



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:18 AM UTC

PDB ID : 6EM9 / pdb_00006em9
EMDB ID : EMD-3895
Title : S.aureus ClpC resting state, asymmetric map
Authors : Carroni, M.; Mogk, A.; Bukau, B.; Franke, K.
Deposited on : 2017-10-01
Resolution : 8.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

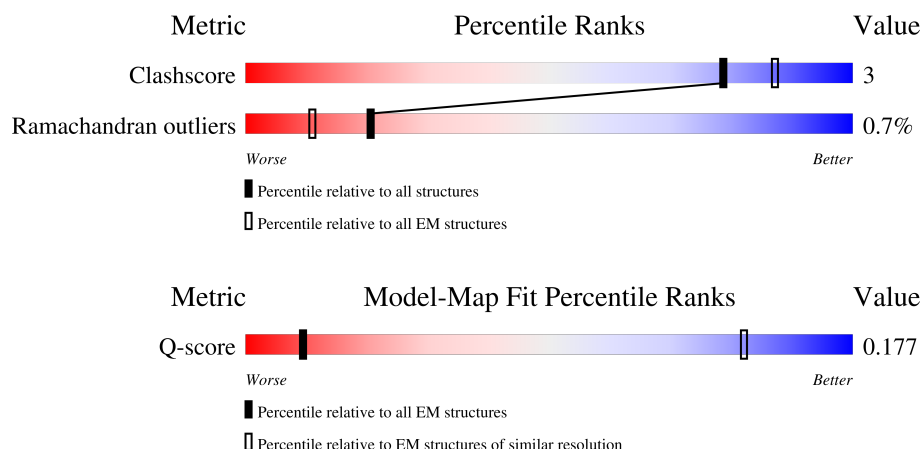
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 8.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	298 (7.90 - 8.90)

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

Mol	Chain	Length	Quality of chain
1	A	818	
1	B	818	
1	C	818	
1	D	818	
1	E	818	

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Mol	Chain	Length	Quality of chain
1	F	818	
1	G	818	
1	H	818	
1	I	818	
1	L	818	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25512 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.

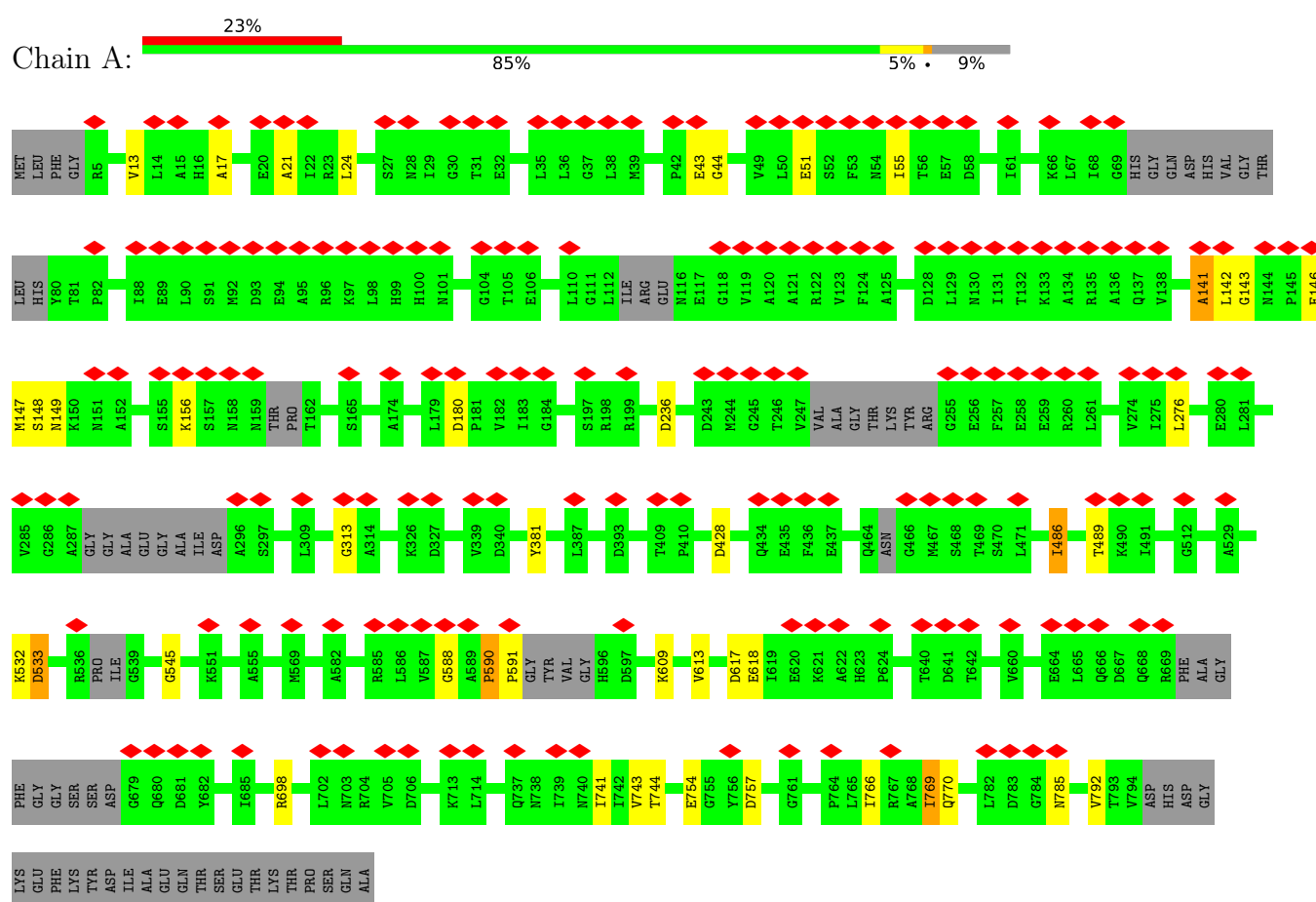
- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpC.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	B	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	C	602	Total	C	N	O	0	0
			2408	1204	602	602		
1	D	436	Total	C	N	O	0	0
			1744	872	436	436		
1	E	664	Total	C	N	O	0	0
			2656	1328	664	664		
1	F	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	G	744	Total	C	N	O	0	0
			2976	1488	744	744		
1	I	436	Total	C	N	O	0	0
			1744	872	436	436		
1	H	602	Total	C	N	O	0	0
			2408	1204	602	602		
1	L	662	Total	C	N	O	0	0
			2648	1324	662	662		

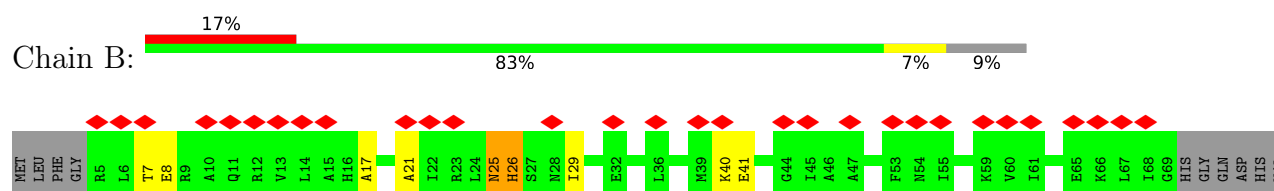
3 Residue-property plots

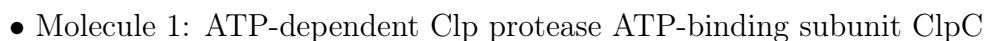
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

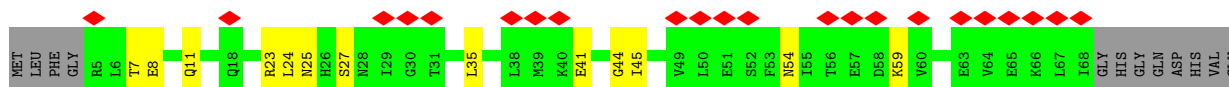
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

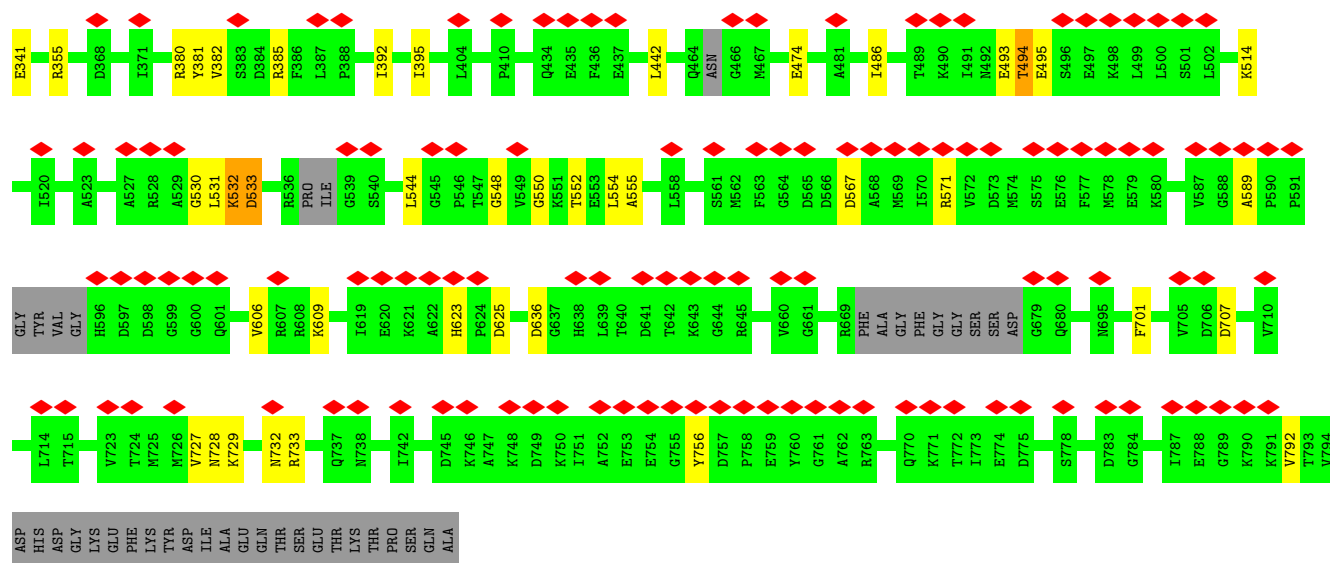


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC

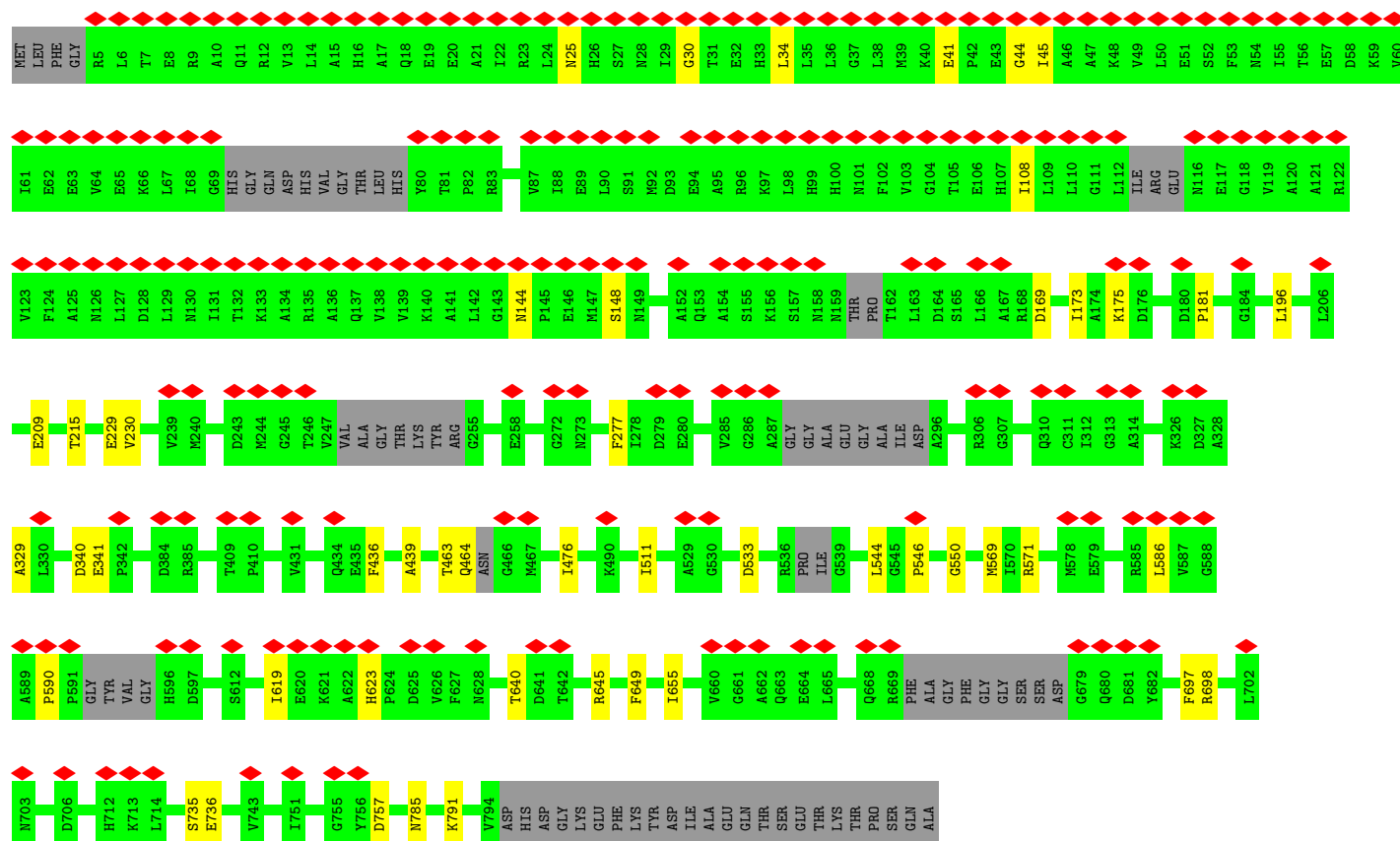
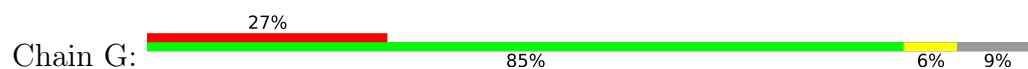






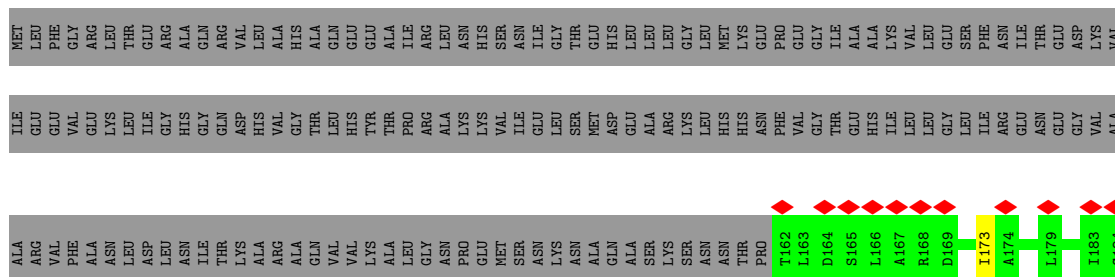
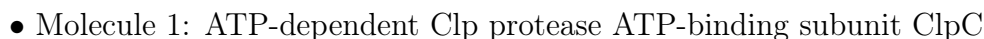


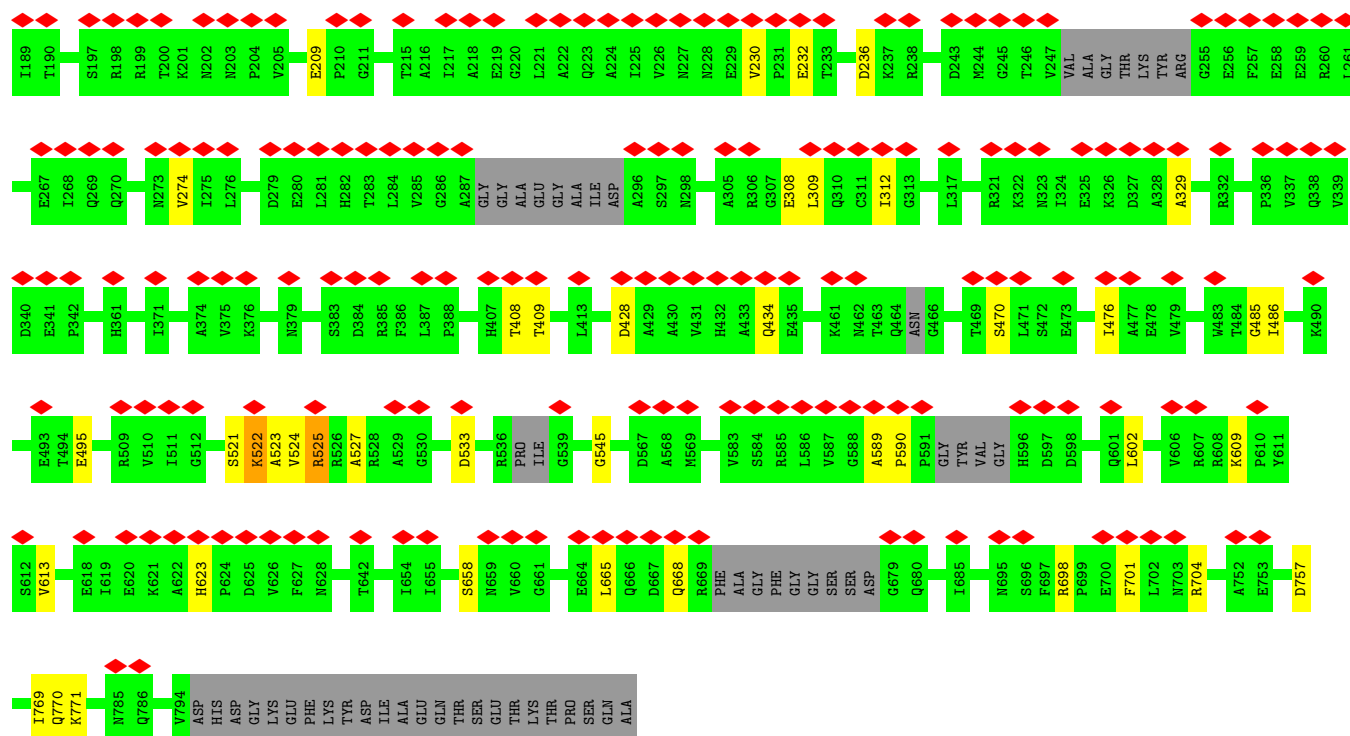
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC



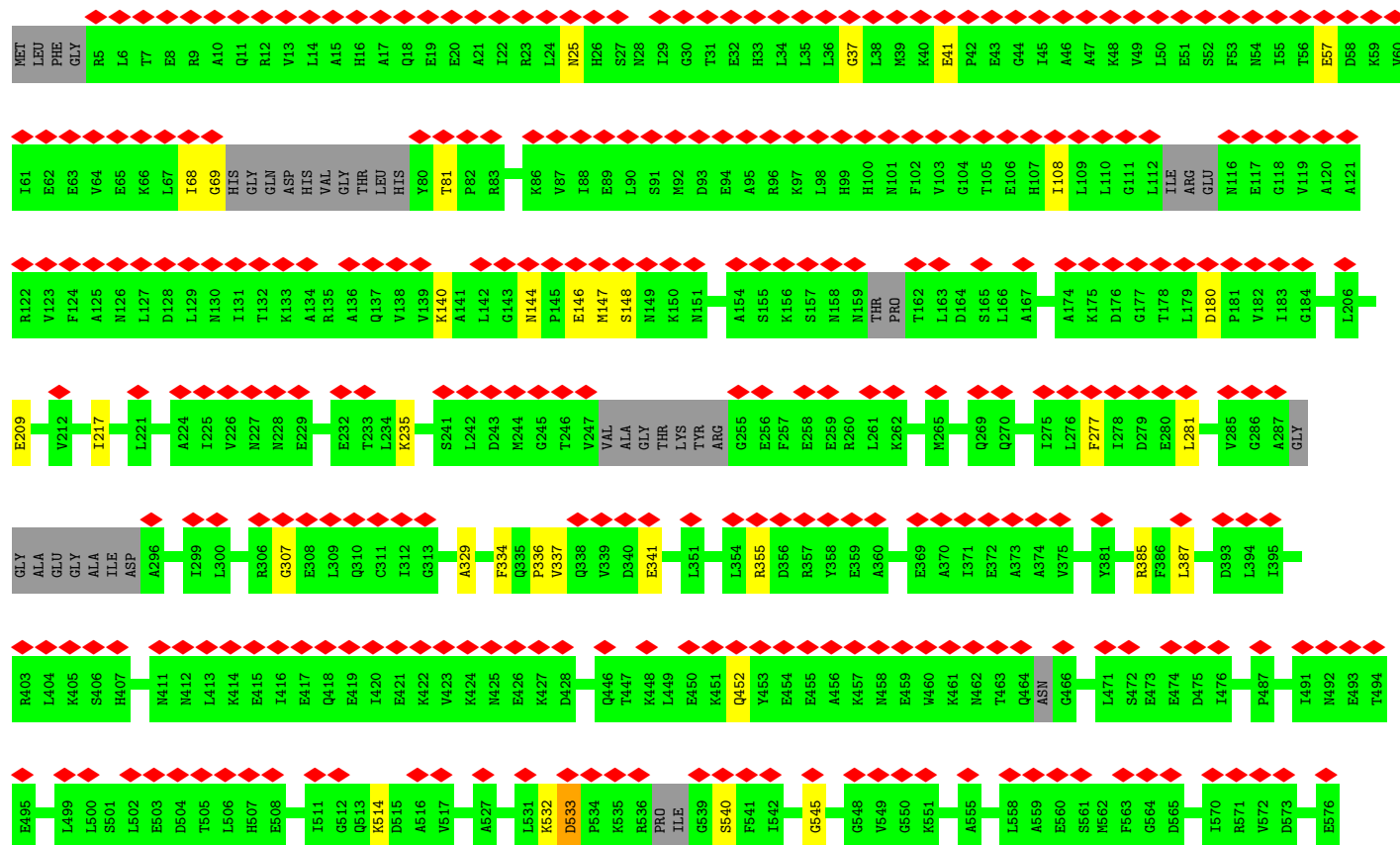
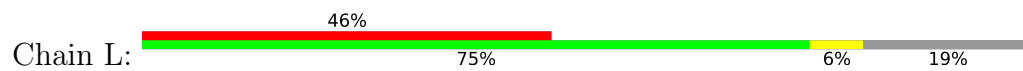
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC







• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.958	Depositor
Minimum map value	-1.477	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	0.92	1/2960 (0.0%)	1.59	36/3672 (1.0%)
1	B	0.94	1/2959 (0.0%)	1.63	54/3669 (1.5%)
1	C	0.94	0/2395	1.66	42/2971 (1.4%)
1	D	1.09	10/1734 (0.6%)	1.75	33/2150 (1.5%)
1	E	0.87	0/2641	1.75	57/3275 (1.7%)
1	F	0.96	2/2960 (0.1%)	1.76	67/3672 (1.8%)
1	G	0.92	0/2959	1.63	48/3669 (1.3%)
1	H	0.90	0/2395	1.68	42/2971 (1.4%)
1	I	1.02	9/1734 (0.5%)	1.68	29/2150 (1.3%)
1	L	0.85	0/2634	1.67	55/3268 (1.7%)
All	All	0.93	23/25371 (0.1%)	1.68	463/31467 (1.5%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	459	GLU	CA-C	10.25	1.62	1.52
1	D	458	ASN	CA-C	8.71	1.64	1.53
1	D	459	GLU	N-CA	7.65	1.55	1.46
1	I	458	ASN	CA-C	7.21	1.62	1.52
1	D	403	ARG	CA-C	6.96	1.61	1.52
1	I	403	ARG	CA-C	6.71	1.61	1.52
1	D	404	LEU	CA-C	6.70	1.58	1.52
1	I	402	VAL	CA-C	6.65	1.59	1.52
1	I	459	GLU	N-CA	6.53	1.54	1.46
1	D	406	SER	CA-C	6.17	1.61	1.52
1	D	402	VAL	CA-C	6.16	1.60	1.52
1	F	495	GLU	N-CA	6.14	1.54	1.46
1	I	405	LYS	CA-C	5.84	1.60	1.52
1	F	494	THR	CA-C	5.71	1.60	1.52
1	D	460	TRP	N-CA	5.60	1.53	1.46
1	I	406	SER	CA-C	5.60	1.60	1.52
1	A	148	SER	N-CA	5.45	1.53	1.46
1	I	459	GLU	CA-C	5.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	ASN	CA-C	5.25	1.58	1.52
1	I	404	LEU	CA-C	5.22	1.59	1.52
1	D	785	ASN	CA-C	5.21	1.57	1.52
1	D	405	LYS	CA-C	5.20	1.59	1.52
1	I	387	LEU	CA-C	5.12	1.57	1.52

All (463) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	402	VAL	N-CA-C	18.11	127.13	111.56
1	C	525	ARG	N-CA-C	12.98	138.45	110.80
1	E	130	ASN	N-CA-C	12.66	124.77	110.97
1	I	402	VAL	N-CA-C	12.23	122.39	112.12
1	C	526	ARG	N-CA-C	11.73	127.78	113.23
1	D	460	TRP	N-CA-C	11.64	125.42	111.33
1	I	460	TRP	N-CA-C	11.10	124.76	111.33
1	F	732	ASN	N-CA-C	10.75	126.53	113.41
1	F	27	SER	N-CA-C	10.57	122.89	111.36
1	H	525	ARG	N-CA-C	-10.38	101.17	114.04
1	A	545	GLY	CA-C-N	10.20	130.00	120.21
1	A	545	GLY	C-N-CA	10.20	130.00	120.21
1	I	405	LYS	N-CA-C	10.13	121.91	111.07
1	I	458	ASN	N-CA-C	10.01	128.63	113.61
1	D	458	ASN	N-CA-C	9.83	127.38	112.54
1	D	461	LYS	N-CA-C	9.59	122.94	111.33
1	F	733	ARG	N-CA-C	9.59	125.34	112.30
1	C	230	VAL	CA-C-N	9.52	129.46	120.03
1	C	230	VAL	C-N-CA	9.52	129.46	120.03
1	I	461	LYS	N-CA-C	9.31	122.60	111.33
1	F	552	THR	N-CA-C	-9.29	101.11	111.14
1	A	533	ASP	CA-C-N	9.28	129.02	119.56
1	A	533	ASP	C-N-CA	9.28	129.02	119.56
1	A	766	ILE	N-CA-C	9.25	119.30	110.42
1	E	533	ASP	CA-C-N	9.21	129.44	119.87
1	E	533	ASP	C-N-CA	9.21	129.44	119.87
1	B	578	MET	N-CA-C	8.98	121.89	111.11
1	E	641	ASP	N-CA-C	8.94	123.70	110.48
1	G	571	ARG	N-CA-C	8.93	123.01	108.99
1	E	642	THR	N-CA-C	-8.89	102.84	114.31
1	L	700	GLU	N-CA-C	-8.80	104.59	114.62
1	F	233	THR	N-CA-C	8.80	124.36	111.96
1	L	545	GLY	CA-C-N	8.75	128.69	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	545	GLY	C-N-CA	8.75	128.69	120.03
1	F	341	GLU	CA-C-N	8.72	128.66	120.03
1	F	341	GLU	C-N-CA	8.72	128.66	120.03
1	H	668	GLN	N-CA-C	-8.67	100.39	112.45
1	E	239	VAL	N-CA-C	8.58	115.39	106.21
1	F	756	TYR	N-CA-C	8.57	122.83	110.24
1	I	403	ARG	N-CA-C	8.52	123.48	112.41
1	B	8	GLU	N-CA-C	8.46	123.44	113.20
1	A	741	ILE	N-CA-C	8.45	120.28	107.77
1	E	25	ASN	N-CA-C	8.45	123.15	111.74
1	C	545	GLY	CA-C-N	8.44	128.94	119.92
1	C	545	GLY	C-N-CA	8.44	128.94	119.92
1	G	533	ASP	CA-C-N	8.44	128.16	119.56
1	G	533	ASP	C-N-CA	8.44	128.16	119.56
1	I	638	HIS	N-CA-C	8.42	122.07	108.76
1	L	638	HIS	N-CA-C	8.33	121.74	109.07
1	A	588	GLY	N-CA-C	8.29	117.75	110.21
1	H	230	VAL	N-CA-C	8.23	116.86	107.89
1	G	108	ILE	N-CA-C	-8.22	102.80	110.53
1	E	27	SER	N-CA-C	8.20	123.10	113.18
1	D	785	ASN	N-CA-C	8.13	123.02	112.12
1	C	274	VAL	N-CA-C	8.09	119.02	108.35
1	E	41	GLU	CA-C-N	8.07	128.26	119.87
1	E	41	GLU	C-N-CA	8.07	128.26	119.87
1	A	146	GLU	N-CA-C	8.07	120.60	109.54
1	G	41	GLU	CA-C-N	8.07	128.26	119.87
1	G	41	GLU	C-N-CA	8.07	128.26	119.87
1	L	540	SER	N-CA-C	8.03	119.22	108.38
1	L	108	ILE	N-CA-C	-8.02	102.44	110.62
1	F	138	VAL	N-CA-C	-7.94	104.98	111.81
1	F	493	GLU	N-CA-C	7.93	122.30	112.47
1	H	545	GLY	CA-C-N	7.92	128.36	120.52
1	H	545	GLY	C-N-CA	7.92	128.36	120.52
1	D	403	ARG	N-CA-C	7.84	125.38	113.61
1	G	30	GLY	N-CA-C	7.82	117.33	110.21
1	G	619	ILE	N-CA-C	7.82	117.77	110.42
1	E	148	SER	N-CA-C	7.80	120.92	109.07
1	D	533	ASP	CA-C-N	7.74	127.45	119.56
1	D	533	ASP	C-N-CA	7.74	127.45	119.56
1	H	698	ARG	CA-C-N	7.72	127.43	119.56
1	H	698	ARG	C-N-CA	7.72	127.43	119.56
1	D	462	ASN	N-CA-C	7.71	120.31	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	ASP	CA-C-N	7.67	127.34	119.82
1	B	533	ASP	C-N-CA	7.67	127.34	119.82
1	A	24	LEU	N-CA-C	7.62	122.07	111.56
1	C	500	LEU	N-CA-C	-7.60	101.89	112.45
1	C	229	GLU	N-CA-C	7.60	120.92	110.06
1	G	697	PHE	N-CA-C	7.60	121.87	109.72
1	L	140	LYS	N-CA-C	-7.58	103.10	111.36
1	A	149	ASN	N-CA-C	7.54	123.44	109.56
1	I	401	LYS	N-CA-C	7.53	122.23	112.89
1	E	531	LEU	N-CA-C	7.52	121.79	111.71
1	D	406	SER	N-CA-C	7.52	126.81	110.80
1	F	131	ILE	N-CA-C	7.52	117.56	111.62
1	L	657	THR	N-CA-C	7.52	119.46	108.86
1	B	412	ASN	N-CA-C	-7.43	102.86	112.23
1	H	589	ALA	CA-C-N	7.43	128.03	120.38
1	H	589	ALA	C-N-CA	7.43	128.03	120.38
1	G	209	GLU	CA-C-N	7.41	127.86	120.52
1	G	209	GLU	C-N-CA	7.41	127.86	120.52
1	A	698	ARG	CA-C-N	7.41	127.76	119.32
1	A	698	ARG	C-N-CA	7.41	127.76	119.32
1	D	484	THR	N-CA-C	-7.39	104.24	113.55
1	F	380	ARG	N-CA-C	7.36	122.97	113.18
1	H	665	LEU	N-CA-C	-7.35	104.30	113.20
1	F	41	GLU	CA-C-N	7.32	127.02	119.56
1	F	41	GLU	C-N-CA	7.32	127.02	119.56
1	H	757	ASP	CA-C-N	7.31	127.02	119.56
1	H	757	ASP	C-N-CA	7.31	127.02	119.56
1	G	169	ASP	N-CA-C	7.31	120.88	110.14
1	E	545	GLY	CA-C-N	7.26	127.21	120.03
1	E	545	GLY	C-N-CA	7.26	127.21	120.03
1	F	382	VAL	N-CA-C	7.20	120.47	108.81
1	E	35	LEU	N-CA-C	-7.17	102.48	112.45
1	C	623	HIS	CA-C-N	7.12	126.83	119.56
1	C	623	HIS	C-N-CA	7.12	126.83	119.56
1	E	362	HIS	N-CA-C	-7.10	104.49	113.72
1	E	640	THR	N-CA-C	7.08	120.22	110.24
1	C	668	GLN	N-CA-C	-7.07	102.99	111.69
1	D	709	ILE	N-CA-C	7.05	118.04	108.17
1	B	130	ASN	N-CA-C	7.03	118.94	111.28
1	B	329	ALA	N-CA-C	-7.01	104.36	113.12
1	C	209	GLU	CA-C-N	7.01	127.18	120.31
1	C	209	GLU	C-N-CA	7.01	127.18	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	THR	CA-C-N	7.00	128.59	119.84
1	E	81	THR	C-N-CA	7.00	128.59	119.84
1	D	628	ASN	N-CA-C	-6.99	103.09	111.69
1	A	147	MET	N-CA-C	6.92	118.71	111.03
1	G	640	THR	N-CA-C	-6.92	100.05	110.28
1	H	428	ASP	N-CA-C	-6.91	103.68	111.07
1	B	306	ARG	N-CA-C	-6.89	106.06	114.75
1	H	476	ILE	N-CA-C	-6.89	102.63	112.35
1	A	769	ILE	N-CA-C	6.88	117.67	110.72
1	D	609	LYS	CA-C-N	6.88	127.03	119.87
1	D	609	LYS	C-N-CA	6.88	127.03	119.87
1	I	533	ASP	CA-C-N	6.88	126.58	119.56
1	I	533	ASP	C-N-CA	6.88	126.58	119.56
1	H	230	VAL	CA-C-N	6.88	126.85	120.03
1	H	230	VAL	C-N-CA	6.88	126.85	120.03
1	H	236	ASP	N-CA-C	-6.88	103.00	111.40
1	B	545	GLY	CA-C-N	6.87	126.83	120.03
1	B	545	GLY	C-N-CA	6.87	126.83	120.03
1	F	495	GLU	N-CA-C	6.86	125.42	110.80
1	C	428	ASP	N-CA-C	-6.84	103.90	111.36
1	L	533	ASP	CA-C-N	6.83	126.52	119.82
1	L	533	ASP	C-N-CA	6.83	126.52	119.82
1	E	274	VAL	N-CA-C	6.82	119.86	108.81
1	B	29	ILE	N-CA-C	6.81	113.50	106.21
1	E	533	ASP	N-CA-C	6.81	119.38	109.71
1	L	387	LEU	N-CA-C	6.80	122.10	113.25
1	L	180	ASP	CA-C-N	6.79	126.76	120.03
1	L	180	ASP	C-N-CA	6.79	126.76	120.03
1	D	401	LYS	N-CA-C	6.78	120.81	112.54
1	C	329	ALA	N-CA-C	-6.77	103.04	112.45
1	E	474	GLU	N-CA-C	6.76	118.65	111.28
1	H	329	ALA	N-CA-C	-6.72	103.11	112.45
1	L	609	LYS	CA-C-N	6.71	126.34	119.56
1	L	609	LYS	C-N-CA	6.71	126.34	119.56
1	C	658	SER	N-CA-C	6.70	119.51	108.99
1	L	341	GLU	CA-C-N	6.70	126.66	119.76
1	L	341	GLU	C-N-CA	6.70	126.66	119.76
1	F	149	ASN	N-CA-C	6.68	120.76	111.74
1	G	215	THR	N-CA-C	-6.67	104.08	111.82
1	H	409	THR	N-CA-C	6.65	119.27	109.62
1	E	323	ASN	CA-C-N	6.64	133.92	121.97
1	E	323	ASN	C-N-CA	6.64	133.92	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ASP	CA-C-N	6.63	126.59	120.03
1	B	180	ASP	C-N-CA	6.63	126.59	120.03
1	L	355	ARG	N-CA-C	6.62	119.33	111.33
1	L	209	GLU	CA-C-N	6.61	126.78	120.31
1	L	209	GLU	C-N-CA	6.61	126.78	120.31
1	C	665	LEU	N-CA-C	-6.54	105.27	113.18
1	F	392	ILE	N-CA-C	-6.52	105.48	111.67
1	C	216	ALA	N-CA-C	-6.48	104.07	112.23
1	F	355	ARG	N-CA-C	6.48	118.03	110.97
1	F	533	ASP	CA-C-N	6.47	126.16	119.56
1	F	533	ASP	C-N-CA	6.47	126.16	119.56
1	F	103	VAL	N-CA-C	6.46	117.37	108.84
1	L	329	ALA	N-CA-C	-6.43	104.47	112.90
1	H	209	GLU	CA-C-N	6.43	126.95	120.14
1	H	209	GLU	C-N-CA	6.43	126.95	120.14
1	I	462	ASN	N-CA-C	6.41	118.10	107.20
1	D	377	LEU	N-CA-C	-6.40	103.82	111.69
1	H	274	VAL	N-CA-C	6.39	117.91	108.45
1	E	151	ASN	N-CA-C	6.39	116.68	108.24
1	I	549	VAL	N-CA-C	-6.39	107.07	113.20
1	H	312	ILE	CA-C-N	-6.38	109.24	121.05
1	H	312	ILE	C-N-CA	-6.38	109.24	121.05
1	B	40	LYS	N-CA-C	6.38	120.33	112.54
1	I	609	LYS	CA-C-N	6.37	126.50	119.87
1	I	609	LYS	C-N-CA	6.37	126.50	119.87
1	F	329	ALA	N-CA-C	-6.37	103.60	112.45
1	H	533	ASP	CA-C-N	6.36	126.05	119.56
1	H	533	ASP	C-N-CA	6.36	126.05	119.56
1	F	532	LYS	N-CA-C	-6.36	101.06	110.46
1	F	623	HIS	CA-C-N	6.36	126.84	119.47
1	F	623	HIS	C-N-CA	6.36	126.84	119.47
1	G	277	PHE	N-CA-C	6.34	118.82	109.24
1	E	589	ALA	CA-C-N	6.34	126.91	120.38
1	E	589	ALA	C-N-CA	6.34	126.91	120.38
1	C	609	LYS	CA-C-N	6.29	125.91	119.56
1	C	609	LYS	C-N-CA	6.29	125.91	119.56
1	E	23	ARG	N-CA-C	-6.20	105.62	113.43
1	F	530	GLY	CA-C-N	-6.20	112.39	120.44
1	F	530	GLY	C-N-CA	-6.20	112.39	120.44
1	A	609	LYS	CA-C-N	6.17	127.13	120.83
1	A	609	LYS	C-N-CA	6.17	127.13	120.83
1	H	470	SER	N-CA-C	6.17	118.34	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ASP	N-CA-C	-6.17	104.48	111.14
1	H	658	SER	N-CA-C	6.16	118.49	108.76
1	B	609	LYS	CA-C-N	6.15	127.28	120.45
1	B	609	LYS	C-N-CA	6.15	127.28	120.45
1	L	514	LYS	N-CA-C	6.14	117.77	111.14
1	B	365	ASN	N-CA-C	6.14	118.95	108.02
1	H	408	THR	N-CA-C	6.14	116.38	108.34
1	G	698	ARG	CA-C-N	6.12	125.81	119.56
1	G	698	ARG	C-N-CA	6.12	125.81	119.56
1	F	550	GLY	N-CA-C	-6.11	107.23	115.36
1	E	204	PRO	CA-C-N	6.10	128.74	120.63
1	E	204	PRO	C-N-CA	6.10	128.74	120.63
1	A	381	TYR	N-CA-C	6.09	117.71	111.14
1	I	709	ILE	N-CA-C	6.08	116.68	108.17
1	B	761	GLY	N-CA-C	-6.07	101.66	112.58
1	G	229	GLU	N-CA-C	-6.07	104.95	112.90
1	B	470	SER	N-CA-C	6.06	118.53	110.53
1	C	701	PHE	N-CA-C	-6.05	104.01	112.12
1	F	494	THR	N-CA-C	6.05	122.12	114.31
1	L	601	GLN	N-CA-C	-6.04	105.14	113.18
1	D	528	ARG	N-CA-C	6.03	118.49	110.53
1	I	406	SER	N-CA-C	6.03	123.63	110.80
1	G	550	GLY	N-CA-C	-6.02	107.09	114.92
1	B	25	ASN	CA-C-N	-6.01	112.17	120.71
1	B	25	ASN	C-N-CA	-6.01	112.17	120.71
1	F	231	PRO	N-CA-C	6.00	124.25	113.70
1	F	149	ASN	CA-C-N	-5.99	112.48	120.63
1	F	149	ASN	C-N-CA	-5.99	112.48	120.63
1	I	384	ASP	N-CA-C	5.99	122.66	113.19
1	D	459	GLU	N-CA-C	5.98	120.14	112.12
1	D	377	LEU	CA-C-N	5.97	128.55	120.38
1	D	377	LEU	C-N-CA	5.97	128.55	120.38
1	H	701	PHE	N-CA-C	-5.96	104.70	111.14
1	A	769	ILE	CA-C-N	-5.93	112.33	120.28
1	A	769	ILE	C-N-CA	-5.93	112.33	120.28
1	E	128	ASP	N-CA-C	-5.93	98.86	108.41
1	F	609	LYS	CA-C-N	5.93	125.61	119.56
1	F	609	LYS	C-N-CA	5.93	125.61	119.56
1	D	613	VAL	N-CA-C	5.93	116.90	108.42
1	A	785	ASN	N-CA-C	-5.92	104.46	111.03
1	I	367	SER	N-CA-C	5.92	118.31	108.13
1	H	434	GLN	CA-C-N	5.92	131.21	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	434	GLN	C-N-CA	5.92	131.21	121.86
1	H	609	LYS	CA-C-N	5.92	126.03	119.87
1	H	609	LYS	C-N-CA	5.92	126.03	119.87
1	B	361	HIS	N-CA-C	5.91	120.02	112.34
1	F	130	ASN	N-CA-C	5.90	118.47	111.33
1	F	339	VAL	N-CA-C	-5.90	99.77	108.85
1	G	329	ALA	N-CA-C	-5.90	104.25	112.45
1	A	143	GLY	N-CA-C	5.88	122.11	110.77
1	D	638	HIS	N-CA-C	5.88	123.32	110.80
1	G	25	ASN	N-CA-C	5.87	119.52	111.54
1	C	613	VAL	CA-C-N	-5.86	115.46	123.14
1	C	613	VAL	C-N-CA	-5.86	115.46	123.14
1	I	401	LYS	CA-C-N	-5.85	116.63	122.77
1	I	401	LYS	C-N-CA	-5.85	116.63	122.77
1	L	57	GLU	N-CA-C	5.83	118.42	111.71
1	C	347	THR	N-CA-C	-5.83	104.83	111.07
1	I	613	VAL	N-CA-C	5.83	116.75	108.42
1	G	645	ARG	N-CA-C	5.82	118.03	109.24
1	E	335	GLN	CA-C-N	5.82	125.72	119.85
1	E	335	GLN	C-N-CA	5.82	125.72	119.85
1	D	402	VAL	CA-C-O	-5.81	115.15	120.73
1	L	41	GLU	CA-C-N	5.81	125.48	119.56
1	L	41	GLU	C-N-CA	5.81	125.48	119.56
1	C	569	MET	N-CA-C	5.80	118.99	109.76
1	L	452	GLN	N-CA-C	5.80	118.31	110.88
1	H	173	ILE	N-CA-C	-5.79	104.68	111.00
1	F	606	VAL	N-CA-C	-5.79	107.21	111.90
1	A	13	VAL	N-CA-C	-5.78	104.72	110.62
1	L	81	THR	CA-C-N	5.78	126.17	119.47
1	L	81	THR	C-N-CA	5.78	126.17	119.47
1	L	704	ARG	N-CA-C	-5.76	105.45	112.88
1	G	569	MET	CA-C-N	5.76	130.19	122.93
1	G	569	MET	C-N-CA	5.76	130.19	122.93
1	B	26	HIS	N-CA-C	-5.72	101.93	110.23
1	C	757	ASP	CA-C-N	5.72	126.99	119.84
1	C	757	ASP	C-N-CA	5.72	126.99	119.84
1	F	37	GLY	CA-C-N	5.71	128.19	120.65
1	F	37	GLY	C-N-CA	5.71	128.19	120.65
1	B	181	PRO	CA-C-N	5.70	129.07	120.75
1	B	181	PRO	C-N-CA	5.70	129.07	120.75
1	B	387	LEU	N-CA-C	5.69	120.23	112.55
1	G	173	ILE	N-CA-C	-5.67	104.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	623	HIS	CA-C-N	5.67	126.05	119.47
1	E	623	HIS	C-N-CA	5.67	126.05	119.47
1	E	534	PRO	N-CA-C	5.66	120.99	114.03
1	G	34	LEU	N-CA-C	-5.65	104.60	112.45
1	F	81	THR	CA-C-N	5.64	126.89	119.84
1	F	81	THR	C-N-CA	5.64	126.89	119.84
1	A	55	ILE	N-CA-C	5.64	115.97	107.80
1	I	484	THR	N-CA-C	-5.64	106.76	113.97
1	L	277	PHE	N-CA-C	5.64	118.91	109.95
1	B	568	ALA	N-CA-C	-5.63	106.38	113.20
1	A	276	LEU	N-CA-C	5.63	117.91	108.73
1	B	7	THR	N-CA-C	-5.63	103.48	110.41
1	C	532	LYS	N-CA-C	-5.63	102.69	110.35
1	F	589	ALA	CA-C-N	5.63	126.18	120.38
1	F	589	ALA	C-N-CA	5.63	126.18	120.38
1	F	209	GLU	N-CA-C	5.61	117.75	109.50
1	B	623	HIS	CA-C-N	5.60	125.97	119.47
1	B	623	HIS	C-N-CA	5.60	125.97	119.47
1	E	612	SER	N-CA-C	5.59	117.34	108.79
1	G	511	ILE	N-CA-C	5.59	116.53	110.21
1	G	586	LEU	CA-C-N	-5.59	115.60	122.93
1	G	586	LEU	C-N-CA	-5.59	115.60	122.93
1	L	337	VAL	CA-C-N	-5.58	113.92	122.62
1	L	337	VAL	C-N-CA	-5.58	113.92	122.62
1	C	173	ILE	N-CA-C	-5.57	105.09	110.72
1	I	624	PRO	CA-C-N	5.57	132.18	121.54
1	I	624	PRO	C-N-CA	5.57	132.18	121.54
1	B	587	VAL	N-CA-C	-5.56	101.86	109.37
1	F	385	ARG	N-CA-C	5.55	118.61	109.85
1	F	531	LEU	N-CA-C	-5.54	105.14	111.07
1	B	364	ILE	N-CA-C	5.54	115.58	108.82
1	B	468	SER	N-CA-C	5.53	120.91	113.72
1	F	544	LEU	N-CA-C	-5.53	101.32	109.62
1	L	25	ASN	N-CA-C	5.53	119.20	111.74
1	A	180	ASP	CA-C-N	5.52	125.50	120.03
1	A	180	ASP	C-N-CA	5.52	125.50	120.03
1	L	147	MET	N-CA-C	5.52	118.06	111.71
1	L	385	ARG	CA-C-N	5.51	129.39	121.50
1	L	385	ARG	C-N-CA	5.51	129.39	121.50
1	G	655	ILE	N-CA-C	5.50	116.04	108.12
1	B	550	GLY	CA-C-N	-5.49	112.37	120.28
1	B	550	GLY	C-N-CA	-5.49	112.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	569	MET	N-CA-C	5.48	118.06	108.52
1	F	234	LEU	N-CA-C	5.48	118.47	109.76
1	F	28	ASN	CA-C-N	-5.47	115.93	122.22
1	F	28	ASN	C-N-CA	-5.47	115.93	122.22
1	F	567	ASP	N-CA-C	5.47	119.95	113.12
1	B	612	SER	N-CA-C	5.44	116.55	108.60
1	E	242	LEU	N-CA-C	5.43	118.09	109.24
1	A	757	ASP	CA-C-N	5.42	125.76	119.47
1	A	757	ASP	C-N-CA	5.42	125.76	119.47
1	L	235	LYS	N-CA-C	-5.39	105.41	111.28
1	G	148	SER	N-CA-C	5.38	116.32	108.14
1	B	757	ASP	CA-C-N	5.37	124.98	119.56
1	B	757	ASP	C-N-CA	5.37	124.98	119.56
1	F	442	LEU	N-CA-C	-5.36	105.36	111.14
1	C	217	ILE	N-CA-C	-5.34	105.32	110.72
1	L	307	GLY	CA-C-N	5.34	131.13	122.53
1	L	307	GLY	C-N-CA	5.34	131.13	122.53
1	C	696	SER	N-CA-C	-5.34	107.78	114.56
1	F	727	VAL	N-CA-C	-5.33	107.62	113.43
1	A	313	GLY	N-CA-C	-5.33	105.27	112.57
1	G	785	ASN	N-CA-C	-5.33	106.84	113.55
1	H	613	VAL	CA-C-N	-5.33	116.20	123.12
1	H	613	VAL	C-N-CA	-5.33	116.20	123.12
1	D	432	HIS	N-CA-C	5.32	117.08	111.28
1	I	575	SER	N-CA-C	-5.32	106.74	113.18
1	L	146	GLU	CA-C-N	5.32	127.94	120.28
1	L	146	GLU	C-N-CA	5.32	127.94	120.28
1	C	514	LYS	N-CA-C	-5.32	105.89	112.38
1	E	24	LEU	CA-C-N	5.30	129.67	122.19
1	E	24	LEU	C-N-CA	5.30	129.67	122.19
1	I	787	ILE	N-CA-C	5.30	116.54	108.80
1	F	474	GLU	N-CA-C	5.30	117.06	111.28
1	G	791	LYS	N-CA-C	5.30	116.90	108.79
1	H	485	GLY	N-CA-C	-5.30	105.92	112.33
1	E	149	ASN	N-CA-C	5.29	121.76	113.72
1	C	474	GLU	N-CA-C	5.29	117.04	111.28
1	G	757	ASP	CA-C-N	5.28	124.89	119.56
1	G	757	ASP	C-N-CA	5.28	124.89	119.56
1	B	366	ILE	N-CA-C	5.28	116.79	109.29
1	D	757	ASP	CA-C-N	5.28	125.59	119.47
1	D	757	ASP	C-N-CA	5.28	125.59	119.47
1	E	59	LYS	N-CA-C	-5.28	105.11	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	VAL	N-CA-C	5.27	115.64	107.78
1	B	277	PHE	N-CA-C	5.27	117.84	109.24
1	G	649	PHE	N-CA-C	5.27	117.44	111.11
1	D	575	SER	N-CA-C	-5.27	106.80	113.18
1	E	566	ASP	N-CA-C	-5.27	105.71	111.82
1	H	602	LEU	N-CA-C	5.27	120.57	113.72
1	L	217	ILE	N-CA-C	-5.27	105.26	111.00
1	H	704	ARG	N-CA-C	-5.26	106.54	113.17
1	B	232	GLU	N-CA-C	5.24	117.05	110.91
1	F	707	ASP	CA-C-N	-5.24	115.93	122.48
1	F	707	ASP	C-N-CA	-5.24	115.93	122.48
1	B	233	THR	N-CA-C	-5.24	105.10	112.12
1	A	236	ASP	N-CA-C	-5.23	105.72	112.68
1	G	623	HIS	CA-C-N	5.22	124.89	119.56
1	G	623	HIS	C-N-CA	5.22	124.89	119.56
1	F	792	VAL	N-CA-C	5.22	115.08	107.88
1	F	144	ASN	N-CA-C	5.21	121.34	109.81
1	A	51	GLU	N-CA-C	-5.21	105.60	111.28
1	G	476	ILE	N-CA-C	-5.21	105.46	110.72
1	H	623	HIS	CA-C-N	5.21	125.51	119.47
1	H	623	HIS	C-N-CA	5.21	125.51	119.47
1	L	336	PRO	CA-C-N	5.21	130.18	122.94
1	L	336	PRO	C-N-CA	5.21	130.18	122.94
1	C	723	VAL	N-CA-C	-5.20	105.47	110.72
1	G	230	VAL	CA-C-N	5.20	125.20	120.21
1	G	230	VAL	C-N-CA	5.20	125.20	120.21
1	E	127	LEU	N-CA-C	5.20	117.83	110.50
1	E	183	ILE	N-CA-C	5.20	115.79	108.36
1	F	625	ASP	N-CA-C	-5.20	105.53	111.14
1	F	548	GLY	N-CA-C	5.19	125.48	113.18
1	F	514	LYS	N-CA-C	5.19	116.93	111.28
1	G	144	ASN	CA-C-N	5.18	124.85	119.56
1	G	144	ASN	C-N-CA	5.18	124.85	119.56
1	G	196	LEU	N-CA-C	5.18	117.67	111.71
1	F	701	PHE	N-CA-C	-5.18	105.53	111.07
1	C	708	ILE	CA-C-N	-5.18	116.27	122.90
1	C	708	ILE	C-N-CA	-5.18	116.27	122.90
1	I	658	SER	N-CA-C	5.17	117.24	109.23
1	B	501	SER	CA-C-N	5.17	127.16	120.44
1	B	501	SER	C-N-CA	5.17	127.16	120.44
1	F	636	ASP	N-CA-C	5.16	120.73	113.56
1	C	533	ASP	CA-C-N	5.16	124.82	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	533	ASP	C-N-CA	5.16	124.82	119.56
1	B	148	SER	N-CA-C	5.14	116.11	108.60
1	D	743	VAL	N-CA-C	-5.14	101.18	108.58
1	F	107	HIS	N-CA-C	-5.14	106.16	112.90
1	C	387	LEU	N-CA-C	5.14	119.93	113.25
1	E	209	GLU	CA-C-N	5.14	126.27	119.84
1	E	209	GLU	C-N-CA	5.14	126.27	119.84
1	C	741	ILE	N-CA-C	5.12	115.28	108.11
1	G	175	LYS	N-CA-C	5.12	116.86	111.28
1	B	463	THR	N-CA-C	-5.12	106.72	113.17
1	D	607	ARG	N-CA-C	5.11	120.25	112.54
1	I	585	ARG	N-CA-C	-5.11	106.74	113.12
1	E	540	SER	N-CA-C	5.10	117.00	108.99
1	E	336	PRO	N-CA-C	5.09	119.47	111.38
1	A	613	VAL	CA-C-N	-5.09	116.50	123.12
1	A	613	VAL	C-N-CA	-5.09	116.50	123.12
1	C	699	PRO	N-CA-C	-5.09	107.22	113.84
1	D	741	ILE	CA-C-N	-5.09	116.50	123.12
1	D	741	ILE	C-N-CA	-5.09	116.50	123.12
1	L	37	GLY	N-CA-C	-5.09	101.12	113.18
1	L	334	PHE	N-CA-C	5.09	118.41	110.32
1	I	344	VAL	N-CA-C	5.08	115.31	110.53
1	B	701	PHE	N-CA-C	-5.08	105.20	111.40
1	E	491	ILE	N-CA-C	5.07	116.17	111.45
1	B	230	VAL	CA-C-N	5.07	126.18	119.84
1	B	230	VAL	C-N-CA	5.07	126.18	119.84
1	E	655	ILE	N-CA-C	5.07	114.77	106.72
1	E	315	THR	N-CA-C	5.06	114.92	108.24
1	A	754	GLU	N-CA-C	5.06	117.57	111.40
1	E	568	ALA	N-CA-C	-5.06	107.11	113.28
1	L	307	GLY	N-CA-C	-5.06	108.27	115.30
1	E	11	GLN	N-CA-C	-5.06	107.18	113.55
1	B	156	LYS	N-CA-C	5.05	118.22	111.75
1	L	148	SER	N-CA-C	5.05	116.73	108.55
1	B	340	ASP	N-CA-C	5.05	114.95	108.34
1	D	766	ILE	N-CA-C	-5.04	105.58	110.42
1	E	24	LEU	N-CA-C	-5.04	107.13	113.28
1	L	144	ASN	CA-C-N	5.04	124.70	119.56
1	L	144	ASN	C-N-CA	5.04	124.70	119.56
1	B	41	GLU	CA-C-N	5.04	126.13	119.84
1	B	41	GLU	C-N-CA	5.04	126.13	119.84
1	F	395	ILE	N-CA-C	-5.04	105.80	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	259	GLU	N-CA-C	5.02	116.83	111.36
1	F	728	ASN	N-CA-C	-5.01	106.99	113.01
1	L	281	LEU	N-CA-C	5.01	116.20	107.93
1	B	660	VAL	N-CA-C	-5.01	107.50	111.81
1	L	610	PRO	N-CA-C	5.01	120.12	113.86
1	E	155	SER	N-CA-C	5.00	114.76	108.45
1	G	181	PRO	N-CA-C	-5.00	103.90	111.41
1	L	693	LEU	CA-C-N	5.00	128.69	120.63
1	L	693	LEU	C-N-CA	5.00	128.69	120.63
1	G	544	LEU	N-CA-C	5.00	116.67	108.52

There are no chirality outliers.

There are no planarity outliers.

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	2976	0	790	9	0
1	B	2976	0	789	11	0
1	C	2408	0	638	13	0
1	D	1744	0	458	20	0
1	E	2656	0	703	7	0
1	F	2976	0	790	6	0
1	G	2976	0	789	5	0
1	H	2408	0	638	12	0
1	I	1744	0	458	13	0
1	L	2648	0	704	5	0
All	All	25512	0	6757	90	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 3.

All (90) 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:C:523:ALA:CA	1:D:776:ASN:CA	1.96	1.43
1:C:523:ALA:CA	1:D:776:ASN:C	2.04	1.29
1:C:523:ALA:C	1:D:776:ASN:C	2.13	1.17
1:C:523:ALA:CA	1:D:776:ASN:O	1.95	1.13
1:C:523:ALA:O	1:D:776:ASN:C	2.00	1.05
1:H:523:ALA:CA	1:H:527:ALA:H	1.76	0.98
1:C:523:ALA:C	1:D:776:ASN:CA	2.38	0.97
1:H:523:ALA:O	1:H:527:ALA:N	1.95	0.97
1:H:523:ALA:C	1:H:527:ALA:H	1.77	0.91
1:C:523:ALA:O	1:D:777:LEU:N	2.12	0.81
1:C:523:ALA:O	1:D:777:LEU:CA	2.41	0.69
1:H:521:SER:O	1:H:522:LYS:O	2.14	0.66
1:I:405:LYS:H	1:I:460:TRP:H	1.46	0.64
1:C:224:ALA:O	1:C:226:VAL:N	2.32	0.63
1:D:403:ARG:N	1:D:459:GLU:O	2.36	0.59
1:H:523:ALA:CA	1:H:527:ALA:N	2.57	0.59
1:F:381:TYR:O	1:F:494:THR:N	2.36	0.59
1:I:711:PHE:O	1:I:712:HIS:C	2.44	0.59
1:H:521:SER:O	1:H:522:LYS:C	2.48	0.57
1:E:44:GLY:O	1:E:45:ILE:C	2.48	0.56
1:I:403:ARG:N	1:I:459:GLU:O	2.39	0.55
1:L:68:ILE:O	1:L:69:GLY:C	2.49	0.54
1:D:405:LYS:N	1:D:459:GLU:H	2.05	0.54
1:L:532:LYS:O	1:L:533:ASP:C	2.51	0.54
1:D:405:LYS:H	1:D:460:TRP:H	1.56	0.53
1:I:404:LEU:O	1:I:458:ASN:N	2.40	0.53
1:G:340:ASP:O	1:G:341:GLU:C	2.51	0.53
1:E:532:LYS:N	1:F:729:LYS:O	2.43	0.51
1:G:44:GLY:O	1:G:45:ILE:C	2.53	0.51
1:I:404:LEU:C	1:I:459:GLU:H	2.19	0.51
1:A:141:ALA:O	1:A:142:LEU:C	2.52	0.51
1:D:711:PHE:O	1:D:712:HIS:C	2.54	0.51
1:F:532:LYS:O	1:F:533:ASP:C	2.53	0.51
1:C:523:ALA:O	1:D:776:ASN:O	2.29	0.51
1:D:404:LEU:H	1:D:459:GLU:C	2.18	0.50
1:I:404:LEU:H	1:I:459:GLU:C	2.19	0.50
1:E:81:THR:O	1:E:83:ARG:N	2.45	0.50
1:G:735:SER:O	1:G:736:GLU:C	2.53	0.50
1:E:587:VAL:N	1:F:571:ARG:O	2.45	0.49
1:I:404:LEU:O	1:I:457:LYS:N	2.45	0.49
1:B:436:PHE:O	1:B:437:GLU:C	2.55	0.49
1:C:532:LYS:O	1:C:533:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LEU:C	1:D:459:GLU:H	2.20	0.49
1:H:523:ALA:C	1:H:525:ARG:N	2.69	0.48
1:I:405:LYS:N	1:I:459:GLU:H	2.11	0.48
1:A:532:LYS:O	1:A:533:ASP:C	2.55	0.47
1:B:735:SER:O	1:B:736:GLU:C	2.57	0.47
1:G:463:THR:O	1:G:464:GLN:C	2.57	0.47
1:B:17:ALA:O	1:B:21:ALA:N	2.48	0.47
1:H:308:GLU:O	1:H:309:LEU:C	2.57	0.47
1:H:523:ALA:C	1:H:525:ARG:H	2.23	0.47
1:B:80:TYR:O	1:B:81:THR:C	2.58	0.46
1:I:623:HIS:O	1:I:624:PRO:C	2.59	0.46
1:A:486:ILE:O	1:A:489:THR:N	2.49	0.45
1:A:43:GLU:O	1:A:44:GLY:C	2.59	0.45
1:H:769:ILE:O	1:H:770:GLN:C	2.57	0.45
1:L:627:PHE:O	1:L:631:LEU:N	2.50	0.45
1:B:25:ASN:O	1:B:26:HIS:C	2.57	0.44
1:A:743:VAL:O	1:A:744:THR:C	2.58	0.44
1:L:584:SER:O	1:L:601:GLN:N	2.50	0.44
1:H:769:ILE:O	1:H:771:LYS:N	2.50	0.44
1:E:574:MET:O	1:E:578:MET:N	2.50	0.44
1:I:622:ALA:O	1:I:623:HIS:C	2.60	0.44
1:C:535:LYS:O	1:C:536:ARG:O	2.36	0.43
1:D:438:ASN:O	1:D:439:ALA:C	2.61	0.43
1:F:81:THR:O	1:F:83:ARG:N	2.51	0.43
1:D:402:VAL:N	1:D:459:GLU:O	2.52	0.43
1:I:463:THR:O	1:I:464:GLN:C	2.61	0.43
1:A:17:ALA:O	1:A:21:ALA:N	2.51	0.42
1:A:769:ILE:O	1:A:770:GLN:C	2.58	0.42
1:G:436:PHE:O	1:G:439:ALA:N	2.52	0.42
1:E:80:TYR:O	1:E:81:THR:C	2.61	0.42
1:E:7:THR:O	1:E:8:GLU:C	2.62	0.42
1:D:463:THR:O	1:D:464:GLN:C	2.61	0.42
1:B:395:ILE:O	1:B:396:ASP:C	2.61	0.42
1:D:581:HIS:O	1:D:585:ARG:N	2.54	0.41
1:I:661:GLY:O	1:I:662:ALA:C	2.63	0.41
1:B:112:LEU:O	1:B:118:GLY:N	2.53	0.41
1:B:213:GLY:O	1:B:214:LYS:C	2.63	0.41
1:B:550:GLY:O	1:B:551:LYS:C	2.63	0.41
1:I:402:VAL:N	1:I:459:GLU:O	2.53	0.41
1:H:770:GLN:O	1:H:771:LYS:C	2.63	0.41
1:C:554:LEU:O	1:C:555:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:LEU:O	1:F:555:ALA:C	2.63	0.41
1:D:774:GLU:O	1:D:775:ASP:C	2.64	0.41
1:L:614:ILE:O	1:L:655:ILE:N	2.50	0.41
1:B:486:ILE:O	1:B:487:PRO:C	2.64	0.40
1:A:590:PRO:O	1:A:591:PRO:C	2.63	0.40
1:A:617:ASP:O	1:A:618:GLU:C	2.61	0.40
1:B:512:GLY:O	1:B:513:GLN:C	2.64	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	712/818 (87%)	672 (94%)	36 (5%)	4 (1%)	21	59
1	B	710/818 (87%)	661 (93%)	47 (7%)	2 (0%)	36	72
1	C	576/818 (70%)	548 (95%)	22 (4%)	6 (1%)	12	49
1	D	416/818 (51%)	393 (94%)	19 (5%)	4 (1%)	12	49
1	E	634/818 (78%)	601 (95%)	26 (4%)	7 (1%)	11	46
1	F	712/818 (87%)	660 (93%)	48 (7%)	4 (1%)	21	59
1	G	710/818 (87%)	684 (96%)	24 (3%)	2 (0%)	36	72
1	H	576/818 (70%)	546 (95%)	24 (4%)	6 (1%)	12	49
1	I	416/818 (51%)	391 (94%)	21 (5%)	4 (1%)	12	49
1	L	634/818 (78%)	605 (95%)	28 (4%)	1 (0%)	43	78
All	All	6096/8180 (74%)	5761 (94%)	295 (5%)	40 (1%)	20	56

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	ILE
1	C	495	GLU
1	D	590	PRO
1	E	324	ILE
1	E	589	ALA
1	E	590	PRO
1	G	590	PRO
1	I	590	PRO
1	H	522	LYS
1	H	590	PRO
1	L	590	PRO
1	A	590	PRO
1	B	590	PRO
1	C	224	ALA
1	D	625	ASP
1	F	303	ALA
1	I	625	ASP
1	H	495	GLU
1	C	590	PRO
1	E	82	PRO
1	G	546	PRO
1	I	546	PRO
1	A	156	LYS
1	A	486	ILE
1	D	546	PRO
1	F	211	GLY
1	H	232	GLU
1	B	486	ILE
1	C	525	ARG
1	D	486	ILE
1	E	54	ASN
1	F	486	ILE
1	I	406	SER
1	H	486	ILE
1	A	141	ALA
1	E	232	GLU
1	H	524	VAL
1	C	486	ILE
1	E	212	VAL
1	F	82	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	7
1	G	7
1	F	6
1	C	6
1	H	6
1	A	6
1	D	5
1	I	5
1	E	5
1	L	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	487:PRO	C	488:LEU	N	22.78
1	I	487:PRO	C	488:LEU	N	21.40
1	I	410:PRO	C	411:ASN	N	21.31
1	D	410:PRO	C	411:ASN	N	19.73
1	F	712:HIS	C	713:LYS	N	19.70
1	L	487:PRO	C	488:LEU	N	17.16
1	F	487:PRO	C	488:LEU	N	16.20
1	L	410:PRO	C	411:ASN	N	15.13
1	C	410:PRO	C	411:ASN	N	15.01
1	H	410:PRO	C	411:ASN	N	14.95
1	E	410:PRO	C	411:ASN	N	14.12
1	E	342:PRO	C	343:SER	N	13.10
1	E	487:PRO	C	488:LEU	N	12.43
1	I	712:HIS	C	713:LYS	N	12.16
1	D	736:GLU	C	737:GLN	N	10.99
1	F	410:PRO	C	411:ASN	N	10.73
1	B	410:PRO	C	411:ASN	N	10.48
1	D	712:HIS	C	713:LYS	N	10.43
1	G	410:PRO	C	411:ASN	N	10.24
1	F	45:ILE	C	46:ALA	N	9.52
1	L	437:GLU	C	438:ASN	N	8.91
1	A	437:GLU	C	438:ASN	N	7.87
1	B	487:PRO	C	488:LEU	N	7.71
1	H	712:HIS	C	713:LYS	N	7.15
1	F	437:GLU	C	438:ASN	N	6.93
1	A	410:PRO	C	411:ASN	N	6.82
1	D	437:GLU	C	438:ASN	N	6.55
1	A	487:PRO	C	488:LEU	N	6.39
1	C	712:HIS	C	713:LYS	N	6.30
1	C	437:GLU	C	438:ASN	N	6.14
1	B	45:ILE	C	46:ALA	N	6.13
1	H	437:GLU	C	438:ASN	N	5.98
1	I	736:GLU	C	737:GLN	N	5.94
1	F	736:GLU	C	737:GLN	N	5.75
1	A	45:ILE	C	46:ALA	N	5.68
1	G	45:ILE	C	46:ALA	N	5.61
1	G	342:PRO	C	343:SER	N	5.56
1	I	437:GLU	C	438:ASN	N	5.51
1	G	712:HIS	C	713:LYS	N	4.94
1	E	45:ILE	C	46:ALA	N	4.85
1	B	437:GLU	C	438:ASN	N	4.80
1	B	342:PRO	C	343:SER	N	4.65
1	C	342:PRO	C	343:SER	N	4.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	736:GLU	C	737:GLN	N	4.22
1	E	437:GLU	C	438:ASN	N	4.07
1	G	736:GLU	C	737:GLN	N	4.07
1	B	736:GLU	C	737:GLN	N	4.06
1	H	342:PRO	C	343:SER	N	4.05
1	C	736:GLU	C	737:GLN	N	4.04
1	H	736:GLU	C	737:GLN	N	3.98
1	B	712:HIS	C	713:LYS	N	3.90
1	A	712:HIS	C	713:LYS	N	3.83
1	H	487:PRO	C	488:LEU	N	3.66
1	G	437:GLU	C	438:ASN	N	3.55
1	L	45:ILE	C	46:ALA	N	3.45
1	G	487:PRO	C	488:LEU	N	3.21
1	C	487:PRO	C	488:LEU	N	3.20

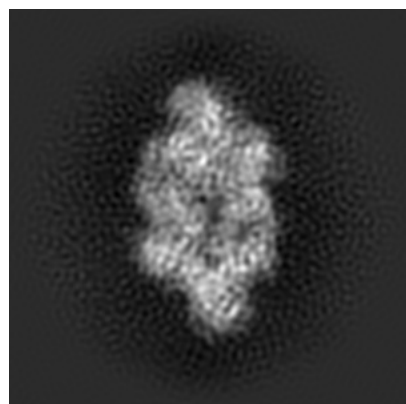
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3895. These allow visual inspection of the internal detail of the map and identification of artifacts.

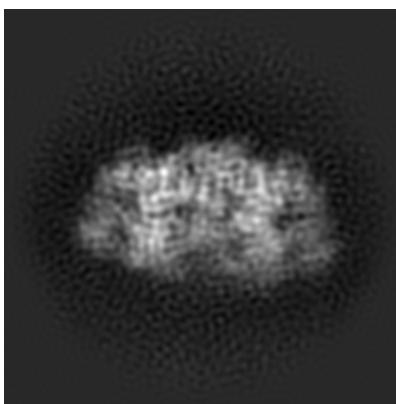
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

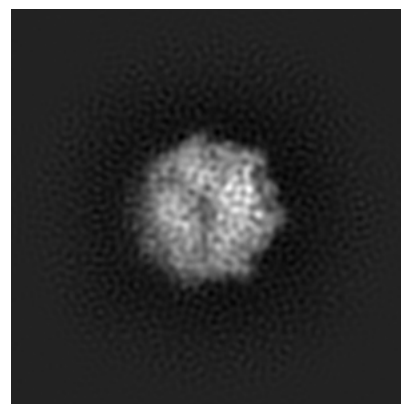
6.1.1 Primary map



X

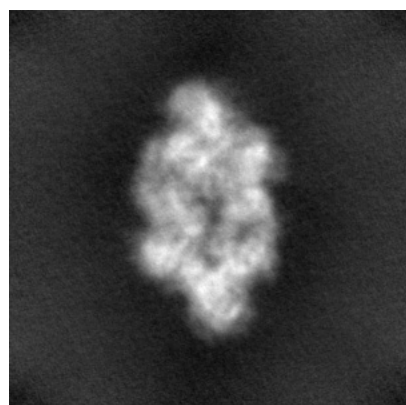


Y

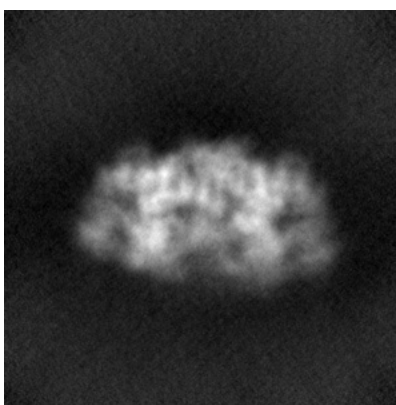


Z

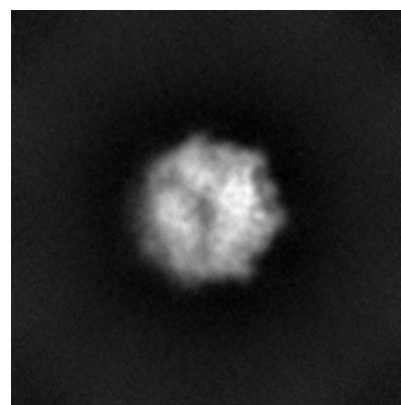
6.1.2 Raw map



X



Y

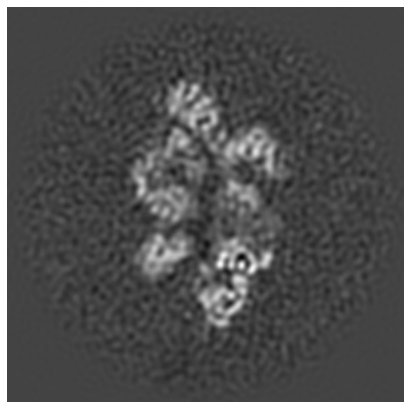


Z

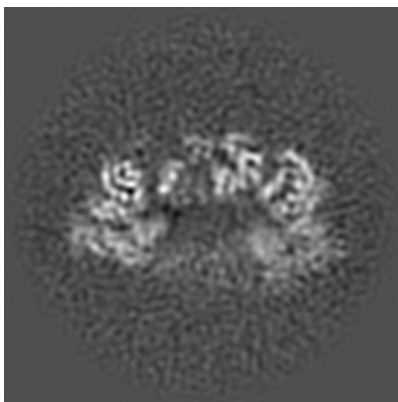
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

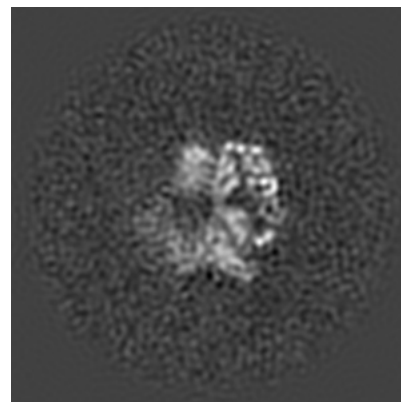
6.2.1 Primary map



X Index: 150

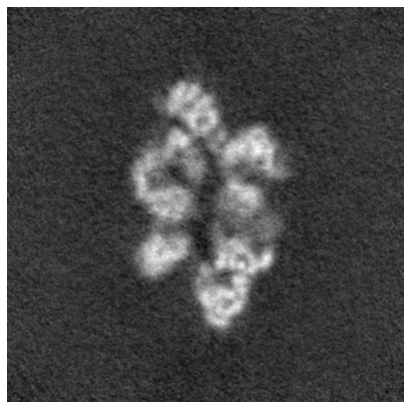


Y Index: 150

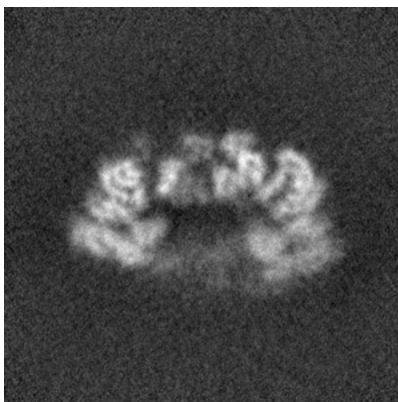


Z Index: 150

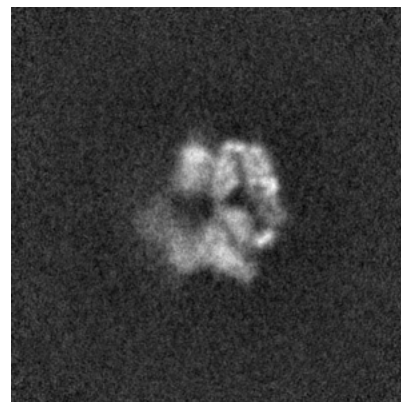
6.2.2 Raw map



X Index: 150



Y Index: 150

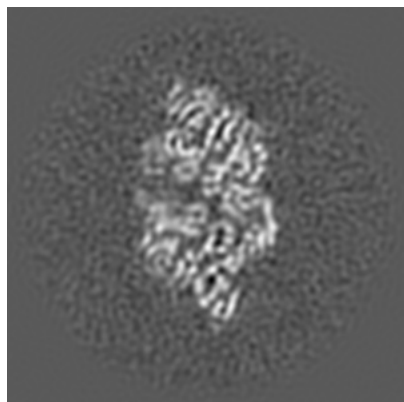


Z Index: 150

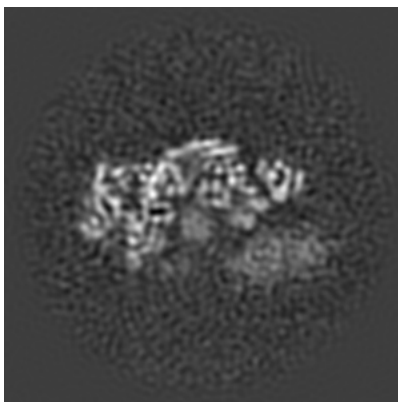
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

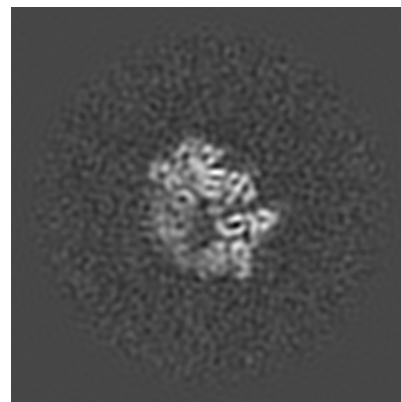
6.3.1 Primary map



X Index: 163

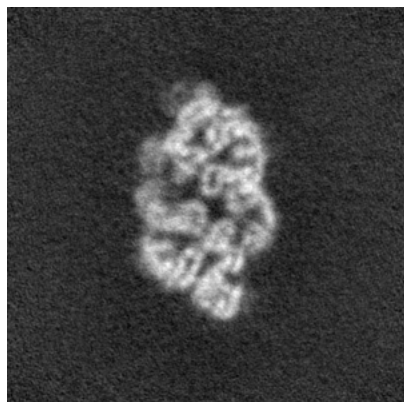


Y Index: 166

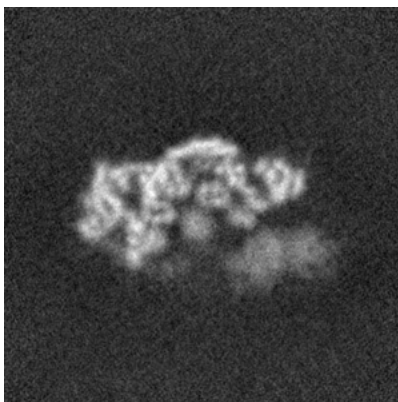


Z Index: 105

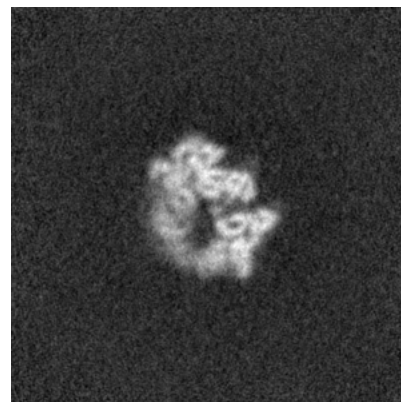
6.3.2 Raw map



X Index: 167



Y Index: 165

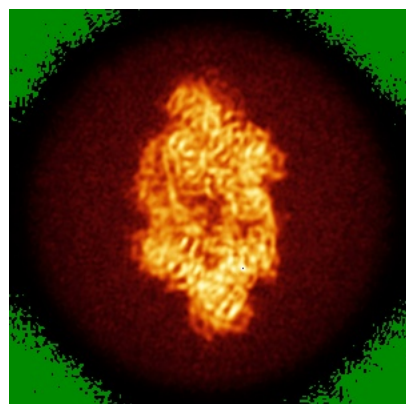


Z Index: 106

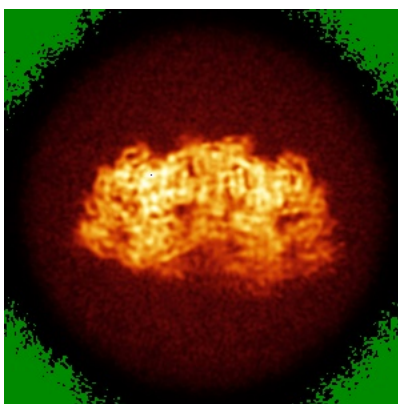
The images above show the largest variance slices of the map in three orthogonal directions.

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

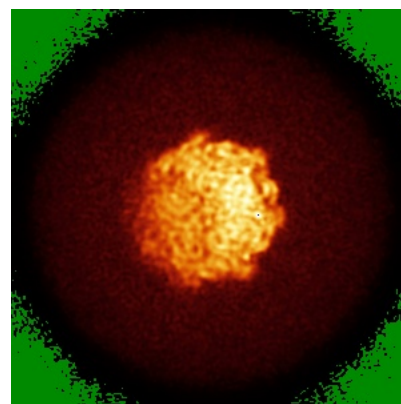
6.4.1 Primary map



X

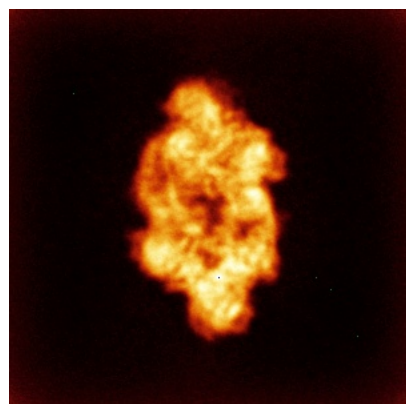


Y

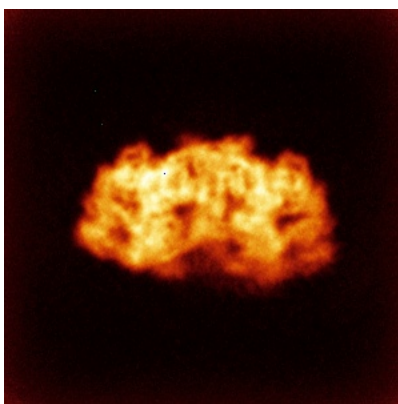


Z

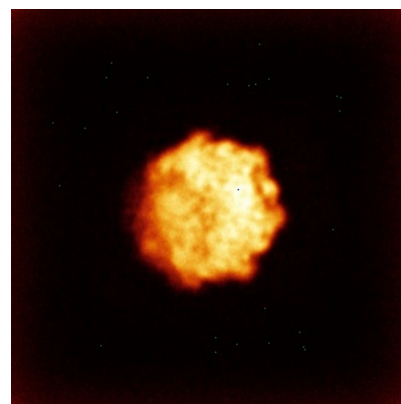
6.4.2 Raw map



X



Y



Z

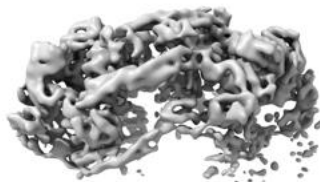
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

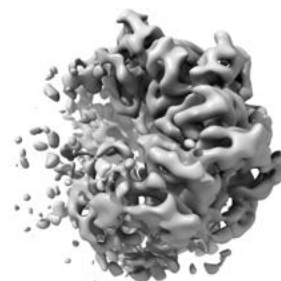
6.5.1 Primary map



X



Y



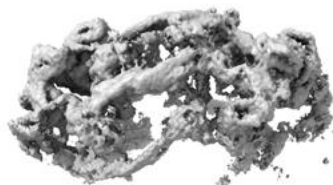
Z

The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

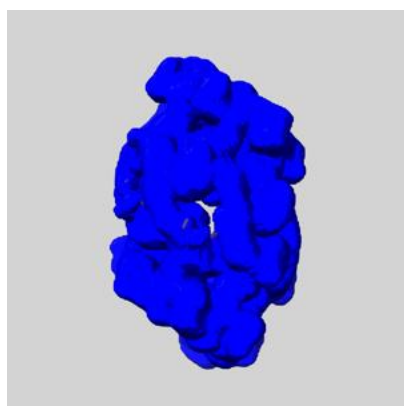
6.6 Mask visualisation [i](#)

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

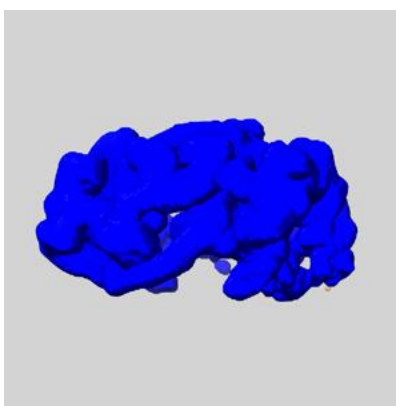
A mask typically either:

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

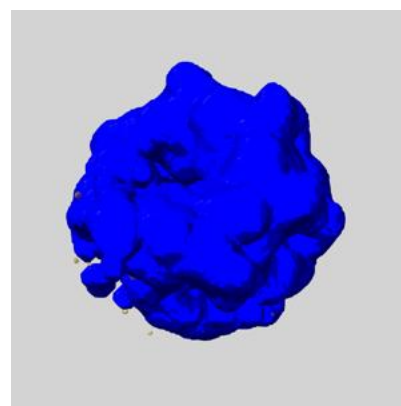
6.6.1 emd_3895_msk_1.map [i](#)



X



Y

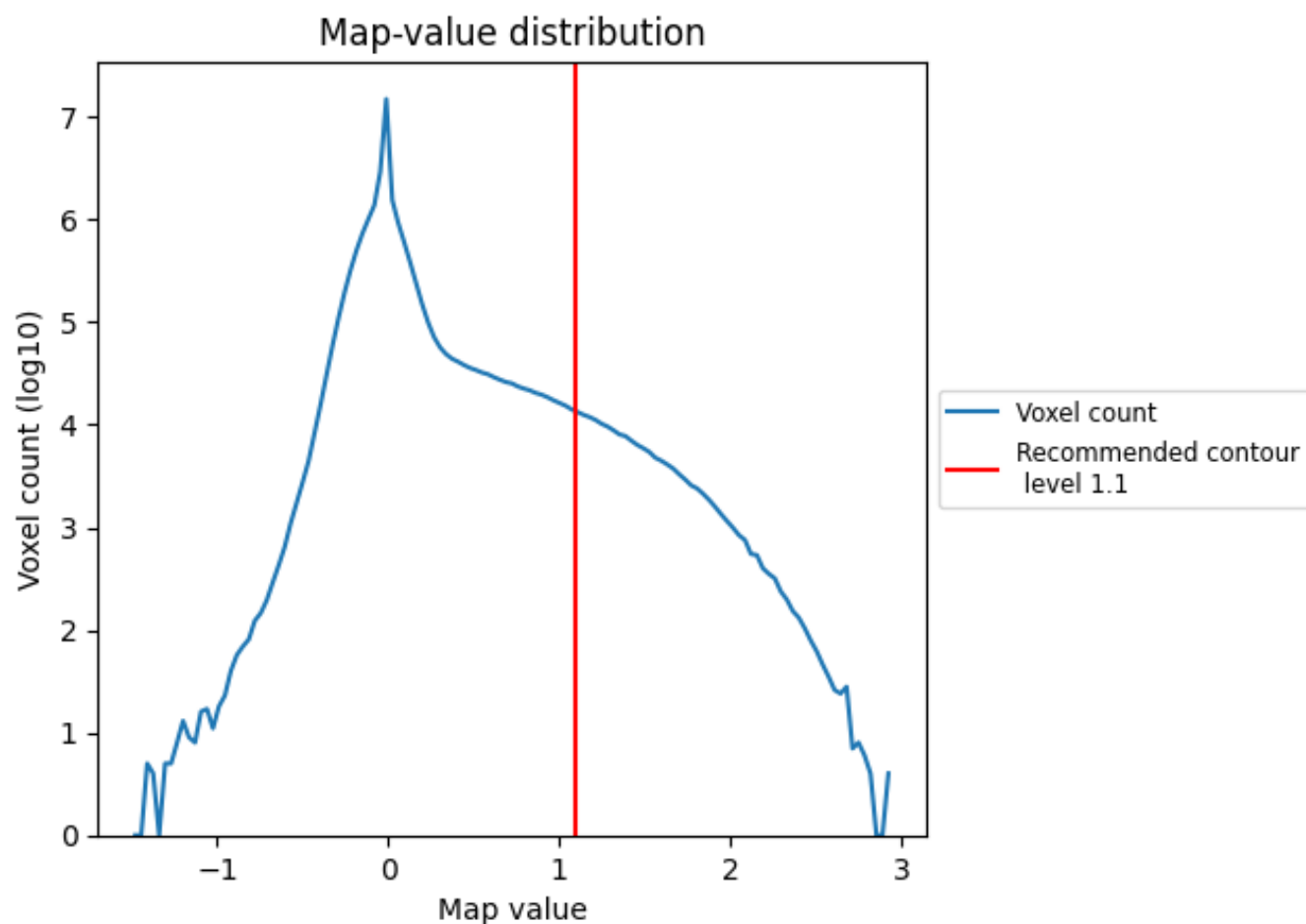


Z

7 Map analysis [i](#)

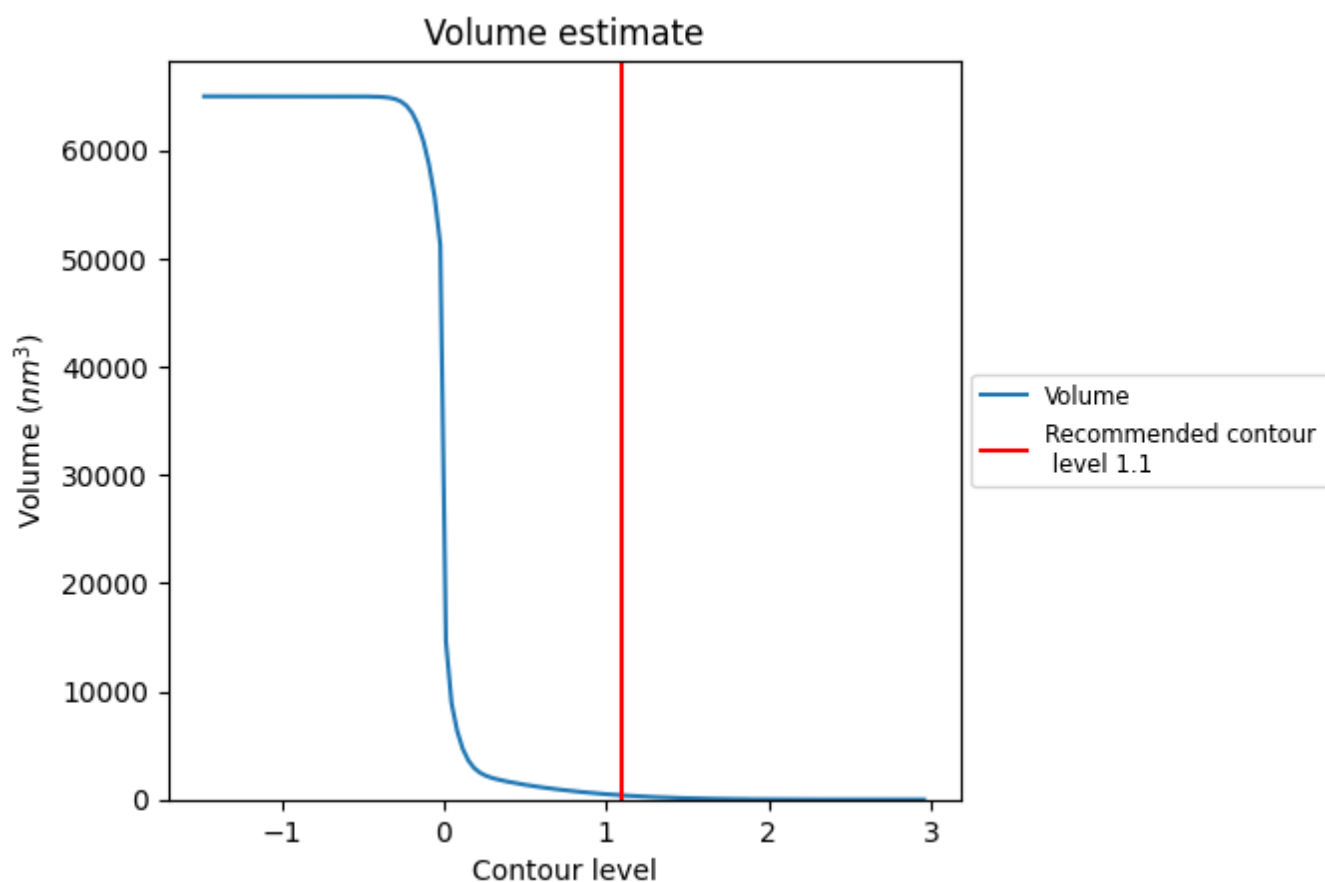
This section contains the results of statistical analysis of the map.

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.

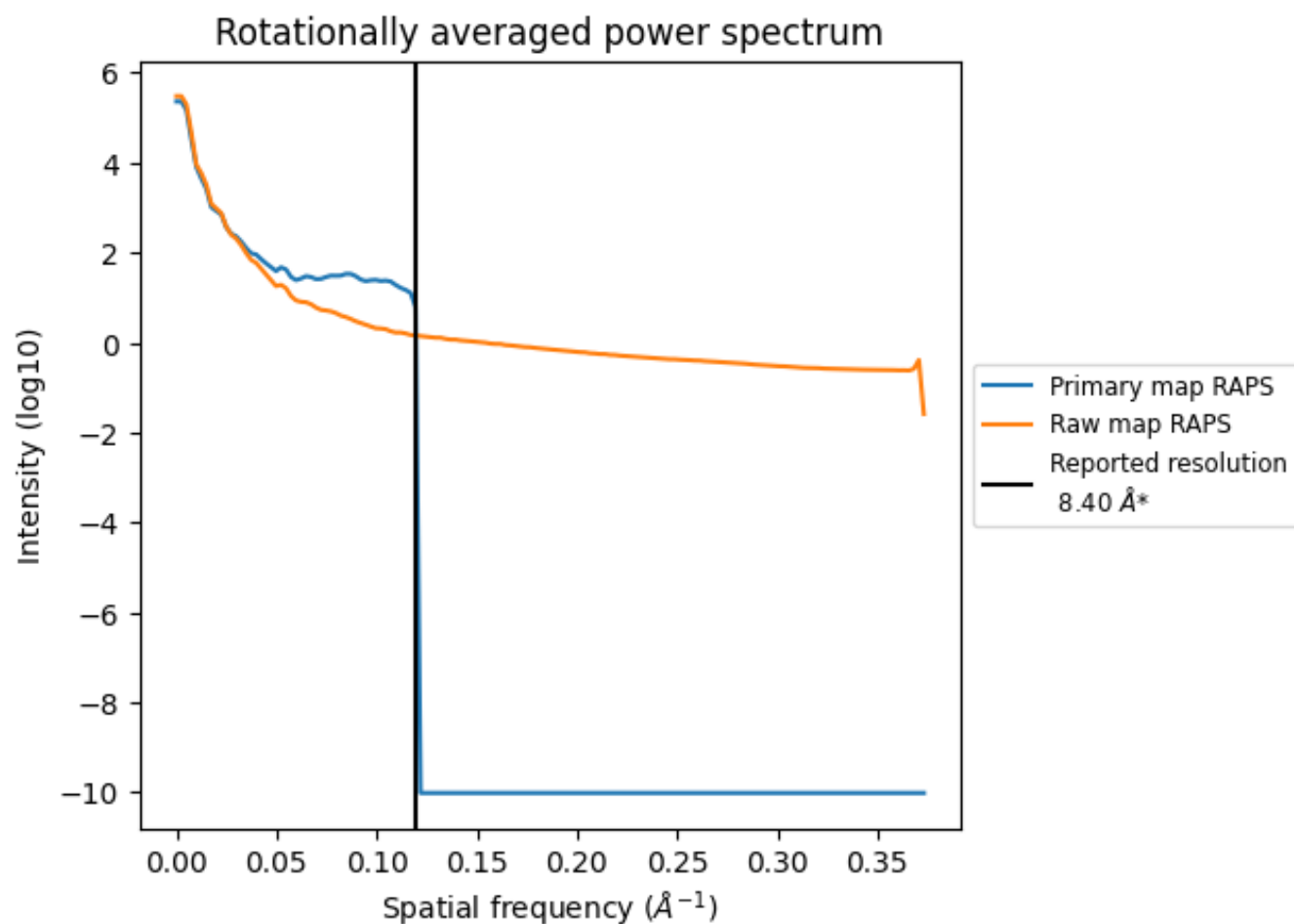
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm³; this corresponds to an approximate mass of 354 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

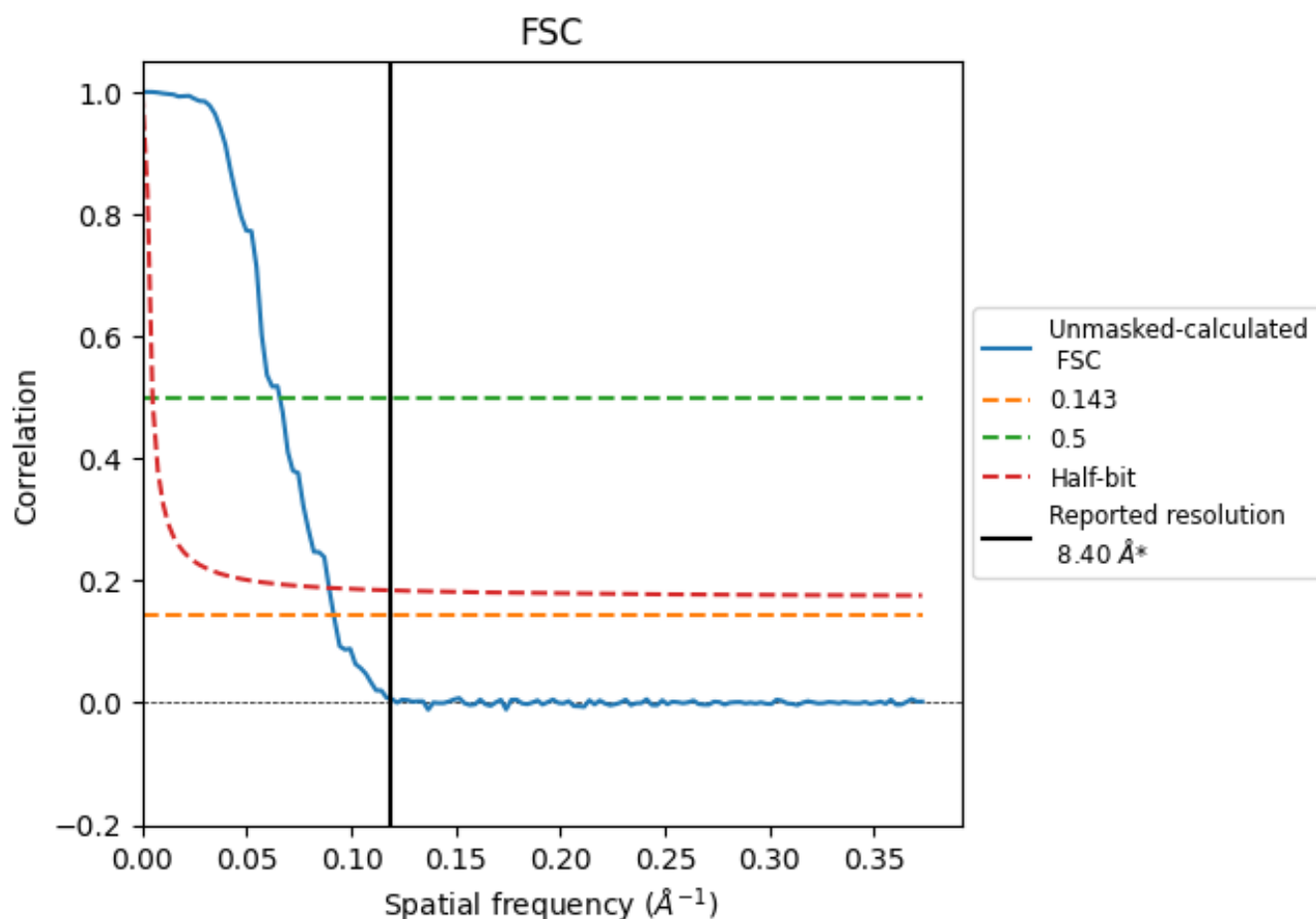


*Reported resolution corresponds to spatial frequency of 0.119 $\text{\AA}^{-1}$

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 0.119 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

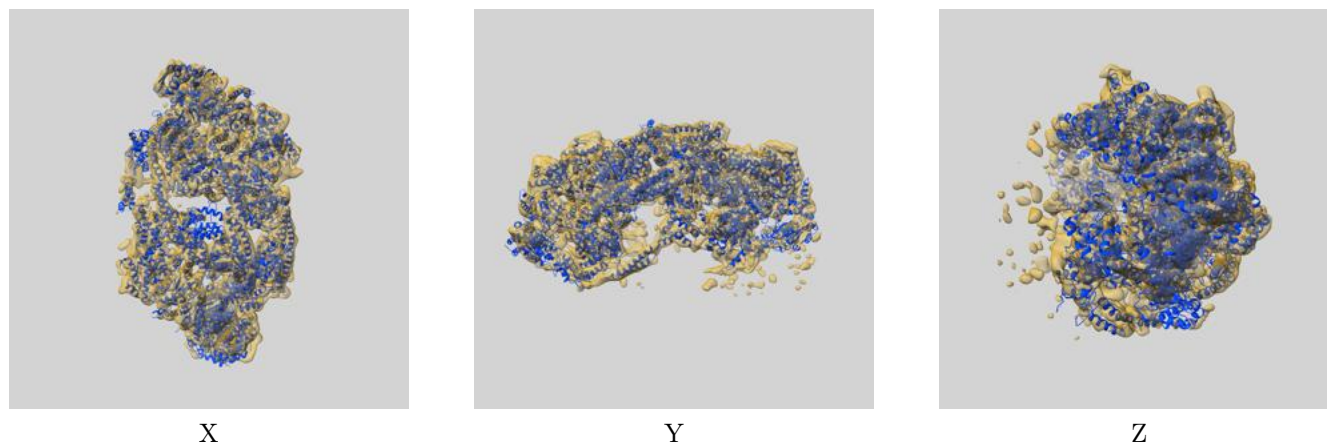
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.91	15.22	11.20

*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 10.91 differs from the reported value 8.4 by more than 10 %

9 Map-model fit [i](#)

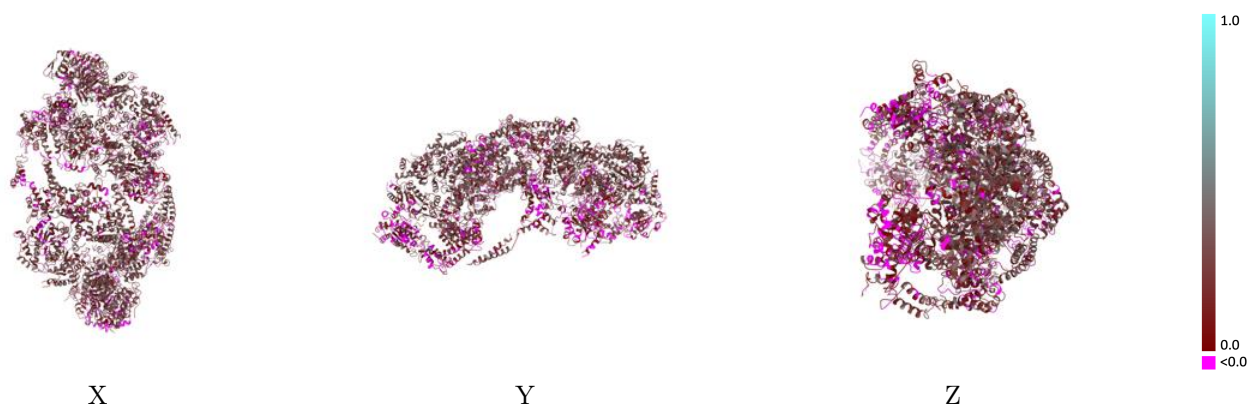
This section contains information regarding the fit between EMDB map EMD-3895 and PDB model 6EM9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



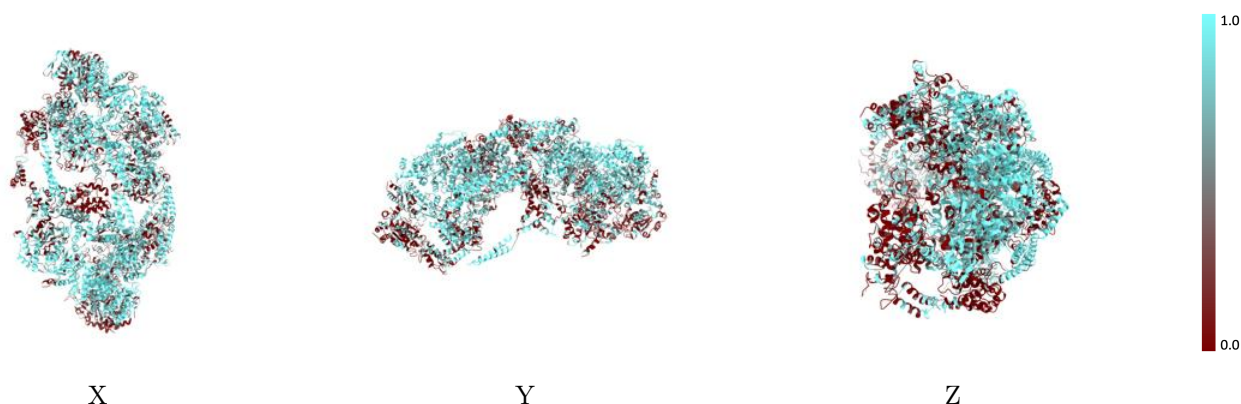
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



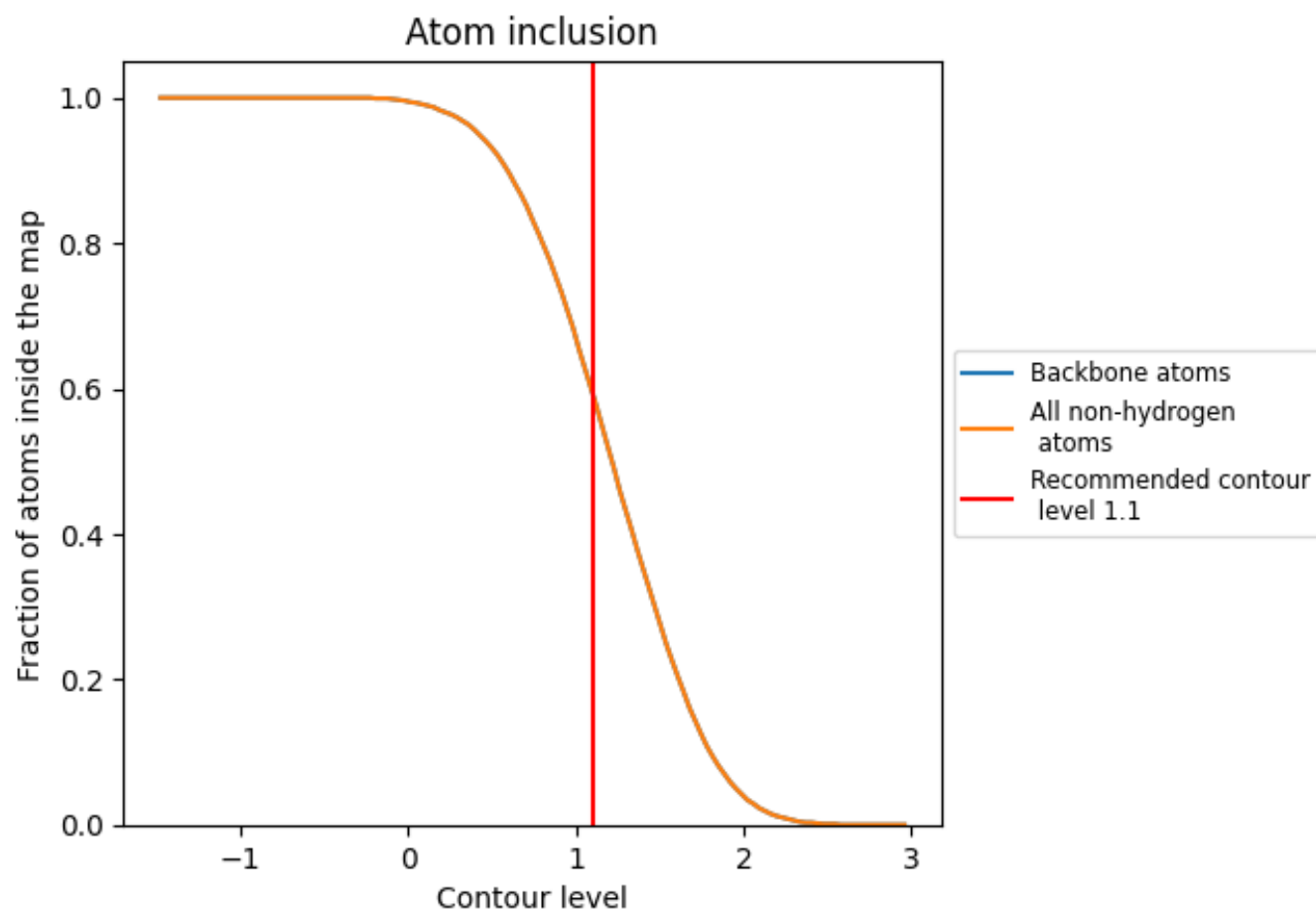
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.1770
A	0.7080	0.2150
B	0.7720	0.2240
C	0.7400	0.2200
D	0.3120	0.0630
E	0.4580	0.1080
F	0.6700	0.1960
G	0.6620	0.2260
H	0.6200	0.1880
I	0.3690	0.1190
L	0.3890	0.1440

1.0
0.0
<0.0