Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 11:25 AM EST

PDB ID	:	3DTP
EMDB ID	:	EMD-1950
Title	:	Tarantula heavy meromyosin obtained by flexible docking to Tarantula muscle thick filament Cryo-EM 3D-MAP
Authors	:	Alamo, L.; Wriggers, W.; Pinto, A.; Bartoli, F.; Salazar, L.; Zhao, F.Q.; Craig, R.; Padron, R.
Deposited on	:	2008-07-15
Resolution	:	20.00 Å(reported)
Based on initial models	:	1I84, 1B7T, 2FXM

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:

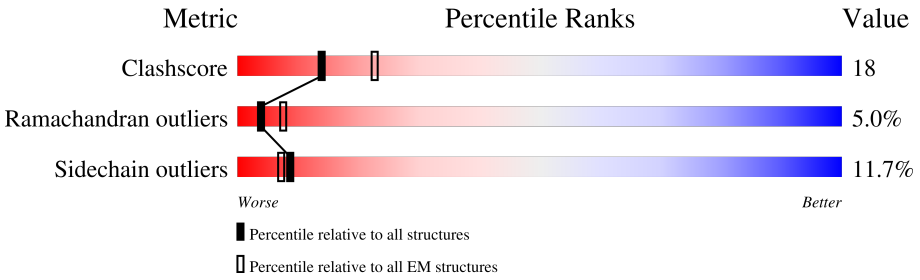
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 20.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	971	85% 56% 32% 8%
2	B	973	40% 49% 37% 9%
3	C	150	68% 73% 23%
3	D	150	34% 47% 42% 8%
4	E	196	99% 57% 36% 6%
4	F	196	100% 43% 34% 15% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25293 atoms, of which 4713 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myosin-11,Myosin-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	938	Total	C	H	N	O	S	0	0
			9360	4819	1759	1312	1432	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	see sequence_details	UNP P10587

- Molecule 2 is a protein called Myosin-11,Myosin-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	940	Total	C	H	N	O	S	0	0
			9379	4828	1764	1315	1434	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	see sequence_details	UNP P10587

- Molecule 3 is a protein called Myosin light polypeptide 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		
3	D	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		

- Molecule 4 is a protein called Myosin II regulatory light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		

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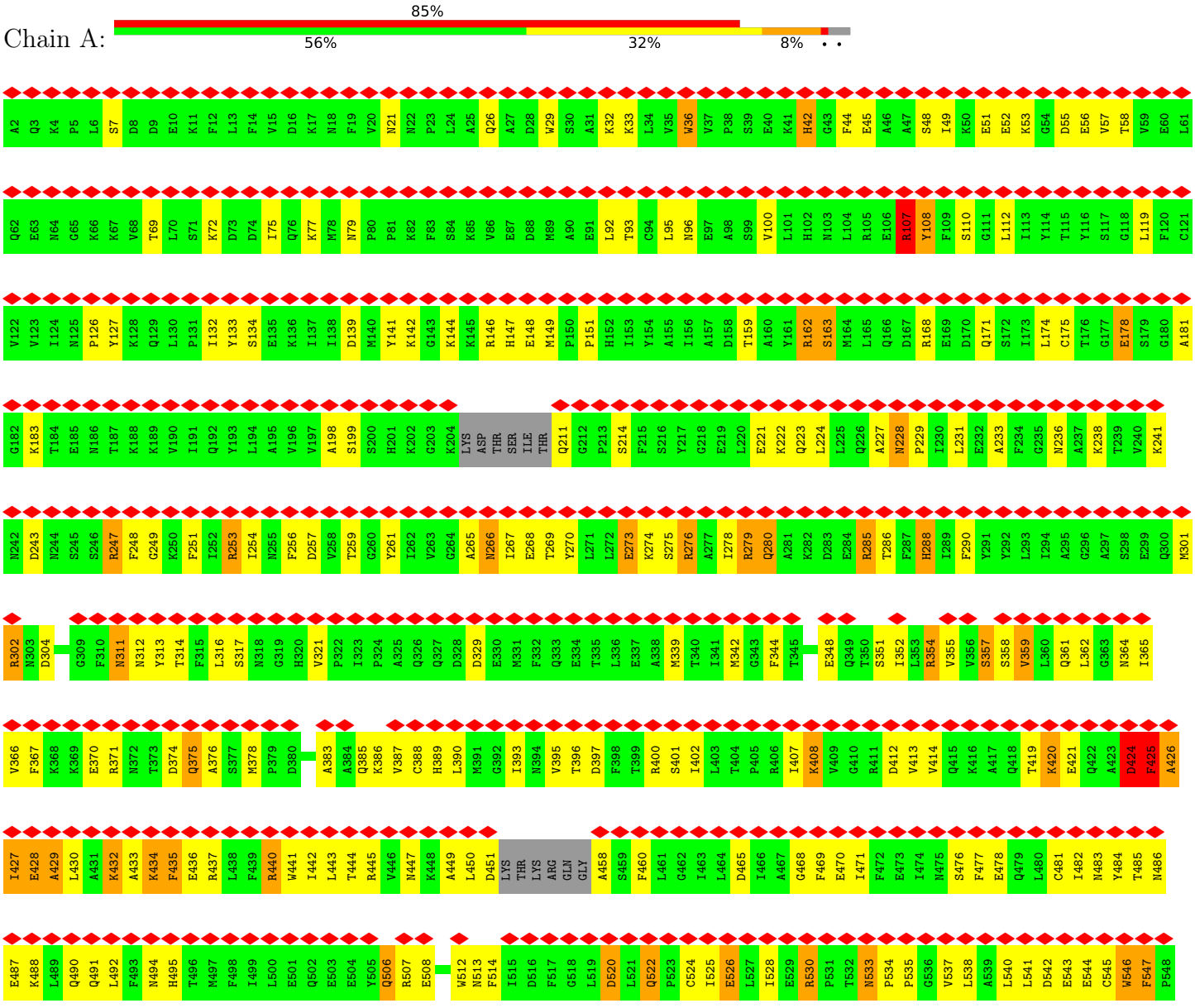
Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		

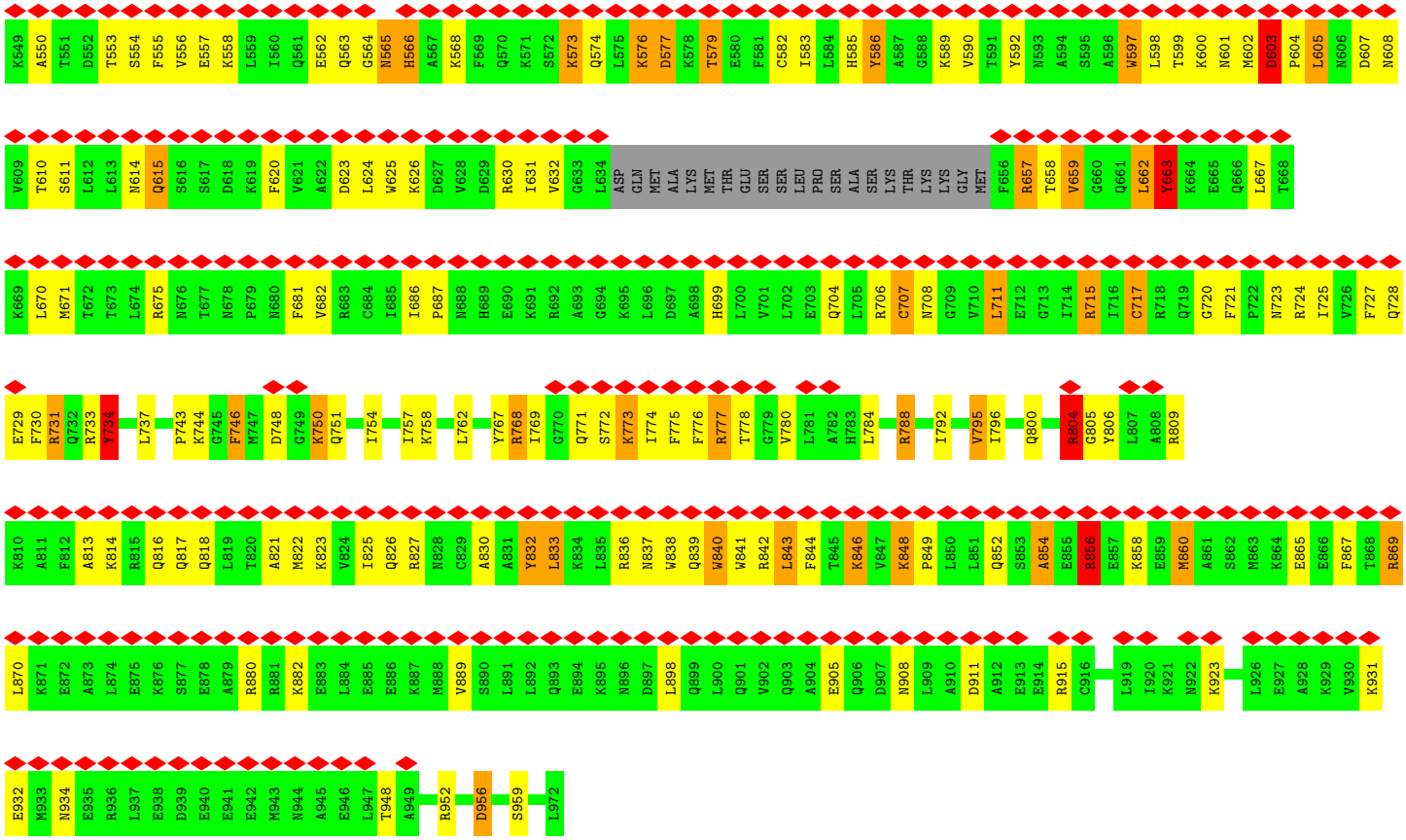
3 Residue-property plots (i)

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

- Molecule 1: Myosin-11,Myosin-7

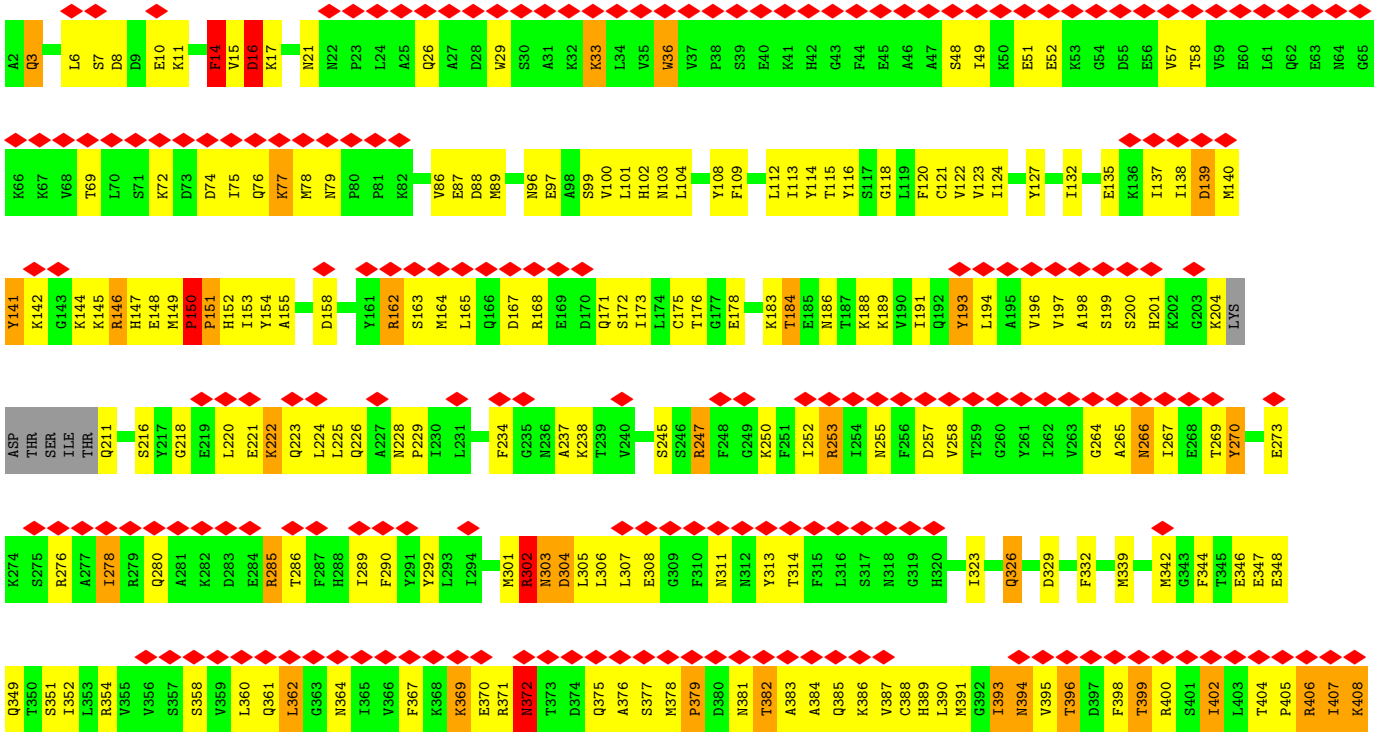
Chain A:

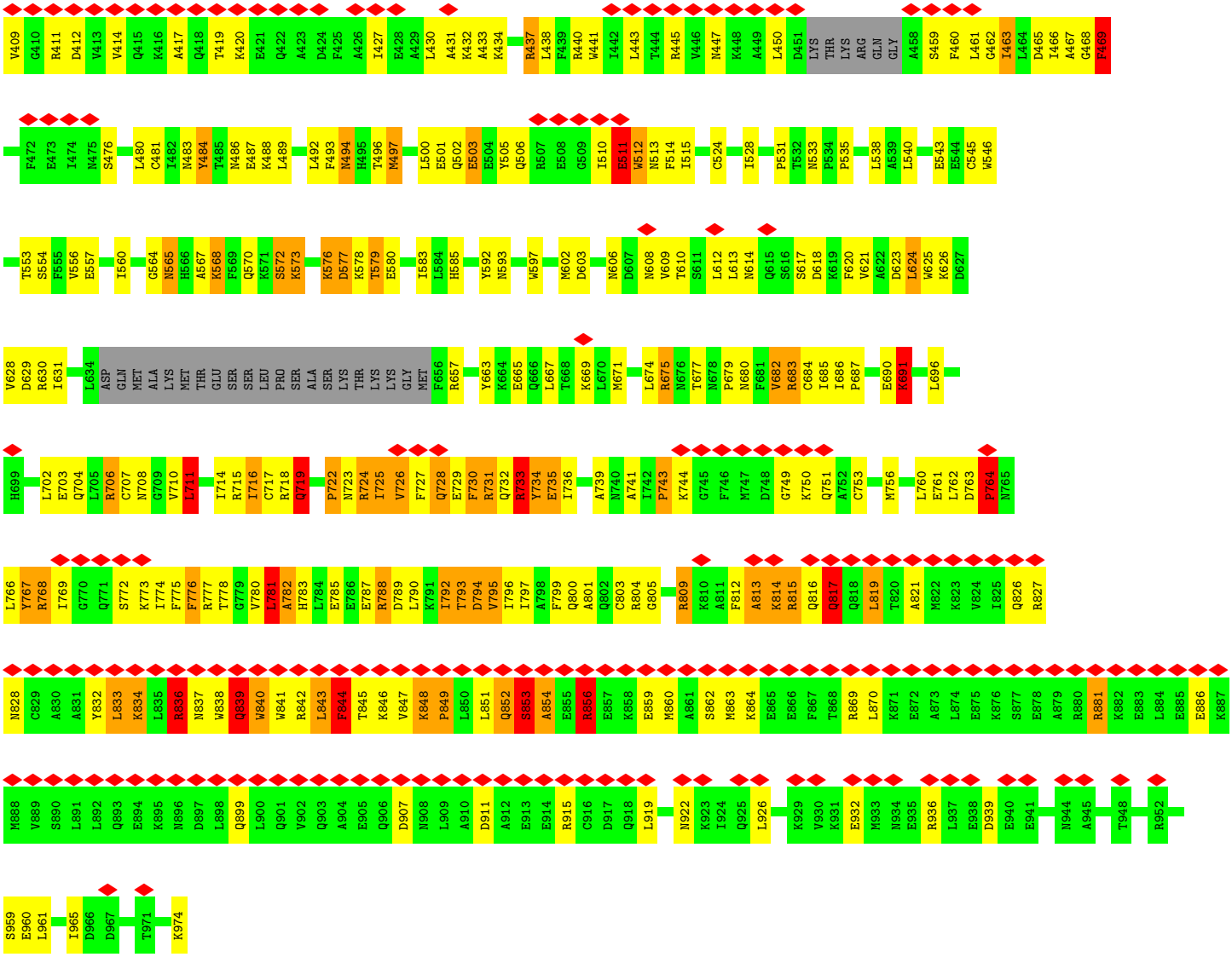




• Molecule 2: Myosin-11,Myosin-7

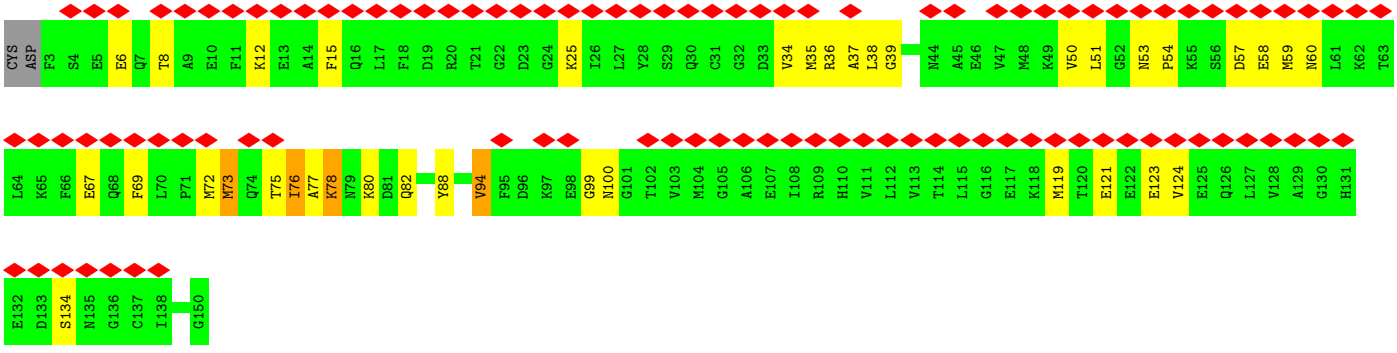
Chain B:





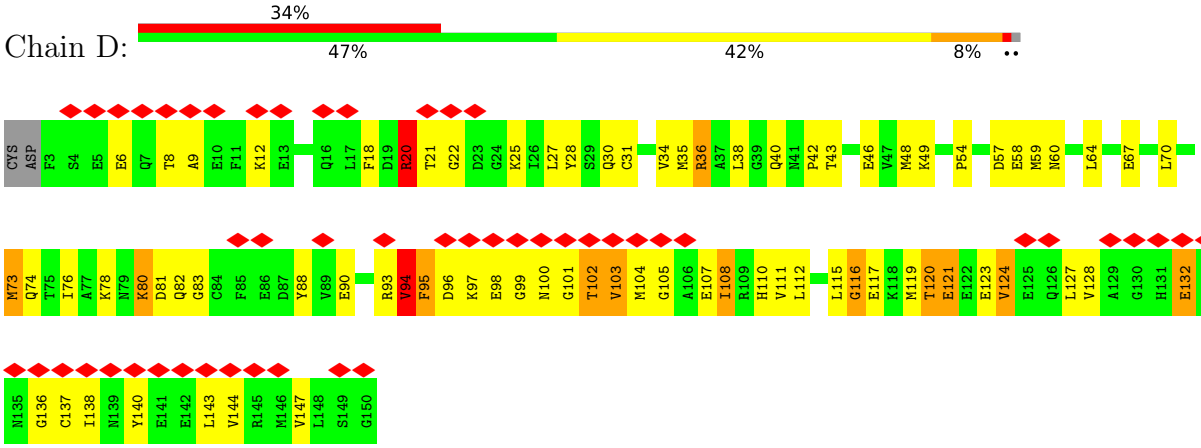
• Molecule 3: Myosin light polypeptide 6

Chain C:



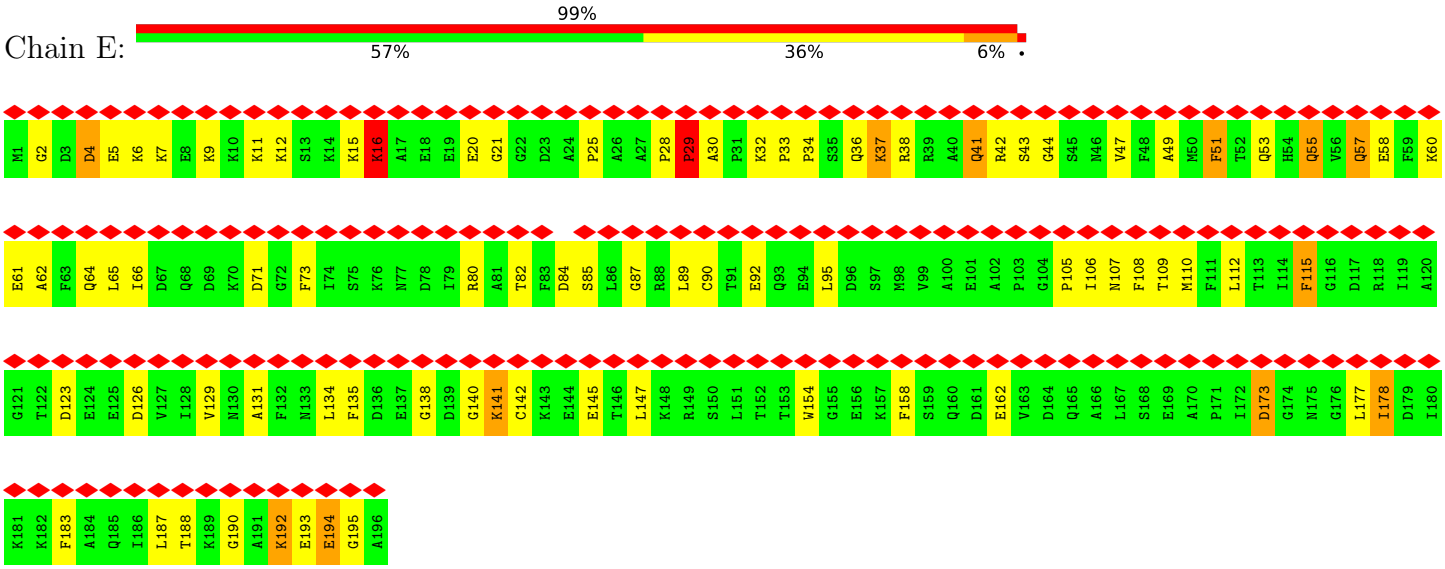
• Molecule 3: Myosin light polypeptide 6

Chain D:



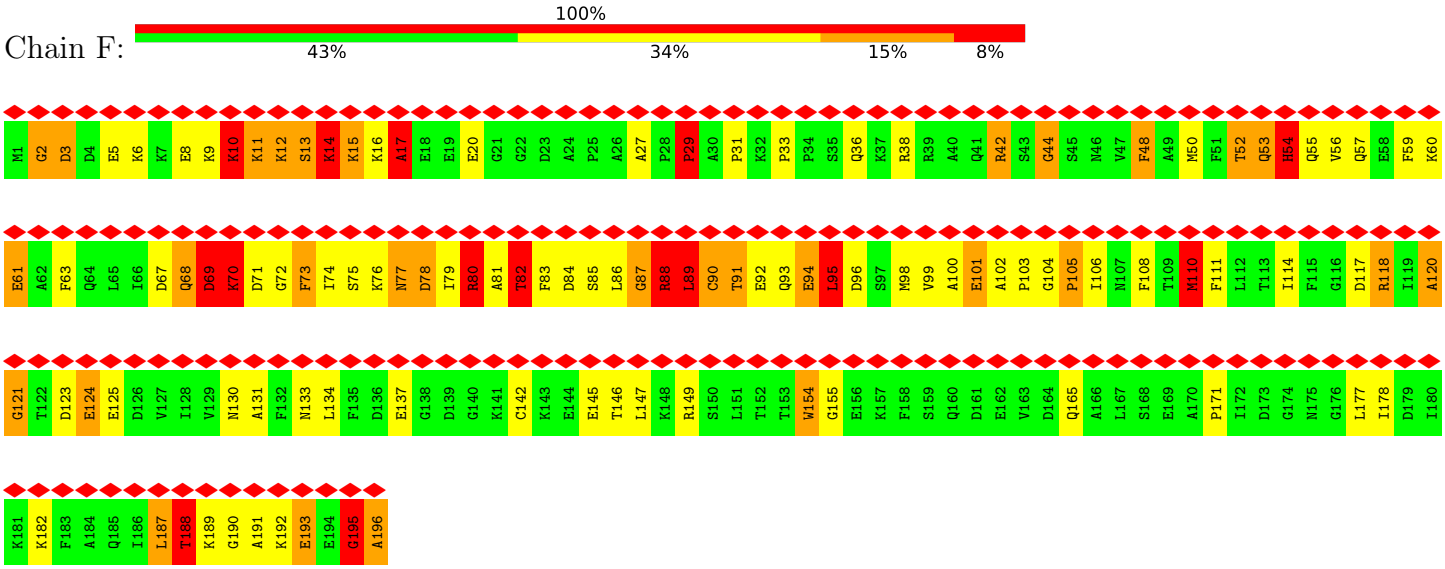
• Molecule 4: Myosin II regulatory light chain

Chain E:



• Molecule 4: Myosin II regulatory light chain

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	15504	Depositor
Resolution determination method	Not provided	
CTF correction method	no corrected	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1950	Depositor
Maximum defocus (nm)	1950	Depositor
Magnification	35000	Depositor
Image detector	Not provided	
Maximum map value	247.077	Depositor
Minimum map value	-0.037	Depositor
Average map value	10.023	Depositor
Map value standard deviation	28.567	Depositor
Recommended contour level	25.0	Depositor
Map size (Å)	620, 620, 620.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.48, 2.48, 2.482	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.66	0/7730	1.43	79/10402 (0.8%)
2	B	0.66	0/7744	1.42	75/10420 (0.7%)
3	C	0.63	0/1175	1.19	2/1575 (0.1%)
3	D	0.65	0/1175	1.33	5/1575 (0.3%)
4	E	0.65	0/1546	1.34	10/2071 (0.5%)
4	F	0.68	0/1546	1.57	21/2071 (1.0%)
All	All	0.66	0/20916	1.41	192/28114 (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	22
2	B	0	31
3	D	0	7
4	E	0	3
4	F	0	16
All	All	0	79

There are no bond length outliers.

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	107	ARG	NE-CZ-NH1	11.80	126.20	120.30
3	C	36	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	A	285	ARG	NE-CZ-NH1	10.09	125.34	120.30
2	B	484	TYR	CB-CG-CD2	-9.55	115.27	121.00
1	A	441	TRP	CD1-CG-CD2	8.99	113.49	106.30
2	B	441	TRP	CD1-CG-CD2	8.75	113.30	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	154	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	A	428	GLU	CA-CB-CG	8.62	132.35	113.40
2	B	840	TRP	CD1-CG-CD2	8.60	113.18	106.30
4	E	154	TRP	CD1-CG-CD2	8.54	113.14	106.30
2	B	546	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	A	597	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	546	TRP	CD1-CG-CD2	8.43	113.04	106.30
2	B	512	TRP	CD1-CG-CD2	8.33	112.96	106.30
2	B	838	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	827	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	302	ARG	NE-CZ-NH2	-8.23	116.19	120.30
2	B	441	TRP	CE2-CD2-CG	-8.22	100.72	107.30
1	A	840	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	A	36	TRP	CD1-CG-CD2	8.17	112.83	106.30
2	B	36	TRP	CE2-CD2-CG	-8.15	100.78	107.30
1	A	445	ARG	NE-CZ-NH2	-8.15	116.23	120.30
4	F	14	LYS	N-CA-C	8.11	132.90	111.00
1	A	625	TRP	CD1-CG-CD2	8.02	112.72	106.30
2	B	840	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	36	TRP	CE2-CD2-CG	-7.93	100.95	107.30
1	A	841	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	A	441	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	597	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	B	597	TRP	CD1-CG-CD2	7.84	112.57	106.30
2	B	546	TRP	CE2-CD2-CG	-7.84	101.03	107.30
2	B	841	TRP	CD1-CG-CD2	7.76	112.51	106.30
2	B	625	TRP	CD1-CG-CD2	7.75	112.50	106.30
2	B	29	TRP	CD1-CG-CD2	7.75	112.50	106.30
4	E	42	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	856	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	546	TRP	CE2-CD2-CG	-7.70	101.14	107.30
2	B	512	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	A	838	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	788	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	804	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	B	841	TRP	CE2-CD2-CG	-7.62	101.21	107.30
4	E	154	TRP	CE2-CD2-CG	-7.57	101.24	107.30
2	B	838	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	734	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	A	512	TRP	CE2-CD2-CG	-7.56	101.25	107.30
2	B	715	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	29	TRP	CD1-CG-CD2	7.54	112.33	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	840	TRP	CE2-CD2-CG	-7.54	101.27	107.30
2	B	597	TRP	CE2-CD2-CG	-7.53	101.28	107.30
2	B	29	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	512	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	A	777	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	838	TRP	CE2-CD2-CG	-7.39	101.39	107.30
2	B	781	LEU	CA-C-N	-7.38	100.96	117.20
4	F	154	TRP	CD1-CG-CD2	7.36	112.19	106.30
2	B	253	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	B	36	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	A	253	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	29	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	625	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	841	TRP	CE2-CD2-CG	-7.20	101.54	107.30
2	B	394	ASN	CA-C-N	-7.20	101.37	117.20
3	D	36	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	B	625	TRP	CE2-CD2-CG	-7.14	101.58	107.30
3	D	94	VAL	CA-CB-CG1	7.10	121.55	110.90
1	A	731	ARG	NE-CZ-NH2	-7.04	116.78	120.30
4	E	16	LYS	CA-CB-CG	7.04	128.88	113.40
1	A	425	PHE	N-CA-CB	6.97	123.15	110.60
2	B	285	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	663	TYR	CB-CG-CD2	-6.96	116.83	121.00
2	B	782	ALA	N-CA-CB	-6.88	100.46	110.10
1	A	428	GLU	N-CA-CB	6.88	122.98	110.60
4	F	91	THR	CA-C-N	6.86	132.28	117.20
1	A	228	ASN	N-CA-C	6.80	129.37	111.00
2	B	437	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	B	302	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	276	ARG	NE-CZ-NH1	6.56	123.58	120.30
4	F	195	GLY	O-C-N	-6.55	112.21	122.70
1	A	788	ARG	NE-CZ-NH2	-6.54	117.03	120.30
4	E	192	LYS	O-C-N	-6.54	112.24	122.70
1	A	276	ARG	NE-CZ-NH2	-6.52	117.04	120.30
3	D	93	ARG	NE-CZ-NH1	6.50	123.55	120.30
4	F	154	TRP	CE2-CD2-CG	-6.49	102.11	107.30
2	B	441	TRP	CB-CG-CD1	-6.47	118.59	127.00
4	E	16	LYS	N-CA-CB	6.42	122.16	110.60
1	A	869	ARG	NE-CZ-NH2	-6.41	117.10	120.30
2	B	469	PHE	CA-C-N	-6.34	103.25	117.20
1	A	425	PHE	CA-C-N	6.33	131.13	117.20
1	A	253	ARG	NE-CZ-NH1	6.31	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	196	ALA	N-CA-C	6.29	127.98	111.00
2	B	809	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	733	ARG	NE-CZ-NH2	6.23	123.41	120.30
2	B	468	GLY	CA-C-N	-6.23	103.50	117.20
3	D	20	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	B	856	ARG	N-CA-C	6.18	127.70	111.00
4	F	195	GLY	CA-C-N	6.18	130.80	117.20
2	B	484	TYR	CB-CG-CD1	6.16	124.70	121.00
2	B	869	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	36	TRP	CG-CD2-CE3	6.09	139.39	133.90
1	A	428	GLU	OE1-CD-OE2	-6.09	115.99	123.30
4	E	80	ARG	NE-CZ-NH2	6.09	123.34	120.30
2	B	512	TRP	CB-CG-CD1	-6.08	119.10	127.00
2	B	484	TYR	CA-CB-CG	6.03	124.86	113.40
2	B	36	TRP	CB-CG-CD1	-5.97	119.25	127.00
1	A	659	VAL	CB-CA-C	-5.95	100.11	111.40
1	A	659	VAL	CA-CB-CG2	5.90	119.76	110.90
2	B	836	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	279	ARG	CA-CB-CG	5.90	126.38	113.40
2	B	706	ARG	NE-CZ-NH2	-5.90	117.35	120.30
4	F	54	HIS	CA-CB-CG	5.89	123.62	113.60
4	F	54	HIS	N-CA-CB	5.87	121.16	110.60
2	B	881	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	B	441	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	A	285	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	168	ARG	NE-CZ-NH1	5.75	123.17	120.30
4	F	94	GLU	CA-CB-CG	5.74	126.03	113.40
1	A	795	VAL	O-C-N	-5.74	113.52	122.70
4	E	57	GLN	CA-C-N	-5.73	104.60	117.20
4	F	187	LEU	N-CA-C	5.72	126.44	111.00
2	B	856	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	465	ASP	CA-C-N	-5.70	104.65	117.20
4	F	14	LYS	CA-C-N	5.69	129.72	117.20
2	B	718	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	795	VAL	CA-CB-CG1	5.68	119.42	110.90
2	B	253	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	36	TRP	CB-CG-CD1	-5.66	119.64	127.00
1	A	273	GLU	N-CA-CB	5.66	120.79	110.60
4	F	188	THR	N-CA-C	5.65	126.25	111.00
3	C	88	TYR	CB-CG-CD2	-5.65	117.61	121.00
4	F	82	THR	CA-CB-CG2	5.63	120.28	112.40
1	A	465	ASP	CB-CG-OD1	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	A	168	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	546	TRP	CB-CG-CD1	-5.54	119.79	127.00
2	B	718	ARG	NE-CZ-NH2	-5.54	117.53	120.30
4	F	73	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	440	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	441	TRP	CG-CD1-NE1	-5.51	104.59	110.10
3	D	124	VAL	CA-CB-CG2	5.50	119.16	110.90
1	A	659	VAL	N-CA-CB	5.49	123.59	111.50
2	B	840	TRP	CG-CD2-CE3	5.49	138.84	133.90
2	B	624	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	795	VAL	N-CA-C	5.46	125.74	111.00
2	B	795	VAL	CA-C-N	5.46	129.21	117.20
2	B	718	ARG	CA-CB-CG	5.43	125.34	113.40
2	B	840	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	827	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	B	14	PHE	CB-CA-C	-5.38	99.64	110.40
1	A	424	ASP	O-C-N	-5.37	114.10	122.70
1	A	227	ALA	N-CA-C	5.37	125.48	111.00
1	A	750	LYS	CA-CB-CG	5.35	125.17	113.40
2	B	841	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	A	838	TRP	CG-CD2-CE3	5.34	138.71	133.90
4	F	80	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	512	TRP	CB-CG-CD1	-5.31	120.09	127.00
2	B	838	TRP	CG-CD2-CE3	5.30	138.67	133.90
2	B	838	TRP	CG-CD1-NE1	-5.29	104.81	110.10
2	B	463	ILE	CA-C-N	5.27	128.80	117.20
1	A	248	PHE	CA-C-N	5.26	126.73	116.20
1	A	441	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	777	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	827	ARG	CA-CB-CG	5.24	124.93	113.40
4	E	154	TRP	CG-CD1-NE1	-5.24	104.86	110.10
4	F	80	ARG	NE-CZ-NH2	5.23	122.91	120.30
2	B	711	LEU	CA-CB-CG	5.22	127.30	115.30
2	B	839	GLN	N-CA-C	5.21	125.08	111.00
1	A	706	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	B	150	PRO	N-CA-CB	-5.19	96.89	102.60
2	B	406	ARG	CA-CB-CG	5.18	124.81	113.40
1	A	520	ASP	N-CA-C	-5.18	97.02	111.00
2	B	840	TRP	CG-CD1-NE1	-5.16	104.94	110.10
4	F	89	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	229	PRO	N-CA-C	5.15	125.49	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	869	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	675	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	530	ARG	NE-CZ-NH2	-5.13	117.74	120.30
4	F	87	GLY	CA-C-N	5.12	128.47	117.20
2	B	441	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	441	TRP	CG-CD2-CE3	5.11	138.50	133.90
2	B	936	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	546	TRP	CG-CD2-CE3	5.09	138.48	133.90
2	B	546	TRP	CG-CD2-CE3	5.08	138.48	133.90
1	A	806	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	512	TRP	CG-CD2-CE3	5.05	138.45	133.90
2	B	726	VAL	CG1-CB-CG2	-5.05	102.81	110.90
2	B	597	TRP	CG-CD2-CE3	5.05	138.44	133.90
4	F	73	PHE	CB-CG-CD2	5.05	124.33	120.80
1	A	408	LYS	CA-CB-CG	5.03	124.46	113.40
4	E	192	LYS	CA-C-N	5.03	128.26	117.20
4	F	91	THR	O-C-N	-5.02	114.67	122.70

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	108	TYR	Sidechain
1	A	127	TYR	Sidechain
1	A	133	TYR	Sidechain
1	A	249	GLY	Peptide
1	A	270	TYR	Sidechain
1	A	276	ARG	Sidechain
1	A	313	TYR	Sidechain
1	A	354	ARG	Sidechain
1	A	359	VAL	Peptide
1	A	362	LEU	Peptide
1	A	424	ASP	Peptide
1	A	427	ILE	Peptide
1	A	432	LYS	Peptide
1	A	663	TYR	Sidechain
1	A	715	ARG	Sidechain
1	A	734	TYR	Sidechain
1	A	746	PHE	Sidechain
1	A	768	ARG	Sidechain
1	A	773	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	804	ARG	Sidechain
1	A	832	TYR	Sidechain
2	B	116	TYR	Sidechain
2	B	127	TYR	Sidechain
2	B	141	TYR	Sidechain
2	B	146	ARG	Sidechain
2	B	193	TYR	Sidechain
2	B	211	GLN	Peptide
2	B	270	TYR	Sidechain
2	B	276	ARG	Sidechain
2	B	302	ARG	Sidechain
2	B	313	TYR	Sidechain
2	B	372	ASN	Peptide
2	B	377	SER	Peptide
2	B	467	ALA	Peptide
2	B	630	ARG	Sidechain
2	B	657	ARG	Sidechain
2	B	683	ARG	Peptide
2	B	691	LYS	Peptide
2	B	719	GLN	Peptide
2	B	733	ARG	Sidechain
2	B	734	TYR	Sidechain
2	B	767	TYR	Sidechain
2	B	768	ARG	Sidechain
2	B	776	PHE	Sidechain
2	B	781	LEU	Peptide
2	B	792	ILE	Peptide
2	B	815	ARG	Sidechain
2	B	817	GLN	Peptide
2	B	832	TYR	Sidechain
2	B	844	PHE	Peptide
2	B	848	LYS	Peptide
2	B	915	ARG	Sidechain
3	D	120	THR	Peptide
3	D	20	ARG	Sidechain
3	D	28	TYR	Sidechain
3	D	36	ARG	Sidechain
3	D	67	GLU	Peptide
3	D	95	PHE	Sidechain
3	D	99	GLY	Peptide
4	E	138	GLY	Peptide
4	E	21	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	E	25	PRO	Peptide
4	F	10	LYS	Peptide
4	F	101	GLU	Peptide
4	F	17	ALA	Peptide
4	F	2	GLY	Peptide
4	F	38	ARG	Sidechain
4	F	52	THR	Peptide
4	F	53	GLN	Peptide
4	F	54	HIS	Peptide
4	F	68	GLN	Peptide
4	F	69	ASP	Peptide
4	F	70	LYS	Peptide
4	F	71	ASP	Peptide
4	F	78	ASP	Peptide
4	F	80	ARG	Peptide
4	F	88	ARG	Peptide
4	F	89	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7601	1759	7638	233	0
2	B	7615	1764	7656	339	0
3	C	1160	251	1126	17	0
3	D	1160	251	1126	56	0
4	E	1522	344	1492	58	0
4	F	1522	344	1492	109	0
All	All	20580	4713	20530	721	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 18.

All (721) 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)
4:E:12:LYS:HA	4:F:68:GLN:HG3	1.41	1.03
2:B:178:GLU:HA	2:B:469:PHE:HB3	1.42	1.01
2:B:375:GLN:HA	2:B:419:THR:HA	1.43	0.99
2:B:238:LYS:HB3	2:B:285:ARG:HB2	1.43	0.99
2:B:856:ARG:HA	2:B:859:GLU:HB2	1.47	0.95
1:A:273:GLU:HA	1:A:478:GLU:HG2	1.46	0.94
4:F:88:ARG:HD2	4:F:89:LEU:HB2	1.46	0.94
1:A:728:GLN:HG3	2:B:395:VAL:HB	1.46	0.94
1:A:33:LYS:HB3	1:A:49:ILE:HB	1.52	0.90
2:B:122:VAL:HA	2:B:683:ARG:HB2	1.52	0.88
2:B:147:HIS:HB3	2:B:782:ALA:HB3	1.54	0.88
2:B:118:GLY:HA3	2:B:717:CYS:HB3	1.54	0.88
4:E:9:LYS:HD3	4:F:81:ALA:HA	1.58	0.84
2:B:729:GLU:HG2	3:D:107:GLU:HG2	1.60	0.84
1:A:367:PHE:HB2	1:A:424:ASP:HB2	1.60	0.83
1:A:487:GLU:HG3	1:A:525:ILE:HG12	1.58	0.83
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.61	0.82
2:B:123:VAL:HG21	2:B:682:VAL:HG12	1.62	0.81
2:B:732:GLN:HB3	3:D:94:VAL:HA	1.63	0.81
2:B:731:ARG:HB2	2:B:753:CYS:HB2	1.63	0.80
2:B:736:ILE:HG12	2:B:795:VAL:HB	1.63	0.79
1:A:822:MET:HA	1:A:825:ILE:HD12	1.65	0.79
4:E:142:CYS:HB3	4:E:147:LEU:HD21	1.62	0.79
4:E:57:GLN:HG3	4:E:58:GLU:HG3	1.65	0.77
2:B:123:VAL:HG11	2:B:186:ASN:HD21	1.50	0.76
2:B:3:GLN:HG3	2:B:17:LYS:HD3	1.67	0.76
2:B:15:VAL:HG12	2:B:112:LEU:HD13	1.68	0.75
4:F:3:ASP:HA	4:F:6:LYS:HB2	1.66	0.75
2:B:727:PHE:HB2	2:B:774:ILE:HB	1.69	0.75
2:B:524:CYS:HB2	2:B:568:LYS:HD3	1.70	0.74
3:D:20:ARG:HH21	3:D:27:LEU:HD11	1.54	0.73
2:B:33:LYS:HB3	2:B:49:ILE:HB	1.68	0.73
1:A:355:VAL:HA	1:A:358:SER:HB2	1.68	0.73
4:F:60:LYS:HA	4:F:63:PHE:HB2	1.69	0.73
1:A:231:LEU:HD21	1:A:442:ILE:HG13	1.69	0.72
1:A:792:ILE:HD12	3:C:94:VAL:HG13	1.72	0.72
2:B:801:ALA:HB2	3:D:43:THR:HG22	1.72	0.72
1:A:610:THR:HG21	1:A:631:ILE:HG13	1.73	0.71
4:F:54:HIS:HB3	4:F:57:GLN:HB2	1.72	0.71
3:D:83:GLY:HA3	3:D:88:TYR:HE2	1.54	0.71
1:A:428:GLU:HB2	1:A:432:LYS:HE3	1.71	0.71
2:B:382:THR:HA	2:B:385:GLN:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:HA	1:A:443:LEU:HD21	1.73	0.70
4:F:11:LYS:HB3	4:F:104:GLY:HA3	1.73	0.70
3:D:119:MET:HB3	3:D:123:GLU:HB2	1.73	0.70
1:A:428:GLU:O	1:A:432:LYS:HG2	1.90	0.70
1:A:754:ILE:HA	1:A:757:ILE:HB	1.74	0.70
1:A:860:MET:SD	2:B:863:MET:SD	2.90	0.70
2:B:496:THR:HB	2:B:679:PRO:HG3	1.73	0.70
4:E:6:LYS:HE2	4:E:32:LYS:HA	1.72	0.70
2:B:402:ILE:HG12	2:B:427:ILE:HD13	1.74	0.70
1:A:840:TRP:HA	4:E:195:GLY:HA3	1.73	0.70
2:B:265:ALA:HB3	2:B:450:LEU:HB3	1.72	0.70
1:A:424:ASP:HA	1:A:427:ILE:HG22	1.74	0.69
2:B:138:ILE:HG21	2:B:196:VAL:HG13	1.74	0.69
1:A:352:ILE:HA	1:A:355:VAL:HB	1.73	0.69
4:F:52:THR:HG21	4:F:56:VAL:HB	1.72	0.69
2:B:124:ILE:HG13	2:B:685:ILE:HB	1.74	0.69
4:F:111:PHE:HA	4:F:114:ILE:HG12	1.75	0.68
1:A:491:GLN:HB2	1:A:525:ILE:HD12	1.74	0.68
2:B:843:LEU:HA	4:F:192:LYS:HA	1.76	0.68
4:F:74:ILE:HB	4:F:106:ILE:HB	1.76	0.68
1:A:339:MET:SD	1:A:352:ILE:HG21	2.34	0.67
2:B:176:THR:OG1	2:B:683:ARG:HA	1.95	0.67
2:B:269:THR:HG22	2:B:443:LEU:HD22	1.76	0.67
2:B:671:MET:SD	2:B:674:LEU:HD12	2.35	0.67
1:A:524:CYS:SG	1:A:585:HIS:HA	2.34	0.67
3:D:95:PHE:HB2	3:D:103:VAL:HG13	1.77	0.67
1:A:437:ARG:HA	1:A:440:ARG:HB2	1.77	0.67
2:B:164:MET:HE2	2:B:171:GLN:HG3	1.76	0.66
1:A:898:LEU:HD21	2:B:899:GLN:HE21	1.60	0.66
2:B:789:ASP:HB3	3:D:116:GLY:HA2	1.78	0.66
2:B:763:ASP:HB3	2:B:766:LEU:HD12	1.77	0.66
4:F:15:LYS:HG2	4:F:102:ALA:HA	1.76	0.66
3:D:54:PRO:HB2	3:D:59:MET:HG2	1.78	0.66
4:F:11:LYS:HA	4:F:103:PRO:O	1.96	0.66
2:B:393:ILE:HD11	2:B:398:PHE:HD1	1.61	0.66
1:A:768:ARG:HB3	1:A:775:PHE:HB2	1.78	0.65
2:B:76:GLN:HB3	2:B:96:ASN:HD21	1.61	0.65
2:B:704:GLN:HA	2:B:707:CYS:SG	2.36	0.65
1:A:880:ARG:HB3	2:B:881:ARG:HD2	1.77	0.65
2:B:671:MET:HG3	2:B:675:ARG:NH1	2.10	0.65
2:B:817:GLN:HB2	4:F:134:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:797:ILE:HG12	3:D:117:GLU:HG2	1.79	0.65
3:D:80:LYS:HD2	3:D:81:ASP:H	1.62	0.65
1:A:139:ASP:HA	1:A:142:LYS:HB2	1.77	0.65
4:F:80:ARG:HD2	4:F:95:LEU:HD21	1.79	0.64
3:D:95:PHE:HD1	3:D:107:GLU:HG3	1.61	0.64
2:B:362:LEU:HD13	2:B:431:ALA:HA	1.78	0.64
1:A:49:ILE:HG23	1:A:57:VAL:HG11	1.79	0.64
1:A:53:LYS:HB2	1:A:56:GLU:HB2	1.80	0.64
4:F:106:ILE:HA	4:F:110:MET:HB3	1.78	0.64
1:A:447:ASN:HA	1:A:450:LEU:HB2	1.80	0.64
2:B:554:SER:HA	2:B:557:GLU:HG2	1.80	0.64
4:F:68:GLN:NE2	4:F:78:ASP:HB2	2.14	0.63
2:B:278:ILE:HG12	2:B:432:LYS:HE2	1.81	0.63
3:C:54:PRO:HB2	3:C:59:MET:HG2	1.81	0.63
4:F:78:ASP:O	4:F:82:THR:HB	1.99	0.63
2:B:503:GLU:HA	2:B:506:GLN:HB2	1.81	0.62
1:A:658:THR:O	1:A:662:LEU:HB3	1.99	0.62
2:B:173:ILE:HG12	2:B:680:ASN:HB2	1.82	0.62
3:D:70:LEU:HG	3:D:74:GLN:HE21	1.65	0.62
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.82	0.62
2:B:535:PRO:HB2	2:B:540:LEU:HG	1.82	0.62
1:A:407:ILE:HG13	1:A:414:VAL:HB	1.82	0.61
3:C:54:PRO:HB3	3:C:58:GLU:HG2	1.80	0.61
3:D:111:VAL:HG13	3:D:115:LEU:HD22	1.82	0.61
2:B:610:THR:HG22	2:B:628:VAL:HG22	1.81	0.61
1:A:425:PHE:CE2	1:A:428:GLU:HG3	2.35	0.61
1:A:729:GLU:HG3	2:B:396:THR:HB	1.83	0.61
2:B:859:GLU:HB3	2:B:863:MET:SD	2.41	0.61
1:A:771:GLN:O	2:B:379:PRO:HA	1.99	0.61
2:B:223:GLN:HB3	2:B:342:MET:SD	2.41	0.61
2:B:266:ASN:HA	2:B:447:ASN:OD1	2.00	0.61
2:B:146:ARG:HB2	2:B:723:ASN:OD1	2.01	0.61
2:B:184:THR:O	2:B:188:LYS:HE3	2.01	0.61
2:B:49:ILE:HG23	2:B:57:VAL:HG11	1.83	0.61
2:B:735:GLU:HA	2:B:756:MET:HE1	1.83	0.61
1:A:426:ALA:HA	1:A:429:ALA:HB3	1.82	0.60
1:A:485:THR:HG23	1:A:667:LEU:HD11	1.82	0.60
2:B:238:LYS:HD3	2:B:285:ARG:HD3	1.83	0.60
2:B:845:THR:HB	4:F:189:LYS:HA	1.83	0.60
4:F:130:ASN:HA	4:F:133:ASN:HB3	1.82	0.60
2:B:153:ILE:HG12	2:B:186:ASN:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:4:ASP:HA	4:E:7:LYS:HD2	1.83	0.60
4:E:37:LYS:HB2	4:F:89:LEU:HD21	1.84	0.60
4:F:13:SER:HA	4:F:15:LYS:N	2.17	0.60
4:F:44:GLY:O	4:F:120:ALA:HA	2.01	0.60
4:E:66:ILE:HA	4:E:82:THR:HG21	1.82	0.60
2:B:852:GLN:O	2:B:853:SER:HB2	2.02	0.60
1:A:667:LEU:O	1:A:671:MET:HB2	2.01	0.59
1:A:817:GLN:HG3	4:E:134:LEU:HB3	1.84	0.59
4:F:8:GLU:HA	4:F:11:LYS:HD2	1.83	0.59
1:A:492:LEU:HD22	1:A:671:MET:SD	2.43	0.59
2:B:804:ARG:NH2	3:D:119:MET:SD	2.75	0.59
4:E:61:GLU:HA	4:E:64:GLN:OE1	2.03	0.59
1:A:175:CYS:SG	1:A:682:VAL:HB	2.43	0.59
1:A:275:SER:OG	1:A:600:LYS:HE2	2.02	0.59
1:A:119:LEU:HB2	1:A:717:CYS:SG	2.43	0.59
2:B:164:MET:SD	2:B:459:SER:HB2	2.43	0.59
2:B:510:ILE:HD12	2:B:768:ARG:HG2	1.84	0.58
2:B:301:MET:HA	2:B:304:ASP:HB2	1.84	0.58
2:B:354:ARG:HB2	2:B:390:LEU:HD22	1.85	0.58
2:B:735:GLU:HA	2:B:756:MET:CE	2.32	0.58
3:D:104:MET:HB3	3:D:107:GLU:HB3	1.85	0.58
2:B:843:LEU:HD13	4:F:196:ALA:HB3	1.85	0.58
3:D:42:PRO:HB3	3:D:76:ILE:HG21	1.86	0.58
2:B:727:PHE:HA	2:B:730:PHE:HB2	1.85	0.58
2:B:437:ARG:HB3	2:B:624:LEU:HB3	1.85	0.58
1:A:290:PHE:HD1	1:A:316:LEU:HD21	1.69	0.58
1:A:707:CYS:SG	1:A:708:ASN:N	2.77	0.58
1:A:870:LEU:HB3	2:B:870:LEU:HB3	1.86	0.58
1:A:163:SER:HB3	1:A:171:GLN:NE2	2.18	0.57
2:B:793:THR:HA	2:B:797:ILE:HB	1.84	0.57
1:A:77:LYS:H	1:A:77:LYS:HD2	1.68	0.57
3:C:38:LEU:HD12	3:C:73:MET:HG3	1.86	0.57
2:B:483:ASN:HA	2:B:486:ASN:HB2	1.85	0.57
4:F:14:LYS:HB3	4:F:103:PRO:HB2	1.86	0.57
4:F:69:ASP:HB2	4:F:73:PHE:HB2	1.85	0.57
1:A:576:LYS:HD2	1:A:577:ASP:H	1.70	0.57
1:A:856:ARG:NH2	2:B:856:ARG:HB3	2.20	0.57
1:A:911:ASP:HB3	1:A:915:ARG:HH21	1.68	0.57
4:E:62:ALA:HA	4:E:65:LEU:HB2	1.87	0.57
1:A:107:ARG:HG2	1:A:112:LEU:HB2	1.85	0.57
1:A:723:ASN:HB2	1:A:776:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:614:ASN:HB2	2:B:628:VAL:HG21	1.87	0.56
2:B:726:VAL:HA	2:B:773:LYS:HA	1.87	0.56
4:F:117:ASP:HA	4:F:120:ALA:HB3	1.87	0.56
2:B:388:CYS:HA	2:B:391:MET:HB2	1.85	0.56
1:A:141:TYR:HA	1:A:149:MET:HG3	1.88	0.56
2:B:306:LEU:HB3	2:B:386:LYS:HE3	1.87	0.56
1:A:556:VAL:HB	1:A:579:THR:HG22	1.87	0.56
1:A:842:ARG:NH1	4:E:194:GLU:HB2	2.21	0.56
2:B:194:LEU:HD12	2:B:198:ALA:HB2	1.86	0.56
2:B:576:LYS:HD2	2:B:577:ASP:H	1.70	0.56
1:A:605:LEU:HD21	1:A:662:LEU:HD22	1.87	0.56
2:B:137:ILE:O	2:B:141:TYR:HB2	2.06	0.56
2:B:140:MET:HB3	2:B:149:MET:HE1	1.88	0.56
1:A:553:THR:HA	1:A:579:THR:HG21	1.87	0.56
1:A:573:LYS:H	1:A:573:LYS:HD2	1.70	0.56
2:B:223:GLN:HG2	2:B:342:MET:HA	1.87	0.56
2:B:614:ASN:ND2	2:B:626:LYS:HA	2.21	0.55
1:A:108:TYR:HE1	1:A:126:PRO:HA	1.72	0.55
2:B:821:ALA:HB1	4:F:131:ALA:HA	1.89	0.55
2:B:833:LEU:H	2:B:833:LEU:HD22	1.72	0.55
1:A:274:LYS:HB2	1:A:432:LYS:HB2	1.88	0.55
2:B:580:GLU:HB3	2:B:593:ASN:HD22	1.72	0.55
1:A:144:LYS:HD2	1:A:148:GLU:HB2	1.89	0.55
2:B:173:ILE:O	2:B:463:ILE:HA	2.06	0.55
1:A:247:ARG:HG3	1:A:273:GLU:HB3	1.88	0.54
2:B:768:ARG:HB3	2:B:775:PHE:HB2	1.89	0.54
4:E:38:ARG:HG2	4:F:88:ARG:HD3	1.90	0.54
1:A:351:SER:HA	1:A:354:ARG:HG2	1.88	0.54
2:B:722:PRO:HD2	2:B:777:ARG:HA	1.88	0.54
4:E:90:CYS:HB2	4:E:95:LEU:HG	1.89	0.54
1:A:809:ARG:HB3	3:C:37:ALA:HA	1.89	0.54
2:B:306:LEU:HD11	2:B:389:HIS:HD2	1.72	0.54
4:E:112:LEU:HA	4:E:115:PHE:HB2	1.89	0.54
2:B:502:GLN:HG2	2:B:512:TRP:CD1	2.41	0.54
4:F:9:LYS:HG2	4:F:12:LYS:HB2	1.89	0.54
4:E:16:LYS:HB3	4:F:68:GLN:O	2.08	0.54
1:A:253:ARG:O	1:A:265:ALA:HA	2.08	0.54
2:B:492:LEU:HD13	2:B:675:ARG:HH21	1.73	0.54
1:A:402:ILE:HG12	1:A:427:ILE:HD13	1.90	0.54
2:B:253:ARG:O	2:B:265:ALA:HA	2.08	0.54
2:B:845:THR:HG21	4:F:188:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:MET:SD	3:C:76:ILE:HD12	2.47	0.54
2:B:610:THR:HG21	2:B:631:ILE:HG13	1.89	0.54
3:D:18:PHE:HB3	3:D:30:GLN:NE2	2.21	0.54
1:A:814:LYS:O	1:A:817:GLN:HG2	2.08	0.54
1:A:491:GLN:HB2	1:A:525:ILE:CD1	2.38	0.53
1:A:734:TYR:HB3	1:A:737:LEU:HD12	1.89	0.53
2:B:99:SER:HA	2:B:102:HIS:HB3	1.91	0.53
2:B:732:GLN:CB	3:D:94:VAL:HA	2.38	0.53
1:A:545:CYS:SG	1:A:602:MET:SD	3.02	0.53
2:B:731:ARG:HD2	2:B:756:MET:HE3	1.90	0.53
2:B:768:ARG:O	2:B:774:ILE:HA	2.08	0.53
2:B:814:LYS:HD3	4:F:137:GLU:HA	1.89	0.53
3:D:132:GLU:HB2	3:D:136:GLY:HA2	1.90	0.53
2:B:323:ILE:HG21	2:B:326:GLN:NE2	2.23	0.53
4:F:8:GLU:O	4:F:11:LYS:HB2	2.09	0.53
1:A:528:ILE:HG12	1:A:538:LEU:HG	1.91	0.53
1:A:704:GLN:HA	1:A:707:CYS:SG	2.48	0.53
1:A:800:GLN:O	1:A:804:ARG:HG3	2.08	0.53
2:B:496:THR:HA	2:B:500:LEU:HB2	1.91	0.53
1:A:818:GLN:O	1:A:821:ALA:HB3	2.09	0.53
2:B:247:ARG:HG3	2:B:273:GLU:HB3	1.91	0.53
2:B:846:LYS:NZ	4:F:191:ALA:HA	2.23	0.53
1:A:178:GLU:O	1:A:183:LYS:NZ	2.41	0.53
1:A:582:CYS:HA	1:A:590:VAL:O	2.09	0.53
2:B:844:PHE:HB3	2:B:845:THR:HG23	1.90	0.53
2:B:433:ALA:O	2:B:437:ARG:HG2	2.08	0.53
1:A:266:ASN:HA	1:A:447:ASN:OD1	2.08	0.53
4:F:42:ARG:NH1	4:F:121:GLY:O	2.42	0.53
1:A:830:ALA:HA	1:A:833:LEU:HD22	1.90	0.52
1:A:839:GLN:HA	4:E:194:GLU:HG2	1.91	0.52
1:A:728:GLN:HE22	2:B:385:GLN:HG3	1.74	0.52
4:F:68:GLN:HB2	4:F:78:ASP:CG	2.30	0.52
1:A:33:LYS:O	1:A:48:SER:HA	2.09	0.52
2:B:191:ILE:HG23	2:B:224:LEU:HG	1.91	0.52
2:B:788:ARG:HG2	2:B:792:ILE:HG12	1.91	0.52
2:B:101:LEU:HD13	2:B:702:LEU:HD13	1.91	0.52
1:A:750:LYS:HG3	1:A:769:ILE:HG21	1.91	0.52
2:B:145:LYS:HB3	2:B:782:ALA:HB1	1.90	0.52
2:B:252:ILE:HB	2:B:463:ILE:HB	1.91	0.52
3:C:8:THR:O	3:C:12:LYS:HG3	2.09	0.52
4:F:106:ILE:HD13	4:F:114:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LEU:HD11	2:B:613:LEU:HD11	1.91	0.52
2:B:480:LEU:HD23	2:B:481:CYS:SG	2.50	0.52
1:A:49:ILE:HD11	1:A:75:ILE:HD12	1.92	0.52
2:B:674:LEU:HA	2:B:677:THR:OG1	2.09	0.52
4:F:69:ASP:CB	4:F:73:PHE:HB2	2.40	0.52
1:A:198:ALA:O	1:A:261:TYR:HA	2.09	0.52
1:A:425:PHE:CD2	1:A:428:GLU:HG3	2.45	0.51
4:F:106:ILE:HD13	4:F:114:ILE:HD13	1.91	0.51
2:B:764:PRO:HA	2:B:767:TYR:HE2	1.75	0.51
3:D:111:VAL:HA	3:D:115:LEU:HD13	1.91	0.51
4:F:73:PHE:O	4:F:74:ILE:HG13	2.10	0.51
2:B:150:PRO:O	2:B:155:ALA:HB2	2.10	0.51
2:B:809:ARG:NH2	3:D:40:GLN:O	2.43	0.51
3:C:15:PHE:HD2	3:C:34:VAL:HG11	1.74	0.51
4:E:73:PHE:HA	4:E:107:ASN:HA	1.91	0.51
4:F:177:LEU:HD11	4:F:182:LYS:HD2	1.92	0.51
2:B:800:GLN:O	2:B:804:ARG:HG3	2.10	0.51
2:B:819:LEU:HD12	3:D:22:GLY:HA2	1.92	0.51
4:E:109:THR:OG1	4:F:70:LYS:HB3	2.10	0.51
1:A:814:LYS:HE3	4:E:134:LEU:O	2.10	0.51
1:A:425:PHE:O	1:A:429:ALA:N	2.44	0.51
2:B:545:CYS:SG	2:B:602:MET:HB2	2.51	0.51
2:B:735:GLU:N	2:B:756:MET:SD	2.84	0.51
2:B:466:ILE:HD13	2:B:489:LEU:HD23	1.92	0.51
2:B:172:SER:HA	2:B:462:GLY:O	2.10	0.50
2:B:583:ILE:HG12	2:B:592:TYR:HE2	1.76	0.50
2:B:671:MET:HG3	2:B:675:ARG:HH12	1.76	0.50
3:D:54:PRO:HB3	3:D:58:GLU:HG2	1.92	0.50
1:A:42:HIS:HD2	1:A:45:GLU:HB3	1.75	0.50
1:A:433:ALA:HA	1:A:436:GLU:HB2	1.92	0.50
2:B:183:LYS:HG2	2:B:466:ILE:HG13	1.92	0.50
1:A:931:LYS:HA	1:A:934:ASN:HD22	1.76	0.50
2:B:405:PRO:HB3	2:B:606:ASN:HD21	1.76	0.50
4:E:51:PHE:HB3	4:F:61:GLU:HG3	1.94	0.50
1:A:49:ILE:HG23	1:A:57:VAL:CG1	2.42	0.50
1:A:233:ALA:O	1:A:288:HIS:HB2	2.11	0.50
1:A:507:ARG:HG2	2:B:372:ASN:ND2	2.26	0.50
2:B:494:ASN:N	2:B:494:ASN:HD22	2.09	0.50
4:F:83:PHE:HB3	4:F:88:ARG:O	2.10	0.50
1:A:537:VAL:HG13	1:A:555:PHE:HZ	1.76	0.50
2:B:148:GLU:O	2:B:150:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:PHE:HB3	2:B:360:LEU:HD21	1.94	0.50
3:D:108:ILE:HD12	3:D:128:VAL:HG12	1.94	0.50
1:A:821:ALA:HB1	4:E:131:ALA:HA	1.94	0.49
2:B:222:LYS:O	2:B:226:GLN:HG2	2.11	0.49
2:B:511:GLU:O	2:B:768:ARG:NH1	2.45	0.49
2:B:919:LEU:HA	2:B:922:ASN:HB3	1.94	0.49
4:E:60:LYS:HE2	4:F:60:LYS:HD3	1.94	0.49
1:A:36:TRP:HA	1:A:45:GLU:O	2.12	0.49
2:B:141:TYR:HB3	2:B:193:TYR:HE2	1.77	0.49
4:E:62:ALA:O	4:E:66:ILE:HB	2.11	0.49
1:A:367:PHE:CE1	1:A:427:ILE:HG21	2.47	0.49
1:A:767:TYR:CD1	1:A:769:ILE:HG12	2.47	0.49
1:A:351:SER:HB3	1:A:390:LEU:HD11	1.94	0.49
1:A:370:GLU:HB2	1:A:376:ALA:HA	1.94	0.49
2:B:152:HIS:HB3	2:B:155:ALA:H	1.77	0.49
2:B:358:SER:HB3	2:B:390:LEU:HB2	1.94	0.49
2:B:727:PHE:HB3	2:B:772:SER:O	2.13	0.49
2:B:766:LEU:HD13	2:B:780:VAL:HG21	1.94	0.49
1:A:659:VAL:HA	1:A:662:LEU:HD23	1.94	0.49
2:B:141:TYR:HB3	2:B:193:TYR:CE2	2.47	0.49
2:B:617:SER:HB2	3:C:99:GLY:HA3	1.94	0.49
2:B:620:PHE:O	2:B:624:LEU:HG	2.13	0.49
2:B:881:ARG:HH11	2:B:881:ARG:HG2	1.78	0.49
3:D:140:TYR:O	3:D:144:VAL:HG23	2.13	0.49
1:A:119:LEU:HD12	1:A:717:CYS:SG	2.52	0.49
1:A:238:LYS:HG3	1:A:243:ASP:HA	1.95	0.49
2:B:734:TYR:CD2	2:B:788:ARG:HD3	2.47	0.49
2:B:847:VAL:HG12	2:B:851:LEU:HD21	1.94	0.49
4:F:78:ASP:HA	4:F:81:ALA:HB3	1.94	0.49
1:A:367:PHE:O	1:A:420:LYS:HG3	2.13	0.49
1:A:729:GLU:OE2	2:B:396:THR:HA	2.12	0.49
4:E:141:LYS:HE2	4:E:178:ILE:HB	1.94	0.49
2:B:813:ALA:O	2:B:816:GLN:HG2	2.12	0.49
4:F:75:SER:HA	4:F:105:PRO:HA	1.94	0.49
1:A:223:GLN:NE2	1:A:449:ALA:HB1	2.28	0.49
2:B:74:ASP:O	2:B:76:GLN:HG3	2.12	0.49
4:E:82:THR:HA	4:E:85:SER:OG	2.11	0.49
2:B:302:ARG:HA	2:B:307:LEU:HD12	1.94	0.48
2:B:851:LEU:HA	4:E:53:GLN:NE2	2.28	0.48
3:C:121:GLU:HA	3:C:124:VAL:HG22	1.95	0.48
4:F:79:ILE:HG23	4:F:83:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:9:LYS:NZ	4:F:80:ARG:HA	2.27	0.48
1:A:956:ASP:O	1:A:959:SER:HB3	2.14	0.48
2:B:150:PRO:HB2	2:B:151:PRO:HD2	1.96	0.48
2:B:404:THR:HG22	2:B:417:ALA:HA	1.95	0.48
2:B:731:ARG:HD2	2:B:756:MET:CE	2.43	0.48
1:A:603:ASP:O	1:A:605:LEU:HD22	2.13	0.48
1:A:813:ALA:HA	1:A:816:GLN:OE1	2.13	0.48
2:B:138:ILE:HG23	2:B:197:VAL:HG23	1.94	0.48
2:B:178:GLU:O	2:B:183:LYS:NZ	2.46	0.48
2:B:108:TYR:HD1	2:B:113:ILE:HG22	1.77	0.48
2:B:727:PHE:CE1	2:B:769:ILE:HD12	2.49	0.48
2:B:805:GLY:O	2:B:809:ARG:HG2	2.14	0.48
1:A:533:ASN:HB3	1:A:534:PRO:HD2	1.96	0.48
1:A:889:VAL:HG11	2:B:258:VAL:HG22	1.95	0.48
2:B:730:PHE:CD1	2:B:774:ILE:HG21	2.47	0.48
1:A:383:ALA:HA	1:A:386:LYS:HD2	1.95	0.48
1:A:583:ILE:HD11	1:A:592:TYR:HE2	1.79	0.48
3:D:8:THR:HG22	3:D:12:LYS:HE3	1.96	0.48
1:A:174:LEU:O	1:A:681:PHE:HA	2.13	0.48
1:A:848:LYS:H	1:A:849:PRO:HD2	1.77	0.48
1:A:95:LEU:HD22	1:A:100:VAL:HG22	1.96	0.47
1:A:421:GLU:O	1:A:425:PHE:HB2	2.14	0.47
1:A:547:PHE:HB3	1:A:550:ALA:HB2	1.97	0.47
1:A:301:MET:HA	1:A:304:ASP:HB2	1.96	0.47
1:A:522:GLN:O	1:A:526:GLU:HG2	2.15	0.47
2:B:123:VAL:HG11	2:B:186:ASN:ND2	2.24	0.47
2:B:364:ASN:HB2	2:B:383:ALA:HA	1.96	0.47
1:A:583:ILE:O	1:A:589:LYS:HA	2.14	0.47
2:B:339:MET:HB3	2:B:344:PHE:HB2	1.96	0.47
2:B:480:LEU:HG	2:B:528:ILE:HD11	1.95	0.47
1:A:923:LYS:HG2	2:B:926:LEU:HD11	1.96	0.47
2:B:789:ASP:OD1	3:D:115:LEU:HA	2.14	0.47
2:B:800:GLN:NE2	3:D:112:LEU:HA	2.29	0.47
3:D:127:LEU:HD11	3:D:147:VAL:HG12	1.96	0.47
1:A:236:ASN:O	1:A:288:HIS:HD2	1.98	0.47
1:A:542:ASP:O	1:A:545:CYS:SG	2.72	0.47
2:B:7:SER:H	2:B:10:GLU:HB2	1.79	0.47
2:B:854:ALA:O	4:F:55:GLN:HB2	2.14	0.47
2:B:135:GLU:HA	2:B:138:ILE:HB	1.97	0.47
2:B:358:SER:OG	2:B:434:LYS:NZ	2.48	0.47
4:E:20:GLU:HG2	4:E:110:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:90:CYS:HA	4:F:94:GLU:HB2	1.96	0.47
1:A:483:ASN:HB2	1:A:592:TYR:OH	2.14	0.47
2:B:104:LEU:HD12	2:B:710:VAL:HG11	1.97	0.47
2:B:792:ILE:HD12	2:B:796:ILE:HB	1.97	0.47
4:F:15:LYS:N	4:F:103:PRO:HD2	2.29	0.47
1:A:269:THR:O	1:A:440:ARG:NH1	2.47	0.47
1:A:274:LYS:HG3	1:A:432:LYS:HD3	1.97	0.47
1:A:524:CYS:SG	1:A:585:HIS:ND1	2.88	0.47
2:B:358:SER:O	2:B:362:LEU:HD12	2.15	0.47
2:B:726:VAL:HG13	2:B:772:SER:O	2.14	0.47
4:F:48:PHE:HB2	4:F:56:VAL:HG23	1.96	0.47
1:A:275:SER:CB	1:A:600:LYS:HE2	2.45	0.47
1:A:365:ILE:HA	1:A:378:MET:HE1	1.97	0.47
1:A:905:GLU:HA	1:A:908:ASN:ND2	2.30	0.47
2:B:237:ALA:HB3	2:B:247:ARG:HD3	1.96	0.47
2:B:323:ILE:HG21	2:B:326:GLN:HE21	1.80	0.47
4:F:106:ILE:CD1	4:F:114:ILE:HG21	2.44	0.47
1:A:256:PHE:O	1:A:458:ALA:N	2.47	0.46
1:A:275:SER:HA	1:A:432:LYS:HZ3	1.80	0.46
1:A:432:LYS:HE2	1:A:432:LYS:HB3	1.74	0.46
2:B:58:THR:HA	2:B:69:THR:HA	1.97	0.46
2:B:121:CYS:O	2:B:123:VAL:HG23	2.15	0.46
2:B:840:TRP:HB3	4:F:118:ARG:HG2	1.96	0.46
3:D:34:VAL:O	3:D:38:LEU:HG	2.14	0.46
3:D:40:GLN:HG3	3:D:42:PRO:HG3	1.97	0.46
2:B:846:LYS:O	2:B:849:PRO:HD2	2.15	0.46
4:E:33:PRO:O	4:E:36:GLN:HG3	2.15	0.46
4:F:2:GLY:O	4:F:5:GLU:HB3	2.15	0.46
2:B:505:TYR:HB3	2:B:510:ILE:HG12	1.97	0.46
3:D:105:GLY:O	3:D:108:ILE:HG22	2.15	0.46
2:B:815:ARG:O	3:D:18:PHE:HA	2.15	0.46
1:A:58:THR:HA	1:A:69:THR:HA	1.97	0.46
1:A:843:LEU:HA	4:E:192:LYS:HA	1.97	0.46
2:B:707:CYS:SG	2:B:708:ASN:N	2.88	0.46
2:B:764:PRO:HA	2:B:767:TYR:CE2	2.50	0.46
2:B:178:GLU:CA	2:B:469:PHE:HB3	2.29	0.46
3:D:80:LYS:HD2	3:D:81:ASP:N	2.28	0.46
4:F:98:MET:HE3	4:F:101:GLU:HB2	1.98	0.46
1:A:734:TYR:CE1	1:A:784:LEU:HB3	2.51	0.46
1:A:762:LEU:HD21	1:A:784:LEU:HD11	1.98	0.46
2:B:783:HIS:CE1	2:B:787:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:ALA:CB	3:D:43:THR:HG22	2.43	0.46
2:B:833:LEU:HD23	2:B:834:LYS:NZ	2.30	0.46
2:B:839:GLN:OE1	4:F:88:ARG:HB3	2.15	0.46
4:E:84:ASP:HB2	4:E:89:LEU:HD21	1.97	0.46
4:F:88:ARG:CD	4:F:89:LEU:HB2	2.32	0.46
2:B:497:MET:HA	2:B:501:GLU:HB3	1.97	0.46
3:D:119:MET:HB2	3:D:124:VAL:HG12	1.98	0.46
4:E:92:GLU:HA	4:E:95:LEU:HD12	1.97	0.46
1:A:355:VAL:O	1:A:359:VAL:HG23	2.15	0.46
1:A:607:ASP:HA	1:A:610:THR:HB	1.98	0.46
2:B:176:THR:HG1	2:B:683:ARG:HA	1.80	0.46
2:B:406:ARG:HB3	2:B:608:ASN:HD21	1.79	0.46
2:B:842:ARG:HB2	4:F:191:ALA:CB	2.45	0.46
4:F:56:VAL:HG12	4:F:108:PHE:CZ	2.51	0.46
1:A:846:LYS:HZ3	4:E:193:GLU:CD	2.19	0.46
2:B:376:ALA:HB3	2:B:420:LYS:HB2	1.98	0.45
2:B:725:ILE:HG21	2:B:781:LEU:HD11	1.98	0.45
2:B:144:LYS:HB3	2:B:149:MET:HG3	1.98	0.45
2:B:438:LEU:HA	2:B:624:LEU:HD22	1.97	0.45
2:B:510:ILE:HG21	2:B:775:PHE:CE1	2.51	0.45
3:D:101:GLY:HA2	3:D:140:TYR:HE2	1.81	0.45
1:A:484:TYR:HD2	1:A:663:TYR:HE2	1.65	0.45
1:A:541:LEU:HA	1:A:544:GLU:HB2	1.98	0.45
1:A:711:LEU:HD22	1:A:711:LEU:H	1.81	0.45
2:B:488:LYS:O	2:B:492:LEU:N	2.50	0.45
1:A:604:PRO:HA	1:A:657:ARG:O	2.16	0.45
2:B:252:ILE:O	2:B:462:GLY:HA2	2.16	0.45
3:D:98:GLU:H	3:D:100:ASN:ND2	2.14	0.45
4:F:59:PHE:N	4:F:59:PHE:CD2	2.84	0.45
2:B:690:GLU:O	2:B:691:LYS:HB3	2.16	0.45
4:F:42:ARG:HH22	4:F:124:GLU:H	1.65	0.45
1:A:387:VAL:HG22	1:A:434:LYS:HD2	1.99	0.45
1:A:603:ASP:HB2	1:A:659:VAL:HA	1.99	0.45
2:B:141:TYR:CD2	2:B:149:MET:SD	3.10	0.45
2:B:572:SER:HB3	2:B:580:GLU:O	2.17	0.45
2:B:669:LYS:HE3	2:B:669:LYS:HB2	1.73	0.45
3:C:51:LEU:HD13	3:C:59:MET:SD	2.56	0.45
4:E:106:ILE:HA	4:E:110:MET:HB3	1.99	0.45
1:A:254:ILE:O	1:A:460:PHE:HA	2.17	0.45
2:B:768:ARG:HA	2:B:768:ARG:HD3	1.79	0.45
1:A:506:GLN:OE1	1:A:514:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ARG:NH1	1:A:662:LEU:HB2	2.31	0.45
2:B:375:GLN:HG3	2:B:419:THR:HG22	1.99	0.45
2:B:497:MET:HA	2:B:501:GLU:CB	2.47	0.45
2:B:753:CYS:HA	2:B:756:MET:SD	2.56	0.45
3:C:69:PHE:HA	3:C:72:MET:SD	2.56	0.45
4:F:54:HIS:CB	4:F:57:GLN:HB2	2.44	0.45
1:A:490:GLN:NE2	1:A:494:ASN:HD21	2.15	0.45
1:A:614:ASN:ND2	1:A:626:LYS:HA	2.32	0.45
1:A:856:ARG:HH22	2:B:856:ARG:HB3	1.82	0.45
2:B:687:PRO:HB2	2:B:696:LEU:HA	2.00	0.45
2:B:753:CYS:HA	2:B:756:MET:HG2	1.99	0.45
4:E:6:LYS:HZ1	4:E:34:PRO:HG3	1.82	0.45
1:A:42:HIS:HB2	1:A:44:PHE:O	2.18	0.44
1:A:762:LEU:HD11	1:A:784:LEU:HD21	1.98	0.44
2:B:158:ASP:HB2	2:B:193:TYR:OH	2.17	0.44
2:B:787:GLU:HG2	2:B:790:LEU:HD22	1.99	0.44
1:A:361:GLN:HA	1:A:364:ASN:HB2	1.99	0.44
1:A:526:GLU:HA	1:A:530:ARG:HB2	1.99	0.44
2:B:108:TYR:HD2	2:B:696:LEU:HD12	1.82	0.44
2:B:167:ASP:HB2	2:B:773:LYS:HE2	1.99	0.44
3:D:35:MET:HG2	3:D:73:MET:SD	2.57	0.44
1:A:429:ALA:HB2	1:A:603:ASP:HA	2.00	0.44
1:A:724:ARG:HB2	1:A:773:LYS:HD3	1.98	0.44
2:B:72:LYS:HA	2:B:75:ILE:HG12	1.98	0.44
2:B:199:SER:CB	2:B:221:GLU:HG2	2.48	0.44
2:B:367:PHE:CE1	2:B:378:MET:HB2	2.52	0.44
2:B:430:LEU:HD11	2:B:613:LEU:CD1	2.47	0.44
2:B:573:LYS:H	2:B:573:LYS:HD2	1.82	0.44
2:B:776:PHE:HB2	2:B:781:LEU:HB2	1.99	0.44
2:B:842:ARG:HB2	4:F:191:ALA:HB3	2.00	0.44
4:F:9:LYS:HA	4:F:12:LYS:N	2.31	0.44
4:F:12:LYS:O	4:F:15:LYS:HB2	2.17	0.44
1:A:375:GLN:HA	1:A:419:THR:HA	1.99	0.44
1:A:948:THR:O	1:A:952:ARG:HG2	2.17	0.44
2:B:6:LEU:HB2	2:B:11:LYS:HG3	2.00	0.44
2:B:120:PHE:HD2	2:B:683:ARG:HG3	1.82	0.44
2:B:218:GLY:O	2:B:222:LYS:NZ	2.49	0.44
4:F:130:ASN:O	4:F:134:LEU:HG	2.18	0.44
1:A:823:LYS:HA	1:A:826:GLN:OE1	2.17	0.44
1:A:854:ALA:O	1:A:858:LYS:HG3	2.18	0.44
2:B:36:TRP:CD1	2:B:78:MET:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:VAL:HG13	2:B:88:ASP:O	2.18	0.44
2:B:826:GLN:HE22	4:F:155:GLY:HA3	1.81	0.44
4:E:11:LYS:HB2	4:F:77:ASN:CB	2.47	0.44
1:A:663:TYR:O	1:A:667:LEU:HB2	2.18	0.44
2:B:120:PHE:CD1	2:B:497:MET:HG2	2.51	0.44
2:B:250:LYS:HD2	2:B:267:ILE:HG23	1.98	0.44
3:C:34:VAL:O	3:C:38:LEU:HG	2.18	0.44
4:E:5:GLU:HG3	4:E:6:LYS:N	2.33	0.44
1:A:357:SER:O	1:A:361:GLN:HB2	2.17	0.44
2:B:407:ILE:HB	2:B:408:LYS:H	1.69	0.44
3:D:21:THR:HA	4:F:154:TRP:HZ2	1.82	0.44
1:A:159:THR:O	1:A:163:SER:HB2	2.17	0.44
1:A:477:PHE:HB3	1:A:600:LYS:HD3	1.99	0.44
2:B:556:VAL:O	2:B:560:ILE:HG12	2.18	0.44
3:D:9:ALA:HA	3:D:12:LYS:HD2	1.99	0.44
1:A:311:ASN:N	1:A:311:ASN:HD22	2.15	0.44
1:A:605:LEU:HD23	1:A:630:ARG:HH12	1.82	0.44
2:B:225:LEU:O	2:B:229:PRO:HD2	2.18	0.44
2:B:839:GLN:HA	4:F:88:ARG:HB2	1.98	0.44
3:C:75:THR:HA	3:C:78:LYS:HZ1	1.83	0.44
1:A:470:GLU:HG2	1:A:482:ILE:HG21	2.00	0.43
1:A:540:LEU:HD21	1:A:562:GLU:HG3	2.00	0.43
2:B:220:LEU:O	2:B:223:GLN:HB2	2.19	0.43
2:B:270:TYR:O	2:B:440:ARG:NH2	2.51	0.43
2:B:578:LYS:HG2	2:B:593:ASN:ND2	2.33	0.43
3:D:103:VAL:HG12	3:D:138:ILE:HB	2.00	0.43
4:E:158:PHE:HB3	4:E:162:GLU:HB2	2.00	0.43
1:A:265:ALA:O	1:A:450:LEU:HB3	2.17	0.43
1:A:428:GLU:HB2	1:A:432:LYS:CE	2.46	0.43
1:A:825:ILE:HG13	4:E:131:ALA:HB1	2.00	0.43
2:B:86:VAL:HG22	2:B:87:GLU:H	1.83	0.43
2:B:153:ILE:HD11	2:B:173:ILE:HG21	2.00	0.43
3:C:119:MET:HB3	3:C:123:GLU:HB2	1.99	0.43
4:E:37:LYS:HD2	4:F:89:LEU:HD22	2.00	0.43
4:F:79:ILE:HG22	4:F:99:VAL:HA	1.99	0.43
4:F:130:ASN:HB3	4:F:134:LEU:HG	2.00	0.43
2:B:114:TYR:CD2	2:B:123:VAL:HG22	2.53	0.43
1:A:554:SER:HA	1:A:557:GLU:HG2	2.00	0.43
2:B:732:GLN:CA	3:D:94:VAL:HA	2.48	0.43
1:A:285:ARG:HD2	1:A:321:VAL:O	2.17	0.43
1:A:420:LYS:HB3	1:A:421:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:795:VAL:O	2:B:799:PHE:N	2.51	0.43
1:A:541:LEU:HD11	1:A:598:LEU:HA	2.01	0.43
1:A:746:PHE:HE1	2:B:303:ASN:HA	1.83	0.43
2:B:497:MET:O	2:B:716:ILE:HG12	2.18	0.43
3:D:140:TYR:HA	3:D:143:LEU:HB3	2.01	0.43
1:A:540:LEU:HD22	1:A:558:LYS:HD3	2.00	0.43
1:A:725:ILE:O	1:A:774:ILE:N	2.52	0.43
2:B:145:LYS:NZ	2:B:789:ASP:OD2	2.52	0.43
2:B:391:MET:HB3	2:B:393:ILE:HG23	2.01	0.43
2:B:817:GLN:HG3	4:F:134:LEU:HB3	2.00	0.43
2:B:839:GLN:O	4:F:195:GLY:HA3	2.19	0.43
2:B:853:SER:HB3	4:F:54:HIS:O	2.19	0.43
4:F:9:LYS:O	4:F:10:LYS:NZ	2.51	0.43
1:A:758:LYS:NZ	1:A:762:LEU:O	2.51	0.43
2:B:800:GLN:HE21	3:D:119:MET:HG2	1.84	0.43
1:A:733:ARG:HG2	1:A:788:ARG:HD3	2.00	0.43
2:B:834:LYS:H	2:B:834:LYS:HD2	1.84	0.43
1:A:805:GLY:O	1:A:809:ARG:HG2	2.18	0.43
2:B:393:ILE:HD11	2:B:398:PHE:CD1	2.47	0.43
2:B:407:ILE:O	2:B:408:LYS:NZ	2.52	0.43
2:B:860:MET:O	2:B:864:LYS:HG2	2.18	0.43
3:D:102:THR:HB	3:D:137:CYS:HB3	2.00	0.43
1:A:842:ARG:HB3	4:E:194:GLU:HB3	2.01	0.42
2:B:11:LYS:NZ	2:B:16:ASP:OD2	2.52	0.42
2:B:17:LYS:HE3	2:B:87:GLU:HG3	2.02	0.42
2:B:139:ASP:HA	2:B:142:LYS:HB2	2.00	0.42
2:B:785:GLU:CD	2:B:788:ARG:HH21	2.22	0.42
4:E:41:GLN:NE2	4:F:87:GLY:O	2.52	0.42
2:B:15:VAL:O	2:B:17:LYS:HG3	2.18	0.42
2:B:351:SER:O	2:B:354:ARG:HG2	2.19	0.42
1:A:437:ARG:HD2	1:A:440:ARG:HD2	2.01	0.42
1:A:603:ASP:HB2	1:A:659:VAL:CA	2.49	0.42
1:A:731:ARG:HH11	2:B:385:GLN:NE2	2.17	0.42
1:A:908:ASN:O	1:A:911:ASP:HB2	2.19	0.42
2:B:14:PHE:CD2	2:B:150:PRO:HG3	2.54	0.42
2:B:663:TYR:O	2:B:667:LEU:N	2.53	0.42
2:B:840:TRP:HA	4:F:195:GLY:HA3	2.00	0.42
1:A:162:ARG:CZ	1:A:162:ARG:HA	2.49	0.42
1:A:238:LYS:HD3	1:A:285:ARG:HD3	2.02	0.42
1:A:429:ALA:O	1:A:433:ALA:HB3	2.19	0.42
2:B:741:ALA:O	2:B:743:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:ALA:HB1	4:E:66:ILE:HD13	2.01	0.42
4:F:12:LYS:HE2	4:F:105:PRO:O	2.19	0.42
1:A:367:PHE:HE1	1:A:378:MET:SD	2.43	0.42
2:B:711:LEU:O	2:B:714:ILE:HB	2.19	0.42
2:B:842:ARG:HD2	4:F:193:GLU:HB2	2.00	0.42
1:A:547:PHE:HB3	1:A:550:ALA:CB	2.48	0.42
1:A:601:ASN:C	1:A:659:VAL:HG23	2.40	0.42
2:B:115:THR:O	2:B:121:CYS:HA	2.19	0.42
2:B:163:SER:OG	2:B:724:ARG:HG3	2.20	0.42
2:B:618:ASP:HB3	2:B:621:VAL:HG23	2.01	0.42
2:B:683:ARG:NH2	2:B:708:ASN:OD1	2.52	0.42
2:B:732:GLN:HB3	3:D:94:VAL:C	2.40	0.42
4:E:60:LYS:HB2	4:E:60:LYS:NZ	2.35	0.42
1:A:251:PHE:O	1:A:267:ILE:HA	2.20	0.42
1:A:602:MET:HG3	1:A:604:PRO:HD3	2.02	0.42
2:B:502:GLN:OE1	2:B:514:PHE:HA	2.19	0.42
2:B:685:ILE:HD12	2:B:704:GLN:HB3	2.01	0.42
2:B:716:ILE:O	2:B:719:GLN:HG2	2.20	0.42
2:B:732:GLN:HB3	3:D:94:VAL:CA	2.41	0.42
2:B:292:TYR:HB3	2:B:332:PHE:HB2	2.00	0.42
2:B:788:ARG:O	2:B:792:ILE:HG12	2.20	0.42
2:B:814:LYS:HE3	2:B:814:LYS:O	2.19	0.42
3:C:53:ASN:N	3:C:54:PRO:HD3	2.34	0.42
3:D:120:THR:O	3:D:124:VAL:HG13	2.20	0.42
4:F:76:LYS:HA	4:F:102:ALA:O	2.20	0.42
1:A:491:GLN:HE22	1:A:520:ASP:HA	1.85	0.42
2:B:339:MET:SD	2:B:349:GLN:HG2	2.60	0.42
2:B:409:VAL:HB	2:B:414:VAL:HG21	2.02	0.42
4:F:16:LYS:H	4:F:100:ALA:HB1	1.85	0.42
2:B:842:ARG:HG3	4:F:193:GLU:HB2	2.01	0.42
2:B:846:LYS:HZ3	4:F:191:ALA:HA	1.83	0.42
3:D:101:GLY:HA2	3:D:140:TYR:CE2	2.54	0.42
4:E:141:LYS:NZ	4:E:173:ASP:O	2.51	0.42
1:A:477:PHE:CZ	1:A:481:CYS:SG	3.13	0.41
1:A:486:ASN:HB3	1:A:586:TYR:OH	2.19	0.41
2:B:97:GLU:CD	2:B:706:ARG:HH21	2.24	0.41
2:B:398:PHE:O	2:B:402:ILE:HB	2.20	0.41
2:B:398:PHE:HA	2:B:609:VAL:HG23	2.02	0.41
2:B:728:GLN:OE1	2:B:749:GLY:HA3	2.20	0.41
3:D:95:PHE:CD2	3:D:108:ILE:HG12	2.55	0.41
4:E:5:GLU:HG3	4:E:6:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:37:LYS:HD2	4:F:89:LEU:CD2	2.50	0.41
1:A:844:PHE:HB2	4:E:190:GLY:O	2.20	0.41
2:B:171:GLN:O	2:B:461:LEU:HA	2.19	0.41
2:B:387:VAL:HG12	2:B:391:MET:SD	2.60	0.41
2:B:400:ARG:HH21	2:B:400:ARG:HD3	1.71	0.41
3:D:46:GLU:O	3:D:49:LYS:HB3	2.21	0.41
4:E:15:LYS:HB2	4:F:69:ASP:OD2	2.20	0.41
4:E:43:SER:HA	4:F:193:GLU:O	2.20	0.41
4:F:91:THR:OG1	4:F:93:GLN:HB3	2.21	0.41
1:A:611:SER:O	1:A:615:GLN:NE2	2.53	0.41
3:D:48:MET:SD	3:D:54:PRO:HD2	2.60	0.41
4:F:16:LYS:N	4:F:100:ALA:O	2.53	0.41
4:F:17:ALA:O	4:F:20:GLU:HB2	2.20	0.41
1:A:361:GLN:HG3	1:A:364:ASN:HB2	2.01	0.41
1:A:444:THR:HG21	1:A:620:PHE:O	2.20	0.41
2:B:100:VAL:HG21	2:B:711:LEU:HD13	2.02	0.41
2:B:145:LYS:CB	2:B:782:ALA:HB1	2.50	0.41
2:B:255:ASN:HD22	2:B:264:GLY:HA3	1.85	0.41
2:B:800:GLN:NE2	3:D:119:MET:HG2	2.35	0.41
1:A:825:ILE:CG1	4:E:131:ALA:HB1	2.51	0.41
2:B:175:CYS:HB2	2:B:183:LYS:HG3	2.02	0.41
2:B:776:PHE:CD1	2:B:781:LEU:HA	2.55	0.41
4:E:28:PRO:HA	4:E:29:PRO:HD3	1.89	0.41
4:E:30:ALA:HA	4:E:37:LYS:HG2	2.02	0.41
4:E:147:LEU:HD12	4:E:177:LEU:HD23	2.01	0.41
1:A:183:LYS:HZ1	1:A:468:GLY:HA3	1.86	0.41
1:A:397:ASP:HA	1:A:400:ARG:NH1	2.35	0.41
1:A:534:PRO:HA	1:A:535:PRO:HD3	1.82	0.41
1:A:686:ILE:HA	1:A:687:PRO:HD2	1.91	0.41
2:B:115:THR:N	2:B:122:VAL:O	2.54	0.41
2:B:255:ASN:HA	2:B:460:PHE:HA	2.02	0.41
2:B:344:PHE:O	2:B:349:GLN:NE2	2.53	0.41
4:E:2:GLY:HA2	4:F:92:GLU:HG2	2.00	0.41
4:F:74:ILE:HG23	4:F:78:ASP:HB3	2.03	0.41
1:A:241:LYS:NZ	1:A:471:ILE:O	2.51	0.41
2:B:141:TYR:HD1	2:B:193:TYR:OH	2.04	0.41
2:B:234:PHE:CE1	2:B:289:ILE:HG12	2.55	0.41
2:B:609:VAL:O	2:B:612:LEU:HB3	2.20	0.41
2:B:727:PHE:CZ	2:B:750:LYS:HA	2.55	0.41
2:B:736:ILE:HG23	2:B:794:ASP:OD1	2.21	0.41
2:B:859:GLU:O	2:B:863:MET:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:142:CYS:HB3	4:F:147:LEU:HD21	2.02	0.41
4:F:171:PRO:HB2	4:F:178:ILE:HG22	2.01	0.41
1:A:199:SER:HB2	1:A:221:GLU:OE2	2.20	0.41
1:A:602:MET:O	1:A:658:THR:HA	2.20	0.41
2:B:33:LYS:O	2:B:48:SER:HA	2.21	0.41
2:B:49:ILE:HG23	2:B:57:VAL:CG1	2.49	0.41
2:B:348:GLU:O	2:B:352:ILE:HG13	2.21	0.41
4:F:12:LYS:HA	4:F:15:LYS:HG3	2.02	0.41
1:A:58:THR:HG22	1:A:69:THR:OG1	2.21	0.41
1:A:280:GLN:HB2	1:A:317:SER:OG	2.20	0.41
1:A:425:PHE:CD2	1:A:599:THR:HB	2.55	0.41
1:A:603:ASP:HB2	1:A:659:VAL:HG22	2.03	0.41
1:A:744:LYS:HA	2:B:303:ASN:OD1	2.20	0.41
1:A:772:SER:OG	1:A:773:LYS:HE3	2.21	0.41
1:A:832:TYR:HE1	1:A:836:ARG:NH1	2.18	0.41
2:B:89:MET:HB3	2:B:714:ILE:HG12	2.02	0.41
2:B:218:GLY:O	2:B:222:LYS:HB2	2.21	0.41
2:B:305:LEU:HD22	2:B:354:ARG:HB3	2.03	0.41
2:B:381:ASN:O	2:B:385:GLN:N	2.51	0.41
2:B:493:PHE:HD2	2:B:494:ASN:ND2	2.19	0.41
2:B:730:PHE:HA	2:B:733:ARG:HD2	2.03	0.41
4:F:31:PRO:HG2	4:F:36:GLN:NE2	2.36	0.41
1:A:339:MET:HB3	1:A:344:PHE:HD1	1.85	0.41
1:A:432:LYS:HA	1:A:435:PHE:HB2	2.03	0.41
1:A:804:ARG:NH2	3:C:119:MET:SD	2.94	0.41
2:B:141:TYR:HA	2:B:149:MET:SD	2.60	0.41
3:D:31:CYS:HB2	3:D:64:LEU:HD11	2.02	0.41
4:F:42:ARG:NH2	4:F:120:ALA:O	2.54	0.41
1:A:52:GLU:OE1	1:A:72:LYS:NZ	2.53	0.40
1:A:401:SER:HB3	1:A:608:ASN:HB3	2.02	0.40
1:A:476:SER:OG	1:A:600:LYS:NZ	2.54	0.40
2:B:361:GLN:NE2	2:B:364:ASN:ND2	2.69	0.40
2:B:393:ILE:HD13	2:B:613:LEU:HG	2.03	0.40
2:B:961:LEU:O	2:B:965:ILE:HG13	2.22	0.40
4:F:76:LYS:HG3	4:F:103:PRO:HA	2.03	0.40
4:F:195:GLY:HA2	4:F:196:ALA:O	2.21	0.40
1:A:563:GLN:OE1	1:A:566:HIS:HD2	2.04	0.40
2:B:6:LEU:HB3	2:B:10:GLU:HB3	2.02	0.40
2:B:189:LYS:HA	2:B:189:LYS:HD3	1.86	0.40
2:B:308:GLU:HG3	2:B:386:LYS:NZ	2.36	0.40
2:B:399:THR:HA	2:B:402:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:731:ARG:NH1	2:B:749:GLY:HA2	2.36	0.40
4:F:68:GLN:HB2	4:F:78:ASP:OD2	2.21	0.40
4:F:95:LEU:HB3	4:F:96:ASP:H	1.76	0.40
1:A:385:GLN:HA	1:A:395:VAL:HG11	2.03	0.40
2:B:15:VAL:HG22	2:B:87:GLU:HG2	2.02	0.40
2:B:162:ARG:NH2	2:B:165:LEU:HD12	2.37	0.40
2:B:176:THR:O	2:B:684:CYS:HB2	2.22	0.40
2:B:204:LYS:NZ	2:B:216:SER:OG	2.52	0.40
2:B:306:LEU:HD11	2:B:389:HIS:CD2	2.54	0.40
2:B:384:ALA:O	2:B:387:VAL:HB	2.22	0.40
2:B:623:ASP:HA	2:B:626:LYS:HD2	2.03	0.40
4:E:129:VAL:HA	4:E:183:PHE:CD2	2.56	0.40
1:A:348:GLU:O	1:A:352:ILE:HG13	2.21	0.40
1:A:720:GLY:O	1:A:777:ARG:NH1	2.53	0.40
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.51	0.40
1:A:729:GLU:CD	1:A:729:GLU:H	2.25	0.40
2:B:487:GLU:OE1	2:B:585:HIS:HA	2.22	0.40
2:B:736:ILE:HG13	2:B:739:ALA:HB2	2.02	0.40
2:B:788:ARG:O	2:B:792:ILE:N	2.54	0.40
2:B:800:GLN:HA	2:B:803:CYS:SG	2.62	0.40
4:F:27:ALA:O	4:F:29:PRO:HD3	2.20	0.40
4:F:114:ILE:O	4:F:118:ARG:N	2.54	0.40
4:F:146:THR:O	4:F:149:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	930/971 (96%)	740 (80%)	153 (16%)	37 (4%)	3 23
2	B	932/973 (96%)	764 (82%)	127 (14%)	41 (4%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	146/150 (97%)	127 (87%)	12 (8%)	7 (5%)	2 21
3	D	146/150 (97%)	122 (84%)	18 (12%)	6 (4%)	3 23
4	E	194/196 (99%)	158 (81%)	24 (12%)	12 (6%)	1 17
4	F	194/196 (99%)	118 (61%)	52 (27%)	24 (12%)	0 5
All	All	2542/2636 (96%)	2029 (80%)	386 (15%)	127 (5%)	4 20

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	181	ALA
1	A	224	LEU
1	A	429	ALA
1	A	533	ASN
1	A	795	VAL
1	A	848	LYS
2	B	16	ASP
2	B	257	ASP
2	B	369	LYS
2	B	407	ILE
2	B	469	PHE
2	B	533	ASN
2	B	735	GLU
2	B	743	PRO
2	B	793	THR
2	B	794	ASP
2	B	837	ASN
2	B	848	LYS
2	B	853	SER
2	B	856	ARG
3	C	100	ASN
3	D	94	VAL
3	D	97	LYS
3	D	116	GLY
3	D	121	GLU
4	E	29	PRO
4	F	11	LYS
4	F	14	LYS
4	F	53	GLN
4	F	54	HIS
4	F	110	MET

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Mol	Chain	Res	Type
4	F	120	ALA
4	F	123	ASP
4	F	125	GLU
4	F	188	THR
1	A	32	LYS
1	A	134	SER
1	A	371	ARG
1	A	508	GLU
1	A	564	GLY
1	A	605	LEU
1	A	670	LEU
1	A	780	VAL
1	A	846	LYS
1	A	860	MET
2	B	77	LYS
2	B	184	THR
2	B	346	GLU
2	B	393	ILE
2	B	511	GLU
2	B	733	ARG
2	B	762	LEU
2	B	813	ALA
2	B	819	LEU
2	B	836	ARG
2	B	854	ALA
3	C	6	GLU
3	C	57	ASP
3	C	77	ALA
4	E	47	VAL
4	E	49	ALA
4	E	55	GLN
4	E	178	ILE
4	F	15	LYS
4	F	70	LYS
4	F	121	GLY
1	A	257	ASP
1	A	288	HIS
1	A	374	ASP
1	A	426	ALA
1	A	574	GLN
1	A	852	GLN
2	B	151	PRO

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Mol	Chain	Res	Type
2	B	565	ASN
2	B	572	SER
2	B	817	GLN
2	B	839	GLN
3	D	57	ASP
4	E	188	THR
4	E	194	GLU
4	F	3	ASP
4	F	17	ALA
4	F	29	PRO
4	F	190	GLY
1	A	151	PRO
1	A	603	ASP
1	A	632	VAL
1	A	717	CYS
1	A	854	ALA
2	B	362	LEU
2	B	564	GLY
2	B	567	ALA
2	B	579	THR
3	D	6	GLU
4	F	82	THR
4	F	195	GLY
1	A	92	LEU
1	A	93	THR
1	A	132	ILE
1	A	469	PHE
1	A	546	TRP
1	A	565	ASN
2	B	531	PRO
4	E	44	GLY
4	E	141	LYS
4	F	12	LYS
4	F	13	SER
4	F	72	GLY
4	F	95	LEU
2	B	379	PRO
2	B	629	ASP
2	B	722	PRO
2	B	725	ILE
3	C	39	GLY
3	C	94	VAL

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Mol	Chain	Res	Type
4	E	105	PRO
1	A	743	PRO
3	C	76	ILE
4	F	44	GLY
4	F	105	PRO
1	A	393	ILE
1	A	413	VAL
4	E	87	GLY
2	B	132	ILE
4	E	140	GLY
2	B	764	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	828/857 (97%)	741 (90%)	87 (10%)	7 24
2	B	829/858 (97%)	719 (87%)	110 (13%)	4 18
3	C	127/129 (98%)	118 (93%)	9 (7%)	14 39
3	D	127/129 (98%)	113 (89%)	14 (11%)	6 22
4	E	162/162 (100%)	146 (90%)	16 (10%)	8 26
4	F	162/162 (100%)	137 (85%)	25 (15%)	2 14
All	All	2235/2297 (97%)	1974 (88%)	261 (12%)	9 21

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	26	GLN
1	A	42	HIS
1	A	51	GLU
1	A	55	ASP
1	A	79	ASN
1	A	96	ASN

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Mol	Chain	Res	Type
1	A	110	SER
1	A	146	ARG
1	A	147	HIS
1	A	162	ARG
1	A	163	SER
1	A	178	GLU
1	A	211	GLN
1	A	214	SER
1	A	222	LYS
1	A	228	ASN
1	A	247	ARG
1	A	259	THR
1	A	266	ASN
1	A	278	ILE
1	A	279	ARG
1	A	280	GLN
1	A	286	THR
1	A	302	ARG
1	A	311	ASN
1	A	312	ASN
1	A	314	THR
1	A	329	ASP
1	A	342	MET
1	A	357	SER
1	A	366	VAL
1	A	375	GLN
1	A	388	CYS
1	A	389	HIS
1	A	396	THR
1	A	408	LYS
1	A	412	ASP
1	A	420	LYS
1	A	425	PHE
1	A	430	LEU
1	A	434	LYS
1	A	435	PHE
1	A	451	ASP
1	A	488	LYS
1	A	495	HIS
1	A	506	GLN
1	A	513	ASN
1	A	522	GLN

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Mol	Chain	Res	Type
1	A	526	GLU
1	A	543	GLU
1	A	547	PHE
1	A	565	ASN
1	A	566	HIS
1	A	568	LYS
1	A	573	LYS
1	A	576	LYS
1	A	577	ASP
1	A	579	THR
1	A	586	TYR
1	A	597	TRP
1	A	603	ASP
1	A	615	GLN
1	A	623	ASP
1	A	624	LEU
1	A	657	ARG
1	A	662	LEU
1	A	699	HIS
1	A	707	CYS
1	A	711	LEU
1	A	715	ARG
1	A	727	PHE
1	A	730	PHE
1	A	748	ASP
1	A	751	GLN
1	A	778	THR
1	A	796	ILE
1	A	833	LEU
1	A	837	ASN
1	A	843	LEU
1	A	856	ARG
1	A	865	GLU
1	A	867	PHE
1	A	869	ARG
1	A	882	LYS
1	A	932	GLU
1	A	956	ASP
2	B	3	GLN
2	B	8	ASP
2	B	14	PHE
2	B	16	ASP

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Mol	Chain	Res	Type
2	B	21	ASN
2	B	26	GLN
2	B	33	LYS
2	B	51	GLU
2	B	52	GLU
2	B	77	LYS
2	B	79	ASN
2	B	103	ASN
2	B	109	PHE
2	B	139	ASP
2	B	150	PRO
2	B	162	ARG
2	B	200	SER
2	B	201	HIS
2	B	222	LYS
2	B	228	ASN
2	B	245	SER
2	B	247	ARG
2	B	266	ASN
2	B	278	ILE
2	B	280	GLN
2	B	286	THR
2	B	302	ARG
2	B	303	ASN
2	B	304	ASP
2	B	311	ASN
2	B	314	THR
2	B	326	GLN
2	B	329	ASP
2	B	347	GLU
2	B	369	LYS
2	B	370	GLU
2	B	371	ARG
2	B	372	ASN
2	B	382	THR
2	B	394	ASN
2	B	396	THR
2	B	399	THR
2	B	402	ILE
2	B	408	LYS
2	B	411	ARG
2	B	412	ASP

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Mol	Chain	Res	Type
2	B	445	ARG
2	B	476	SER
2	B	484	TYR
2	B	494	ASN
2	B	497	MET
2	B	503	GLU
2	B	511	GLU
2	B	513	ASN
2	B	515	ILE
2	B	538	LEU
2	B	543	GLU
2	B	553	THR
2	B	565	ASN
2	B	568	LYS
2	B	570	GLN
2	B	573	LYS
2	B	576	LYS
2	B	577	ASP
2	B	579	THR
2	B	603	ASP
2	B	665	GLU
2	B	675	ARG
2	B	682	VAL
2	B	686	ILE
2	B	691	LYS
2	B	703	GLU
2	B	711	LEU
2	B	716	ILE
2	B	719	GLN
2	B	724	ARG
2	B	728	GLN
2	B	730	PHE
2	B	731	ARG
2	B	733	ARG
2	B	744	LYS
2	B	751	GLN
2	B	760	LEU
2	B	761	GLU
2	B	764	PRO
2	B	778	THR
2	B	781	LEU
2	B	788	ARG

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Mol	Chain	Res	Type
2	B	812	PHE
2	B	814	LYS
2	B	828	ASN
2	B	833	LEU
2	B	834	LYS
2	B	836	ARG
2	B	839	GLN
2	B	843	LEU
2	B	844	PHE
2	B	849	PRO
2	B	852	GLN
2	B	853	SER
2	B	856	ARG
2	B	862	SER
2	B	886	GLU
2	B	907	ASP
2	B	911	ASP
2	B	932	GLU
2	B	939	ASP
2	B	959	SER
2	B	960	GLU
2	B	974	LYS
3	C	25	LYS
3	C	50	VAL
3	C	60	ASN
3	C	67	GLU
3	C	73	MET
3	C	78	LYS
3	C	80	LYS
3	C	82	GLN
3	C	134	SER
3	D	25	LYS
3	D	60	ASN
3	D	73	MET
3	D	78	LYS
3	D	80	LYS
3	D	82	GLN
3	D	90	GLU
3	D	96	ASP
3	D	102	THR
3	D	103	VAL
3	D	108	ILE

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Mol	Chain	Res	Type
3	D	110	HIS
3	D	121	GLU
3	D	132	GLU
4	E	4	ASP
4	E	16	LYS
4	E	29	PRO
4	E	37	LYS
4	E	41	GLN
4	E	51	PHE
4	E	55	GLN
4	E	71	ASP
4	E	108	PHE
4	E	115	PHE
4	E	123	ASP
4	E	126	ASP
4	E	135	PHE
4	E	145	GLU
4	E	173	ASP
4	E	187	LEU
4	F	10	LYS
4	F	29	PRO
4	F	33	PRO
4	F	42	ARG
4	F	48	PHE
4	F	50	MET
4	F	61	GLU
4	F	67	ASP
4	F	69	ASP
4	F	70	LYS
4	F	77	ASN
4	F	84	ASP
4	F	85	SER
4	F	86	LEU
4	F	88	ARG
4	F	89	LEU
4	F	90	CYS
4	F	95	LEU
4	F	110	MET
4	F	118	ARG
4	F	124	GLU
4	F	145	GLU
4	F	165	GLN

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Mol	Chain	Res	Type
4	F	187	LEU
4	F	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	223	GLN
1	A	311	ASN
1	A	312	ASN
1	A	375	GLN
1	A	494	ASN
1	A	565	ASN
1	A	566	HIS
1	A	614	ASN
1	A	615	GLN
1	A	678	ASN
1	A	680	ASN
1	A	728	GLN
1	A	852	GLN
1	A	908	ASN
1	A	922	ASN
2	B	26	GLN
2	B	186	ASN
2	B	223	GLN
2	B	311	ASN
2	B	326	GLN
2	B	361	GLN
2	B	364	ASN
2	B	372	ASN
2	B	385	GLN
2	B	389	HIS
2	B	494	ASN
2	B	506	GLN
2	B	593	ASN
2	B	608	ASN
2	B	614	ASN
2	B	751	GLN
2	B	800	GLN
2	B	818	GLN
2	B	852	GLN
2	B	899	GLN

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Mol	Chain	Res	Type
3	C	7	GLN
3	C	100	ASN
3	D	16	GLN
3	D	74	GLN
3	D	100	ASN
3	D	135	ASN
4	E	57	GLN
4	F	36	GLN
4	F	46	ASN
4	F	93	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

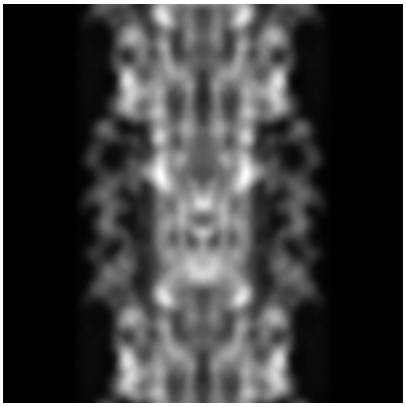
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1950. These allow visual inspection of the internal detail of the map and identification of artifacts.

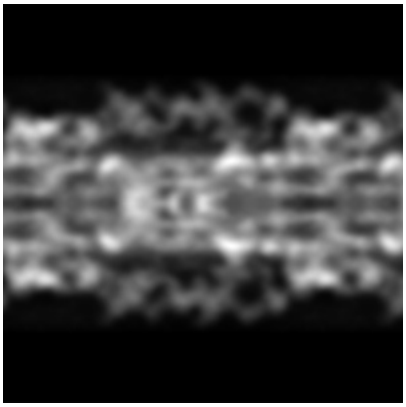
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



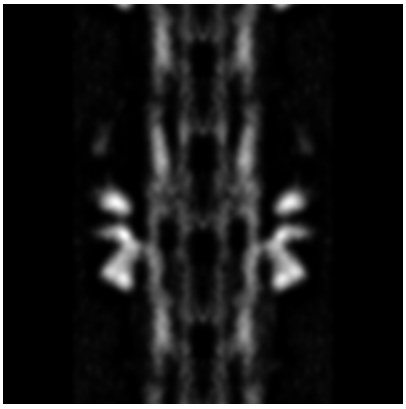
Y

Z

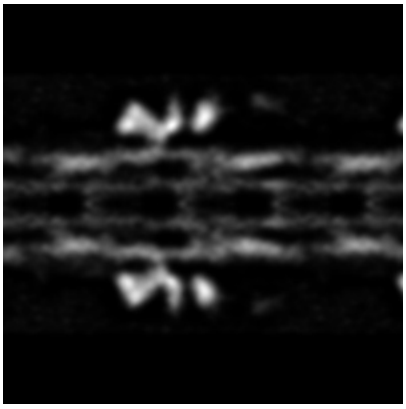
The images above show the map projected in three orthogonal directions.

6.2 Central slices

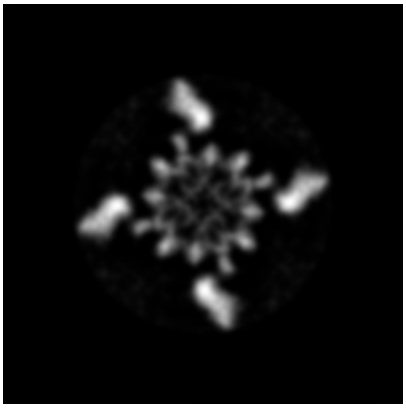
6.2.1 Primary map



X Index: 125



Y Index: 125

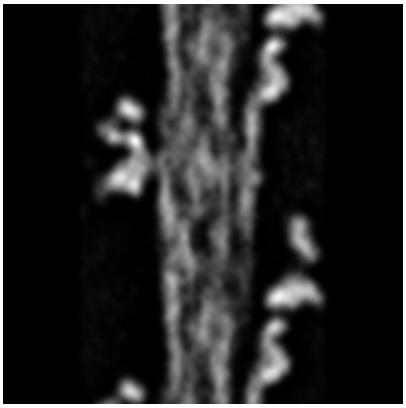


Z Index: 125

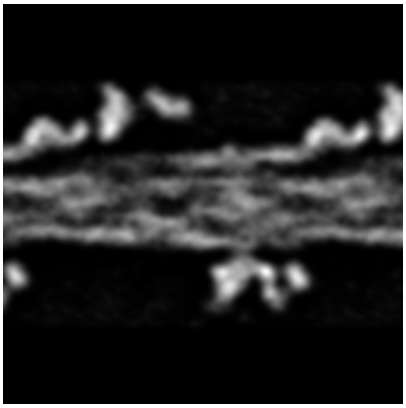
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

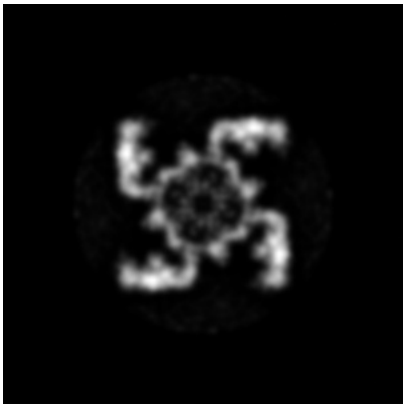
6.3.1 Primary map



X Index: 150



Y Index: 99



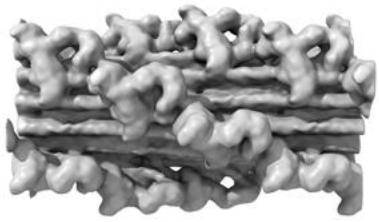
Z Index: 200

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

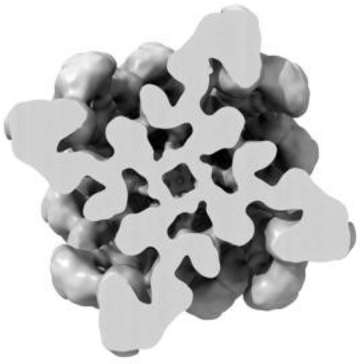
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

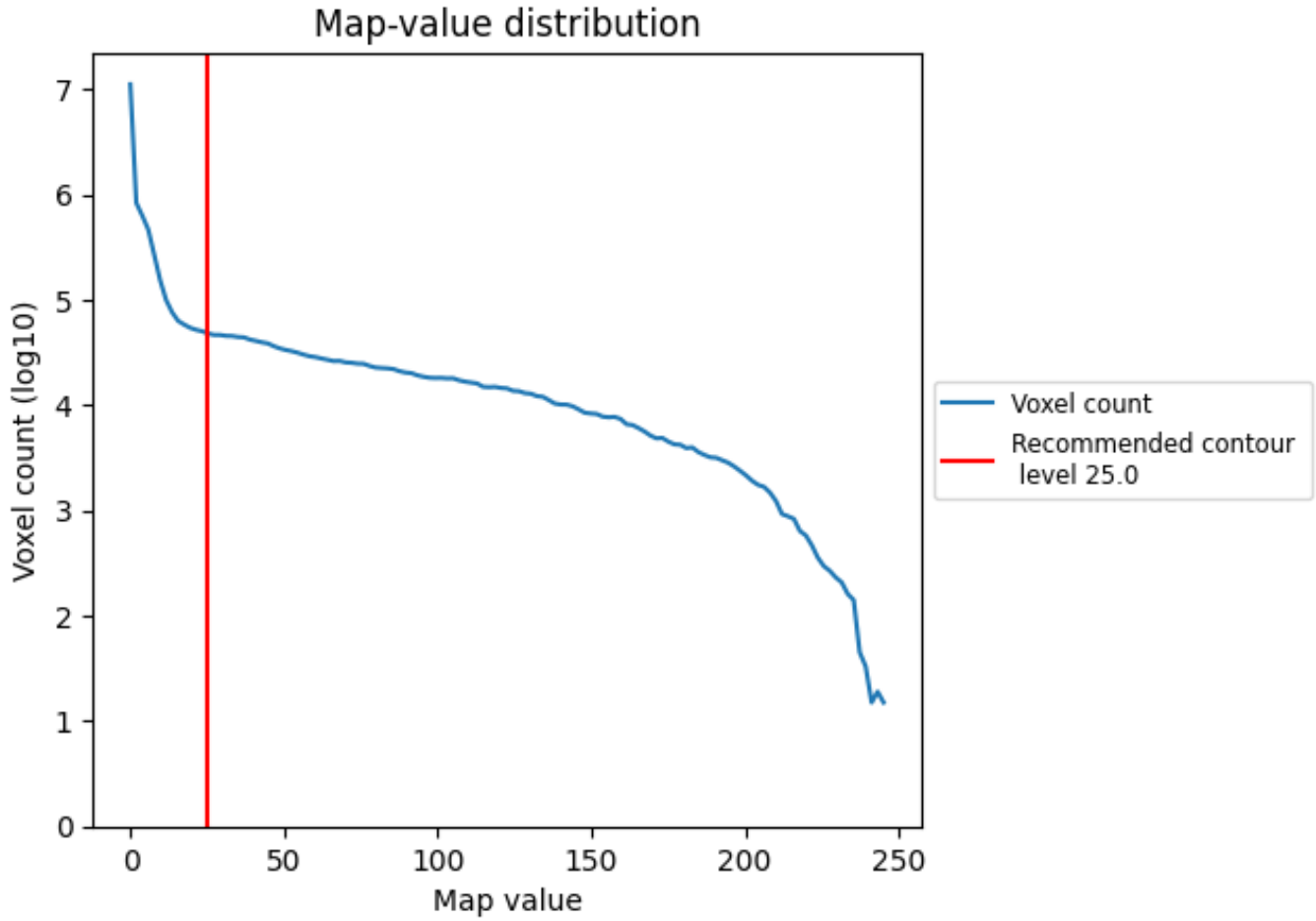
6.5 Mask visualisation (i)

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

7 Map analysis

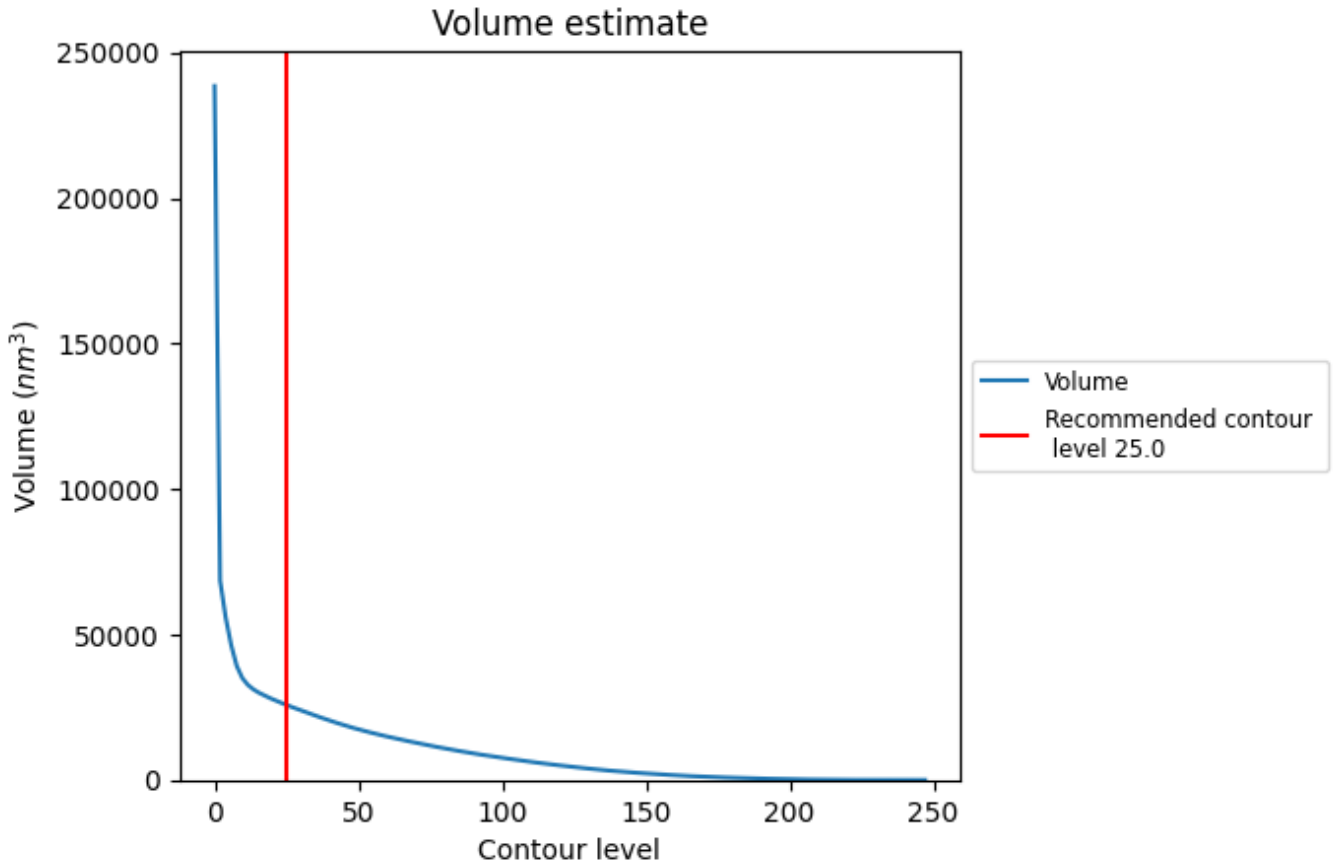
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

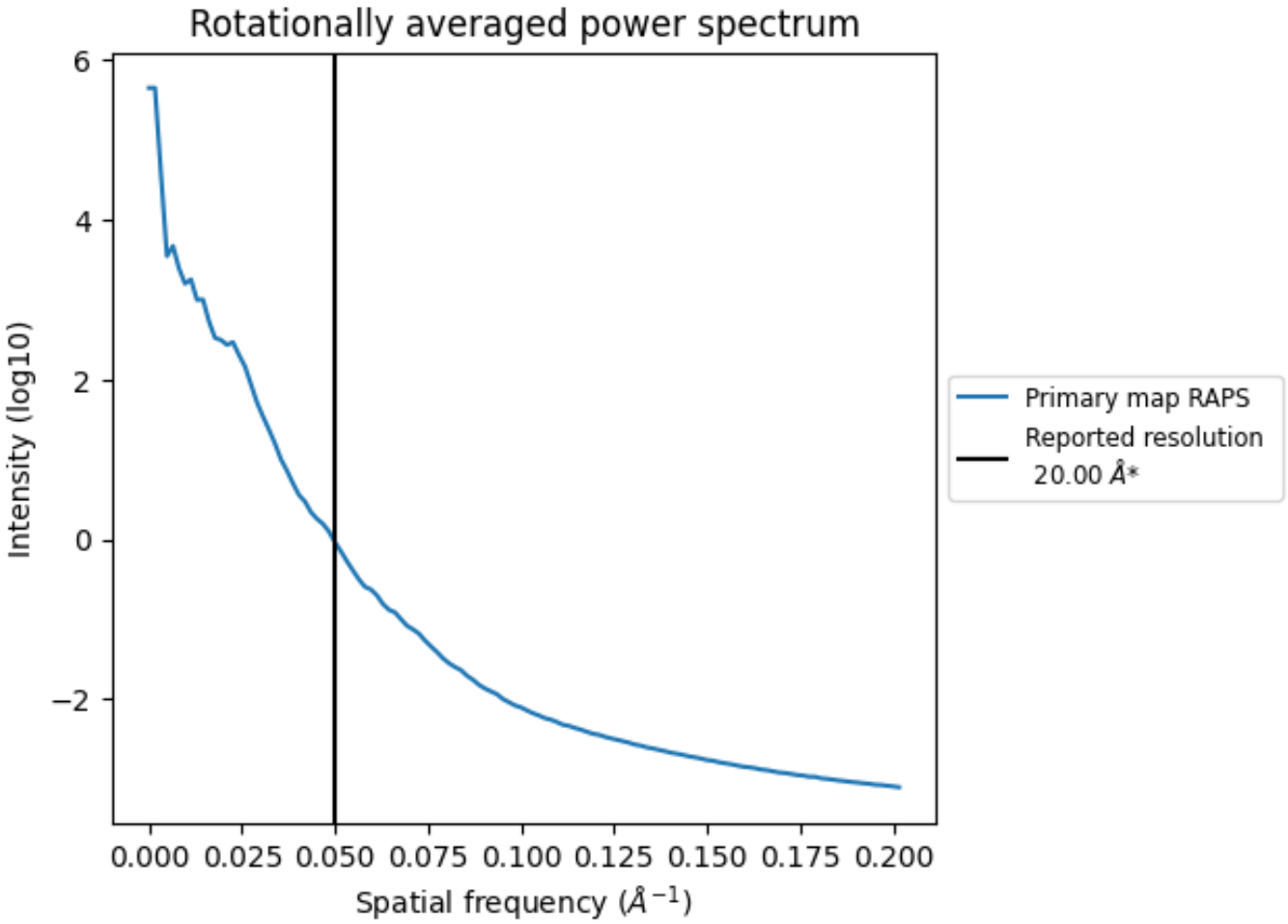
7.2 Volume estimate



The volume at the recommended contour level is 25767 nm^3; this corresponds to an approximate mass of 23276 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 0.050 $Å^{-1}$

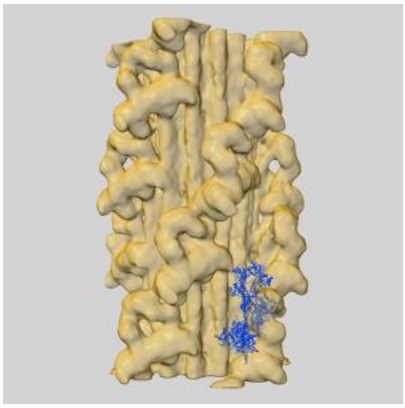
8 Fourier-Shell correlation

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

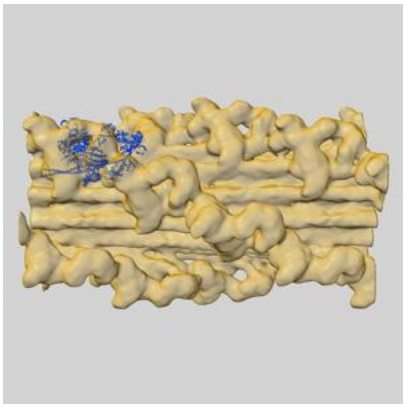
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1950 and PDB model 3DTP. Per-residue inclusion information can be found in section 3 on page 5.

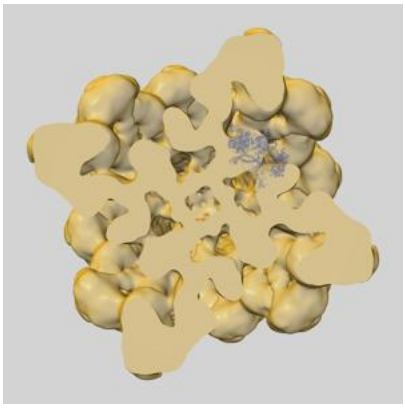
9.1 Map-model overlay



X



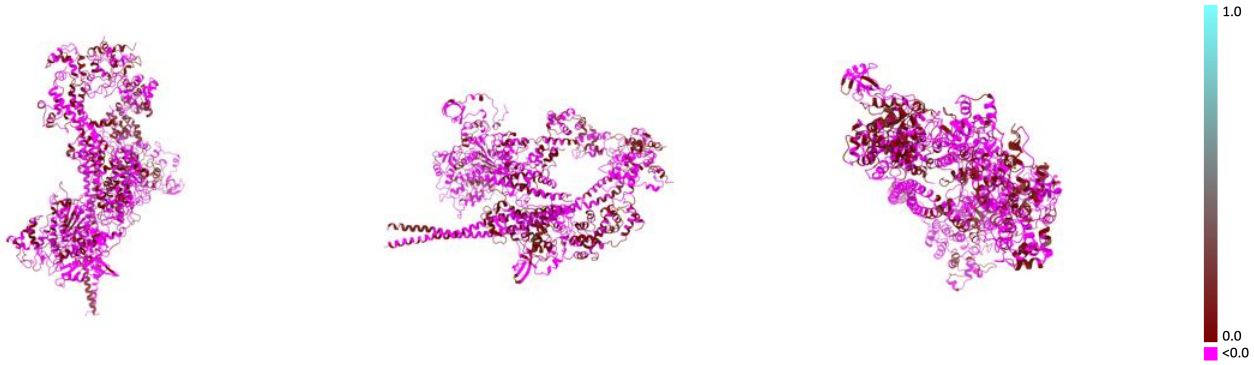
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

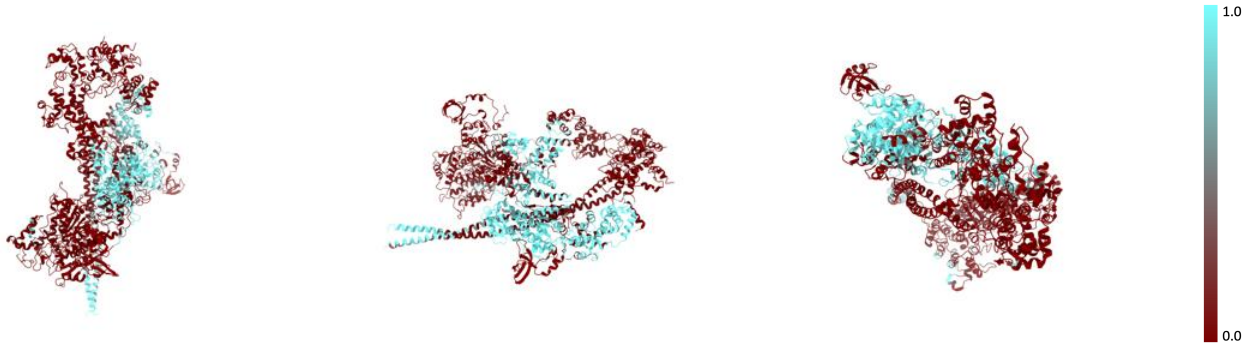
9.2 Q-score mapped to coordinate model



X Y Z

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

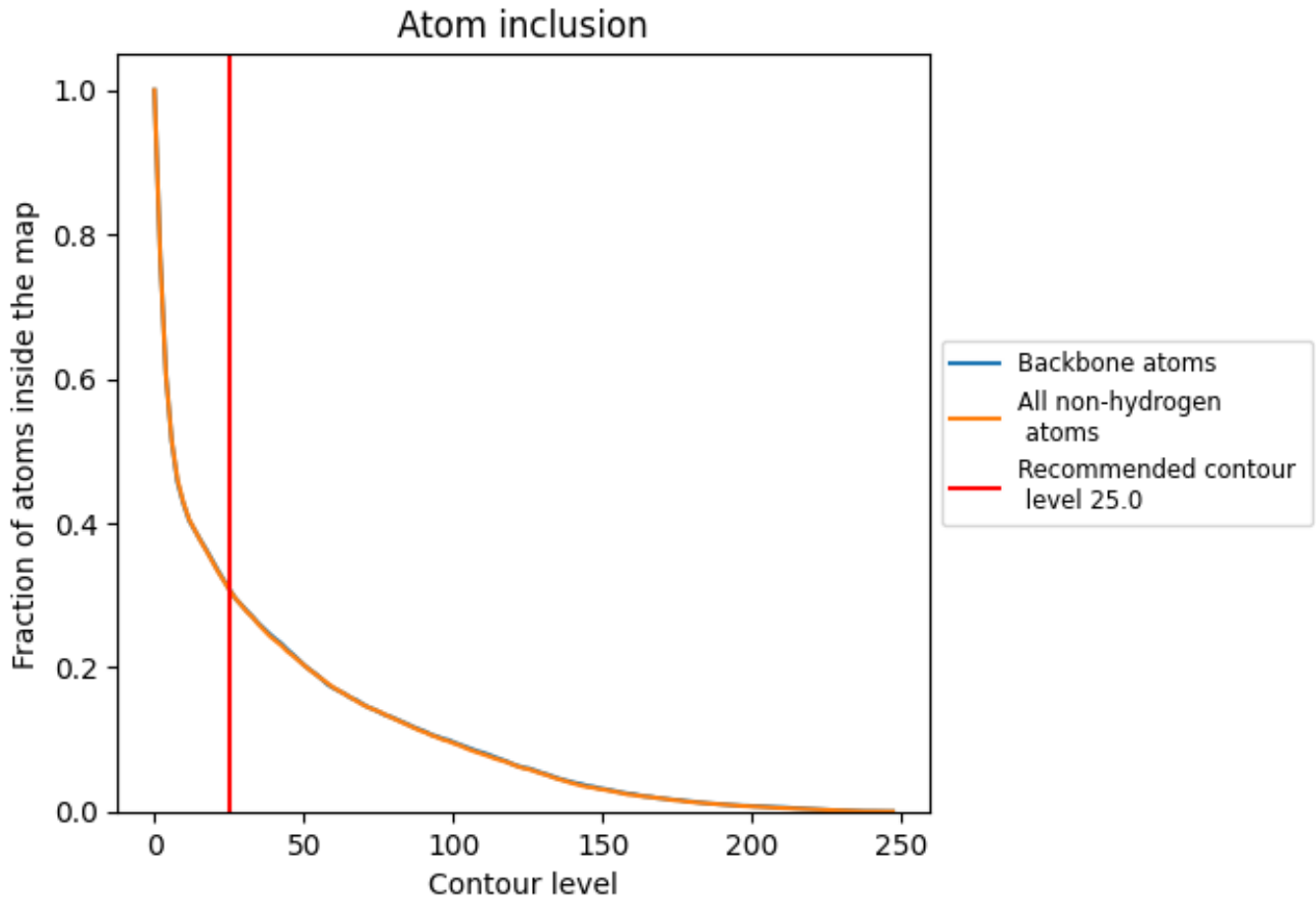
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (25.0).

9.4 Atom inclusion (i)



At the recommended contour level, 31% of all backbone atoms, 31% 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 (25.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3074	-0.0270
A	0.1234	-0.0500
B	0.5666	-0.0170
C	0.2956	-0.0090
D	0.6609	0.0200
E	0.0046	0.0040
F	0.0013	-0.0440