



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:09 AM UTC

PDB ID : 5A5T / pdb_00005a5t
EMDB ID : EMD-3056
Title : Structure of mammalian eIF3 in the context of the 43S preinitiation complex
Authors : des-Georges, A.; Dhote, V.; Kuhn, L.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.; Hashem, Y.
Deposited on : 2015-06-21
Resolution : 6.00 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:

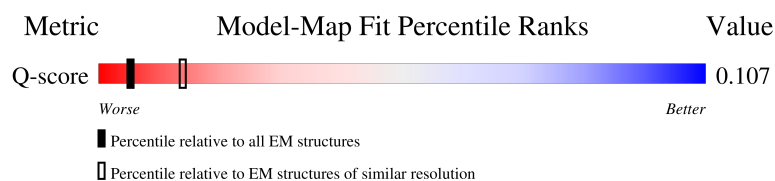
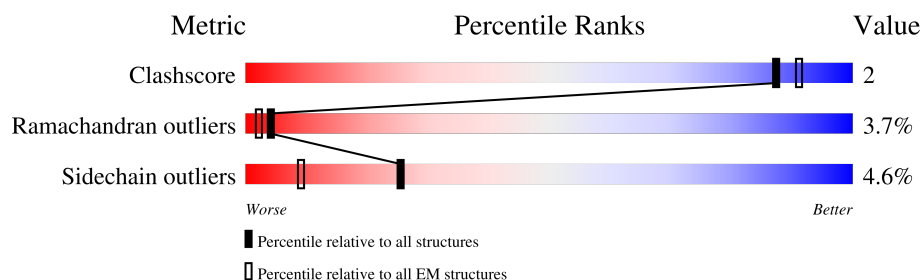
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

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	1362	10% 38% 6% 56%
2	C	843	11% 57% 9% 34%
3	E	445	16% 79% 12% 6%
4	F	364	19% 64% 10% 25%

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Mol	Chain	Length	Quality of chain
5	H	352	34% 73% 17% 8%
6	K	218	49% 89% 10%
7	L	564	38% 55% 9% 34%
8	M	374	20% 83% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25432 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 EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	1
			4935	3107	893	914	21		

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	558	Total	C	N	O	S	0	1
			4529	2842	805	849	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	577	TYR	ALA	conflict	UNP G1U971

- Molecule 3 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	420	Total	C	N	O	S	0	1
			3466	2220	587	639	20		

- Molecule 4 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 5 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 6 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT K.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	216	Total	C	N	O	S	0	1
			1738	1109	286	330	13		

- Molecule 7 is a protein called UNCHARACTERIZED PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	373	Total	C	N	O	S	0	1
			3110	2010	520	563	17		

- Molecule 8 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	366	Total	C	N	O	S	0	1
			2919	1850	494	558	17		

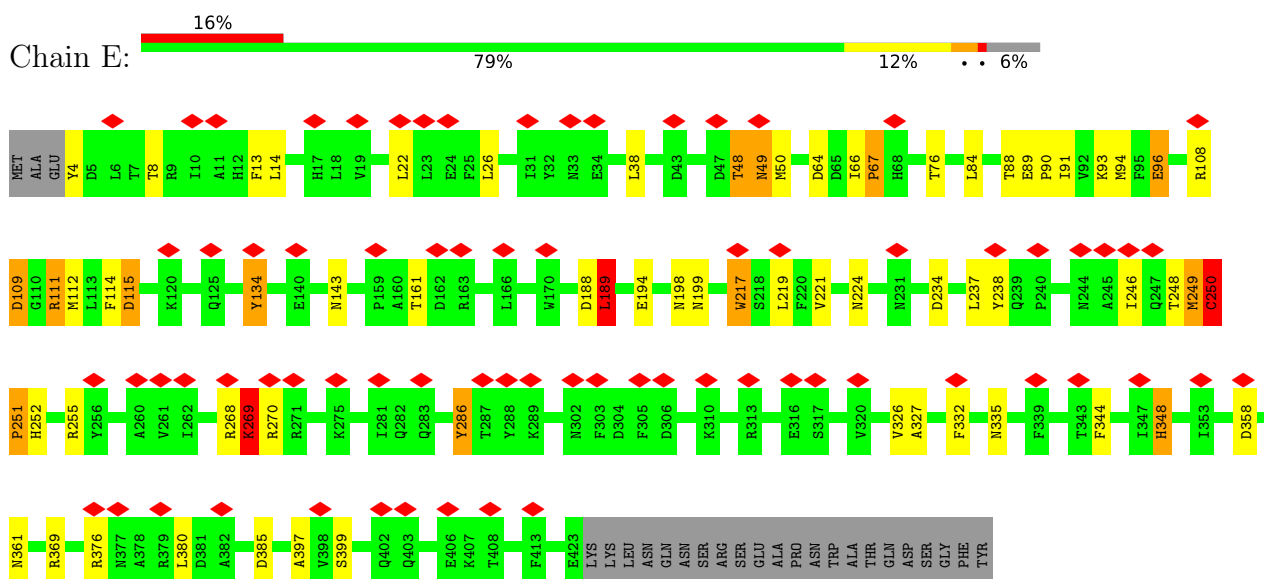
[illegible]

● Molecule 2: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT C

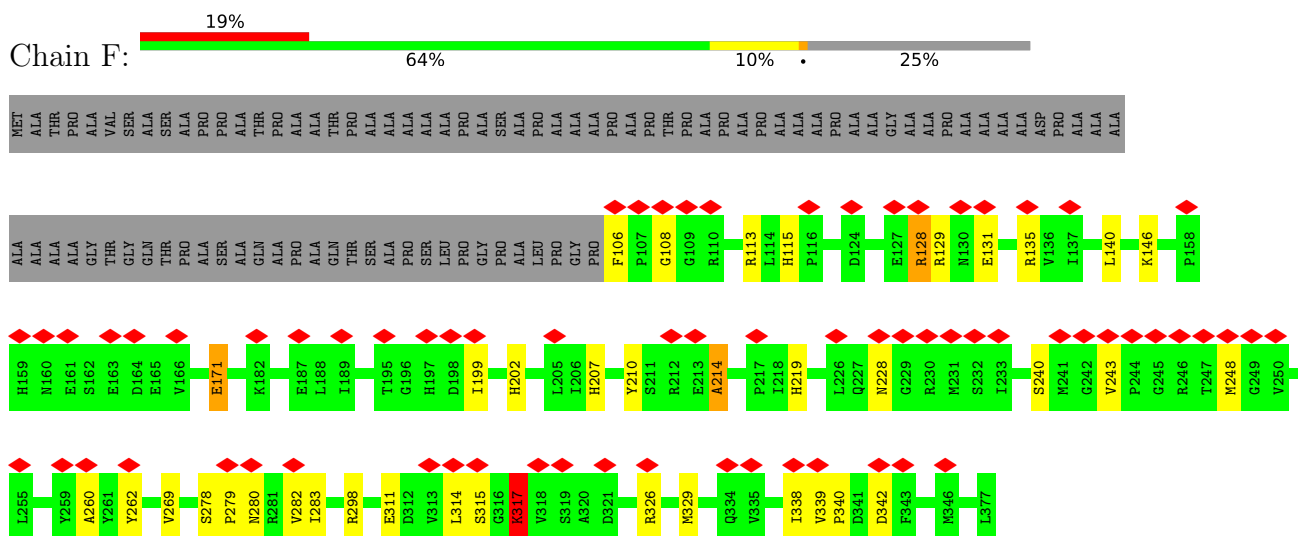


K877	K712	A557	L438	VAL	ALA	VAL	ALA	ASN	MET
GLN	Q713	K558	R439	LYS	LEU	LYS	LEU	LYS	LYS
GLY	F714	D559	Y469	GLU	ALA	GLU	ALA	ASN	ILE
THR	H715	R560	M451	LYS	SER	LYS	SER	ALA	ASP
TVR		T561	D452	PRO	ARG	PRO	ARG	ALA	VAL
GLY	E722	D562	E453	LYS	PHE	LYS	PHE	LYS	THR
GLY	R723		E454	MET	LEU	PHE	LEU	ALA	LYS
TVR		R565			ALA	PHE	ALA	LEU	LYS
PHE	L727	T566	M459	K320	ALA	ALA	ALA	THR	CYS
ARG		C567	D463	E323	PRO	THR	THR	GLU	LEU
ASP					THR		ALA	ARG	GLU
GLN	E731	R581	Y469	H526	GLU	GLU	PRO	GLN	PHE
LYS	W732	W582			ASP	SER	LYS	LYS	LEU
ASP	M733	Y583	H472	Q338	LYS	GLY	GLY	ARG	LEU
TVR	H736			A339	LYS	GLY	GLY	LYS	GLY
GLY		L590	R485	R340	LYS	SER	SER	TVR	LYS
ARG		W591		G341	ALA	LYS	ARG	ASN	ALA
LYS	K742	S592	L490	K342	ALA	LYS	LYS	ARG	TYR
ASN			E491	K343	GLU	PHE	PHE	ASP	GLY
GLU	W746	Q595	E492		LEU	LYS	LEU	PHE	LYS
GLY		D596	K493	D346	LYS	LYS	LYS	GLU	ALA
TVR	H753	W597		R347	ARG	LYS	LYS	SER	LYS
MET					GLU	MET	MET	HIS	SER
ARG	K764	P603	C500	E352	ASP	GLU	GLU	ILE	ILE
GLY	W765	R501	W502		LYS	ASP	LYS	THR	VAL
GLY	W766	W611	Y503	N364	ALA	GLU	ASN	ASN	LYS
TVR	D767			N365	LYS	ASP	TVR	LYS	GLY
ARG		F621	F514	L366	LYS	ASP	GLY	GLN	GLY
GLN	D773	R622	D515		HIS	SER	ASN	ASN	VAL
GLN					ASP	GLU	PRO	PRO	PRO
GLN	R781			G369	ARG	ASP	GLU	GLU	ARG
SER		T626	H519		LYS	SER	SER	GLN	PHE
GLN	S797			D384	LYS	GLY	GLY	SER	TYR
THR			Q522		LYS	ASP	ALA	ILE	ILE
ALA	E805	H630	Q522	N389	LYS	ARG	ASP	ASP	ARG
TVR		N631		L389	LEU	GLY	GLY	GLY	ILE
	F811	A632	P525	A390	ASP	ASP	ALA	ASP	LEU
	E812		P526	T391	GLU	TRP	ALA	ASP	LEU
	L813		E527	Y392	GLU	ASP	ALA	GLY	ASP
		Q648	G528		GLU	THR	ASP	LEU	LEU
		Q649		D410	GLY	GLY	LYS	LEU	LEU
	N828	L650	S529		GLY	GLY	GLY	ASN	ASN
	S829	L651	S530	M415	ASP	ASP	GLY	GLY	LEU
		L652	X531	P416	ASN	THR	THR	GLY	TVR
		R653			GLY	SER	SER	ASP	LEU
	W832	S654	S532	N417	GLY	ASP	SER	SER	ASN
	A833	L655	E533	I418	GLY	ASP	GLY	GLY	GLU
			Q534	F419	TRP	ASP	SER	SER	LEU
	D836	Q656	Q534		GLU	SER	SER	GLY	TRP
	Q837	Q660	D535	E422	ARG	GLY	GLY	ASP	ASP
			Q536	M423	VAL	GLY	GLY	GLU	LYS
	R846	L679	A537		ARG	GLY	GLY	ASP	GLY
	T847		E538	E427	GLY	GLY	GLY	GLY	GLY
	F848	Y697	N539		VAL	VAL	LYS	ASP	LYS
	P849		E540	M430	PRO	GLN	GLN	GLY	LYS
		S703			LEU	THR	THR	ASP	MET

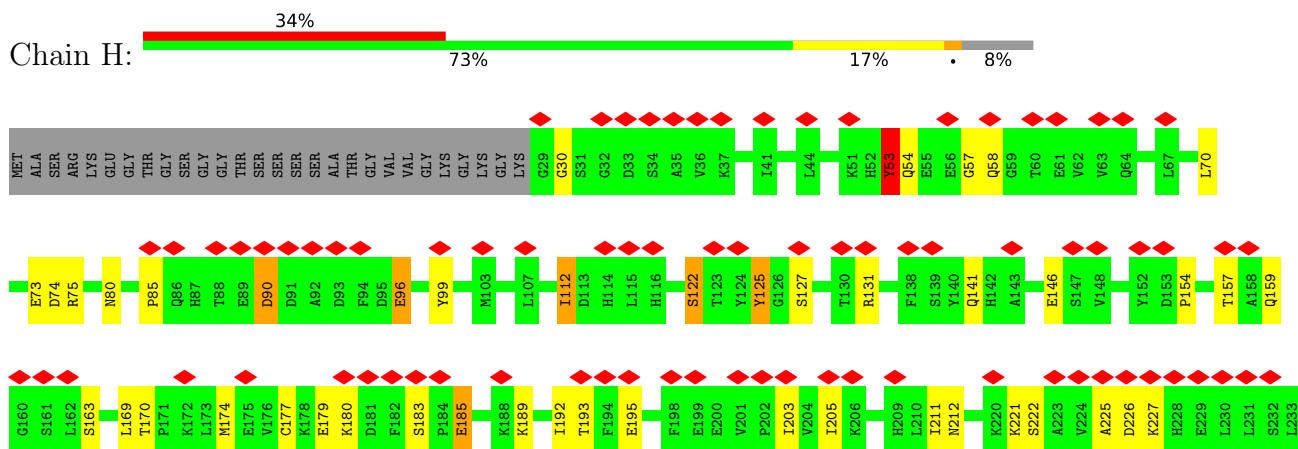
● Molecule 3: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT E

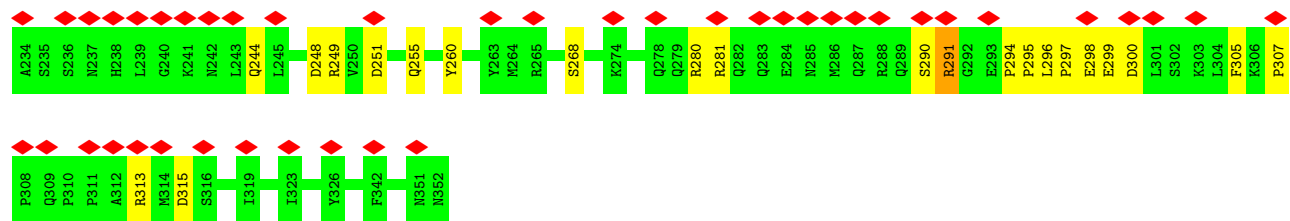


- Molecule 4: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT F

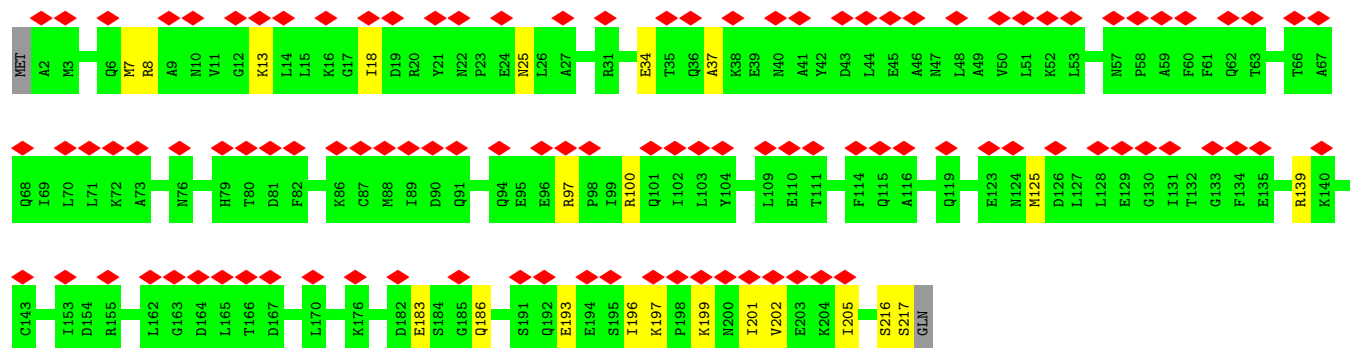
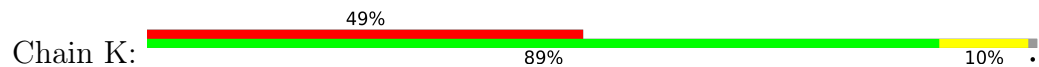


- Molecule 5: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT H

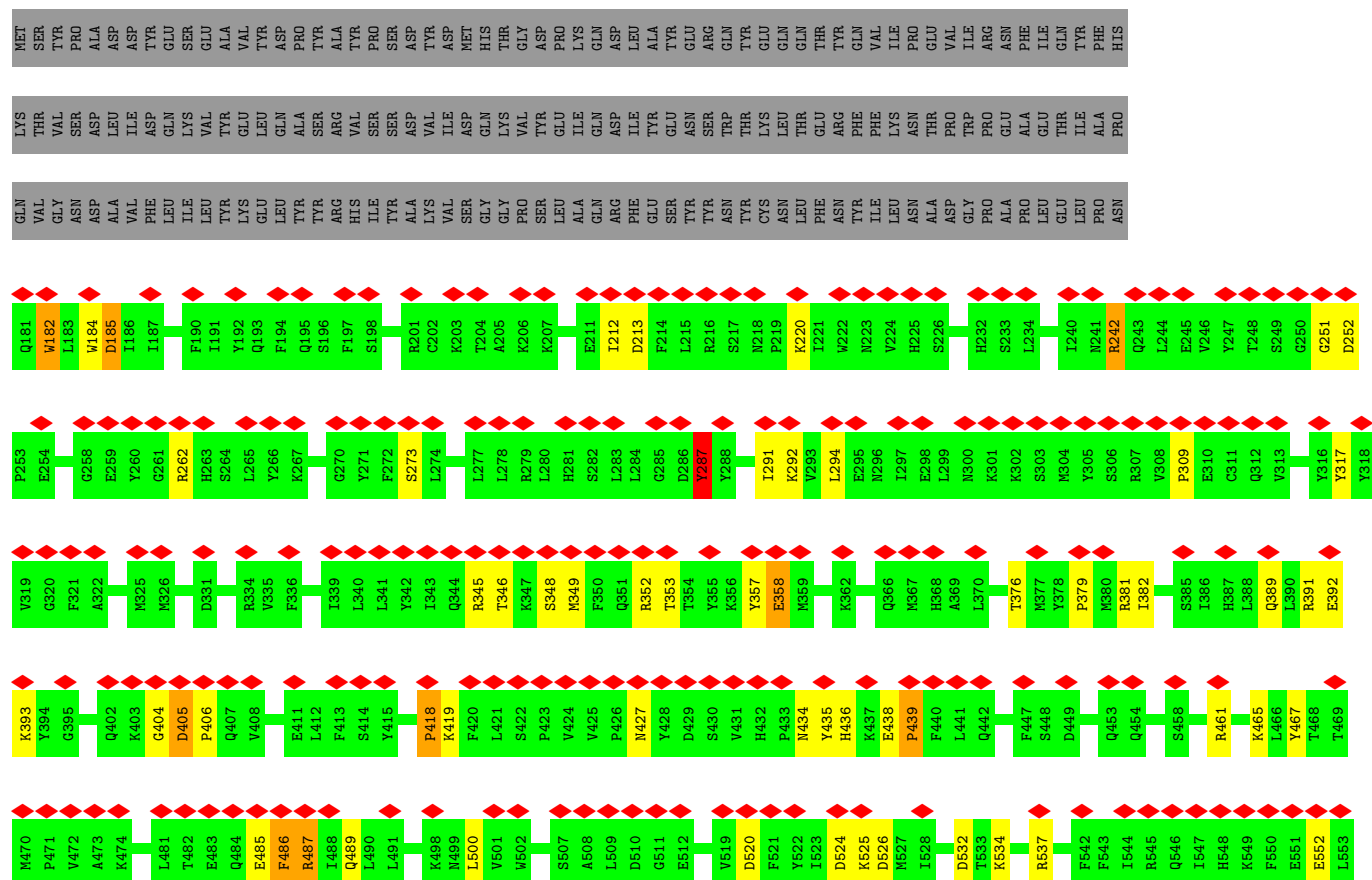




• Molecule 6: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT K

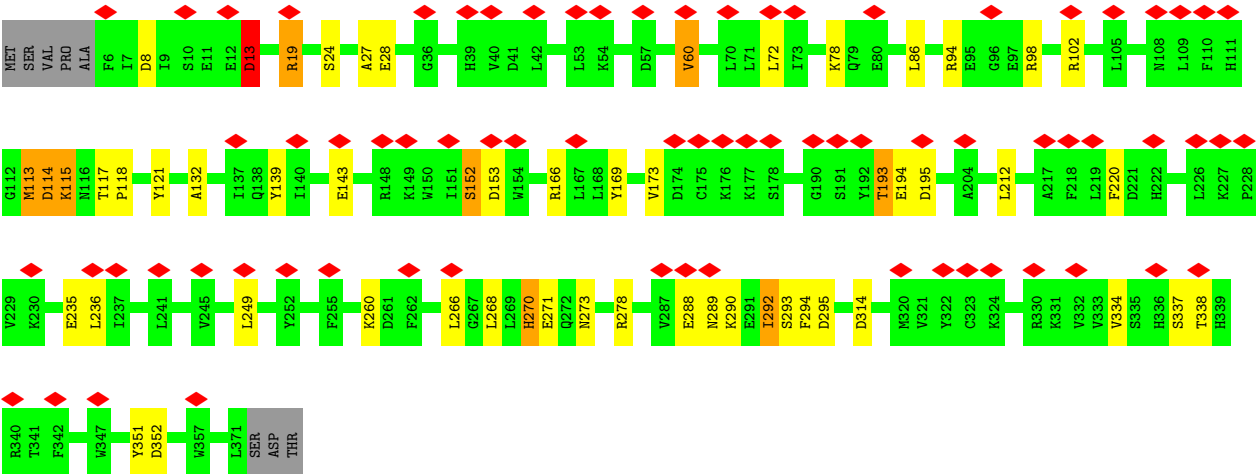
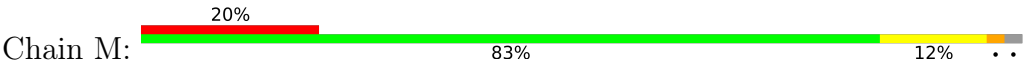


• Molecule 7: UNCHARACTERIZED PROTEIN



ASN
ARG
THR
LEU
PRO
LYS
GLY
GLN
ARG
PRO

● Molecule 8: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT M



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87192	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	30120	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	498.0, 498.0, 498.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.66, 1.66, 1.66	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	0.89	0/5021	1.68	42/6781 (0.6%)
2	C	0.89	0/4608	1.71	57/6219 (0.9%)
3	E	1.84	9/3539 (0.3%)	1.78	48/4788 (1.0%)
4	F	0.86	0/2149	1.65	18/2920 (0.6%)
5	H	0.87	0/2675	1.64	40/3609 (1.1%)
6	K	0.84	0/1773	1.61	14/2398 (0.6%)
7	L	0.87	1/3186 (0.0%)	1.69	38/4298 (0.9%)
8	M	0.86	0/2964	1.75	40/4000 (1.0%)
All	All	1.06	10/25915 (0.0%)	1.70	297/35013 (0.8%)

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	C	1	18
3	E	1	11
4	F	0	6
5	H	1	8
6	K	0	4
7	L	2	12
8	M	1	13
All	All	6	94

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	189	LEU	CB-CG	76.81	3.07	1.53
3	E	217	TRP	CD2-CE3	28.57	1.85	1.40
3	E	251	PRO	C-N	24.81	1.68	1.34
3	E	217	TRP	CE2-CZ2	22.84	1.87	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	217	TRP	CZ2-CH2	22.11	1.79	1.37
3	E	217	TRP	CD2-CE2	21.38	1.77	1.41
3	E	217	TRP	CZ3-CH2	13.98	1.75	1.40
3	E	217	TRP	CE3-CZ3	12.93	1.77	1.38
3	E	250	CYS	CA-C	-6.59	1.44	1.52
7	L	552	GLU	C-N	-5.15	1.26	1.33

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	251	PRO	CA-C-N	19.81	150.42	120.31
3	E	251	PRO	C-N-CA	19.81	150.42	120.31
3	E	250	CYS	O-C-N	-16.05	106.24	121.17
3	E	250	CYS	CA-C-O	-15.20	103.52	121.15
3	E	251	PRO	CA-C-O	14.80	147.53	120.60
8	M	288	GLU	N-CA-C	11.75	123.64	111.07
2	C	391	THR	CA-C-N	10.00	139.70	121.70
2	C	391	THR	C-N-CA	10.00	139.70	121.70
3	E	268	ARG	CA-C-N	9.87	139.47	121.70
3	E	268	ARG	C-N-CA	9.87	139.47	121.70
3	E	268	ARG	N-CA-C	9.44	121.57	111.28
2	C	766	TRP	CA-C-N	9.37	133.77	120.28
2	C	766	TRP	C-N-CA	9.37	133.77	120.28
4	F	128	ARG	N-CA-C	9.36	121.56	111.36
2	C	847	THR	CA-C-N	9.26	138.37	121.70
2	C	847	THR	C-N-CA	9.26	138.37	121.70
3	E	143	ASN	CA-C-N	9.08	138.04	121.70
3	E	143	ASN	C-N-CA	9.08	138.04	121.70
3	E	268	ARG	O-C-N	-8.59	113.01	122.12
6	K	18	ILE	CA-C-N	8.39	132.37	120.28
6	K	18	ILE	C-N-CA	8.39	132.37	120.28
2	C	452	ASP	CA-CB-CG	8.35	120.95	112.60
7	L	357	TYR	CA-C-N	8.26	131.18	120.44
7	L	357	TYR	C-N-CA	8.26	131.18	120.44
3	E	115	ASP	CA-CB-CG	8.23	120.83	112.60
7	L	353	THR	N-CA-C	8.19	120.29	111.36
2	C	847	THR	O-C-N	-8.07	111.85	122.59
4	F	340	PRO	CA-C-N	8.07	131.09	120.28
4	F	340	PRO	C-N-CA	8.07	131.09	120.28
8	M	270	HIS	CA-C-N	8.04	131.05	120.28
8	M	270	HIS	C-N-CA	8.04	131.05	120.28
8	M	294	PHE	CA-C-N	7.85	130.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	294	PHE	C-N-CA	7.85	130.80	120.28
5	H	221	LYS	N-CA-C	7.82	122.28	112.03
7	L	379	PRO	CA-C-N	7.82	135.78	121.70
7	L	379	PRO	C-N-CA	7.82	135.78	121.70
3	E	189	LEU	CD1-CG-CD2	-7.59	94.11	110.80
7	L	486	PHE	CA-C-N	7.56	135.30	121.70
7	L	486	PHE	C-N-CA	7.56	135.30	121.70
1	A	64	SER	N-CA-C	7.52	119.47	111.28
5	H	221	LYS	CA-C-N	7.45	135.10	121.70
5	H	221	LYS	C-N-CA	7.45	135.10	121.70
2	C	451	MET	CA-C-N	7.44	130.11	120.44
2	C	451	MET	C-N-CA	7.44	130.11	120.44
2	C	603	PRO	N-CA-C	7.36	119.68	110.70
3	E	143	ASN	O-C-N	-7.33	113.12	122.21
2	C	704	ASP	CA-CB-CG	-7.24	105.36	112.60
8	M	115	LYS	CA-C-N	7.24	134.73	121.70
8	M	115	LYS	C-N-CA	7.24	134.73	121.70
1	A	389	ASP	CA-CB-CG	-7.16	105.44	112.60
8	M	266	LEU	N-CA-C	7.08	119.08	111.36
2	C	490	LEU	CA-C-N	7.08	134.44	121.70
2	C	490	LEU	C-N-CA	7.08	134.44	121.70
5	H	211	ILE	CA-C-N	7.04	131.38	120.82
5	H	211	ILE	C-N-CA	7.04	131.38	120.82
6	K	125	MET	CA-C-N	6.95	129.48	120.44
6	K	125	MET	C-N-CA	6.95	129.48	120.44
3	E	198	ASN	N-CA-C	6.90	118.80	111.28
3	E	385	ASP	CA-CB-CG	-6.85	105.75	112.60
4	F	342	ASP	CA-CB-CG	6.84	119.44	112.60
8	M	195	ASP	CA-C-N	6.80	133.94	121.70
8	M	195	ASP	C-N-CA	6.80	133.94	121.70
8	M	27	ALA	CA-C-N	6.78	129.37	120.28
8	M	27	ALA	C-N-CA	6.78	129.37	120.28
8	M	288	GLU	O-C-N	-6.73	115.14	122.07
2	C	736	HIS	CA-CB-CG	6.72	120.52	113.80
7	L	184	TRP	CA-C-N	6.72	129.28	120.28
7	L	184	TRP	C-N-CA	6.72	129.28	120.28
8	M	220	PHE	CA-C-N	6.68	129.13	120.44
8	M	220	PHE	C-N-CA	6.68	129.13	120.44
8	M	314	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	239	SER	N-CA-CB	6.60	121.65	110.49
7	L	524	ASP	CA-C-N	6.60	129.13	120.28
7	L	524	ASP	C-N-CA	6.60	129.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	382	ILE	CA-C-N	6.57	129.09	120.28
7	L	382	ILE	C-N-CA	6.57	129.09	120.28
3	E	219	LEU	N-CA-C	6.56	118.09	111.07
7	L	376	THR	CA-C-N	6.52	133.44	121.70
7	L	376	THR	C-N-CA	6.52	133.44	121.70
3	E	188	ASP	CA-CB-CG	-6.50	106.10	112.60
3	E	161	THR	N-CA-C	6.50	118.16	111.14
3	E	189	LEU	CB-CG-CD1	6.48	130.14	110.70
5	H	225	ALA	CA-C-N	6.47	129.83	120.38
5	H	225	ALA	C-N-CA	6.47	129.83	120.38
2	C	562	ASP	CA-CB-CG	-6.41	106.19	112.60
5	H	313	ARG	N-CA-C	6.40	119.92	111.28
7	L	251	GLY	CA-C-N	6.39	128.08	120.09
7	L	251	GLY	C-N-CA	6.39	128.08	120.09
1	A	139	ASP	CA-CB-CG	-6.37	106.23	112.60
8	M	260	LYS	CA-C-N	6.36	128.81	120.28
8	M	260	LYS	C-N-CA	6.36	128.81	120.28
5	H	294	PRO	N-CA-C	6.36	118.45	110.70
2	C	525	PRO	N-CA-C	6.34	118.44	110.70
2	C	434	VAL	CA-C-N	6.34	133.11	121.70
2	C	434	VAL	C-N-CA	6.34	133.11	121.70
3	E	332	PHE	CA-CB-CG	6.34	120.14	113.80
5	H	300	ASP	CA-CB-CG	-6.31	106.29	112.60
7	L	185	ASP	CA-CB-CG	6.28	118.88	112.60
4	F	340	PRO	N-CA-C	6.26	119.98	111.22
8	M	24	SER	CA-C-N	6.25	129.85	119.35
8	M	24	SER	C-N-CA	6.25	129.85	119.35
8	M	13	ASP	CA-C-N	6.24	132.92	121.70
8	M	13	ASP	C-N-CA	6.24	132.92	121.70
4	F	279	PRO	CA-C-N	6.22	132.90	121.70
4	F	279	PRO	C-N-CA	6.22	132.90	121.70
2	C	869	ASN	CA-CB-CG	-6.21	106.39	112.60
1	A	373	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	484	ILE	N-CA-C	6.17	116.95	110.72
8	M	8	ASP	CA-CB-CG	-6.15	106.45	112.60
2	C	343	LYS	N-CA-C	6.12	117.75	111.14
4	F	171	GLU	CB-CG-CD	6.11	122.98	112.60
2	C	490	LEU	O-C-N	-6.04	116.12	123.19
4	F	210	TYR	CA-C-N	6.01	128.33	120.28
4	F	210	TYR	C-N-CA	6.01	128.33	120.28
3	E	198	ASN	CA-C-N	6.00	132.50	121.70
3	E	198	ASN	C-N-CA	6.00	132.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	GLN	N-CA-C	5.97	123.01	109.81
2	C	540	GLU	CA-C-N	5.97	126.74	119.99
2	C	540	GLU	C-N-CA	5.97	126.74	119.99
3	E	91	ILE	N-CA-C	5.97	116.63	110.36
4	F	128	ARG	NE-CZ-NH1	5.97	127.47	121.50
7	L	348	SER	CA-C-N	5.96	132.42	121.70
7	L	348	SER	C-N-CA	5.96	132.42	121.70
8	M	13	ASP	CA-CB-CG	5.93	118.53	112.60
2	C	595	GLN	CA-C-N	5.91	128.20	120.28
2	C	595	GLN	C-N-CA	5.91	128.20	120.28
3	E	49	ASN	O-C-N	-5.91	115.32	123.12
3	E	198	ASN	O-C-N	-5.91	115.86	122.12
5	H	131	ARG	N-CA-C	5.90	117.71	111.28
5	H	296	LEU	N-CA-C	-5.89	102.92	108.22
1	A	404	CYS	CA-C-N	5.87	128.14	120.28
1	A	404	CYS	C-N-CA	5.87	128.14	120.28
8	M	114	ASP	N-CA-CB	-5.83	100.61	110.41
8	M	78	LYS	CA-C-N	5.83	128.41	120.54
8	M	78	LYS	C-N-CA	5.83	128.41	120.54
7	L	532	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	8	PRO	CA-C-N	5.82	128.88	120.38
1	A	8	PRO	C-N-CA	5.82	128.88	120.38
1	A	338	ILE	N-CA-C	5.82	116.56	110.62
6	K	205	ILE	CA-C-N	5.80	128.33	120.38
6	K	205	ILE	C-N-CA	5.80	128.33	120.38
2	C	836	ASP	CA-CB-CG	-5.79	106.81	112.60
3	E	111	ARG	CA-C-N	5.79	128.04	120.28
3	E	111	ARG	C-N-CA	5.79	128.04	120.28
5	H	174	MET	CA-C-N	5.77	128.01	120.28
5	H	174	MET	C-N-CA	5.77	128.01	120.28
3	E	49	ASN	CA-C-N	5.75	132.06	121.70
3	E	49	ASN	C-N-CA	5.75	132.06	121.70
5	H	294	PRO	CA-C-O	-5.75	112.22	120.56
2	C	463	ASP	N-CA-C	5.73	116.19	109.60
7	L	436	HIS	CA-C-N	5.72	127.94	120.28
7	L	436	HIS	C-N-CA	5.72	127.94	120.28
2	C	434	VAL	O-C-N	-5.71	115.43	122.57
3	E	189	LEU	CB-CG-CD2	5.71	127.83	110.70
5	H	192	ILE	N-CA-C	-5.70	107.22	113.43
4	F	228	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	135	GLU	CA-C-N	5.66	132.36	121.54
1	A	135	GLU	C-N-CA	5.66	132.36	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	214	ALA	N-CA-C	5.65	122.30	109.81
3	E	114	PHE	CA-C-N	5.60	128.58	120.79
3	E	114	PHE	C-N-CA	5.60	128.58	120.79
1	A	106	GLU	CA-C-N	5.60	127.78	120.28
1	A	106	GLU	C-N-CA	5.60	127.78	120.28
7	L	353	THR	CA-C-N	5.58	131.74	121.70
7	L	353	THR	C-N-CA	5.58	131.74	121.70
2	C	592	SER	N-CA-C	5.58	117.16	111.14
1	A	422	PRO	CA-C-N	5.57	127.75	120.28
1	A	422	PRO	C-N-CA	5.57	127.75	120.28
3	E	335	ASN	CA-CB-CG	-5.57	107.03	112.60
5	H	159	GLN	N-CA-C	5.57	119.03	111.17
3	E	199	ASN	CA-CB-CG	5.57	118.17	112.60
8	M	152	SER	N-CA-C	5.57	118.39	110.10
2	C	435	ASP	N-CA-CB	5.55	119.94	110.50
4	F	240	SER	CA-C-N	5.54	131.68	121.70
4	F	240	SER	C-N-CA	5.54	131.68	121.70
3	E	48	THR	N-CA-CB	5.54	119.86	110.49
8	M	152	SER	CA-C-N	5.54	127.64	120.44
8	M	152	SER	C-N-CA	5.54	127.64	120.44
2	C	679	LEU	CA-C-N	5.53	127.69	120.28
2	C	679	LEU	C-N-CA	5.53	127.69	120.28
5	H	226	ASP	CA-C-N	5.53	127.95	120.38
5	H	226	ASP	C-N-CA	5.53	127.95	120.38
5	H	297	PRO	CA-C-N	5.51	131.62	121.70
5	H	297	PRO	C-N-CA	5.51	131.62	121.70
2	C	660	GLN	CA-C-N	5.51	127.66	120.28
2	C	660	GLN	C-N-CA	5.51	127.66	120.28
2	C	415	ASN	N-CA-C	5.47	121.90	109.81
1	A	23	LYS	N-CA-C	5.46	118.74	111.75
7	L	485	GLU	O-C-N	-5.46	116.41	122.91
7	L	348	SER	O-C-N	-5.44	116.90	123.27
8	M	193	THR	N-CA-CB	5.43	119.67	110.49
1	A	139	ASP	N-CA-C	5.42	117.18	111.28
5	H	169	LEU	CA-C-N	5.41	128.01	120.65
5	H	169	LEU	C-N-CA	5.41	128.01	120.65
5	H	96	GLU	CA-C-N	5.41	127.87	120.46
5	H	96	GLU	C-N-CA	5.41	127.87	120.46
7	L	212	ILE	N-CA-C	5.40	115.61	110.53
2	C	323	GLU	CB-CG-CD	5.39	121.76	112.60
4	F	262	TYR	N-CA-C	5.38	118.12	110.10
6	K	25	ASN	CA-CB-CG	-5.37	107.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	391	THR	O-C-N	-5.36	114.42	123.00
7	L	486	PHE	O-C-N	-5.36	114.42	123.00
1	A	364	PRO	N-CA-C	5.36	117.23	110.70
6	K	13	LYS	CA-C-N	5.35	127.44	120.28
6	K	13	LYS	C-N-CA	5.35	127.44	120.28
2	C	767	ASP	CA-C-N	5.33	127.96	120.28
2	C	767	ASP	C-N-CA	5.33	127.96	120.28
3	E	13	PHE	CA-CB-CG	-5.32	108.48	113.80
3	E	13	PHE	N-CA-C	5.32	117.16	111.36
1	A	162	ASP	CA-CB-CG	5.31	117.91	112.60
2	C	514	PHE	CA-C-N	5.31	128.78	120.82
2	C	514	PHE	C-N-CA	5.31	128.78	120.82
2	C	711	SER	CA-C-N	5.30	131.67	121.54
2	C	711	SER	C-N-CA	5.30	131.67	121.54
8	M	337	SER	CA-C-N	5.30	131.66	121.54
8	M	337	SER	C-N-CA	5.30	131.66	121.54
3	E	234	ASP	CA-CB-CG	-5.30	107.30	112.60
7	L	353	THR	O-C-N	-5.29	116.12	122.15
2	C	811	PHE	CA-CB-CG	-5.28	108.52	113.80
8	M	86	LEU	CA-C-N	5.28	127.36	120.28
8	M	86	LEU	C-N-CA	5.28	127.36	120.28
7	L	379	PRO	O-C-N	-5.28	116.41	123.06
7	L	391	ARG	CA-C-N	5.28	127.30	120.44
7	L	391	ARG	C-N-CA	5.28	127.30	120.44
1	A	384	VAL	CA-C-N	5.27	124.72	119.24
1	A	384	VAL	C-N-CA	5.27	124.72	119.24
8	M	195	ASP	O-C-N	-5.27	114.82	121.83
4	F	106	PHE	CA-CB-CG	-5.26	108.54	113.80
5	H	298	GLU	N-CA-CB	5.25	119.43	110.50
5	H	244	GLN	CA-C-N	5.23	127.55	120.38
5	H	244	GLN	C-N-CA	5.23	127.55	120.38
1	A	166	ASN	N-CA-C	5.23	121.93	110.80
2	C	773	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	63	LYS	CA-C-N	5.22	127.28	120.28
1	A	63	LYS	C-N-CA	5.22	127.28	120.28
6	K	7	MET	CA-C-N	5.22	127.53	120.38
6	K	7	MET	C-N-CA	5.22	127.53	120.38
2	C	736	HIS	CB-CA-C	-5.21	102.14	110.79
1	A	428	VAL	O-C-N	-5.21	117.08	120.42
5	H	185	GLU	CA-C-N	5.20	127.56	120.54
5	H	185	GLU	C-N-CA	5.20	127.56	120.54
1	A	403	LEU	CA-C-N	5.20	127.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	LEU	C-N-CA	5.20	127.24	120.28
3	E	14	LEU	N-CA-C	5.19	118.28	111.28
3	E	109	ASP	CA-CB-CG	-5.19	107.41	112.60
5	H	307	PRO	N-CA-C	5.18	117.02	110.70
5	H	58	GLN	N-CA-C	5.18	116.93	111.28
2	C	422	GLU	CA-C-N	5.16	129.46	122.07
2	C	422	GLU	C-N-CA	5.16	129.46	122.07
5	H	177	CYS	O-C-N	-5.16	117.00	123.04
1	A	344	MET	CA-C-N	5.15	127.70	120.28
1	A	344	MET	C-N-CA	5.15	127.70	120.28
5	H	122	SER	O-C-N	-5.15	116.12	122.19
4	F	214	ALA	O-C-N	-5.14	115.41	121.32
2	C	736	HIS	CB-CG-CD2	-5.14	124.52	131.20
7	L	526	ASP	CA-CB-CG	-5.13	107.47	112.60
2	C	515	ASP	N-CA-C	5.13	119.84	111.37
3	E	67	PRO	CA-C-N	5.13	129.28	120.71
3	E	67	PRO	C-N-CA	5.13	129.28	120.71
8	M	292	ILE	N-CA-C	5.13	120.01	109.34
3	E	269	LYS	N-CA-CB	5.12	119.21	110.50
1	A	17	GLU	CA-C-N	5.12	127.15	120.28
1	A	17	GLU	C-N-CA	5.12	127.15	120.28
2	C	430	ASN	N-CA-CB	5.12	119.14	110.49
1	A	176	ASP	CA-CB-CG	-5.12	107.48	112.60
5	H	221	LYS	O-C-N	-5.11	117.04	122.30
7	L	465	LYS	CA-C-N	5.11	127.63	120.28
7	L	465	LYS	C-N-CA	5.11	127.63	120.28
5	H	159	GLN	O-C-N	-5.10	116.74	122.86
8	M	273	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	477	HIS	CA-CB-CG	-5.09	108.71	113.80
7	L	287	TYR	CA-C-N	5.09	127.06	120.44
7	L	287	TYR	C-N-CA	5.09	127.06	120.44
3	E	64	ASP	CA-CB-CG	-5.08	107.52	112.60
5	H	177	CYS	CA-C-N	5.08	130.84	121.70
5	H	177	CYS	C-N-CA	5.08	130.84	121.70
2	C	390	ALA	CA-C-N	5.08	130.84	121.70
2	C	390	ALA	C-N-CA	5.08	130.84	121.70
2	C	427	GLU	O-C-N	-5.08	117.01	123.05
6	K	186	GLN	N-CA-C	5.08	116.49	110.19
8	M	212	LEU	CA-C-N	5.08	127.08	120.28
8	M	212	LEU	C-N-CA	5.08	127.08	120.28
2	C	416	PRO	N-CA-C	5.07	122.92	112.47
5	H	53	TYR	N-CA-C	5.06	121.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	HIS	N-CA-CB	5.05	119.03	110.49
3	E	217	TRP	CG-CD1-NE1	5.05	116.77	110.20
6	K	37	ALA	CA-C-N	5.04	127.00	120.44
6	K	37	ALA	C-N-CA	5.04	127.00	120.44
1	A	591	LYS	CA-C-N	5.04	127.29	120.38
1	A	591	LYS	C-N-CA	5.04	127.29	120.38
3	E	8	THR	CA-C-N	5.04	127.04	120.28
3	E	8	THR	C-N-CA	5.04	127.04	120.28
1	A	343	ASP	N-CA-CB	-5.03	103.18	110.47
1	A	328	SER	CA-C-N	5.02	123.40	120.24
1	A	328	SER	C-N-CA	5.02	123.40	120.24
2	C	410	ASP	CA-CB-CG	-5.02	107.58	112.60
5	H	170	THR	N-CA-C	5.02	116.71	109.48

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	513	LYS	CA
3	E	67	PRO	CA
5	H	223	ALA	CA
7	L	418	PRO	CA
7	L	439	PRO	CA
8	M	115	LYS	CA

All (94) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	202	ARG	Sidechain
1	A	300	TYR	Sidechain
1	A	307	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	367	ARG	Sidechain
1	A	438	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	469	ARG	Sidechain
1	A	483	ARG	Sidechain
1	A	489	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	502	ARG	Sidechain
1	A	514	MET	Peptide
1	A	578	ARG	Sidechain
1	A	581	ARG	Sidechain
1	A	589	ARG	Sidechain
1	A	597	ARG	Sidechain
1	A	91	ARG	Sidechain
2	C	320	LYS	Peptide
2	C	347	ARG	Sidechain
2	C	439	ARG	Sidechain
2	C	469	TYR	Sidechain
2	C	485	ARG	Sidechain
2	C	503	TYR	Sidechain
2	C	531	LYS	Peptide
2	C	536	GLN	Peptide
2	C	556	TYR	Sidechain
2	C	565	ARG	Sidechain
2	C	583	TYR	Sidechain
2	C	611	ARG	Sidechain
2	C	622	ARG	Sidechain
2	C	653	ARG	Sidechain
2	C	697	TYR	Sidechain
2	C	708	ARG	Sidechain
2	C	781	ARG	Sidechain
2	C	846	ARG	Sidechain
3	E	108	ARG	Sidechain
3	E	250	CYS	Peptide,Mainchain
3	E	255	ARG	Sidechain
3	E	270	ARG	Sidechain
3	E	286	TYR	Sidechain
3	E	369	ARG	Sidechain
3	E	376	ARG	Sidechain
3	E	4	TYR	Sidechain
3	E	49	ASN	Peptide
3	E	66	ILE	Peptide
4	F	113	ARG	Sidechain
4	F	128	ARG	Peptide,Sidechain
4	F	135	ARG	Sidechain
4	F	298	ARG	Sidechain
4	F	326	ARG	Sidechain
5	H	122	SER	Peptide
5	H	125	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	H	249	ARG	Sidechain
5	H	281	ARG	Sidechain
5	H	290	SER	Peptide
5	H	291	ARG	Sidechain
5	H	75	ARG	Sidechain
5	H	99	TYR	Sidechain
6	K	100	ARG	Sidechain
6	K	139	ARG	Sidechain
6	K	8	ARG	Sidechain
6	K	97	ARG	Sidechain
7	L	242	ARG	Sidechain
7	L	262	ARG	Sidechain
7	L	287	TYR	Sidechain
7	L	317	TYR	Sidechain
7	L	345	ARG	Sidechain
7	L	352	ARG	Sidechain
7	L	405	ASP	Peptide
7	L	434	ASN	Peptide
7	L	438	GLU	Peptide
7	L	467	TYR	Sidechain
7	L	487	ARG	Peptide
7	L	537	ARG	Sidechain
8	M	102	ARG	Sidechain
8	M	114	ASP	Peptide
8	M	121	TYR	Sidechain
8	M	13	ASP	Peptide
8	M	166	ARG	Sidechain
8	M	169	TYR	Sidechain
8	M	19	ARG	Sidechain
8	M	249	LEU	Peptide
8	M	278	ARG	Sidechain
8	M	289	ASN	Peptide
8	M	351	TYR	Sidechain
8	M	94	ARG	Sidechain
8	M	98	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4935	0	5017	3	0
2	C	4529	0	4533	8	0
3	E	3466	0	3446	74	0
4	F	2111	0	2105	3	0
5	H	2624	0	2592	7	0
6	K	1738	0	1706	4	0
7	L	3110	0	3084	6	0
8	M	2919	0	2950	2	0
All	All	25432	0	25433	102	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 2.

All (102) 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)
3:E:217:TRP:CE3	3:E:217:TRP:CZ3	1.77	1.71
3:E:217:TRP:CZ3	3:E:217:TRP:CH2	1.75	1.62
3:E:217:TRP:CE2	3:E:217:TRP:CZ2	1.87	1.60
3:E:217:TRP:CH2	3:E:217:TRP:CZ2	1.79	1.59
3:E:217:TRP:CE3	3:E:217:TRP:CD2	1.86	1.59
3:E:217:TRP:CE2	3:E:217:TRP:CD2	1.77	1.52
3:E:189:LEU:HG	3:E:217:TRP:CD2	1.43	1.52
3:E:38:LEU:CD1	3:E:251:PRO:HD3	1.36	1.52
3:E:251:PRO:C	3:E:252:HIS:N	1.68	1.47
3:E:38:LEU:HD13	3:E:251:PRO:CD	1.43	1.46
3:E:189:LEU:HG	3:E:217:TRP:CE3	1.76	1.21
3:E:38:LEU:CD1	3:E:251:PRO:CD	2.10	1.18
3:E:189:LEU:CG	3:E:217:TRP:CE2	2.28	1.14
3:E:189:LEU:CB	3:E:217:TRP:CD2	2.30	1.13
3:E:189:LEU:CG	3:E:217:TRP:CD2	2.31	1.12
3:E:189:LEU:CB	3:E:217:TRP:CE2	2.31	1.12
3:E:189:LEU:CG	3:E:217:TRP:CE3	2.34	1.09
3:E:251:PRO:HB2	3:E:286:TYR:CE1	1.87	1.09
3:E:189:LEU:CG	3:E:217:TRP:CZ2	2.38	1.07
3:E:189:LEU:CG	3:E:217:TRP:CH2	2.38	1.06
3:E:251:PRO:N	3:E:252:HIS:H	1.53	1.06
3:E:189:LEU:CB	3:E:217:TRP:CZ2	2.39	1.06
3:E:189:LEU:CG	3:E:217:TRP:CZ3	2.41	1.03
3:E:251:PRO:CA	3:E:252:HIS:N	2.21	1.03
3:E:189:LEU:CB	3:E:217:TRP:CE3	2.42	1.02
3:E:189:LEU:CB	3:E:217:TRP:CZ3	2.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:189:LEU:CB	3:E:217:TRP:CH2	2.45	0.98
3:E:251:PRO:CD	3:E:252:HIS:H	1.77	0.96
3:E:251:PRO:HD2	3:E:252:HIS:HB2	1.43	0.95
3:E:189:LEU:HG	3:E:217:TRP:CE2	2.04	0.92
3:E:189:LEU:HB2	3:E:217:TRP:CE3	2.05	0.92
3:E:251:PRO:N	3:E:252:HIS:N	2.18	0.92
3:E:189:LEU:HB3	3:E:217:TRP:CH2	2.06	0.89
3:E:251:PRO:CD	3:E:252:HIS:HB2	2.05	0.85
3:E:38:LEU:HD13	3:E:251:PRO:CG	2.07	0.85
3:E:38:LEU:HD11	3:E:251:PRO:CD	2.04	0.84
3:E:189:LEU:CD1	3:E:217:TRP:CZ3	2.63	0.81
3:E:251:PRO:HB2	3:E:286:TYR:CZ	2.14	0.81
3:E:189:LEU:CD2	3:E:217:TRP:CZ2	2.67	0.77
3:E:38:LEU:CD1	3:E:251:PRO:HD2	2.15	0.77
3:E:38:LEU:HD13	3:E:251:PRO:HD3	0.76	0.76
3:E:189:LEU:CA	3:E:217:TRP:CE2	2.69	0.75
3:E:251:PRO:CG	3:E:252:HIS:HB2	2.18	0.74
3:E:251:PRO:HD2	3:E:252:HIS:CB	2.17	0.74
3:E:251:PRO:CB	3:E:286:TYR:CE1	2.70	0.74
3:E:189:LEU:CD2	3:E:217:TRP:CE2	2.70	0.74
3:E:189:LEU:HB3	3:E:217:TRP:CZ3	2.24	0.73
3:E:251:PRO:CG	3:E:252:HIS:N	2.51	0.73
3:E:189:LEU:HB2	3:E:217:TRP:CD2	2.22	0.73
3:E:38:LEU:HD11	3:E:251:PRO:HD2	1.71	0.68
3:E:251:PRO:CG	3:E:252:HIS:H	2.07	0.67
3:E:251:PRO:HG2	3:E:252:HIS:HB2	1.78	0.66
3:E:251:PRO:HG2	3:E:252:HIS:N	2.10	0.64
7:L:358:GLU:H	7:L:358:GLU:CD	2.04	0.63
3:E:189:LEU:HD22	3:E:217:TRP:CZ2	2.36	0.59
3:E:251:PRO:HB2	3:E:286:TYR:HE1	1.63	0.58
3:E:189:LEU:HA	3:E:217:TRP:CE2	2.38	0.58
3:E:189:LEU:HD23	3:E:217:TRP:CE2	2.39	0.56
3:E:251:PRO:CB	3:E:286:TYR:CZ	2.88	0.54
5:H:227:LYS:HD2	5:H:227:LYS:H	1.72	0.54
3:E:189:LEU:C	3:E:217:TRP:CZ2	2.86	0.53
3:E:251:PRO:HG2	3:E:252:HIS:CB	2.38	0.53
5:H:195:GLU:H	5:H:195:GLU:CD	2.17	0.53
3:E:250:CYS:N	3:E:251:PRO:HA	2.26	0.51
1:A:353:ARG:HH11	5:H:90:ASP:CG	2.19	0.51
6:K:217:SER:N	7:L:534:LYS:HZ1	2.10	0.50
3:E:189:LEU:CD1	3:E:217:TRP:CH2	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:217:SER:N	7:L:534:LYS:NZ	2.60	0.50
1:A:285:LYS:HG2	1:A:292:HIS:CD2	2.46	0.50
3:E:189:LEU:CD1	3:E:217:TRP:CE3	2.94	0.50
6:K:216:SER:C	7:L:534:LYS:HZ1	2.20	0.50
2:C:340:ARG:HE	2:C:384:ASP:CG	2.21	0.49
3:E:249:MET:SD	3:E:251:PRO:HB3	2.53	0.49
6:K:196:ILE:HG13	6:K:197:LYS:H	1.77	0.48
3:E:38:LEU:HD13	3:E:251:PRO:HG3	1.94	0.48
4:F:207:HIS:HE1	4:F:219:HIS:CE1	2.31	0.48
2:C:527:GLU:H	2:C:527:GLU:CD	2.22	0.48
3:E:344:PHE:CE1	3:E:348:HIS:CE1	3.01	0.48
3:E:251:PRO:CB	3:E:252:HIS:N	2.77	0.47
3:E:251:PRO:HG2	3:E:252:HIS:CA	2.45	0.47
3:E:112:MET:HA	3:E:115:ASP:HB2	1.98	0.46
3:E:96:GLU:H	3:E:96:GLU:CD	2.22	0.46
7:L:381:ARG:HH22	7:L:520:ASP:CG	2.24	0.45
2:C:733:MET:HA	2:C:736:HIS:CD2	2.52	0.44
5:H:185:GLU:CD	5:H:189:LYS:HZ1	2.27	0.43
8:M:28:GLU:H	8:M:28:GLU:CD	2.26	0.43
7:L:242:ARG:HA	7:L:427:ASN:HD21	1.83	0.43
3:E:189:LEU:CA	3:E:217:TRP:CZ2	3.01	0.43
2:C:549:GLU:CD	2:C:553:LYS:HZ1	2.28	0.42
2:C:369:GLY:HA3	2:C:419:PHE:CG	2.54	0.42
2:C:877:LYS:N	5:H:280:ARG:NH2	2.66	0.42
3:E:251:PRO:CD	3:E:252:HIS:CB	2.87	0.42
2:C:492:GLU:H	2:C:492:GLU:CD	2.26	0.42
3:E:189:LEU:HD13	3:E:217:TRP:CZ3	2.54	0.42
5:H:179:GLU:CD	5:H:180:LYS:H	2.28	0.42
2:C:805:GLU:H	2:C:805:GLU:CD	2.27	0.41
4:F:311:GLU:CD	4:F:317:LYS:HZ2	2.28	0.41
8:M:271:GLU:H	8:M:271:GLU:CD	2.29	0.41
1:A:486:HIS:CD2	1:A:488:SER:H	2.39	0.41
4:F:207:HIS:CE1	4:F:219:HIS:CE1	3.09	0.40
3:E:111:ARG:HB3	3:E:134:TYR:CZ	2.56	0.40
5:H:30:GLY:H	5:H:74:ASP:CG	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/1362 (44%)	544 (91%)	36 (6%)	18 (3%)	3	22
2	C	556/843 (66%)	512 (92%)	28 (5%)	16 (3%)	3	23
3	E	418/445 (94%)	362 (87%)	37 (9%)	19 (4%)	2	16
4	F	270/364 (74%)	234 (87%)	20 (7%)	16 (6%)	1	13
5	H	322/352 (92%)	277 (86%)	29 (9%)	16 (5%)	1	15
6	K	214/218 (98%)	200 (94%)	12 (6%)	2 (1%)	14	50
7	L	371/564 (66%)	331 (89%)	26 (7%)	14 (4%)	2	19
8	M	364/374 (97%)	320 (88%)	30 (8%)	14 (4%)	2	19
All	All	3113/4522 (69%)	2780 (89%)	218 (7%)	115 (4%)	4	19

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	136	ASP
1	A	166	ASN
1	A	478	CYS
1	A	539	PRO
2	C	392	TYR
2	C	416	PRO
2	C	430	ASN
2	C	712	LYS
3	E	67	PRO
3	E	76	THR
3	E	246	ILE
3	E	399	SER
4	F	214	ALA
4	F	243	VAL
4	F	248	MET
4	F	339	VAL

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Mol	Chain	Res	Type
5	H	154	PRO
5	H	183	SER
5	H	222	SER
7	L	273	SER
7	L	406	PRO
7	L	439	PRO
7	L	489	GLN
7	L	500	LEU
8	M	115	LYS
8	M	117	THR
8	M	268	LEU
8	M	290	LYS
8	M	334	VAL
1	A	21	VAL
1	A	163	LEU
1	A	188	TYR
1	A	311	THR
1	A	501	THR
2	C	326	HIS
2	C	530	SER
2	C	704	ASP
2	C	847	THR
3	E	26	LEU
3	E	88	THR
3	E	238	TYR
3	E	326	VAL
4	F	260	ALA
4	F	315	SER
4	F	338	ILE
5	H	54	GLN
5	H	127	SER
5	H	291	ARG
7	L	294	LEU
8	M	173	VAL
8	M	193	THR
8	M	194	GLU
8	M	292	ILE
8	M	338	THR
1	A	135	GLU
1	A	239	SER
2	C	346	ASP
2	C	529	SER

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Mol	Chain	Res	Type
3	E	48	THR
3	E	50	MET
3	E	237	LEU
3	E	249	MET
3	E	269	LYS
3	E	327	ALA
3	E	397	ALA
4	F	129	ARG
4	F	146	LYS
4	F	314	LEU
4	F	317	LYS
5	H	53	TYR
5	H	57	GLY
5	H	125	TYR
5	H	205	ILE
5	H	305	PHE
7	L	404	GLY
7	L	435	TYR
7	L	486	PHE
8	M	113	MET
1	A	421	GLU
1	A	480	LEU
2	C	655	LEU
2	C	849	PRO
3	E	90	PRO
3	E	380	LEU
5	H	112	ILE
5	H	193	THR
7	L	418	PRO
7	L	487	ARG
1	A	65	HIS
2	C	491	GLU
2	C	653	ARG
3	E	22	LEU
3	E	221	VAL
4	F	131	GLU
4	F	280	ASN
7	L	349	MET
8	M	132	ALA
1	A	344	MET
2	C	707	ARG
5	H	203	ILE

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Mol	Chain	Res	Type
6	K	201	ILE
7	L	182	TRP
8	M	236	LEU
4	F	278	SER
6	K	202	VAL
1	A	514	MET
2	C	436	GLN
4	F	108	GLY
8	M	60	VAL
5	H	295	PRO
5	H	85	PRO
7	L	291	ILE
1	A	417	GLN
4	F	282	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/1245 (44%)	528 (96%)	23 (4%)	26	48
2	C	70/750 (9%)	68 (97%)	2 (3%)	37	58
3	E	324/406 (80%)	309 (95%)	15 (5%)	24	45
4	F	220/282 (78%)	211 (96%)	9 (4%)	27	48
5	H	293/311 (94%)	274 (94%)	19 (6%)	15	37
6	K	190/193 (98%)	186 (98%)	4 (2%)	47	65
7	L	342/516 (66%)	323 (94%)	19 (6%)	19	40
8	M	327/335 (98%)	312 (95%)	15 (5%)	24	45
All	All	2317/4038 (57%)	2211 (95%)	106 (5%)	25	45

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU

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Mol	Chain	Res	Type
1	A	16	ASN
1	A	45	LYS
1	A	75	LYS
1	A	110	GLN
1	A	136	ASP
1	A	162	ASP
1	A	170	VAL
1	A	179	GLN
1	A	261	SER
1	A	300	TYR
1	A	309	ASN
1	A	323	LEU
1	A	335	ARG
1	A	372	ASN
1	A	397	GLU
1	A	419	GLU
1	A	420	LYS
1	A	434	ASN
1	A	521	ASN
1	A	538	LYS
1	A	583	GLU
1	A	593	GLU
2	C	338	GLN
2	C	352	GLU
3	E	84	LEU
3	E	89	GLU
3	E	93	LYS
3	E	94	MET
3	E	96	GLU
3	E	109	ASP
3	E	134	TYR
3	E	189	LEU
3	E	194	GLU
3	E	224	ASN
3	E	248	THR
3	E	269	LYS
3	E	348	HIS
3	E	358	ASP
3	E	361	ASN
4	F	115	HIS
4	F	140	LEU
4	F	171	GLU

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Mol	Chain	Res	Type
4	F	199	ILE
4	F	202	HIS
4	F	269	VAL
4	F	283	ILE
4	F	317	LYS
4	F	329	MET
5	H	53	TYR
5	H	70	LEU
5	H	73	GLU
5	H	80	ASN
5	H	90	ASP
5	H	96	GLU
5	H	112	ILE
5	H	141	GLN
5	H	146	GLU
5	H	157	THR
5	H	163	SER
5	H	212	ASN
5	H	248	ASP
5	H	251	ASP
5	H	255	GLN
5	H	260	TYR
5	H	268	SER
5	H	299	GLU
5	H	315	ASP
6	K	34	GLU
6	K	183	GLU
6	K	193	GLU
6	K	199	LYS
7	L	182	TRP
7	L	185	ASP
7	L	213	ASP
7	L	220	LYS
7	L	252	ASP
7	L	287	TYR
7	L	292	LYS
7	L	309	PRO
7	L	346	THR
7	L	358	GLU
7	L	389	GLN
7	L	392	GLU
7	L	393	LYS

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Mol	Chain	Res	Type
7	L	405	ASP
7	L	418	PRO
7	L	419	LYS
7	L	439	PRO
7	L	461	ARG
7	L	525	LYS
8	M	13	ASP
8	M	19	ARG
8	M	60	VAL
8	M	72	LEU
8	M	113	MET
8	M	118	PRO
8	M	139	TYR
8	M	143	GLU
8	M	152	SER
8	M	153	ASP
8	M	235	GLU
8	M	270	HIS
8	M	293	SER
8	M	295	ASP
8	M	352	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	44	GLN
1	A	80	GLN
1	A	200	ASN
1	A	213	ASN
1	A	486	HIS
2	C	326	HIS
2	C	359	GLN
3	E	105	GLN
3	E	216	HIS
3	E	354	ASN
3	E	396	ASN
4	F	159	HIS
4	F	207	HIS
5	H	345	GLN
5	H	348	GLN
5	H	352	ASN

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Mol	Chain	Res	Type
6	K	151	GLN
6	K	169	GLN
6	K	192	GLN
7	L	366	GLN
7	L	427	ASN
7	L	443	GLN
7	L	453	GLN
7	L	546	GLN
8	M	14	GLN
8	M	39	HIS
8	M	104	GLN
8	M	116	ASN
8	M	205	HIS
8	M	258	ASN
8	M	336	HIS
8	M	346	GLN
8	M	348	GLN
8	M	366	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	251:PRO	C	252:HIS	N	1.68

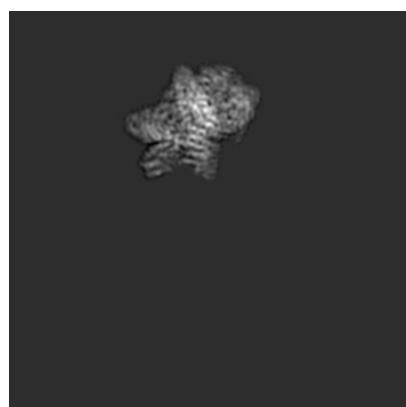
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3056. These allow visual inspection of the internal detail of the map and identification of artifacts.

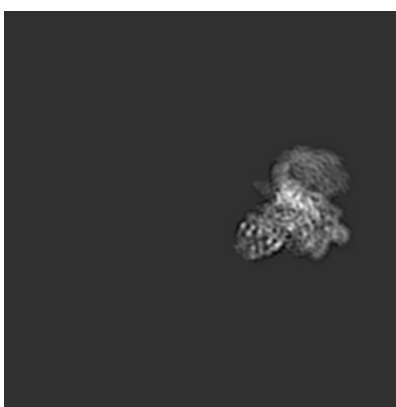
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

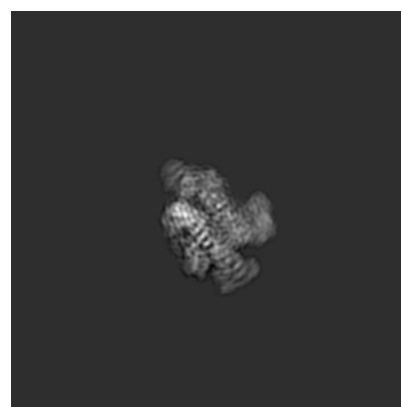
6.1.1 Primary map



X



Y

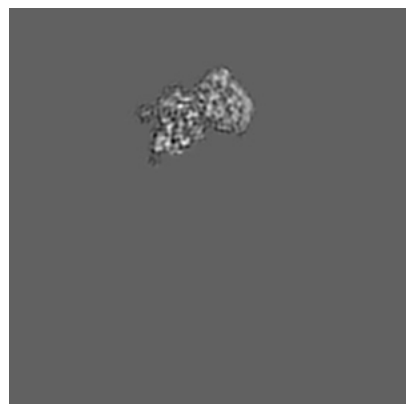


Z

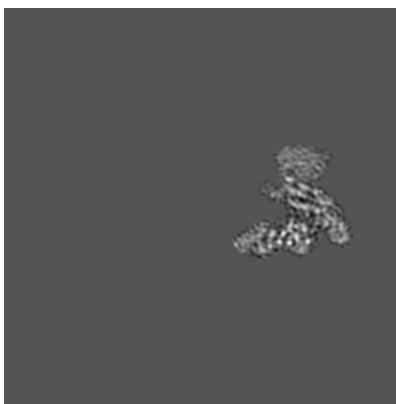
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

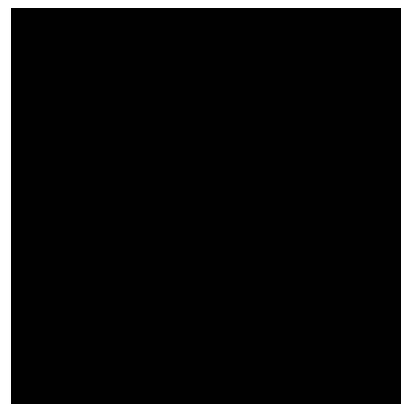
6.2.1 Primary map



X Index: 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: 138



Y Index: 147

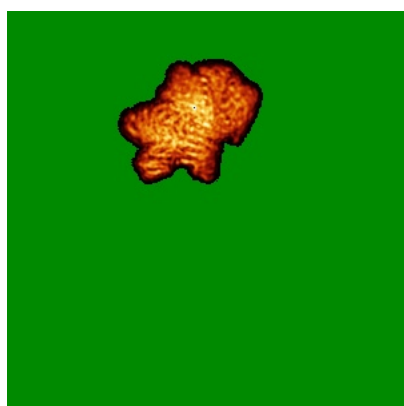


Z Index: 220

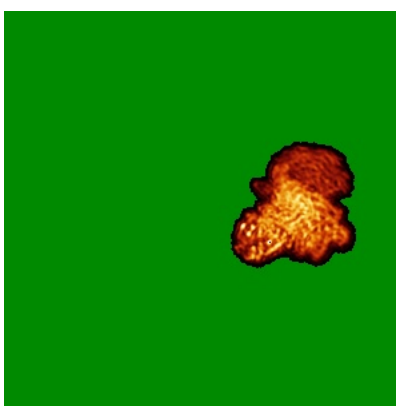
The images above show the largest variance slices of the map in three orthogonal directions.

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

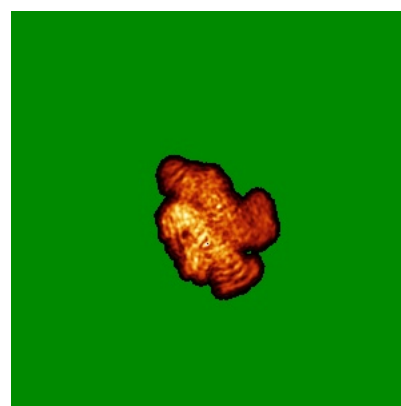
6.4.1 Primary map



X



Y

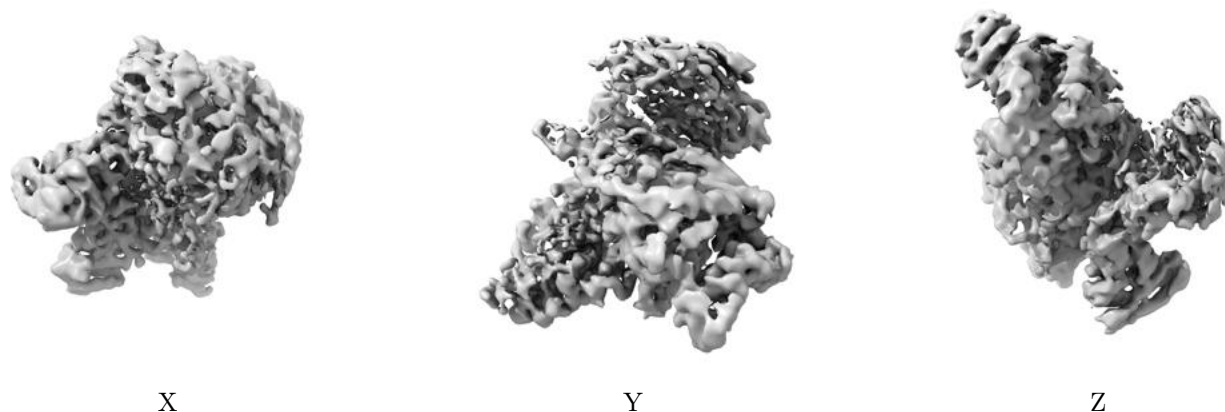


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

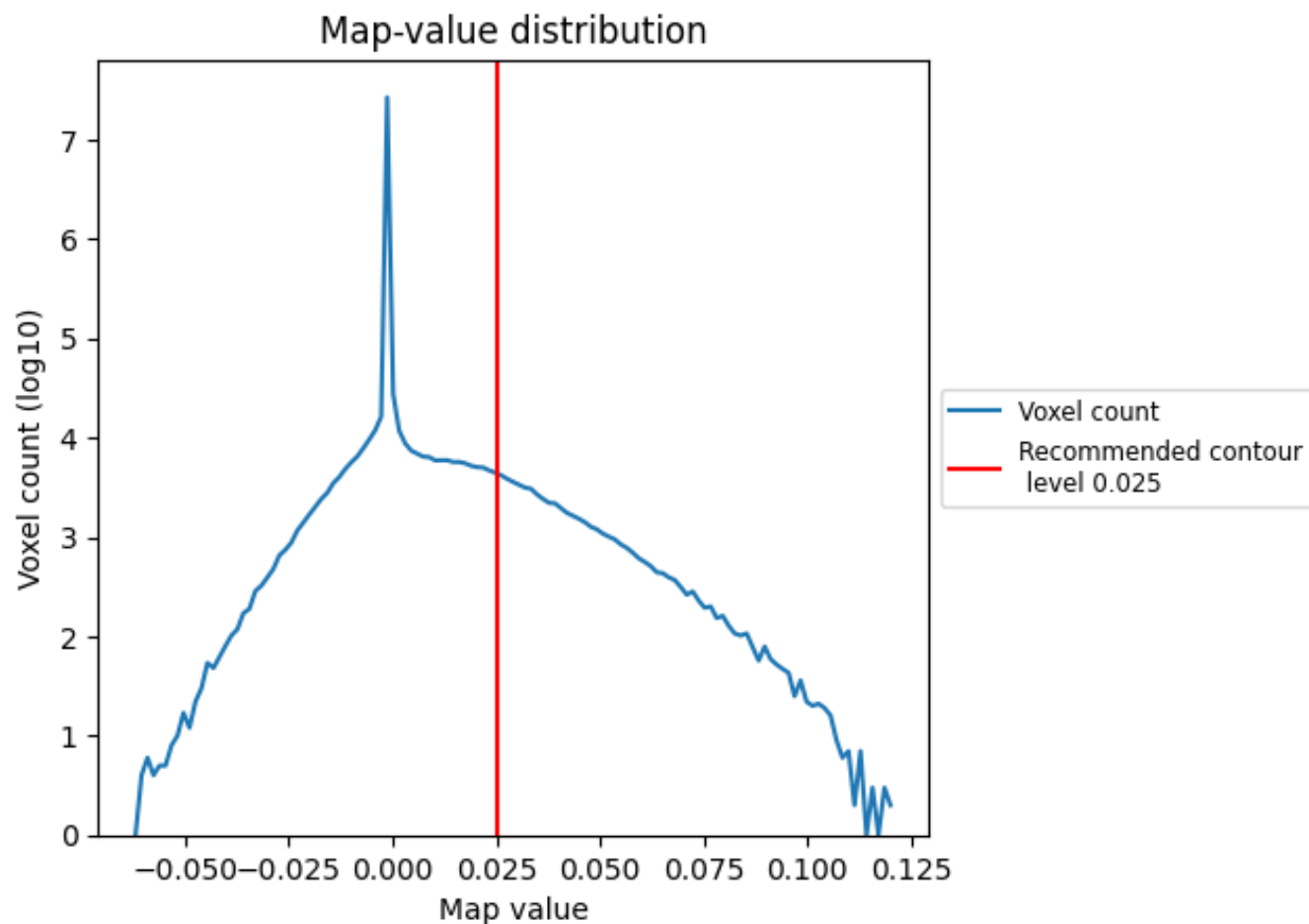
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

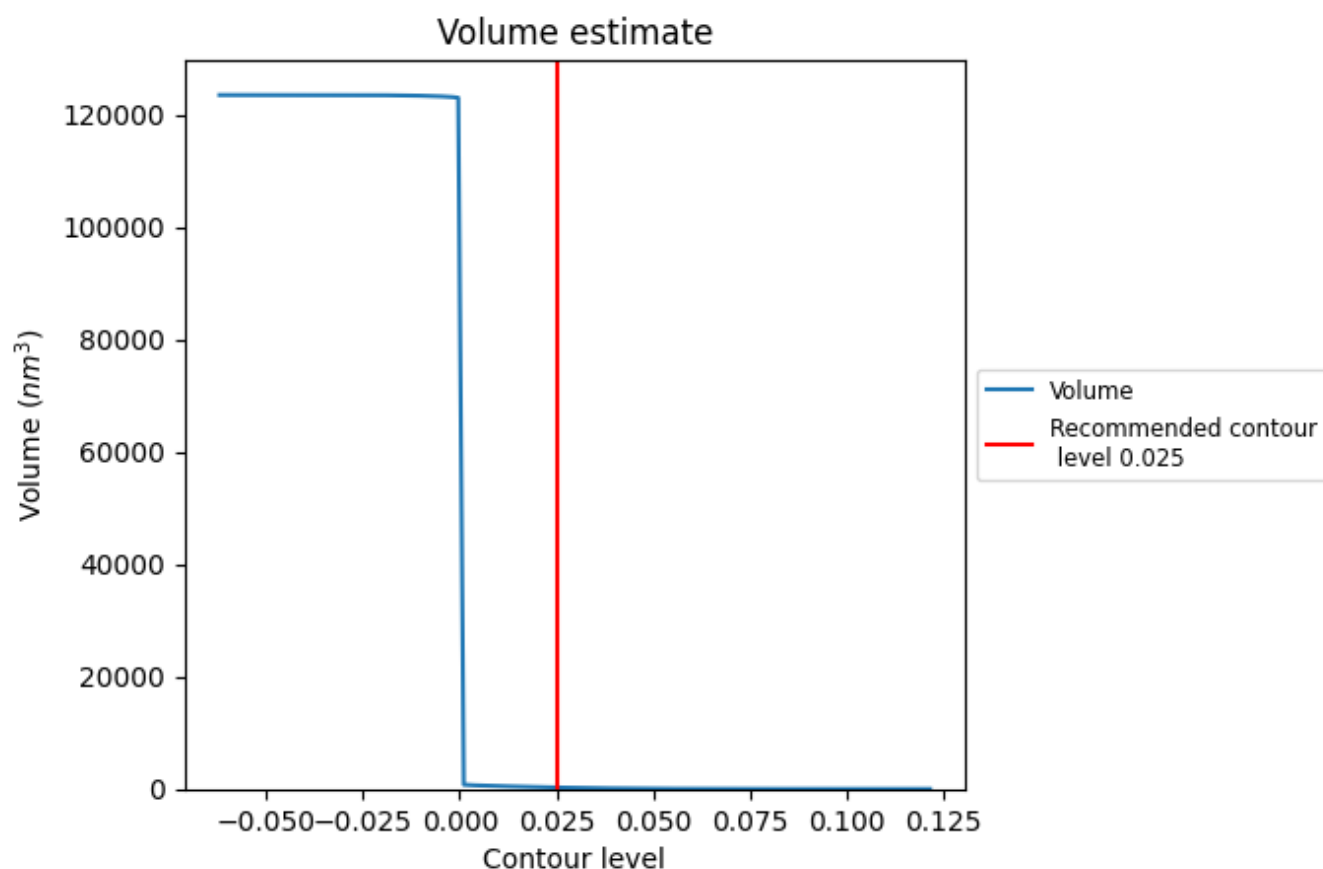
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

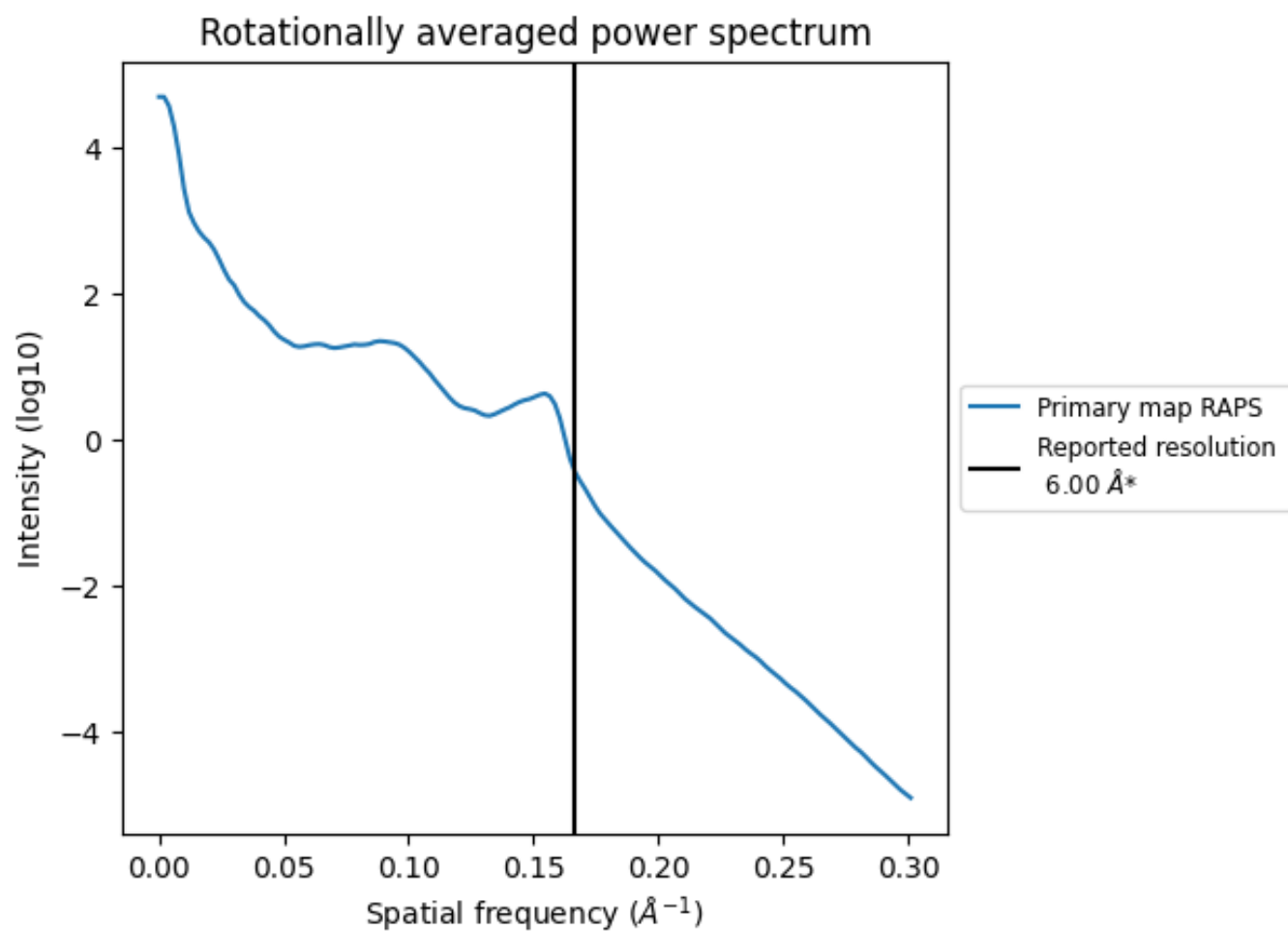
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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 0.167 Å⁻¹

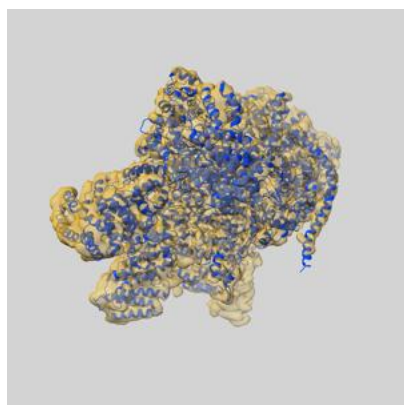
8 Fourier-Shell correlation ⓘ

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

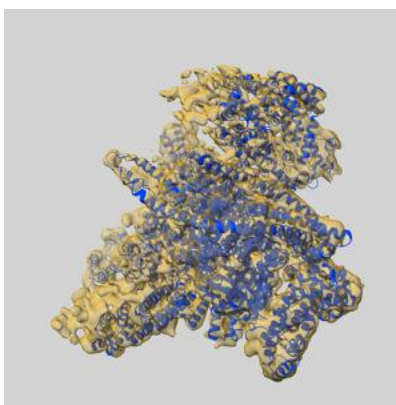
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3056 and PDB model 5A5T. Per-residue inclusion information can be found in section [3](#) on page [6](#).

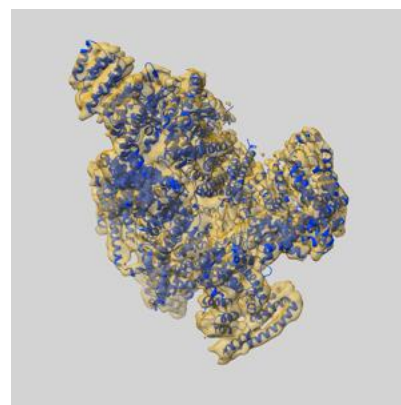
9.1 Map-model overlay [i](#)



X



Y



Z

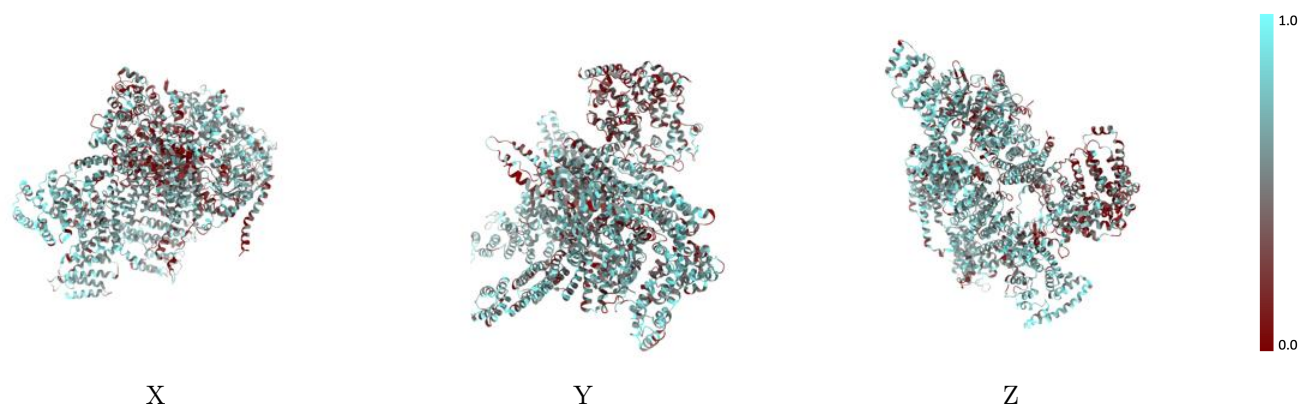
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



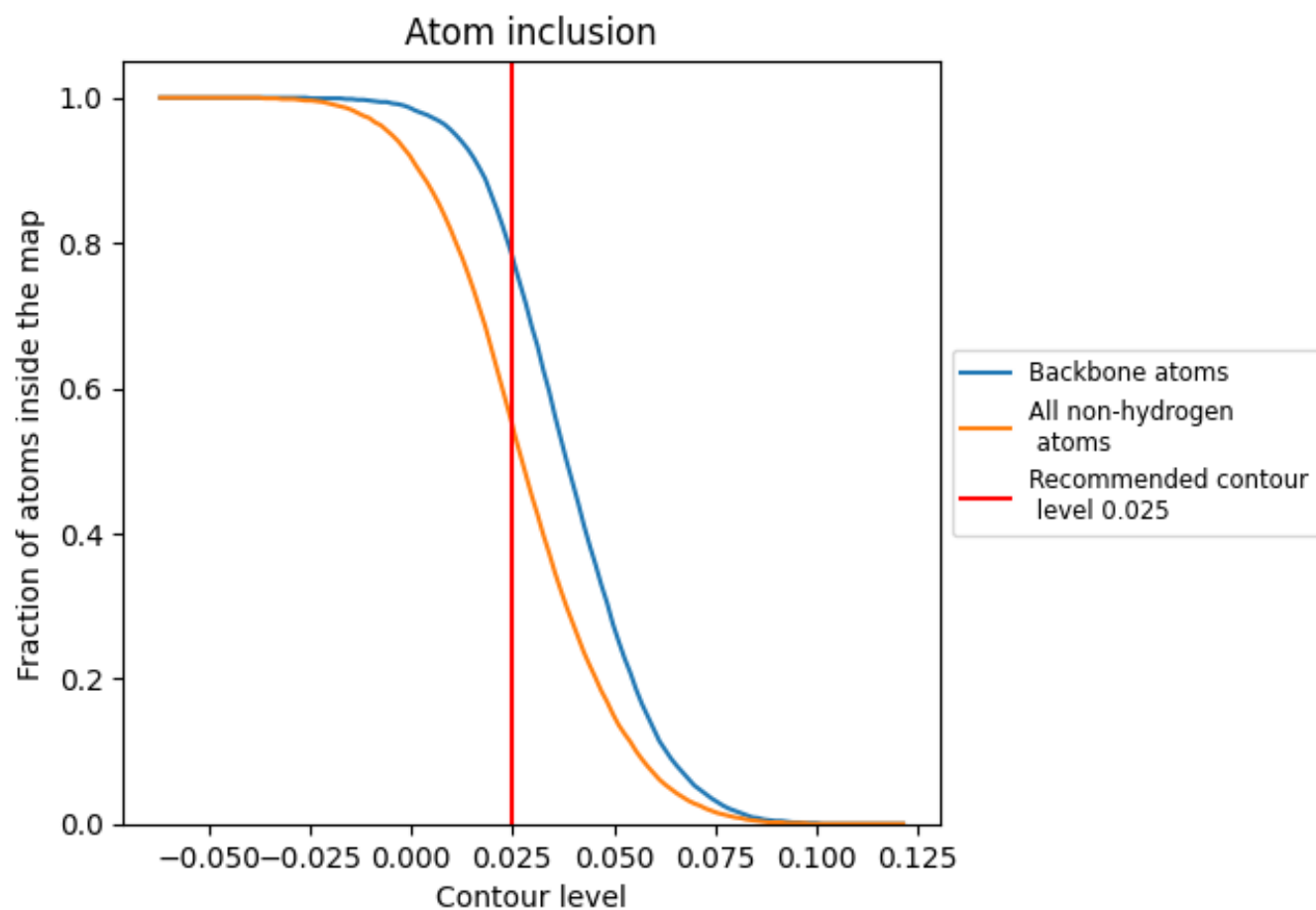
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5490	0.1070
A	0.5850	0.1150
C	0.6150	0.1230
E	0.6360	0.1200
F	0.5490	0.1010
H	0.4750	0.0830
K	0.4360	0.1020
L	0.3580	0.0800
M	0.6150	0.1110

1.0

0.0

<0.0