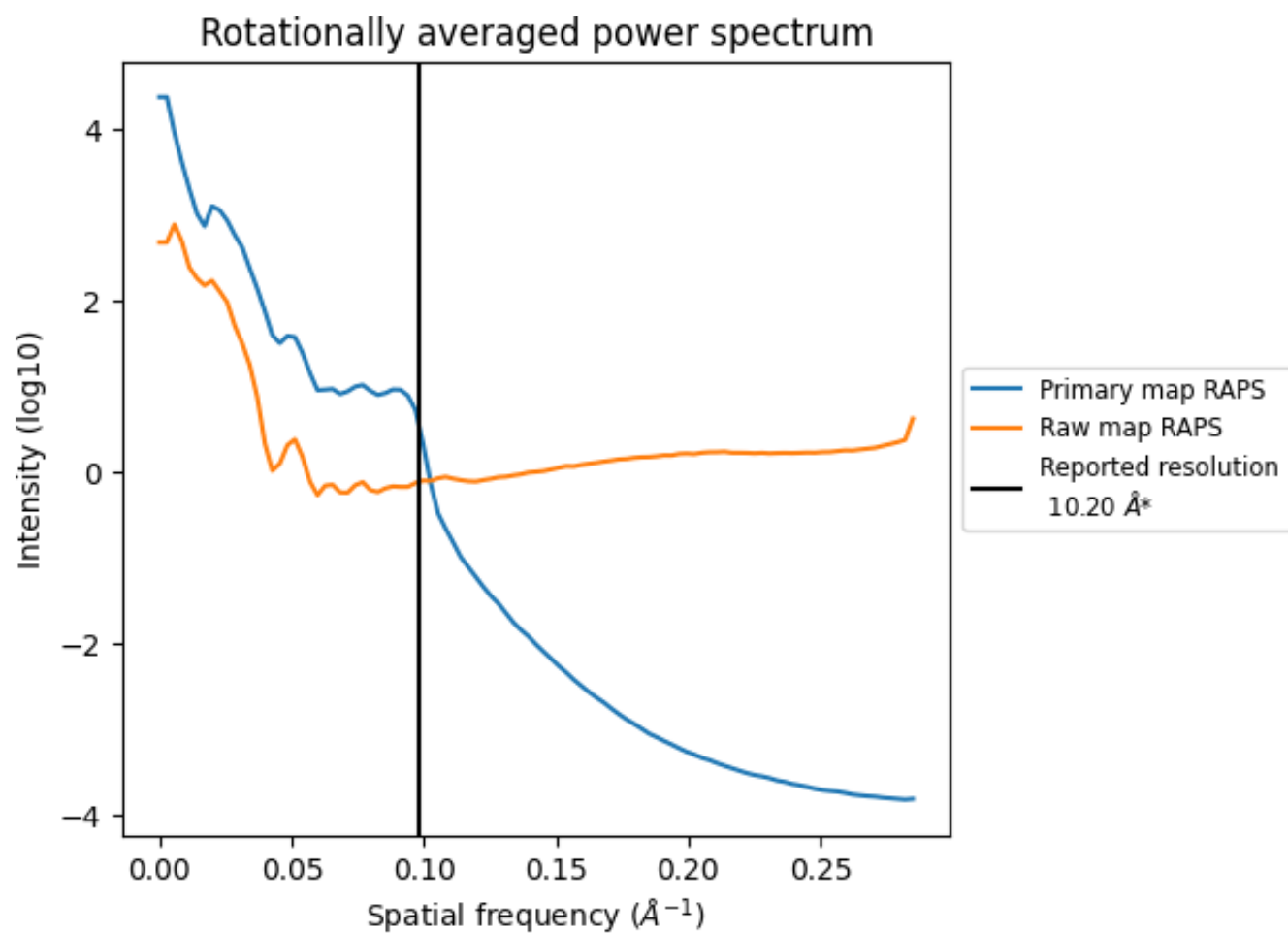


The volume at the recommended contour level is 624 nm<sup>3</sup>; this corresponds to an approximate mass of 564 kDa.

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 [i](#)

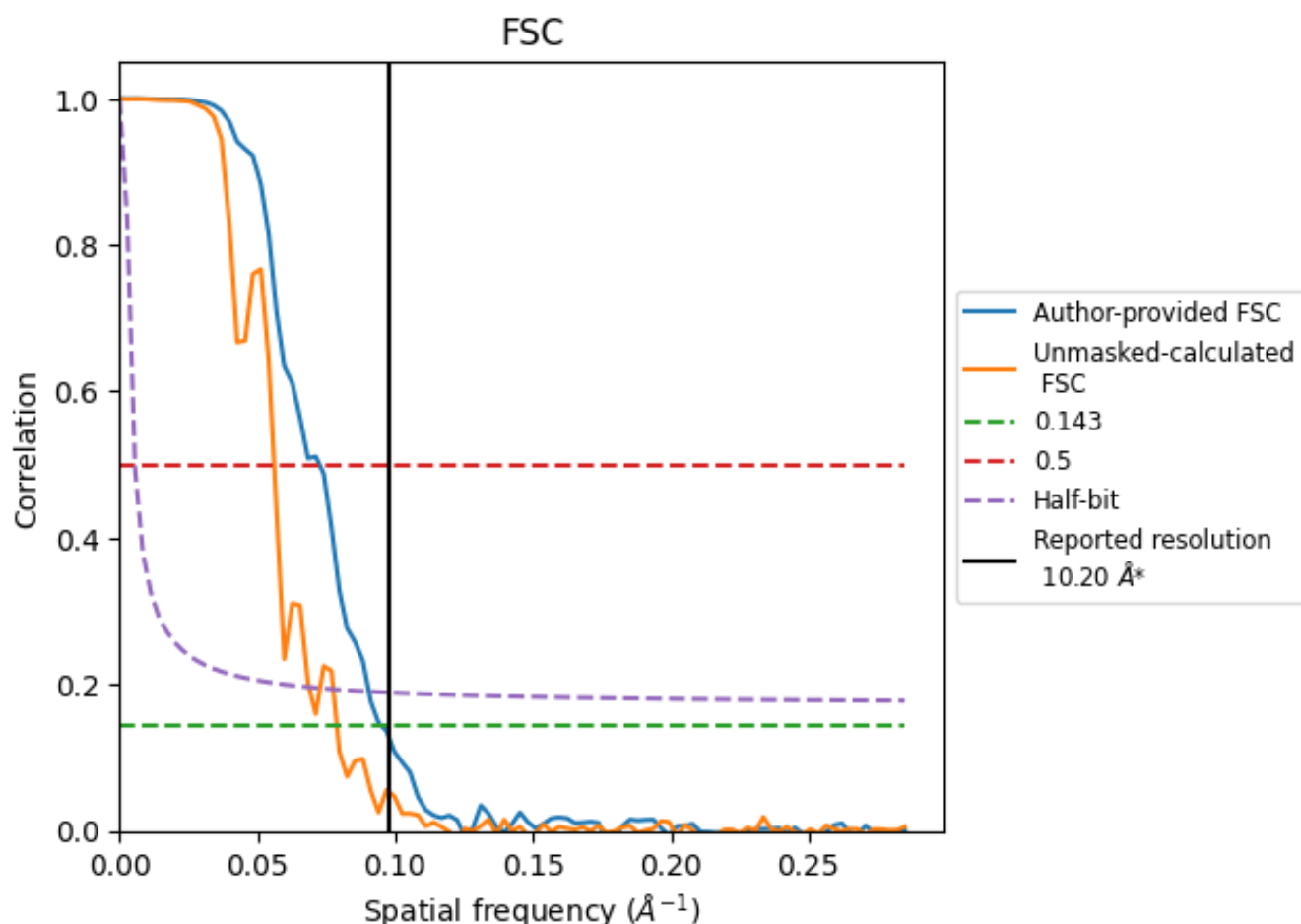


\*Reported resolution corresponds to spatial frequency of 0.098  $\text{\AA}^{-1}$

## 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](#)

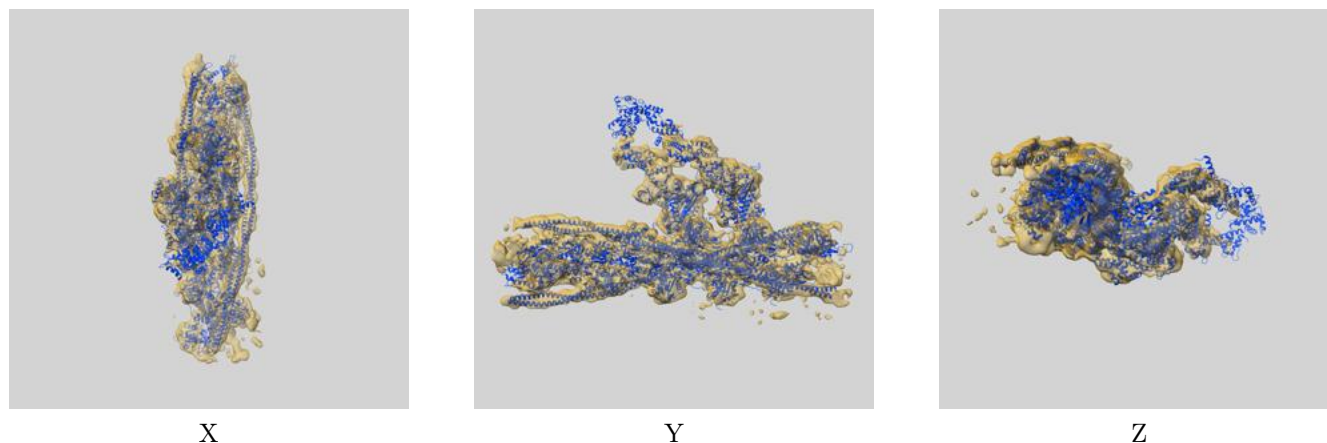
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.20	-	-
Author-provided FSC curve	10.52	13.77	11.05
Unmasked-calculated*	12.67	17.83	14.53

\*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](#)

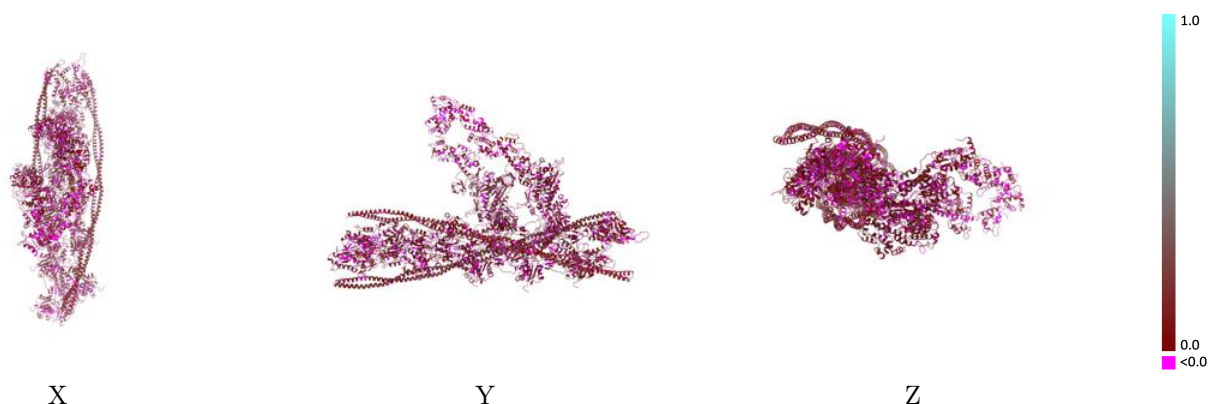
This section contains information regarding the fit between EMDB map EMD-12289 and PDB model 7NEP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



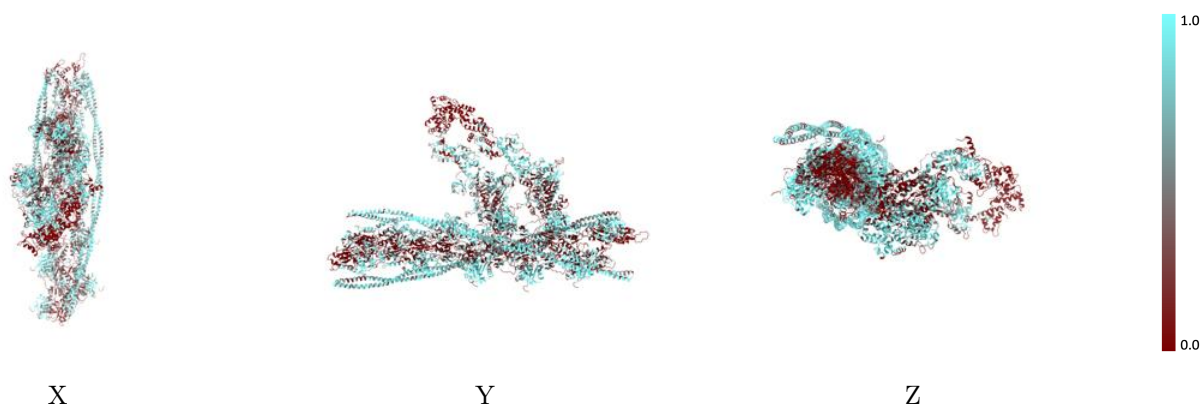
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



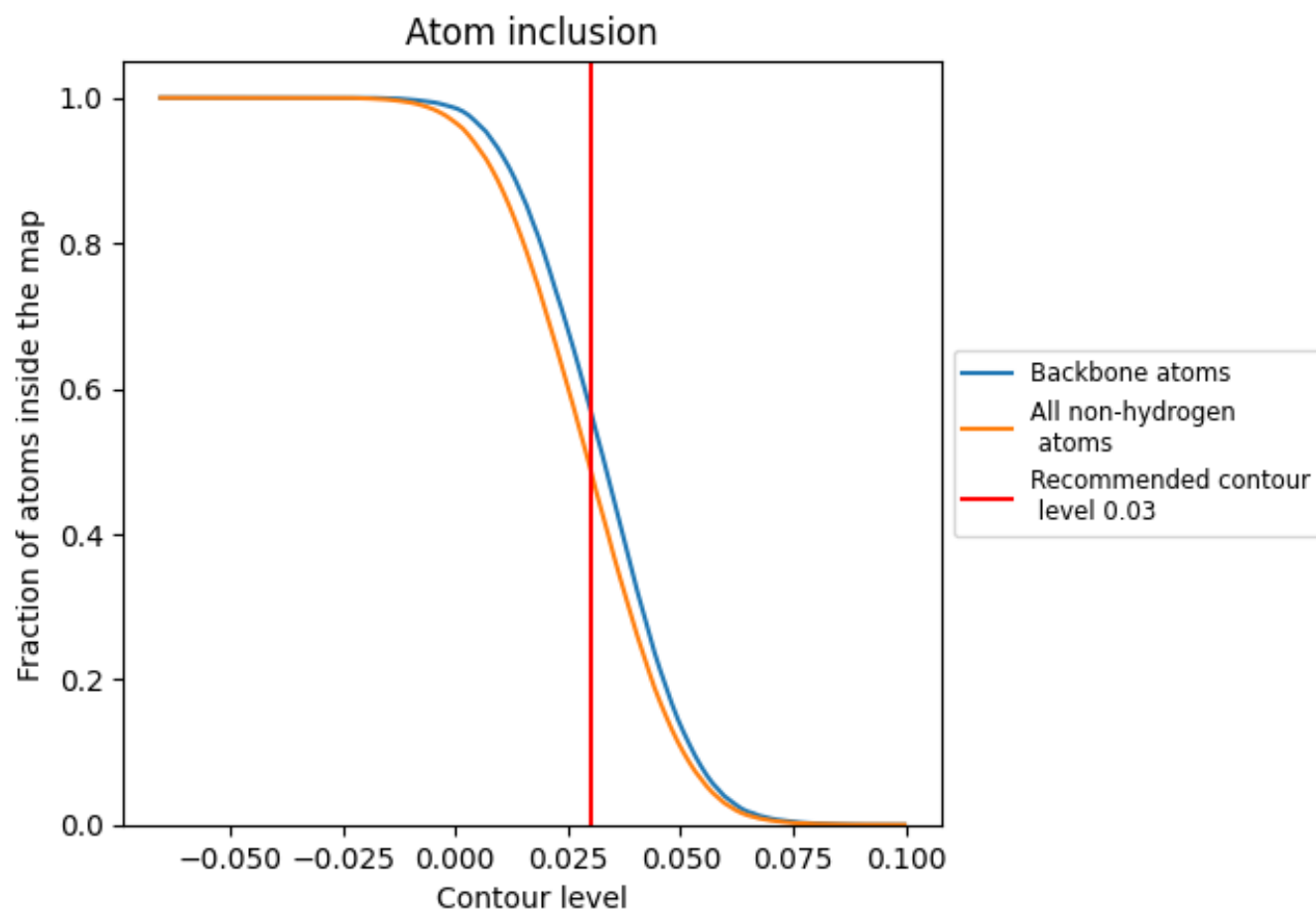
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).













































## 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	 0.4894	 0.0880
A	 0.4482	 0.0930
B	 0.4604	 0.0910
C	 0.4751	 0.0840
D	 0.4657	 0.0880
E	 0.5214	 0.0970
F	 0.4911	 0.0900
G	 0.4827	 0.0920
H	 0.3974	 0.0860
I	 0.4803	 0.0890
J	 0.3242	 0.0700
K	 0.4266	 0.0840
L	 0.5118	 0.0790
M	 0.4771	 0.0690
N	 0.5292	 0.0690
O	 0.5753	 0.0660
P	 0.7535	 0.1300
Q	 0.7481	 0.1430
R	 0.0159	 0.0250
S	 0.0936	 0.0410
T	 0.7698	 0.1340
U	 0.7219	 0.1350

