



Full wwPDB EM Validation Report ⓘ

Oct 8, 2026 – 12:27 PM EDT

PDB ID : 9PBZ / pdb_00009pbz
EMDB ID : EMD-71494
Title : PolII/TFIIF of PIC-Med-SWI/SNF-Nucleosome
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-26
Resolution : 3.60 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:

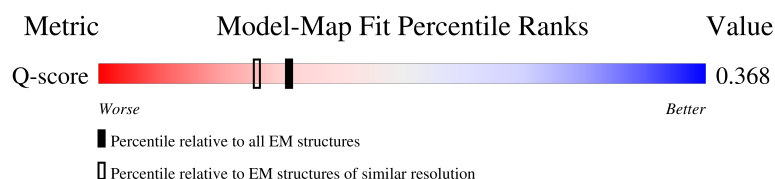
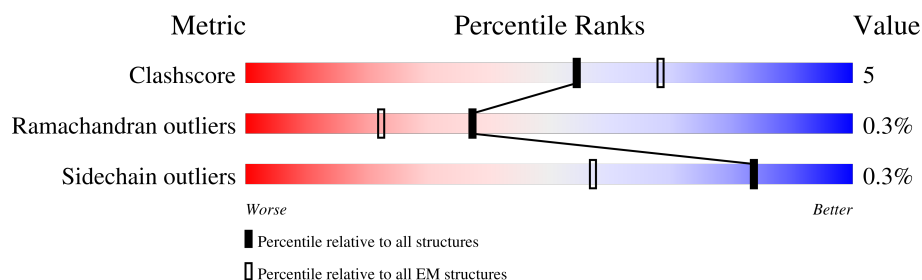
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

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 3.60 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	12797 (3.10 - 4.10)

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	C	318	
2	E	215	
3	F	155	
4	G	171	

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Mol	Chain	Length	Quality of chain
5	I	122	
6	J	70	
7	K	120	
8	L	70	
9	S	309	
10	M	345	
11	B	1224	
12	A	1733	
13	D	221	
14	H	146	
15	Q	735	
16	R	400	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36587 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 DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 9 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	164	Total	C	N	O	S	0	0
			1302	812	230	252	8		

- Molecule 10 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	89	Total	C	N	O	S	0	0
			679	429	112	129	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	1155	Total	C	N	O	S	0	0
			9200	5818	1610	1717	55		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1398	Total	C	N	O	S	0	0
			10996	6931	1926	2078	61		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 15 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	214	Total	C	N	O	S	0	0
			1817	1149	337	324	7		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	198	Total	C	N	O	S	0	0
			1629	1011	293	317	8		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	
17	S	1	Total	Zn	0
			1	1	
17	M	1	Total	Zn	0
			1	1	
17	B	1	Total	Zn	0
			1	1	
17	A	2	Total	Zn	0
			2	2	

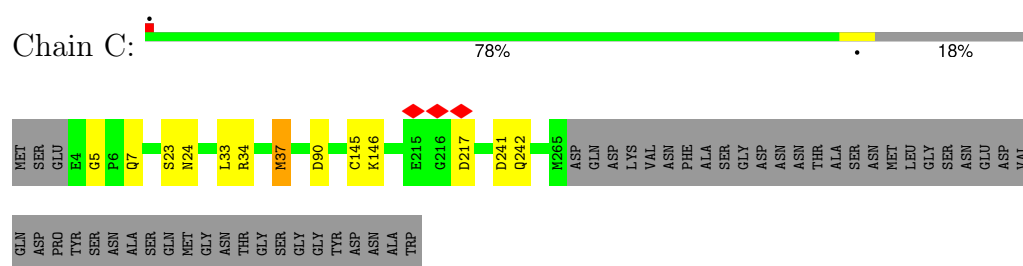
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

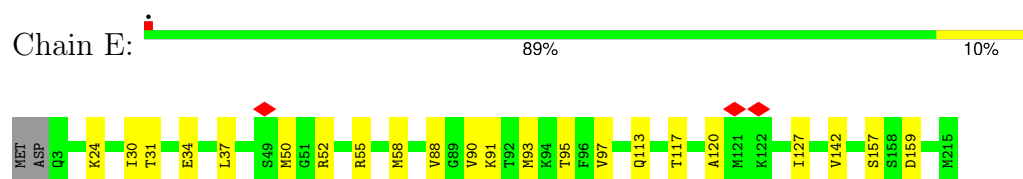
3 Residue-property plots [i](#)

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

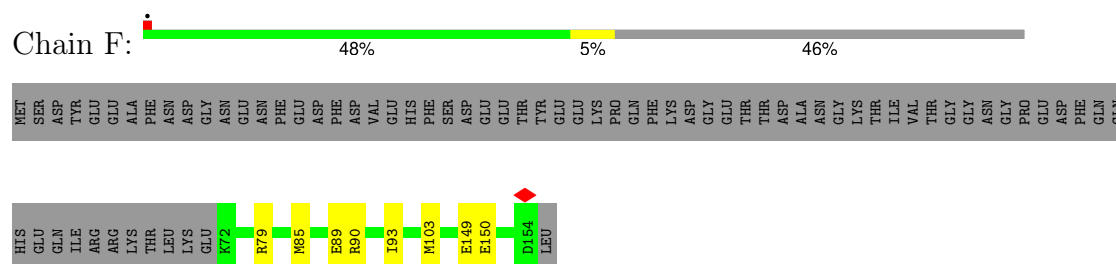
- Molecule 1: DNA-directed RNA polymerase II subunit RPB3



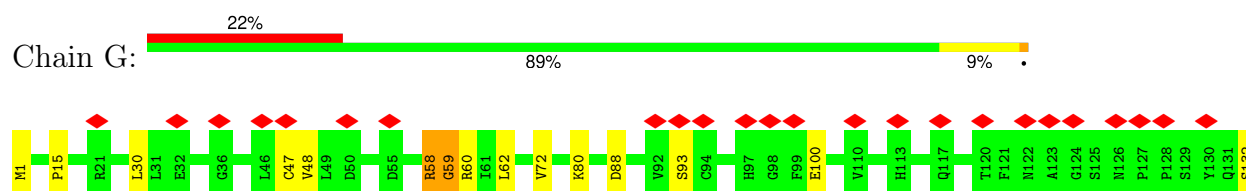
- Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1

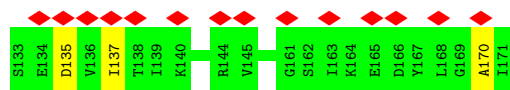


- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

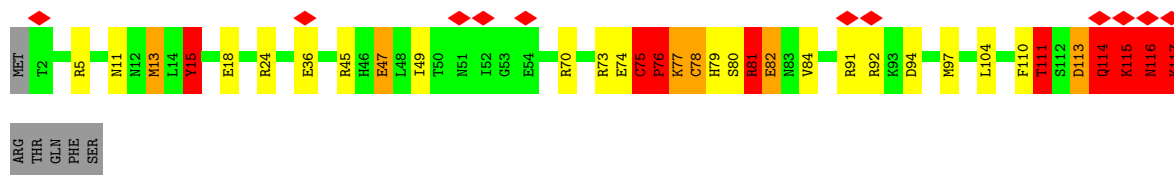


- Molecule 4: DNA-directed RNA polymerase II subunit RPB7

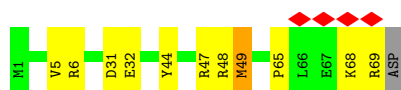
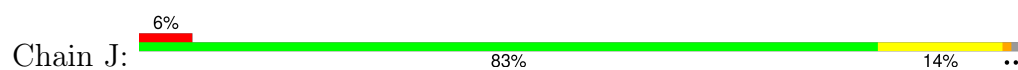




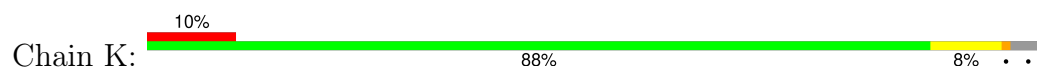
- Molecule 5: DNA-directed RNA polymerase II subunit RPB9



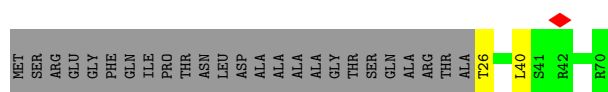
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC5



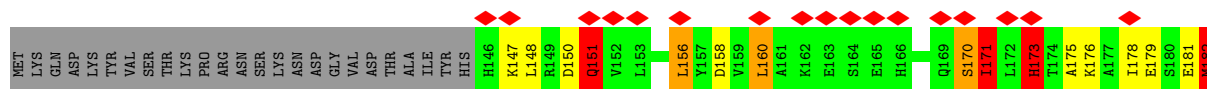
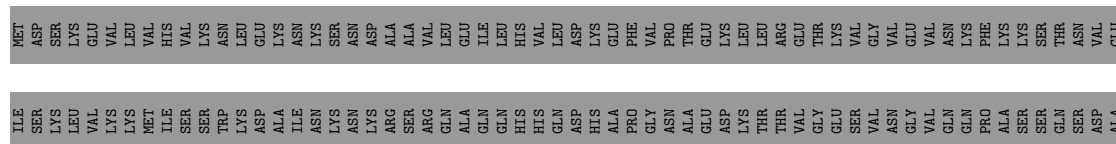
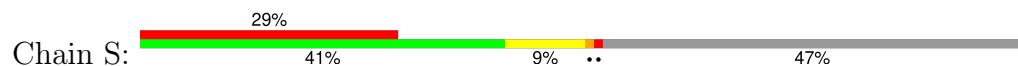
- Molecule 7: DNA-directed RNA polymerase II subunit RPB11

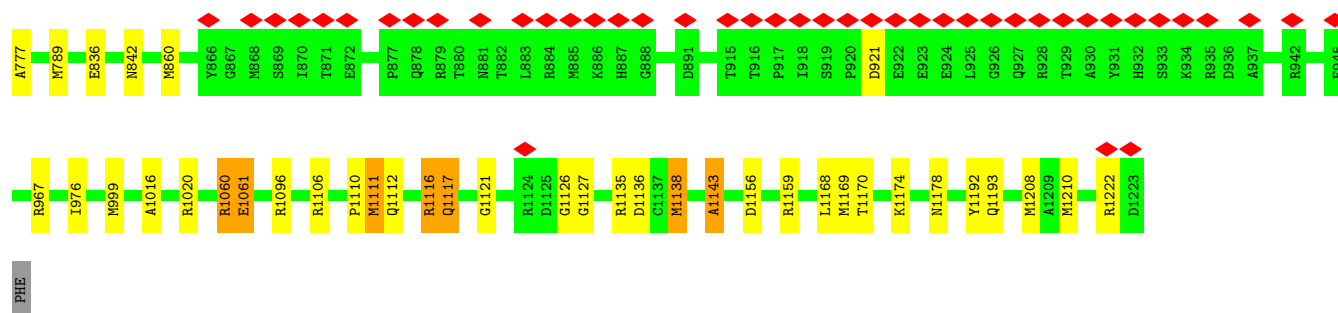


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC4



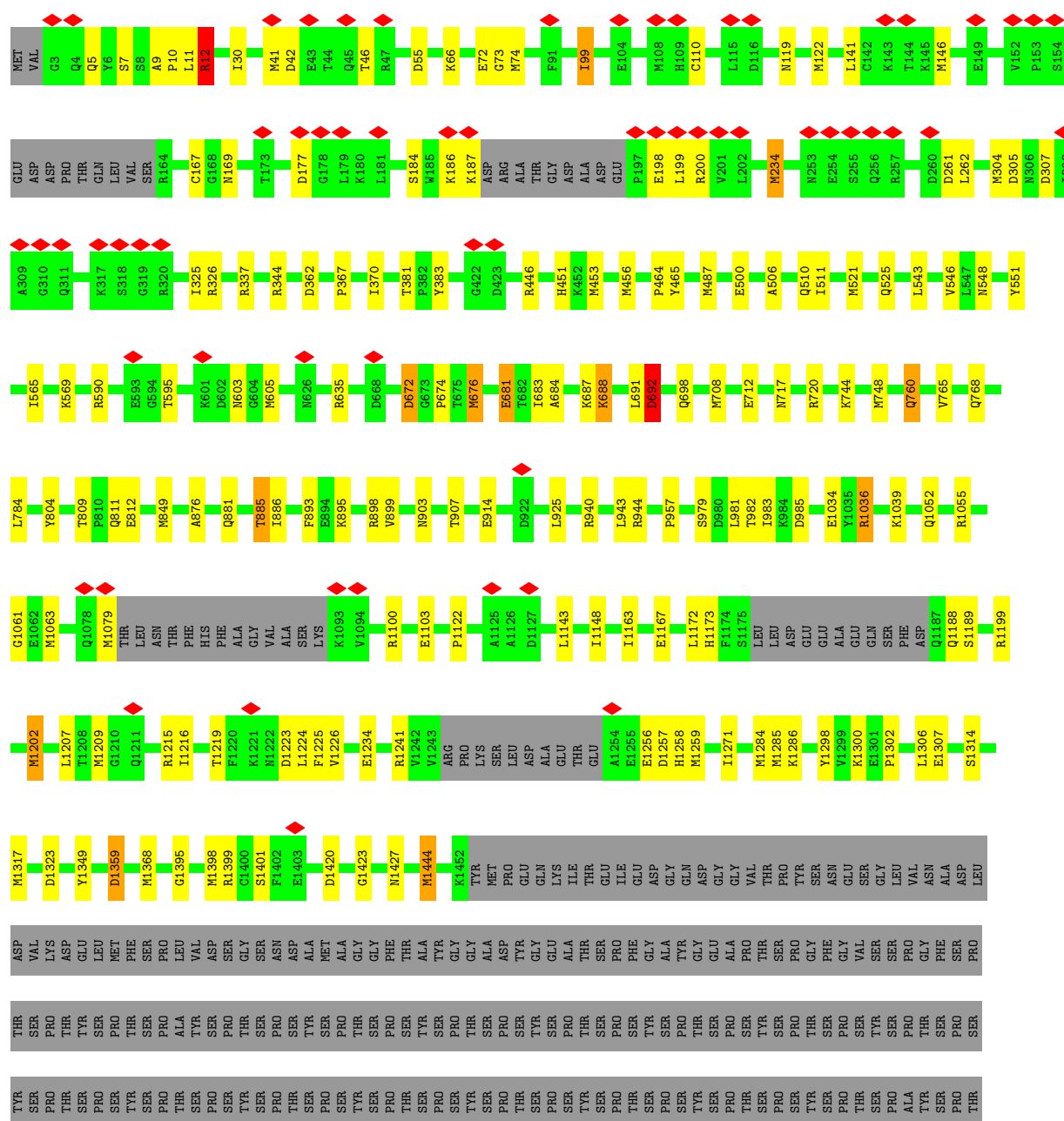
- Molecule 9: Transcription elongation factor S-II

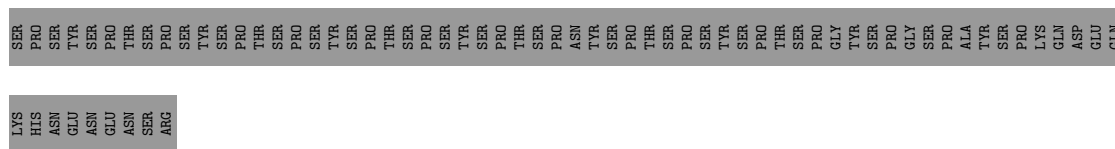




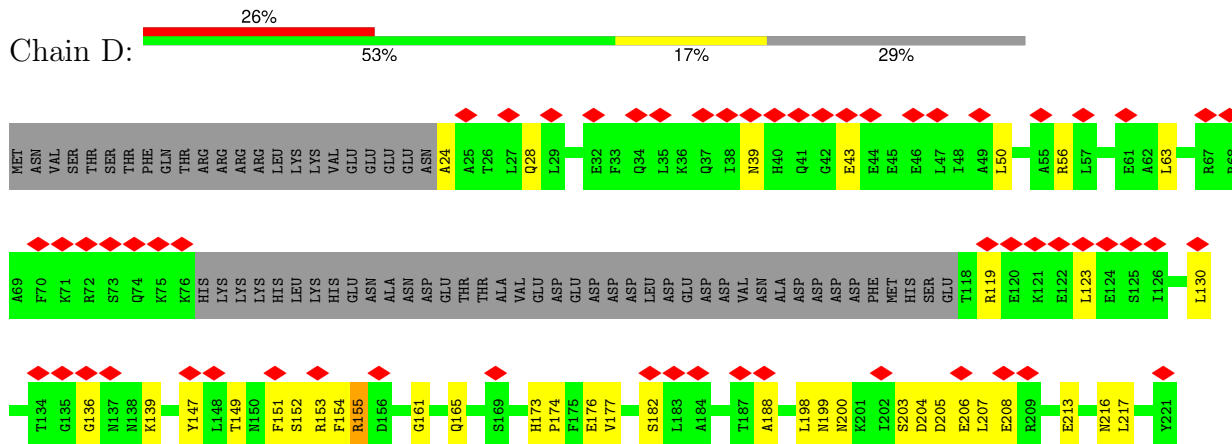
• Molecule 12: DNA-directed RNA polymerase II subunit RPB1

Chain A: 71% 9% 19%

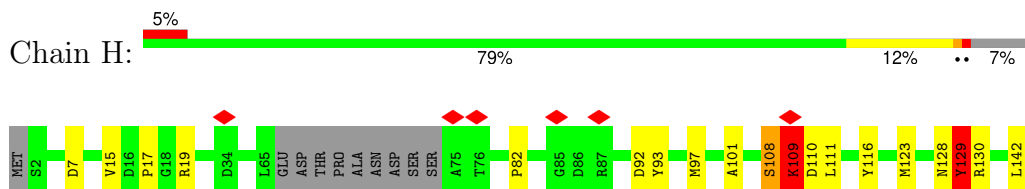




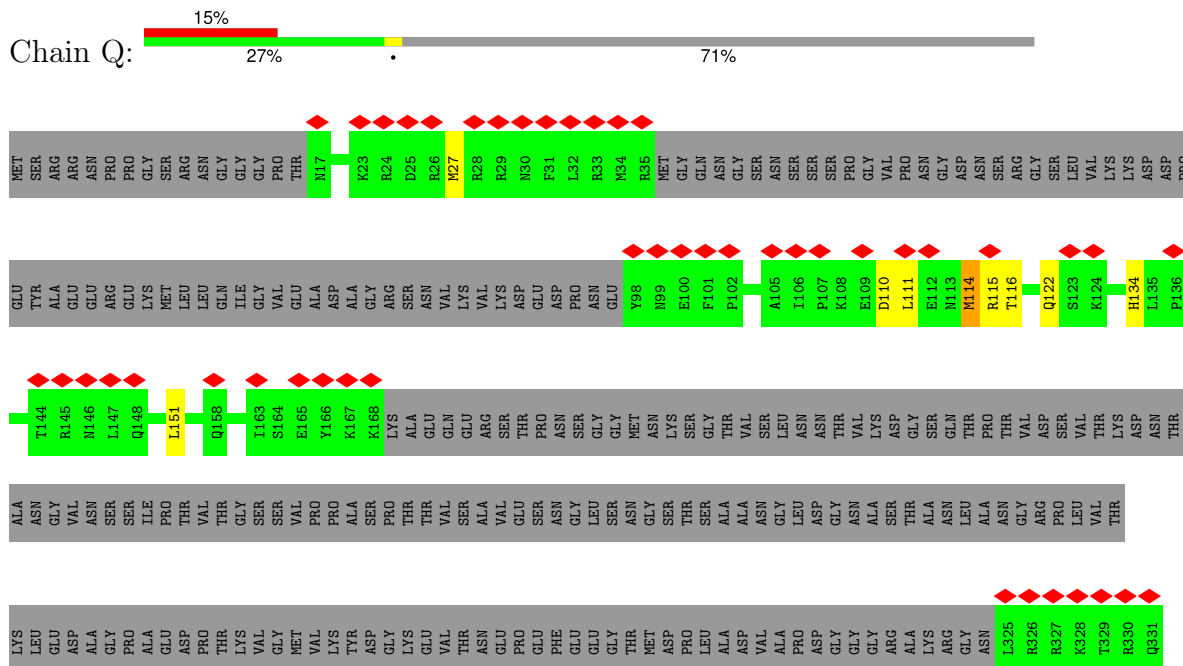
- Molecule 13: DNA-directed RNA polymerase II subunit RPB4



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 15: Transcription initiation factor IIF subunit alpha



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1102224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.688	Depositor
Minimum map value	-2.969	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.419	Depositor
Map size ($\text{\AA}$)	537.6, 537.6, 537.6	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	C	0.45	1/2099 (0.0%)	0.43	1/2845 (0.0%)
2	E	0.31	0/1780	0.47	0/2395
3	F	0.35	0/682	0.49	0/922
4	G	0.46	2/1368 (0.1%)	0.56	0/1844
5	I	2.29	22/962 (2.3%)	2.30	49/1295 (3.8%)
6	J	0.63	2/578 (0.3%)	0.77	2/775 (0.3%)
7	K	0.38	0/942	0.53	1/1272 (0.1%)
8	L	0.19	0/361	0.40	0/478
9	S	1.27	17/1325 (1.3%)	2.17	31/1787 (1.7%)
10	M	0.31	1/687 (0.1%)	0.42	0/927
11	B	0.42	11/9381 (0.1%)	0.63	27/12652 (0.2%)
12	A	0.54	20/11191 (0.2%)	0.72	29/15127 (0.2%)
13	D	0.51	2/1262 (0.2%)	0.63	0/1693
14	H	0.98	10/1107 (0.9%)	1.19	15/1499 (1.0%)
15	Q	0.35	1/1852 (0.1%)	0.43	0/2480
16	R	0.73	5/1652 (0.3%)	0.76	4/2222 (0.2%)
All	All	0.66	94/37229 (0.3%)	0.84	159/50213 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	I	0	10
9	S	1	3
11	B	0	5
12	A	0	7
14	H	1	2
All	All	2	27

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	15	TYR	CZ-OH	46.34	2.35	1.38
5	I	13	MET	SD-CE	28.55	2.50	1.79
12	A	1444	MET	SD-CE	-18.76	1.32	1.79
9	S	173	HIS	CB-CG	-18.67	1.24	1.50
14	H	129	TYR	CA-C	18.10	1.77	1.52
1	C	37	MET	SD-CE	-17.97	1.34	1.79
12	A	99	ILE	CB-CG2	-16.74	0.97	1.52
5	I	116	ASN	CA-C	16.36	1.73	1.52
12	A	688	LYS	CD-CE	-15.23	1.06	1.52
9	S	151	GLN	CA-C	14.95	1.73	1.52
16	R	227	SER	C-O	13.41	1.39	1.23
9	S	173	HIS	CA-CB	-13.02	1.32	1.53
16	R	228	MET	CB-CG	-12.56	1.14	1.52
11	B	1143	ALA	CA-CB	12.10	1.74	1.53
16	R	228	MET	CA-CB	12.09	1.72	1.53
9	S	156	LEU	CG-CD2	11.91	1.91	1.52
16	R	228	MET	N-CA	11.76	1.60	1.46
9	S	160	LEU	CG-CD2	11.22	1.89	1.52
14	H	129	TYR	CG-CD2	11.04	1.62	1.39
5	I	15	TYR	CD2-CE2	-10.94	1.05	1.38
14	H	109	LYS	CD-CE	-10.73	1.20	1.52
11	B	1138	MET	SD-CE	-10.62	1.52	1.79
11	B	1060	ARG	CD-NE	-10.32	1.31	1.46
9	S	173	HIS	CG-ND1	10.06	1.49	1.38
5	I	117	LYS	CB-CG	9.98	1.82	1.52
12	A	676	MET	CA-C	9.95	1.66	1.52
4	G	59	GLY	C-O	-9.81	1.11	1.23
9	S	171	ILE	CB-CG1	-9.55	1.34	1.53
5	I	82	GLU	CA-C	9.43	1.63	1.52
6	J	49	MET	CG-SD	-9.28	1.57	1.80
9	S	156	LEU	CG-CD1	-9.18	1.22	1.52
15	Q	114	MET	SD-CE	-9.08	1.56	1.79
5	I	13	MET	CG-SD	-8.96	1.58	1.80
12	A	683	ILE	C-N	8.62	1.45	1.33
16	R	228	MET	CG-SD	-8.30	1.59	1.80
12	A	234	MET	SD-CE	-8.25	1.58	1.79
5	I	75	CYS	CB-SG	8.01	2.07	1.81
12	A	1202	MET	SD-CE	-7.95	1.59	1.79
9	S	151	GLN	N-CA	-7.82	1.36	1.46
11	B	1060	ARG	CA-CB	7.59	1.65	1.53
12	A	692	ASP	CA-C	7.45	1.62	1.52
14	H	109	LYS	CE-NZ	-7.42	1.27	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	15	TYR	CD1-CE1	-7.37	1.16	1.38
9	S	173	HIS	N-CA	7.34	1.55	1.46
5	I	82	GLU	CG-CD	-7.22	1.33	1.52
12	A	684	ALA	N-CA	7.18	1.55	1.46
5	I	111	THR	CB-CG2	7.11	1.75	1.52
12	A	683	ILE	CA-C	6.87	1.62	1.52
5	I	117	LYS	CE-NZ	-6.81	1.28	1.49
12	A	688	LYS	CB-CG	-6.80	1.32	1.52
14	H	129	TYR	CG-CD1	-6.79	1.25	1.39
9	S	151	GLN	CG-CD	6.73	1.68	1.52
5	I	78	CYS	CA-C	-6.72	1.43	1.52
14	H	129	TYR	N-CA	-6.72	1.37	1.46
5	I	82	GLU	CA-CB	-6.70	1.38	1.53
9	S	160	LEU	CG-CD1	-6.64	1.30	1.52
12	A	676	MET	SD-CE	-6.63	1.62	1.79
5	I	116	ASN	CG-ND2	6.43	1.46	1.33
5	I	78	CYS	CB-SG	-6.22	1.60	1.81
9	S	171	ILE	CA-CB	-6.19	1.46	1.54
12	A	1209	MET	SD-CE	-6.13	1.64	1.79
11	B	1061	GLU	CA-C	6.12	1.60	1.52
4	G	58	ARG	CB-CG	-6.07	1.34	1.52
12	A	12	ARG	CZ-NH2	-6.05	1.25	1.33
5	I	111	THR	CA-C	6.01	1.61	1.53
11	B	1060	ARG	CB-CG	-6.01	1.34	1.52
12	A	1202	MET	CG-SD	-5.89	1.66	1.80
14	H	108	SER	CB-OG	-5.88	1.30	1.42
5	I	116	ASN	N-CA	-5.84	1.38	1.46
11	B	1208	MET	SD-CE	-5.74	1.65	1.79
14	H	109	LYS	N-CA	-5.74	1.38	1.46
12	A	688	LYS	CG-CD	-5.65	1.35	1.52
14	H	108	SER	C-N	-5.63	1.25	1.33
9	S	156	LEU	CB-CG	-5.56	1.42	1.53
13	D	155	ARG	CZ-NH2	-5.54	1.26	1.33
12	A	1359	ASP	CG-OD2	-5.51	1.14	1.25
5	I	77	LYS	CE-NZ	-5.45	1.33	1.49
12	A	692	ASP	CG-OD2	5.42	1.35	1.25
11	B	319	GLU	CD-OE1	-5.41	1.15	1.25
5	I	15	TYR	CE2-CZ	5.40	1.51	1.38
9	S	158	ASP	N-CA	-5.37	1.40	1.46
9	S	160	LEU	CB-CG	-5.35	1.42	1.53
11	B	662	MET	CG-SD	-5.35	1.67	1.80
12	A	688	LYS	CE-NZ	-5.34	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	49	MET	CB-CG	-5.32	1.36	1.52
5	I	94	ASP	CG-OD2	-5.32	1.15	1.25
12	A	885	THR	CB-CG2	-5.31	1.35	1.52
13	D	155	ARG	CD-NE	-5.26	1.38	1.46
11	B	1060	ARG	CZ-NH1	5.21	1.40	1.32
5	I	13	MET	CB-CG	-5.19	1.36	1.52
9	S	182	MET	N-CA	5.18	1.52	1.46
11	B	1061	GLU	CG-CD	-5.11	1.39	1.52
14	H	109	LYS	CG-CD	5.03	1.67	1.52
10	M	141	GLU	CD-OE1	-5.01	1.15	1.25

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	173	HIS	CA-CB-CG	66.13	179.93	113.80
5	I	82	GLU	CB-CG-CD	25.76	156.39	112.60
9	S	156	LEU	CB-CG-CD1	20.84	173.21	110.70
14	H	129	TYR	N-CA-C	-19.64	85.15	112.45
11	B	1060	ARG	CG-CD-NE	19.16	154.15	112.00
12	A	676	MET	CG-SD-CE	18.54	141.69	100.90
16	R	228	MET	CA-CB-CG	-18.09	77.92	114.10
12	A	688	LYS	CG-CD-CE	18.05	152.81	111.30
12	A	692	ASP	N-CA-C	-18.05	90.56	113.12
5	I	117	LYS	CB-CG-CD	-17.59	70.85	111.30
11	B	1060	ARG	CD-NE-CZ	-17.50	99.90	124.40
5	I	78	CYS	CB-CA-C	-16.75	76.21	110.38
9	S	151	GLN	N-CA-C	-16.52	89.49	112.45
14	H	129	TYR	CB-CG-CD1	16.15	145.03	120.80
5	I	82	GLU	N-CA-CB	16.05	136.81	110.32
16	R	228	MET	CB-CG-SD	15.98	160.64	112.70
5	I	116	ASN	CA-CB-CG	15.58	128.18	112.60
6	J	49	MET	CB-CG-SD	15.48	159.13	112.70
5	I	116	ASN	N-CA-C	-15.12	84.97	109.76
9	S	171	ILE	N-CA-CB	-14.86	90.33	110.54
12	A	692	ASP	CA-CB-CG	14.64	127.24	112.60
12	A	676	MET	N-CA-C	-14.56	94.93	111.82
5	I	77	LYS	CD-CE-NZ	14.31	157.69	111.90
12	A	688	LYS	CB-CA-C	14.31	135.77	110.01
5	I	75	CYS	CB-CA-C	-14.02	87.64	109.08
5	I	13	MET	CB-CG-SD	-13.88	71.08	112.70
11	B	19	GLU	CG-CD-OE1	13.78	150.09	118.40
5	I	81	ARG	CA-C-N	-13.59	99.57	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	81	ARG	C-N-CA	-13.59	99.57	121.58
14	H	129	TYR	CG-CD1-CE1	13.42	141.33	121.20
14	H	129	TYR	CB-CG-CD2	-13.04	101.24	120.80
14	H	129	TYR	CD1-CG-CD2	-13.02	98.57	118.10
12	A	688	LYS	CD-CE-NZ	12.63	152.31	111.90
5	I	82	GLU	CB-CA-C	-12.54	92.78	110.34
5	I	116	ASN	CB-CG-ND2	-12.49	97.67	116.40
11	B	19	GLU	CG-CD-OE2	-12.31	90.08	118.40
16	R	227	SER	CA-C-O	-12.19	107.78	121.19
5	I	75	CYS	CA-CB-SG	12.07	142.16	114.40
9	S	156	LEU	CD1-CG-CD2	-11.97	84.46	110.80
5	I	111	THR	OG1-CB-CG2	-11.90	85.51	109.30
9	S	160	LEU	CB-CG-CD1	11.69	145.77	110.70
11	B	19	GLU	CB-CG-CD	11.43	132.03	112.60
9	S	171	ILE	CA-CB-CG1	11.42	129.81	110.40
9	S	160	LEU	CB-CG-CD2	-11.37	76.60	110.70
12	A	692	ASP	OD1-CG-OD2	-11.06	96.36	122.90
9	S	173	HIS	CB-CA-C	-10.98	92.18	110.85
11	B	1116	ARG	CA-C-N	10.96	148.54	121.80
11	B	1116	ARG	C-N-CA	10.96	148.54	121.80
12	A	676	MET	CB-CG-SD	10.51	144.22	112.70
11	B	18	PHE	CB-CG-CD1	10.48	138.52	120.70
9	S	170	SER	CA-CB-OG	10.38	131.85	111.10
11	B	1061	GLU	CB-CG-CD	9.99	129.58	112.60
9	S	182	MET	CG-SD-CE	9.91	122.71	100.90
5	I	82	GLU	N-CA-C	-9.75	91.85	107.93
5	I	82	GLU	CA-CB-CG	9.64	133.39	114.10
9	S	160	LEU	CD1-CG-CD2	-9.58	89.73	110.80
5	I	81	ARG	CD-NE-CZ	-9.57	111.00	124.40
5	I	111	THR	N-CA-C	-9.54	96.22	109.95
5	I	117	LYS	CA-CB-CG	9.45	133.00	114.10
14	H	109	LYS	CB-CG-CD	9.43	132.99	111.30
12	A	681	GLU	CB-CG-CD	9.41	128.60	112.60
12	A	1444	MET	CG-SD-CE	-9.36	80.32	100.90
11	B	1111	MET	CG-SD-CE	-9.31	80.42	100.90
16	R	228	MET	N-CA-CB	9.30	123.50	110.01
5	I	115	LYS	CG-CD-CE	9.29	132.67	111.30
9	S	170	SER	N-CA-C	9.21	122.16	111.11
5	I	77	LYS	CB-CG-CD	9.17	132.38	111.30
9	S	182	MET	N-CA-CB	-9.15	94.16	109.72
14	H	129	TYR	CB-CA-C	-9.11	92.90	110.11
5	I	117	LYS	CD-CE-NZ	9.10	141.01	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	160	LEU	N-CA-CB	9.08	124.28	110.30
5	I	116	ASN	N-CA-CB	8.99	125.36	110.52
5	I	77	LYS	CG-CD-CE	-8.93	90.75	111.30
5	I	78	CYS	N-CA-CB	8.93	124.05	110.30
9	S	182	MET	CB-CA-C	8.90	125.61	110.84
5	I	113	ASP	N-CA-CB	8.74	125.27	110.49
5	I	81	ARG	NE-CZ-NH2	-8.70	111.37	119.20
5	I	77	LYS	CA-CB-CG	-8.65	96.81	114.10
9	S	170	SER	CB-CA-C	8.64	124.64	110.81
9	S	160	LEU	CA-CB-CG	-8.57	86.31	116.30
1	C	37	MET	CG-SD-CE	8.49	119.57	100.90
5	I	117	LYS	CG-CD-CE	8.47	130.78	111.30
11	B	18	PHE	CB-CG-CD2	-8.46	106.33	120.70
9	S	173	HIS	CB-CG-ND1	-8.34	110.20	122.70
5	I	115	LYS	CD-CE-NZ	-8.26	85.47	111.90
9	S	171	ILE	CB-CA-C	8.21	123.22	112.14
11	B	1061	GLU	N-CA-C	-8.15	102.39	111.28
5	I	78	CYS	CA-CB-SG	8.02	132.84	114.40
14	H	129	TYR	N-CA-CB	7.95	122.11	110.26
14	H	109	LYS	N-CA-CB	7.93	123.89	110.49
11	B	662	MET	CG-SD-CE	7.89	118.26	100.90
12	A	99	ILE	CA-CB-CG2	-7.71	97.38	110.50
11	B	1060	ARG	CA-CB-CG	-7.70	98.69	114.10
5	I	76	PRO	N-CA-C	7.59	128.11	112.47
11	B	1060	ARG	CB-CG-CD	7.46	128.46	111.30
12	A	688	LYS	N-CA-CB	-7.45	99.03	110.44
5	I	113	ASP	CA-CB-CG	7.41	120.01	112.60
7	K	8	GLU	CB-CG-CD	7.34	125.08	112.60
5	I	110	PHE	CA-C-N	-7.32	109.73	123.27
5	I	110	PHE	C-N-CA	-7.32	109.73	123.27
9	S	171	ILE	CB-CG1-CD1	-7.28	98.51	113.80
12	A	681	GLU	CG-CD-OE2	-7.24	101.75	118.40
9	S	156	LEU	CB-CG-CD2	-7.22	89.04	110.70
14	H	129	TYR	CA-CB-CG	7.09	126.67	113.90
5	I	13	MET	CA-CB-CG	-7.02	100.05	114.10
11	B	19	GLU	CB-CA-C	7.02	123.61	110.63
6	J	49	MET	CA-CB-CG	-6.98	100.13	114.10
9	S	151	GLN	OE1-CD-NE2	-6.97	115.63	122.60
9	S	170	SER	CA-C-O	-6.87	113.55	120.90
12	A	687	LYS	CA-C-N	-6.77	110.12	122.38
12	A	687	LYS	C-N-CA	-6.77	110.12	122.38
14	H	129	TYR	CD1-CE1-CZ	-6.68	107.57	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	151	GLN	CB-CA-C	-6.62	97.60	110.11
11	B	18	PHE	N-CA-C	-6.58	102.60	112.54
12	A	676	MET	CB-CA-C	-6.46	98.26	110.67
5	I	114	GLN	N-CA-CB	-6.42	99.65	110.49
11	B	19	GLU	N-CA-CB	-6.37	100.41	110.22
12	A	681	GLU	CA-CB-CG	6.36	126.83	114.10
9	S	173	HIS	N-CA-C	-6.29	104.50	111.36
5	I	115	LYS	CA-C-N	-6.10	113.56	122.65
5	I	115	LYS	C-N-CA	-6.10	113.56	122.65
12	A	672	ASP	N-CA-C	6.07	119.03	110.23
12	A	688	LYS	CB-CG-CD	5.99	125.07	111.30
9	S	209	LYS	CA-C-N	5.92	132.35	121.70
9	S	209	LYS	C-N-CA	5.92	132.35	121.70
5	I	75	CYS	N-CA-C	5.85	119.64	109.82
12	A	1163	ILE	CA-CB-CG2	5.74	120.25	110.50
9	S	210	ASN	CA-C-N	5.71	131.99	121.70
9	S	210	ASN	C-N-CA	5.71	131.99	121.70
11	B	662	MET	CB-CG-SD	5.68	129.73	112.70
14	H	109	LYS	N-CA-C	5.67	122.87	110.80
12	A	683	ILE	CA-C-O	-5.65	113.20	120.03
14	H	108	SER	CA-C-N	5.60	132.23	121.54
14	H	108	SER	C-N-CA	5.60	132.23	121.54
12	A	683	ILE	CA-C-N	5.59	133.87	121.80
12	A	683	ILE	C-N-CA	5.59	133.87	121.80
5	I	114	GLN	CB-CG-CD	5.58	122.08	112.60
11	B	1143	ALA	N-CA-CB	5.53	119.82	110.69
5	I	81	ARG	N-CA-CB	-5.51	102.51	112.27
12	A	681	GLU	CG-CD-OE1	5.47	130.99	118.40
11	B	21	GLU	CA-C-O	-5.45	112.72	120.51
5	I	114	GLN	CG-CD-NE2	-5.43	108.25	116.40
14	H	108	SER	N-CA-C	-5.43	101.25	108.74
5	I	82	GLU	CG-CD-OE2	-5.38	106.02	118.40
11	B	322	PHE	CA-C-N	5.33	131.57	121.97
11	B	322	PHE	C-N-CA	5.33	131.57	121.97
12	A	234	MET	CA-CB-CG	5.32	124.75	114.10
5	I	81	ARG	CA-C-O	-5.28	113.54	122.20
11	B	1138	MET	CG-SD-CE	-5.23	89.39	100.90
12	A	681	GLU	OE1-CD-OE2	-5.17	110.50	122.90
11	B	1060	ARG	N-CA-C	-5.14	105.86	111.82
12	A	691	LEU	CA-C-N	-5.12	112.70	122.53
12	A	691	LEU	C-N-CA	-5.12	112.70	122.53
5	I	113	ASP	CA-C-N	5.06	131.20	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	113	ASP	C-N-CA	5.06	131.20	121.54
5	I	114	GLN	OE1-CD-NE2	-5.05	117.55	122.60
9	S	158	ASP	CA-CB-CG	5.03	117.63	112.60
11	B	1117	GLN	N-CA-CB	-5.02	101.44	110.37
11	B	323	VAL	CA-CB-CG1	5.00	118.90	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	S	171	ILE	CB
14	H	109	LYS	CA

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	1036	ARG	Sidechain
12	A	12	ARG	Sidechain
12	A	464	PRO	Peptide
12	A	681	GLU	Sidechain
12	A	688	LYS	Mainchain
12	A	692	ASP	Sidechain
12	A	760	GLN	Peptide
11	B	1060	ARG	Sidechain
11	B	1061	GLU	Sidechain
11	B	19	GLU	Sidechain
11	B	21	GLU	Mainchain
11	B	322	PHE	Peptide
14	H	128	ASN	Peptide
14	H	129	TYR	Sidechain
5	I	114	GLN	Sidechain
5	I	115	LYS	Peptide
5	I	116	ASN	Sidechain
5	I	15	TYR	Sidechain
5	I	70	ARG	Sidechain
5	I	75	CYS	Mainchain
5	I	81	ARG	Sidechain
5	I	82	GLU	Sidechain
5	I	91	ARG	Sidechain
5	I	92	ARG	Sidechain
9	S	150	ASP	Peptide
9	S	151	GLN	Sidechain
9	S	173	HIS	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	C	2061	0	2029	9	0
2	E	1744	0	1772	14	0
3	F	670	0	690	7	0
4	G	1340	0	1357	16	0
5	I	944	0	900	38	0
6	J	569	0	585	8	0
7	K	924	0	934	7	0
8	L	359	0	381	1	0
9	S	1302	0	1295	34	0
10	M	679	0	694	6	0
11	B	9200	0	9193	75	0
12	A	10996	0	11079	120	0
13	D	1253	0	1275	31	0
14	H	1089	0	1062	22	0
15	Q	1817	0	1843	12	0
16	R	1629	0	1619	7	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	M	1	0	0	0	0
17	S	1	0	0	0	0
18	A	1	0	0	0	0
All	All	36587	0	36708	371	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 5.

All (371) 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)
5:I:117:LYS:CB	5:I:117:LYS:CG	1.82	1.57
14:H:129:TYR:C	14:H:129:TYR:CA	1.77	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:111:THR:CB	5:I:111:THR:CG2	1.76	1.55
5:I:117:LYS:CB	5:I:117:LYS:HD3	1.30	1.55
5:I:117:LYS:CB	5:I:117:LYS:CD	1.89	1.48
9:S:156:LEU:CG	9:S:156:LEU:CD2	1.91	1.47
9:S:160:LEU:CG	9:S:160:LEU:CD2	1.89	1.47
12:A:110:CYS:SG	12:A:167:CYS:SG	1.45	1.45
5:I:75:CYS:SG	5:I:75:CYS:CB	2.07	1.43
9:S:160:LEU:CD2	9:S:160:LEU:CB	2.09	1.29
9:S:156:LEU:CD2	9:S:156:LEU:CD1	2.17	1.22
5:I:117:LYS:HD3	5:I:117:LYS:CA	1.80	1.12
9:S:160:LEU:CD2	9:S:160:LEU:CD1	2.29	1.10
9:S:160:LEU:CD2	9:S:160:LEU:HB3	1.81	1.10
14:H:129:TYR:C	14:H:129:TYR:N	2.15	1.05
9:S:156:LEU:CD2	9:S:156:LEU:CB	2.36	1.02
4:G:58:ARG:HH11	12:A:1444:MET:HE2	1.21	1.01
5:I:117:LYS:HD3	5:I:117:LYS:HB2	1.38	1.01
5:I:13:MET:CE	5:I:13:MET:SD	2.50	0.99
9:S:160:LEU:CD2	9:S:160:LEU:HD13	1.89	0.98
9:S:156:LEU:CD2	9:S:156:LEU:HD13	1.94	0.96
14:H:129:TYR:C	14:H:129:TYR:CB	2.37	0.96
16:R:227:SER:C	16:R:228:MET:N	2.24	0.95
5:I:111:THR:CG2	5:I:111:THR:OG1	2.14	0.94
12:A:110:CYS:SG	12:A:167:CYS:CB	2.58	0.92
13:D:152:SER:OG	13:D:155:ARG:NH2	2.05	0.89
5:I:117:LYS:CD	5:I:117:LYS:HB2	1.98	0.85
9:S:160:LEU:HB3	9:S:160:LEU:HD23	1.60	0.83
14:H:93:TYR:HD2	14:H:143:LEU:HB3	1.44	0.82
5:I:117:LYS:HD3	5:I:117:LYS:HA	1.61	0.80
5:I:15:TYR:OH	5:I:15:TYR:CZ	2.35	0.80
3:F:103:MET:HE2	4:G:15:PRO:HG2	1.63	0.79
12:A:1284:MET:HE2	12:A:1306:LEU:HD21	1.65	0.79
12:A:456:MET:HE1	12:A:510:GLN:HB2	1.64	0.78
9:S:156:LEU:CD1	9:S:156:LEU:HD21	2.14	0.78
1:C:34:ARG:HA	1:C:37:MET:HE3	1.67	0.77
5:I:13:MET:SD	5:I:15:TYR:CZ	2.78	0.77
9:S:160:LEU:HD13	9:S:160:LEU:HD21	1.65	0.77
14:H:93:TYR:CD2	14:H:143:LEU:HB3	2.19	0.77
1:C:33:LEU:HG	1:C:37:MET:HE2	1.66	0.77
9:S:156:LEU:HD13	9:S:156:LEU:HD21	1.64	0.76
2:E:142:VAL:HG21	12:A:1317:MET:HE2	1.67	0.75
5:I:80:SER:O	5:I:81:ARG:HG3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:268:MET:HE3	16:R:270:MET:SD	2.27	0.75
11:B:1111:MET:CE	11:B:1117:GLN:H	2.01	0.73
5:I:111:THR:CG2	5:I:111:THR:CA	2.66	0.72
2:E:88:VAL:HG12	2:E:93:MET:HE2	1.72	0.71
12:A:446:ARG:HB2	12:A:487:MET:HE1	1.70	0.71
15:Q:110:ASP:C	15:Q:114:MET:HE3	2.16	0.71
11:B:100:PRO:O	11:B:101:MET:HE2	1.91	0.71
15:Q:110:ASP:O	15:Q:114:MET:HE3	1.91	0.70
5:I:49:ILE:HD13	12:A:1148:ILE:HG23	1.73	0.70
5:I:5:ARG:NH2	5:I:36:GLU:OE1	2.24	0.70
13:D:161:GLY:O	13:D:165:GLN:NE2	2.24	0.70
4:G:58:ARG:NH1	12:A:1444:MET:HE2	2.03	0.69
13:D:153:ARG:NH2	13:D:182:SER:O	2.27	0.68
15:Q:27:MET:SD	15:Q:27:MET:N	2.67	0.68
11:B:1210:MET:HA	12:A:304:MET:HE1	1.76	0.68
15:Q:122:GLN:NE2	15:Q:395:PHE:O	2.27	0.68
13:D:151:PHE:O	13:D:153:ARG:NH1	2.27	0.67
4:G:59:GLY:O	12:A:1444:MET:HE1	1.93	0.67
9:S:156:LEU:CD2	9:S:156:LEU:HB3	2.24	0.67
13:D:203:SER:N	13:D:206:GLU:OE2	2.27	0.67
11:B:766:ARG:CZ	11:B:1020:ARG:HG3	2.25	0.67
7:K:47:ARG:NH1	12:A:548:ASN:OD1	2.29	0.66
4:G:30:LEU:HD11	4:G:72:VAL:HG21	1.77	0.66
11:B:1143:ALA:HB1	12:A:500:GLU:OE1	1.96	0.66
5:I:13:MET:SD	5:I:15:TYR:OH	2.54	0.66
11:B:25:ILE:HD13	11:B:658:ILE:HD11	1.77	0.66
11:B:362:PRO:O	11:B:366:GLN:NE2	2.29	0.65
12:A:1143:LEU:HD23	12:A:1271:ILE:HB	1.79	0.65
2:E:97:VAL:HG13	2:E:127:ILE:HD11	1.78	0.65
3:F:85:MET:HE1	3:F:90:ARG:HB2	1.77	0.65
12:A:903:ASN:O	12:A:907:THR:OG1	2.15	0.65
10:M:26:GLU:O	10:M:28:LYS:NZ	2.31	0.64
13:D:154:PHE:C	13:D:155:ARG:HD2	2.23	0.64
14:H:129:TYR:N	14:H:130:ARG:N	2.46	0.63
12:A:1285:MET:HE1	12:A:1307:GLU:HG2	1.80	0.63
1:C:33:LEU:C	1:C:37:MET:HE2	2.24	0.63
12:A:809:THR:OG1	12:A:812:GLU:OE1	2.16	0.63
12:A:1052:GLN:HG2	12:A:1055:ARG:HH22	1.63	0.62
11:B:330:ALA:O	11:B:334:ILE:HD12	1.98	0.62
12:A:119:ASN:HB3	12:A:122:MET:HE1	1.80	0.62
13:D:213:GLU:N	13:D:213:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:766:ARG:NH2	11:B:1020:ARG:HG3	2.14	0.62
1:C:145:CYS:SG	1:C:146:LYS:N	2.72	0.62
12:A:1395:GLY:O	12:A:1399:ARG:NH2	2.33	0.62
12:A:186:LYS:NZ	12:A:187:LYS:O	2.33	0.62
9:S:181:GLU:HG3	9:S:182:MET:HE2	1.82	0.62
9:S:283:GLN:HB3	9:S:293:LEU:HD13	1.82	0.62
11:B:1138:MET:CE	11:B:1143:ALA:HB3	2.30	0.61
11:B:559:SER:HA	11:B:563:MET:HE3	1.81	0.61
14:H:109:LYS:HE3	14:H:109:LYS:H	1.65	0.61
12:A:167:CYS:O	12:A:169:ASN:ND2	2.33	0.60
13:D:205:ASP:OD1	13:D:206:GLU:N	2.33	0.60
6:J:48:ARG:NH1	6:J:49:MET:SD	2.74	0.60
4:G:58:ARG:HD2	12:A:1444:MET:CE	2.32	0.60
14:H:15:VAL:HG22	14:H:17:PRO:HD3	1.84	0.60
16:R:233:TYR:O	16:R:234:HIS:ND1	2.34	0.60
15:Q:134:HIS:ND1	15:Q:356:ASP:OD2	2.35	0.59
13:D:198:LEU:HD21	13:D:207:LEU:HG	1.83	0.59
9:S:235:ASP:O	9:S:237:ALA:N	2.36	0.59
12:A:881:GLN:NE2	12:A:957:PRO:O	2.35	0.59
12:A:925:LEU:HD13	12:A:983:ILE:HB	1.84	0.59
11:B:230:ALA:O	11:B:261:ARG:NH1	2.36	0.59
5:I:13:MET:HG3	5:I:15:TYR:CE2	2.38	0.58
11:B:747:MET:HE3	11:B:747:MET:HA	1.85	0.58
4:G:1:MET:N	4:G:80:LYS:O	2.36	0.58
12:A:914:GLU:N	12:A:979:SER:O	2.35	0.58
13:D:119:ARG:HH22	13:D:155:ARG:NH2	2.00	0.58
9:S:160:LEU:CB	9:S:160:LEU:HD22	2.25	0.58
4:G:93:SER:OG	4:G:100:GLU:OE2	2.22	0.58
7:K:5:ASP:OD1	7:K:8:GLU:HG3	2.03	0.58
16:R:133:TYR:CD2	16:R:214:ILE:HD11	2.39	0.58
11:B:1159:ARG:NH1	12:A:5:GLN:O	2.37	0.57
12:A:885:THR:HG23	12:A:893:PHE:HE1	1.68	0.57
2:E:90:VAL:HA	2:E:93:MET:HE3	1.87	0.57
1:C:33:LEU:HG	1:C:37:MET:CE	2.35	0.57
11:B:21:GLU:OE1	11:B:22:SER:N	2.37	0.57
9:S:170:SER:HA	9:S:173:HIS:ND1	2.19	0.57
2:E:31:THR:HG23	2:E:34:GLU:H	1.69	0.57
12:A:1167:GLU:N	12:A:1167:GLU:OE1	2.36	0.57
13:D:119:ARG:NH2	13:D:149:THR:OG1	2.38	0.56
11:B:182:SER:OG	11:B:183:GLU:OE1	2.23	0.56
11:B:1111:MET:HE2	11:B:1116:ARG:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:849:MET:HE3	12:A:1061:GLY:HA2	1.88	0.56
10:M:39:SER:OG	10:M:40:GLU:OE1	2.24	0.56
12:A:122:MET:HE3	12:A:141:LEU:HD11	1.86	0.56
12:A:506:ALA:O	12:A:510:GLN:NE2	2.39	0.56
11:B:593:PRO:HA	11:B:596:LEU:CD2	2.35	0.56
11:B:1210:MET:HE1	12:A:325:ILE:HB	1.87	0.56
9:S:285:GLN:HB3	9:S:293:LEU:HD23	1.87	0.55
12:A:982:THR:HG22	12:A:985:ASP:OD2	2.04	0.55
12:A:1256:GLU:HA	12:A:1259:MET:HE2	1.88	0.55
13:D:155:ARG:HD2	13:D:155:ARG:N	2.22	0.55
12:A:456:MET:HE1	12:A:510:GLN:CB	2.35	0.55
6:J:65:PRO:HD2	6:J:68:LYS:HE2	1.89	0.55
11:B:777:ALA:O	11:B:1096:ARG:NH2	2.39	0.55
11:B:323:VAL:HG11	15:Q:412:ARG:HB2	1.87	0.55
5:I:15:TYR:CZ	15:Q:422:ARG:NH1	2.74	0.54
11:B:650:GLU:OE2	11:B:654:ARG:NH2	2.39	0.54
13:D:24:ALA:N	13:D:28:GLN:O	2.39	0.54
9:S:291:GLU:HG2	9:S:292:PRO:HD2	1.89	0.54
10:M:18:LEU:HD22	12:A:66:LYS:HB2	1.89	0.54
11:B:1135:ARG:NH2	11:B:1136:ASP:OD1	2.40	0.54
9:S:188:CYS:SG	9:S:198:ARG:NH2	2.80	0.54
13:D:204:ASP:OD1	13:D:205:ASP:N	2.40	0.54
14:H:19:ARG:O	14:H:19:ARG:NE	2.41	0.54
12:A:981:LEU:HD23	12:A:1039:LYS:HG2	1.90	0.54
2:E:55:ARG:NH1	2:E:113:GLN:OE1	2.41	0.54
12:A:1063:MET:HE3	12:A:1063:MET:HA	1.88	0.53
3:F:85:MET:HE1	3:F:90:ARG:CB	2.37	0.53
11:B:1121:GLY:O	11:B:1126:GLY:N	2.41	0.53
14:H:92:ASP:O	14:H:93:TYR:HD1	1.90	0.53
10:M:138:ASP:O	11:B:451:LYS:NZ	2.31	0.53
12:A:565:ILE:HG13	14:H:97:MET:HE1	1.91	0.53
12:A:708:MET:SD	12:A:712:GLU:HB2	2.49	0.53
12:A:1172:LEU:HD22	12:A:1173:HIS:CE1	2.44	0.53
10:M:132:LYS:HA	10:M:135:MET:HE2	1.91	0.53
11:B:1111:MET:HE1	11:B:1117:GLN:H	1.73	0.53
12:A:337:ARG:NH2	12:A:1401:SER:O	2.42	0.53
13:D:63:LEU:HB3	13:D:130:LEU:HD22	1.91	0.53
16:R:263:MET:HE3	16:R:263:MET:HA	1.91	0.53
11:B:496:ARG:NH2	11:B:540:SER:O	2.42	0.52
14:H:108:SER:OG	14:H:109:LYS:HE3	2.09	0.52
1:C:241:ASP:OD1	1:C:242:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:132:SER:OG	4:G:135:ASP:O	2.23	0.52
11:B:1111:MET:HE3	11:B:1112:GLN:N	2.24	0.52
15:Q:151:LEU:HD23	15:Q:440:ARG:HH22	1.72	0.52
7:K:54:ARG:NH2	14:H:82:PRO:O	2.42	0.52
8:L:26:THR:OG1	8:L:40:LEU:O	2.26	0.52
12:A:744:LYS:HG3	12:A:748:MET:HE2	1.92	0.52
12:A:66:LYS:HG2	12:A:72:GLU:HG2	1.91	0.52
12:A:1349:TYR:HE1	12:A:1368:MET:SD	2.32	0.52
12:A:717:ASN:HD22	12:A:720:ARG:NH2	2.08	0.52
11:B:1168:LEU:C	11:B:1169:MET:HE2	2.35	0.51
5:I:76:PRO:HB2	5:I:77:LYS:HZ2	1.75	0.51
13:D:174:PRO:HA	13:D:177:VAL:HG22	1.93	0.51
13:D:216:ASN:OD1	13:D:217:LEU:N	2.43	0.51
7:K:29:ASN:ND2	7:K:78:THR:O	2.43	0.51
16:R:270:MET:SD	16:R:270:MET:N	2.84	0.51
12:A:1122:PRO:HD3	12:A:1323:ASP:OD1	2.11	0.51
15:Q:137:VAL:HG11	15:Q:352:MET:HE3	1.92	0.51
7:K:39:ASP:OD1	7:K:39:ASP:N	2.43	0.51
11:B:705:MET:H	11:B:710:LEU:HD22	1.76	0.51
12:A:99:ILE:HG21	12:A:234:MET:CE	2.40	0.51
12:A:1202:MET:SD	12:A:1207:LEU:HB2	2.51	0.51
2:E:55:ARG:HA	2:E:58:MET:HE1	1.93	0.51
3:F:79:ARG:NH2	3:F:150:GLU:OE2	2.44	0.50
11:B:101:MET:HG3	16:R:259:VAL:HG21	1.92	0.50
5:I:111:THR:CG2	5:I:111:THR:C	2.84	0.50
11:B:1170:THR:HG21	12:A:30:ILE:HD12	1.93	0.50
12:A:635:ARG:NH2	12:A:876:ALA:O	2.43	0.50
11:B:597:MET:HE3	11:B:617:ARG:HB2	1.91	0.50
11:B:1193:GLN:OE1	12:A:7:SER:OG	2.30	0.50
12:A:1216:ILE:HD11	12:A:1226:VAL:HG11	1.94	0.50
13:D:173:HIS:HB3	13:D:176:GLU:OE1	2.11	0.50
11:B:1106:ARG:NH2	11:B:1110:PRO:O	2.45	0.50
12:A:898:ARG:NH1	12:A:899:VAL:O	2.45	0.50
14:H:129:TYR:C	14:H:129:TYR:CG	2.89	0.50
9:S:175:ALA:HA	9:S:178:ILE:HG12	1.94	0.50
12:A:944:ARG:NE	12:A:1298:TYR:OH	2.45	0.50
12:A:672:ASP:N	12:A:672:ASP:OD1	2.44	0.49
12:A:1188:GLN:NE2	12:A:1189:SER:O	2.44	0.49
1:C:217:ASP:OD1	1:C:217:ASP:N	2.45	0.49
15:Q:115:ARG:NH1	15:Q:345:GLU:OE2	2.45	0.49
11:B:1111:MET:HE2	11:B:1116:ARG:CA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1111:MET:HE1	11:B:1117:GLN:O	2.12	0.49
11:B:21:GLU:O	11:B:22:SER:C	2.56	0.49
11:B:319:GLU:OE1	11:B:319:GLU:N	2.46	0.49
14:H:93:TYR:CE1	14:H:145:ARG:NH1	2.81	0.49
2:E:24:LYS:NZ	2:E:30:ILE:O	2.33	0.49
12:A:1395:GLY:O	12:A:1399:ARG:NH1	2.46	0.49
13:D:136:GLY:O	13:D:139:LYS:NZ	2.28	0.49
11:B:976:ILE:HD12	12:A:465:TYR:HB2	1.94	0.49
13:D:39:ASN:OD1	13:D:43:GLU:N	2.44	0.48
11:B:21:GLU:OE2	11:B:656:GLY:N	2.32	0.48
13:D:119:ARG:NH2	13:D:155:ARG:NH2	2.61	0.48
14:H:108:SER:OG	14:H:109:LYS:CE	2.61	0.48
5:I:76:PRO:HB2	5:I:77:LYS:NZ	2.28	0.48
12:A:146:MET:HE3	12:A:146:MET:O	2.13	0.48
12:A:198:GLU:O	12:A:200:ARG:N	2.47	0.48
4:G:60:ARG:HH21	4:G:62:LEU:HD23	1.79	0.48
11:B:1111:MET:HE3	11:B:1112:GLN:H	1.78	0.48
6:J:69:ARG:HE	6:J:69:ARG:HA	1.78	0.48
14:H:116:TYR:HB2	14:H:123:MET:SD	2.54	0.48
11:B:789:MET:HE3	11:B:967:ARG:HB2	1.96	0.47
12:A:305:ASP:OD1	12:A:305:ASP:N	2.45	0.47
12:A:307:ASP:OD2	12:A:326:ARG:NH1	2.46	0.47
12:A:1199:ARG:NH2	12:A:1234:GLU:O	2.48	0.47
12:A:1215:ARG:NH1	12:A:1219:THR:OG1	2.47	0.47
2:E:157:SER:OG	2:E:159:ASP:OD1	2.29	0.47
13:D:119:ARG:HE	13:D:123:LEU:HD23	1.78	0.47
13:D:152:SER:CB	13:D:155:ARG:HH21	2.23	0.47
14:H:109:LYS:HE3	14:H:109:LYS:N	2.29	0.47
12:A:74:MET:N	12:A:74:MET:HE2	2.30	0.47
2:E:142:VAL:HG21	12:A:1317:MET:CE	2.42	0.47
12:A:590:ARG:CZ	12:A:605:MET:HE1	2.45	0.47
11:B:294:ASP:OD1	11:B:294:ASP:N	2.48	0.46
11:B:860:MET:HE2	11:B:860:MET:HA	1.97	0.46
11:B:26:THR:OG1	11:B:708:GLU:OE2	2.26	0.46
11:B:593:PRO:HA	11:B:596:LEU:HD21	1.98	0.46
3:F:103:MET:HE3	3:F:103:MET:O	2.15	0.46
5:I:77:LYS:H	5:I:77:LYS:HG2	1.58	0.46
5:I:11:ASN:ND2	11:B:296:GLU:OE1	2.48	0.46
9:S:187:ASN:HB2	9:S:228:LEU:HD11	1.97	0.46
12:A:99:ILE:CG2	12:A:234:MET:HE2	2.46	0.46
12:A:1257:ASP:OD1	12:A:1258:HIS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:58:ARG:NH1	12:A:1444:MET:HG2	2.30	0.46
9:S:171:ILE:HD12	9:S:171:ILE:HG21	1.53	0.46
5:I:78:CYS:C	5:I:79:HIS:CG	2.93	0.46
5:I:97:MET:HG3	12:A:698:GLN:HA	1.97	0.46
12:A:1225:PHE:N	12:A:1241:ARG:O	2.49	0.46
1:C:5:GLY:O	1:C:7:GLN:NE2	2.49	0.46
9:S:201:ILE:O	9:S:205:ASN:ND2	2.49	0.46
12:A:362:ASP:OD1	12:A:362:ASP:N	2.48	0.46
2:E:34:GLU:O	2:E:37:LEU:HD23	2.16	0.46
12:A:511:ILE:HA	12:A:521:MET:CE	2.46	0.45
5:I:74:GLU:CG	5:I:81:ARG:HE	2.30	0.45
11:B:836:GLU:OE2	12:A:525:GLN:NE2	2.49	0.45
12:A:885:THR:HG23	12:A:893:PHE:CE1	2.48	0.45
15:Q:111:LEU:HA	15:Q:114:MET:SD	2.56	0.45
12:A:1079:MET:SD	12:A:1359:ASP:OD2	2.75	0.45
12:A:41:MET:HE3	12:A:46:THR:O	2.16	0.45
12:A:381:THR:HG23	12:A:383:TYR:H	1.82	0.45
13:D:56:ARG:HH22	13:D:155:ARG:HG3	1.81	0.45
11:B:842:ASN:HA	11:B:999:MET:HE1	1.99	0.45
11:B:1016:ALA:O	11:B:1020:ARG:HB2	2.17	0.45
11:B:1193:GLN:NE2	12:A:9:ALA:O	2.50	0.45
2:E:117:THR:O	2:E:120:ALA:N	2.50	0.44
4:G:1:MET:HE1	13:D:50:LEU:H	1.82	0.44
11:B:296:GLU:OE1	11:B:296:GLU:N	2.50	0.44
9:S:301:ALA:O	12:A:1300:LYS:NZ	2.49	0.44
11:B:343:ILE:O	11:B:345:LYS:NZ	2.40	0.44
5:I:45:ARG:NH2	5:I:47:GLU:OE1	2.47	0.44
12:A:42:ASP:OD2	12:A:46:THR:OG1	2.35	0.44
6:J:31:ASP:OD1	6:J:31:ASP:N	2.49	0.44
11:B:593:PRO:O	11:B:596:LEU:HG	2.18	0.44
12:A:849:MET:CE	12:A:1061:GLY:HA2	2.47	0.44
12:A:1286:LYS:HD2	12:A:1302:PRO:HB2	1.99	0.44
5:I:73:ARG:HE	5:I:73:ARG:HB3	1.53	0.44
5:I:80:SER:C	5:I:81:ARG:HG3	2.42	0.44
12:A:595:THR:OG1	12:A:603:ASN:ND2	2.51	0.44
12:A:717:ASN:O	12:A:720:ARG:HD3	2.17	0.44
13:D:119:ARG:NH2	13:D:149:THR:O	2.50	0.44
9:S:239:ALA:C	9:S:243:GLN:HE22	2.26	0.44
12:A:234:MET:HB3	12:A:234:MET:HE3	1.62	0.44
12:A:1223:ASP:OD1	12:A:1224:LEU:N	2.51	0.44
15:Q:116:THR:N	15:Q:390:ASP:OD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:176:LYS:O	9:S:179:GLU:HG3	2.17	0.43
9:S:148:LEU:HA	9:S:151:GLN:OE1	2.18	0.43
11:B:1156:ASP:OD1	11:B:1156:ASP:N	2.50	0.43
5:I:81:ARG:HH11	5:I:81:ARG:HD3	1.41	0.43
5:I:114:GLN:H	5:I:115:LYS:HZ3	1.66	0.43
12:A:1100:ARG:NH1	12:A:1103:GLU:OE1	2.51	0.43
9:S:170:SER:HA	9:S:173:HIS:CE1	2.53	0.43
11:B:260:GLY:O	11:B:267:ARG:NH2	2.45	0.43
5:I:18:GLU:OE2	5:I:24:ARG:N	2.52	0.43
7:K:107:THR:O	7:K:111:LEU:HD23	2.19	0.43
12:A:261:ASP:OD1	12:A:262:LEU:N	2.52	0.43
13:D:119:ARG:NH2	13:D:155:ARG:HH22	2.17	0.43
4:G:137:ILE:HG13	4:G:170:ALA:HB2	2.00	0.43
6:J:44:TYR:HA	6:J:47:ARG:HD3	2.00	0.43
11:B:921:ASP:OD1	11:B:921:ASP:N	2.52	0.43
12:A:885:THR:HG22	12:A:940:ARG:HG2	2.01	0.43
12:A:1423:GLY:O	12:A:1427:ASN:ND2	2.51	0.43
4:G:88:ASP:O	13:D:147:TYR:OH	2.31	0.42
3:F:89:GLU:O	3:F:93:ILE:HG23	2.19	0.42
14:H:110:ASP:OD1	14:H:111:LEU:N	2.52	0.42
12:A:1314:SER:O	12:A:1317:MET:HG2	2.20	0.42
9:S:261:ILE:HD12	9:S:261:ILE:H	1.85	0.42
12:A:11:LEU:C	12:A:12:ARG:HD3	2.44	0.42
14:H:7:ASP:OD1	14:H:7:ASP:N	2.53	0.42
2:E:91:LYS:O	2:E:95:THR:HG23	2.20	0.42
11:B:316:PRO:HA	11:B:319:GLU:CD	2.43	0.42
12:A:367:PRO:HG2	12:A:370:ILE:HD12	2.01	0.42
6:J:5:VAL:HG12	6:J:6:ARG:HG2	2.02	0.42
6:J:65:PRO:HB2	6:J:68:LYS:HG2	2.02	0.42
12:A:451:HIS:HD2	12:A:453:MET:HE2	1.85	0.42
7:K:72:LYS:NZ	12:A:551:TYR:OH	2.39	0.42
11:B:1127:GLY:O	12:A:344:ARG:NH1	2.52	0.42
11:B:1192:TYR:CE2	12:A:12:ARG:NH2	2.88	0.42
12:A:55:ASP:OD1	12:A:55:ASP:N	2.46	0.42
12:A:886:ILE:HD13	12:A:943:LEU:HB3	2.02	0.42
4:G:58:ARG:HA	4:G:58:ARG:HD3	1.92	0.41
11:B:593:PRO:HA	11:B:596:LEU:CG	2.50	0.41
9:S:239:ALA:HB1	9:S:243:GLN:HE22	1.83	0.41
11:B:596:LEU:HD12	11:B:597:MET:N	2.35	0.41
11:B:769:TYR:O	11:B:773:MET:HG3	2.19	0.41
11:B:1222:ARG:NH2	12:A:1420:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:760:GLN:HB3	12:A:804:TYR:CE2	2.55	0.41
3:F:149:GLU:OE1	3:F:149:GLU:N	2.51	0.41
4:G:47:CYS:SG	4:G:48:VAL:N	2.93	0.41
11:B:76:GLN:O	11:B:84:ILE:N	2.54	0.41
14:H:101:ALA:HB2	14:H:116:TYR:CE1	2.56	0.41
5:I:74:GLU:HB2	5:I:81:ARG:HH21	1.86	0.41
10:M:30:TYR:HD2	10:M:31:PRO:HA	1.84	0.41
11:B:593:PRO:HA	11:B:596:LEU:HG	2.03	0.41
12:A:10:PRO:HG2	12:A:12:ARG:HH12	1.85	0.41
12:A:184:SER:OG	12:A:199:LEU:HG	2.20	0.41
12:A:768:GLN:OE1	12:A:768:GLN:N	2.45	0.41
11:B:73:GLN:NE2	11:B:74:LEU:O	2.54	0.41
12:A:99:ILE:H	12:A:99:ILE:HG23	1.65	0.41
2:E:50:MET:HE1	2:E:52:ARG:HG2	2.02	0.41
12:A:543:LEU:HA	12:A:546:VAL:HG22	2.02	0.41
12:A:784:LEU:HD21	12:A:811:GLN:HG2	2.02	0.41
13:D:199:ASN:OD1	13:D:200:ASN:N	2.54	0.41
11:B:615:MET:SD	11:B:615:MET:C	3.03	0.41
13:D:119:ARG:HH22	13:D:155:ARG:HH22	1.69	0.41
5:I:78:CYS:C	5:I:79:HIS:CD2	2.99	0.41
6:J:32:GLU:OE1	6:J:32:GLU:N	2.50	0.41
12:A:177:ASP:OD1	12:A:177:ASP:N	2.53	0.41
12:A:895:LYS:HD2	12:A:895:LYS:HA	1.88	0.41
5:I:84:VAL:HG13	5:I:104:LEU:HD11	2.03	0.41
11:B:316:PRO:HA	11:B:319:GLU:OE1	2.21	0.41
14:H:97:MET:HB2	14:H:142:LEU:HB3	2.03	0.41
5:I:97:MET:HE2	5:I:97:MET:HB3	1.89	0.40
11:B:356:LEU:O	11:B:356:LEU:HD23	2.21	0.40
12:A:765:VAL:HG22	12:A:804:TYR:CE2	2.55	0.40
12:A:1398:MET:SD	12:A:1399:ARG:N	2.95	0.40
13:D:188:ALA:HB2	13:D:208:GLU:HB2	2.03	0.40
1:C:23:SER:OG	1:C:24:ASN:N	2.54	0.40
11:B:1174:LYS:O	11:B:1178:ASN:N	2.54	0.40
11:B:1210:MET:HA	12:A:304:MET:CE	2.48	0.40
12:A:10:PRO:HB2	12:A:12:ARG:NH1	2.37	0.40
11:B:21:GLU:CD	11:B:22:SER:N	2.79	0.40
11:B:1111:MET:HE2	11:B:1116:ARG:N	2.37	0.40
9:S:147:LYS:HE3	9:S:147:LYS:HB2	1.94	0.40
12:A:456:MET:CE	12:A:510:GLN:HE21	2.35	0.40
12:A:72:GLU:HB3	12:A:73:GLY:H	1.78	0.40
12:A:1395:GLY:O	12:A:1399:ARG:CZ	2.69	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	C	260/318 (82%)	253 (97%)	6 (2%)	1 (0%)	30	61
2	E	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	F	81/155 (52%)	77 (95%)	4 (5%)	0	100	100
4	G	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
5	I	114/122 (93%)	93 (82%)	17 (15%)	4 (4%)	3	23
6	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
7	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
8	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
9	S	162/309 (52%)	147 (91%)	14 (9%)	1 (1%)	21	54
10	M	85/345 (25%)	83 (98%)	2 (2%)	0	100	100
11	B	1139/1224 (93%)	1109 (97%)	28 (2%)	2 (0%)	43	72
12	A	1386/1733 (80%)	1298 (94%)	84 (6%)	4 (0%)	36	65
13	D	153/221 (69%)	142 (93%)	11 (7%)	0	100	100
14	H	132/146 (90%)	127 (96%)	4 (3%)	1 (1%)	16	49
15	Q	208/735 (28%)	203 (98%)	5 (2%)	0	100	100
16	R	192/400 (48%)	186 (97%)	6 (3%)	0	100	100
All	All	4515/6354 (71%)	4304 (95%)	198 (4%)	13 (0%)	37	65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	76	PRO
5	I	113	ASP
9	S	236	LEU

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Mol	Chain	Res	Type
14	H	109	LYS
11	B	22	SER
12	A	674	PRO
5	I	115	LYS
12	A	1034	GLU
5	I	47	GLU
1	C	90	ASP
12	A	569	LYS
12	A	1036	ARG
11	B	323	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	C	230/274 (84%)	230 (100%)	0	100	100
2	E	195/197 (99%)	195 (100%)	0	100	100
3	F	73/137 (53%)	73 (100%)	0	100	100
4	G	152/152 (100%)	152 (100%)	0	100	100
5	I	110/116 (95%)	107 (97%)	3 (3%)	39	61
6	J	64/65 (98%)	64 (100%)	0	100	100
7	K	99/102 (97%)	99 (100%)	0	100	100
8	L	40/57 (70%)	40 (100%)	0	100	100
9	S	143/274 (52%)	140 (98%)	3 (2%)	47	65
10	M	78/299 (26%)	78 (100%)	0	100	100
11	B	1002/1061 (94%)	1001 (100%)	1 (0%)	88	87
12	A	1221/1520 (80%)	1219 (100%)	2 (0%)	87	85
13	D	139/200 (70%)	139 (100%)	0	100	100
14	H	119/128 (93%)	117 (98%)	2 (2%)	53	69
15	Q	198/641 (31%)	198 (100%)	0	100	100
16	R	187/363 (52%)	186 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4050/5586 (72%)	4038 (100%)	12 (0%)	84 83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	111	THR
5	I	116	ASN
5	I	117	LYS
9	S	151	GLN
9	S	171	ILE
9	S	182	MET
11	B	662	MET
12	A	676	MET
12	A	692	ASP
14	H	109	LYS
14	H	129	TYR
16	R	228	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	131	HIS
1	C	151	GLN
2	E	104	ASN
4	G	14	HIS
4	G	53	ASN
4	G	102	GLN
4	G	122	ASN
5	I	23	ASN
5	I	79	HIS
5	I	83	ASN
5	I	108	HIS
6	J	53	HIS
9	S	243	GLN
10	M	19	ASN
11	B	206	ASN
11	B	236	HIS
11	B	583	ASN
11	B	770	GLN
11	B	958	GLN
11	B	984	HIS

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Mol	Chain	Res	Type
11	B	1065	GLN
12	A	171	GLN
12	A	213	HIS
12	A	256	GLN
12	A	287	HIS
12	A	451	HIS
12	A	525	GLN
12	A	650	GLN
12	A	660	ASN
12	A	717	ASN
12	A	786	HIS
12	A	838	GLN
12	A	862	ASN
12	A	996	ASN
12	A	1188	GLN
12	A	1232	ASN
13	D	143	ASN
13	D	165	GLN
14	H	139	ASN
15	Q	369	ASN
16	R	67	GLN
16	R	232	ASN
16	R	265	HIS

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](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
11	B	1
16	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1155:SER	C	1156:ASP	N	3.18
1	R	227:SER	C	228:MET	N	2.24

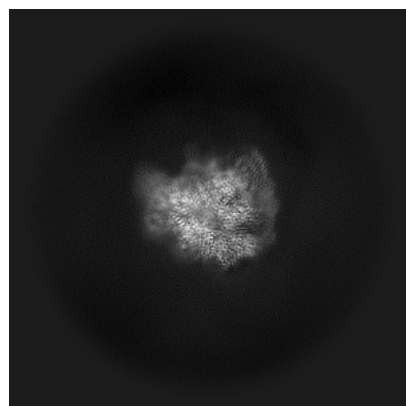
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71494. These allow visual inspection of the internal detail of the map and identification of artifacts.

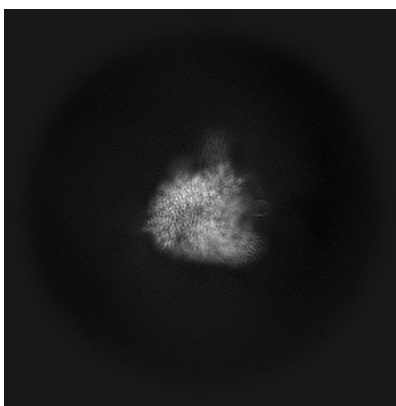
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

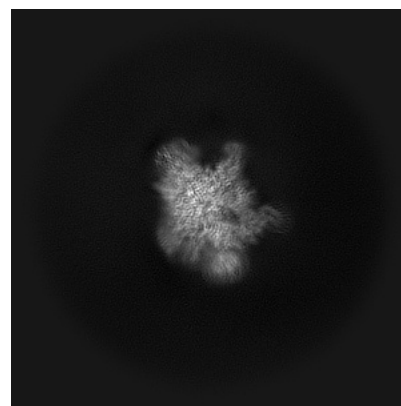
6.1.1 Primary map



X

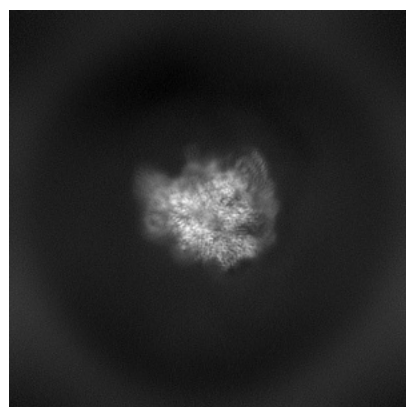


Y

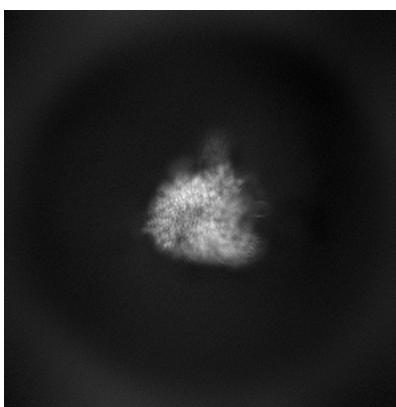


Z

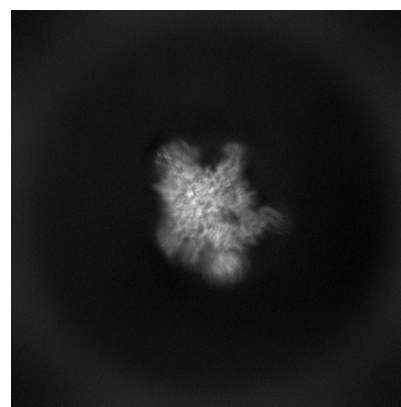
6.1.2 Raw map



X



Y

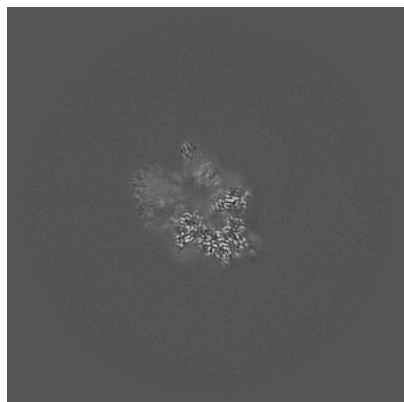


Z

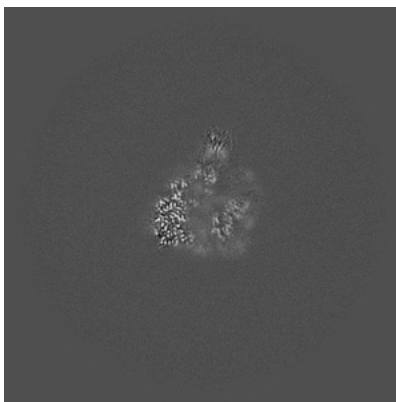
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

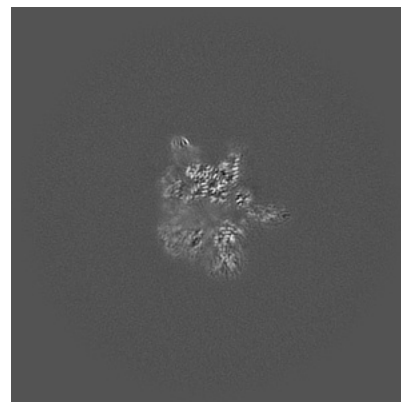
6.2.1 Primary map



X Index: 192

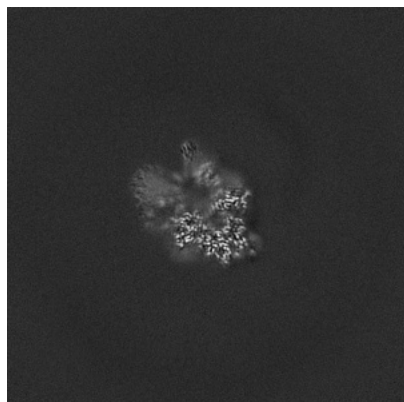


Y Index: 192

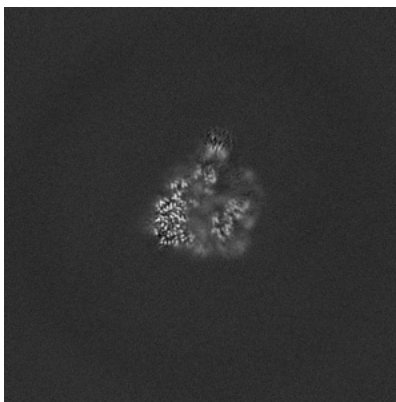


Z Index: 192

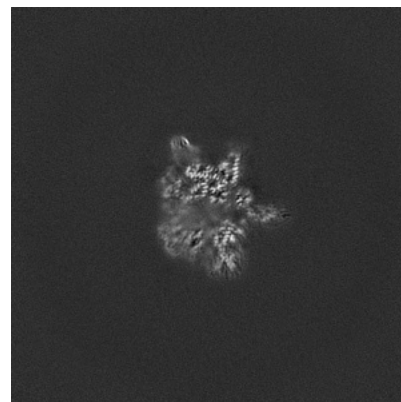
6.2.2 Raw map



X Index: 192



Y Index: 192

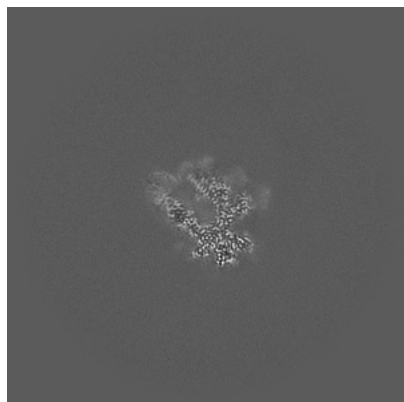


Z Index: 192

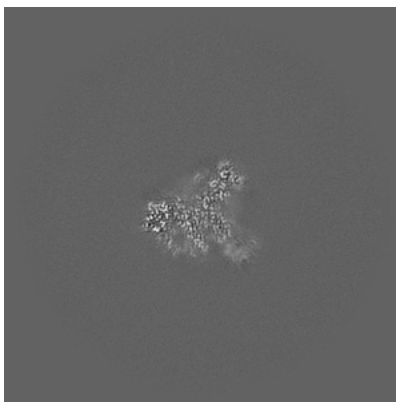
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

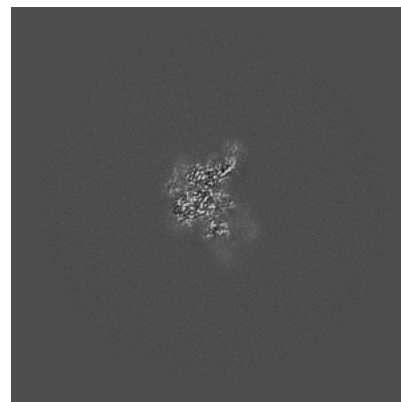
6.3.1 Primary map



X Index: 178

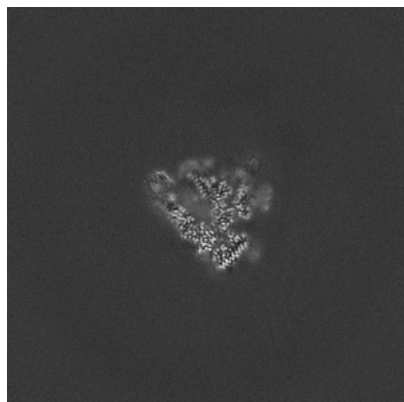


Y Index: 209

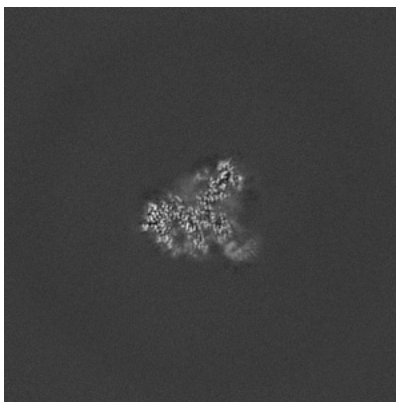


Z Index: 160

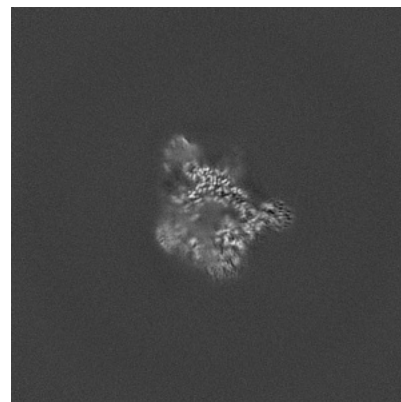
6.3.2 Raw map



X Index: 173



Y Index: 208

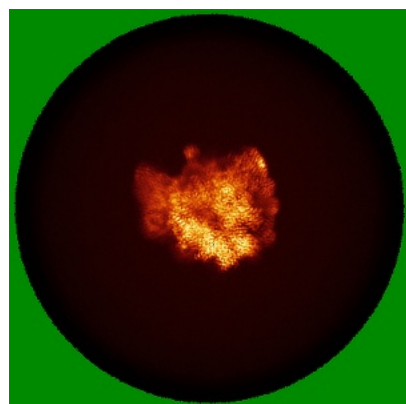


Z Index: 199

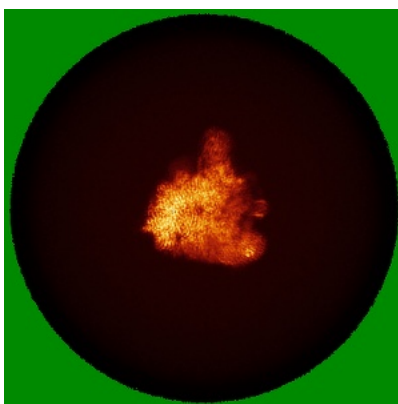
The images above show the largest variance slices of the map in three orthogonal directions.

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

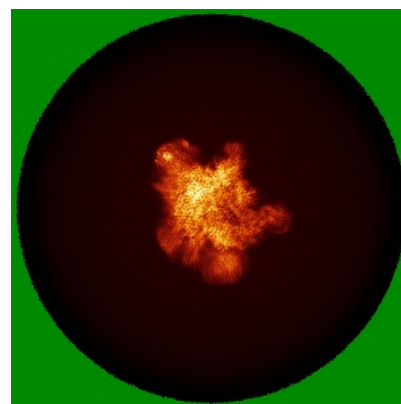
6.4.1 Primary map



X

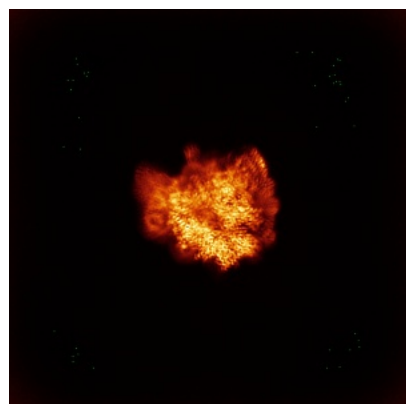


Y

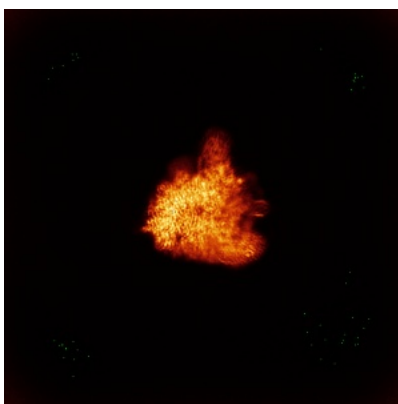


Z

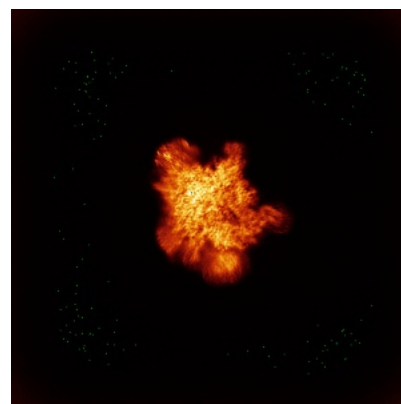
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.419. 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



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.

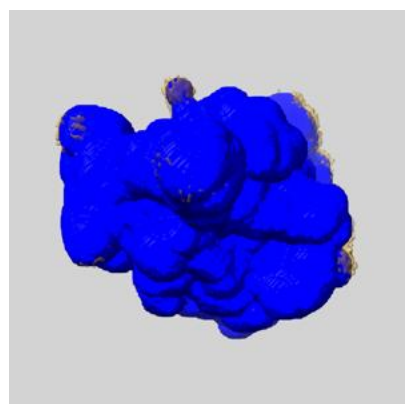
6.6 Mask visualisation [i](#)

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

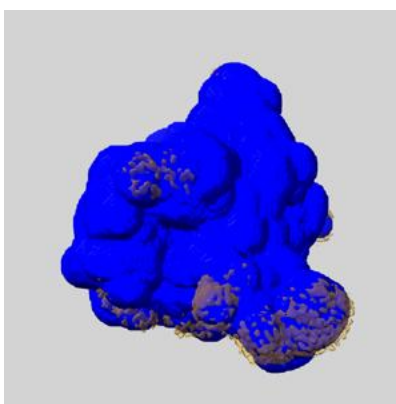
A mask typically either:

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

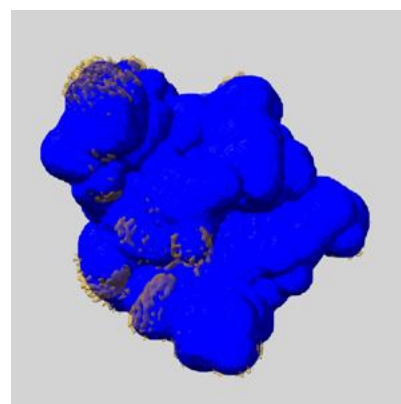
6.6.1 emd_71494_msk_1.map [i](#)



X



Y

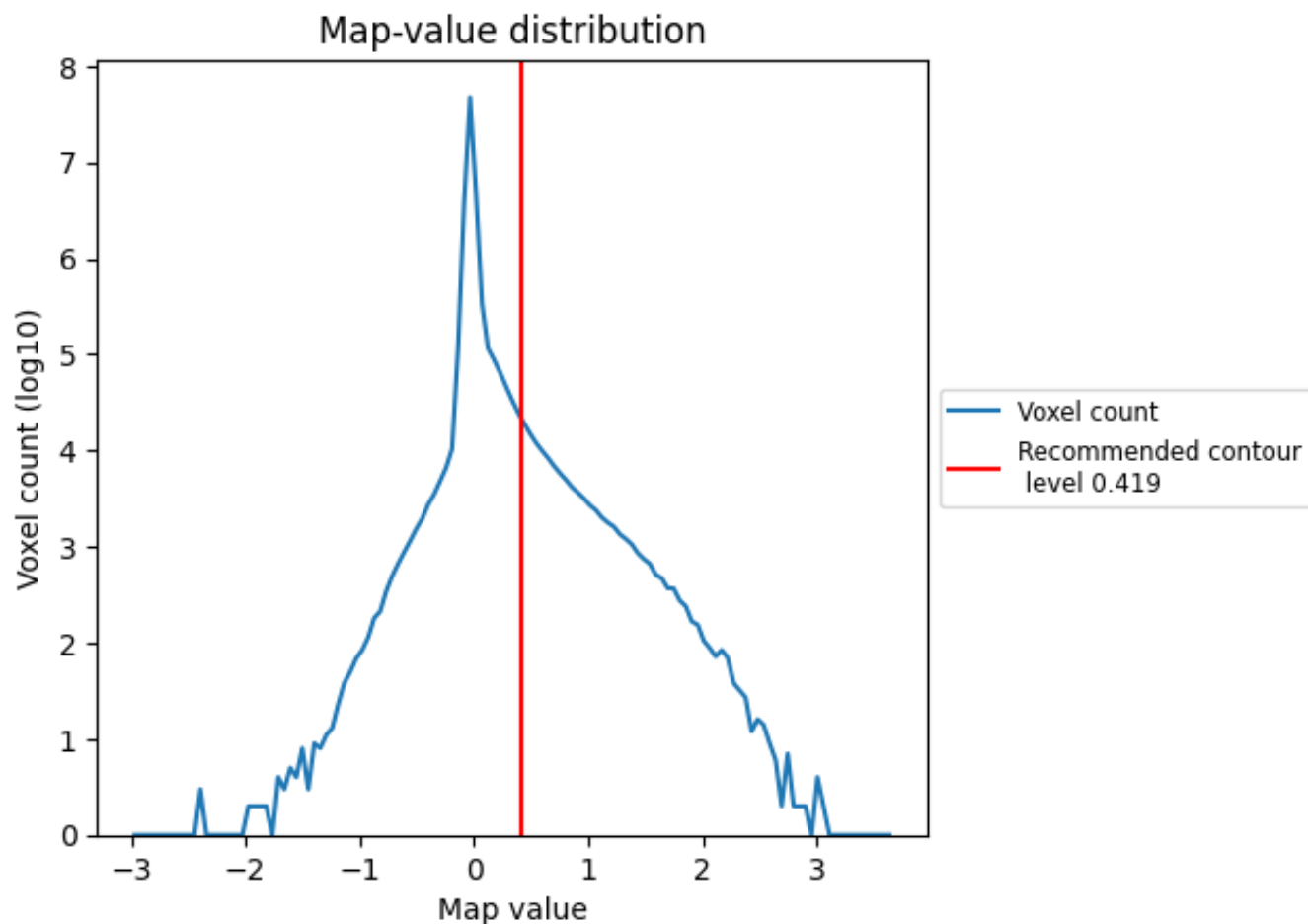


Z

7 Map analysis [i](#)

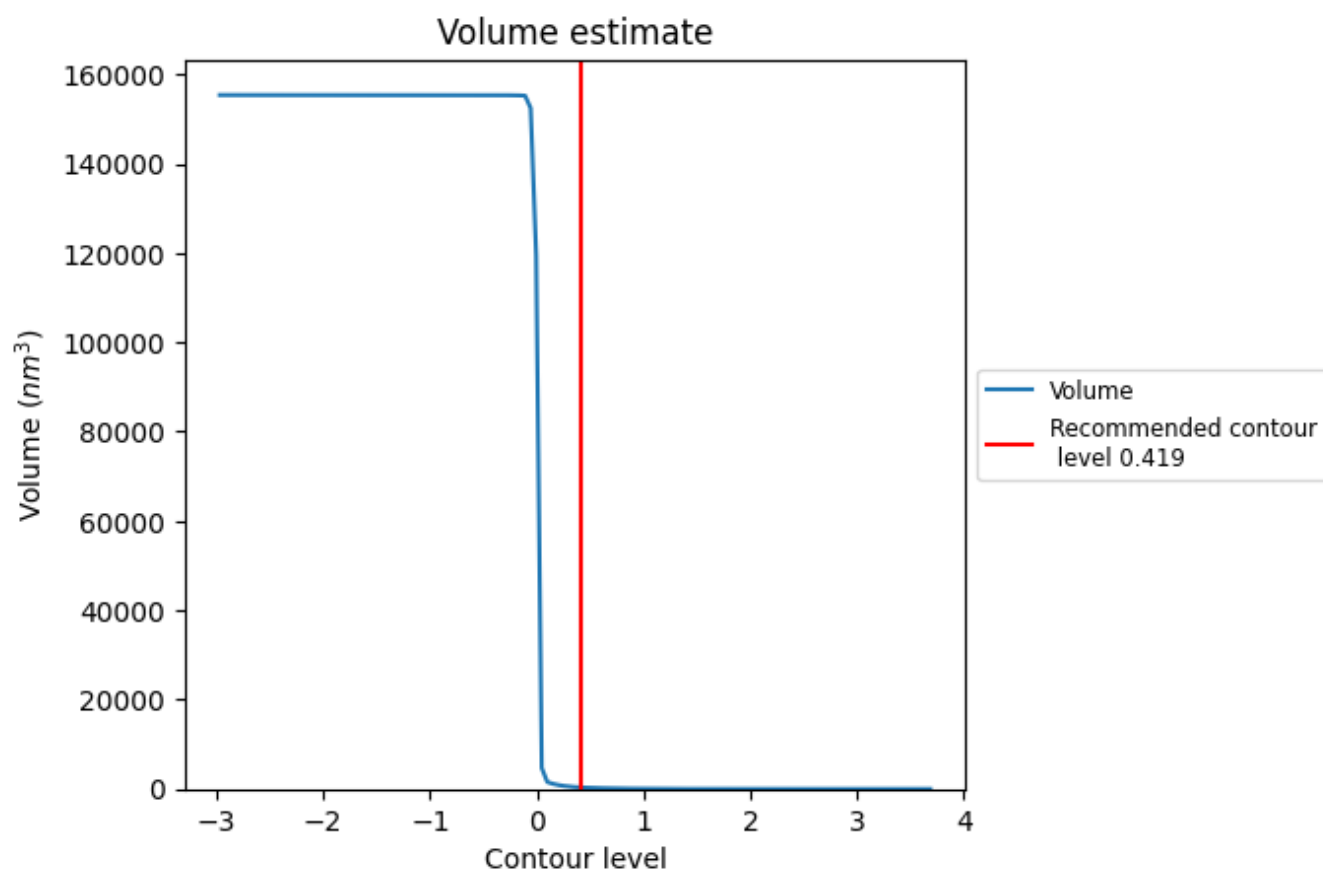
This section contains the results of statistical analysis of the map.

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.

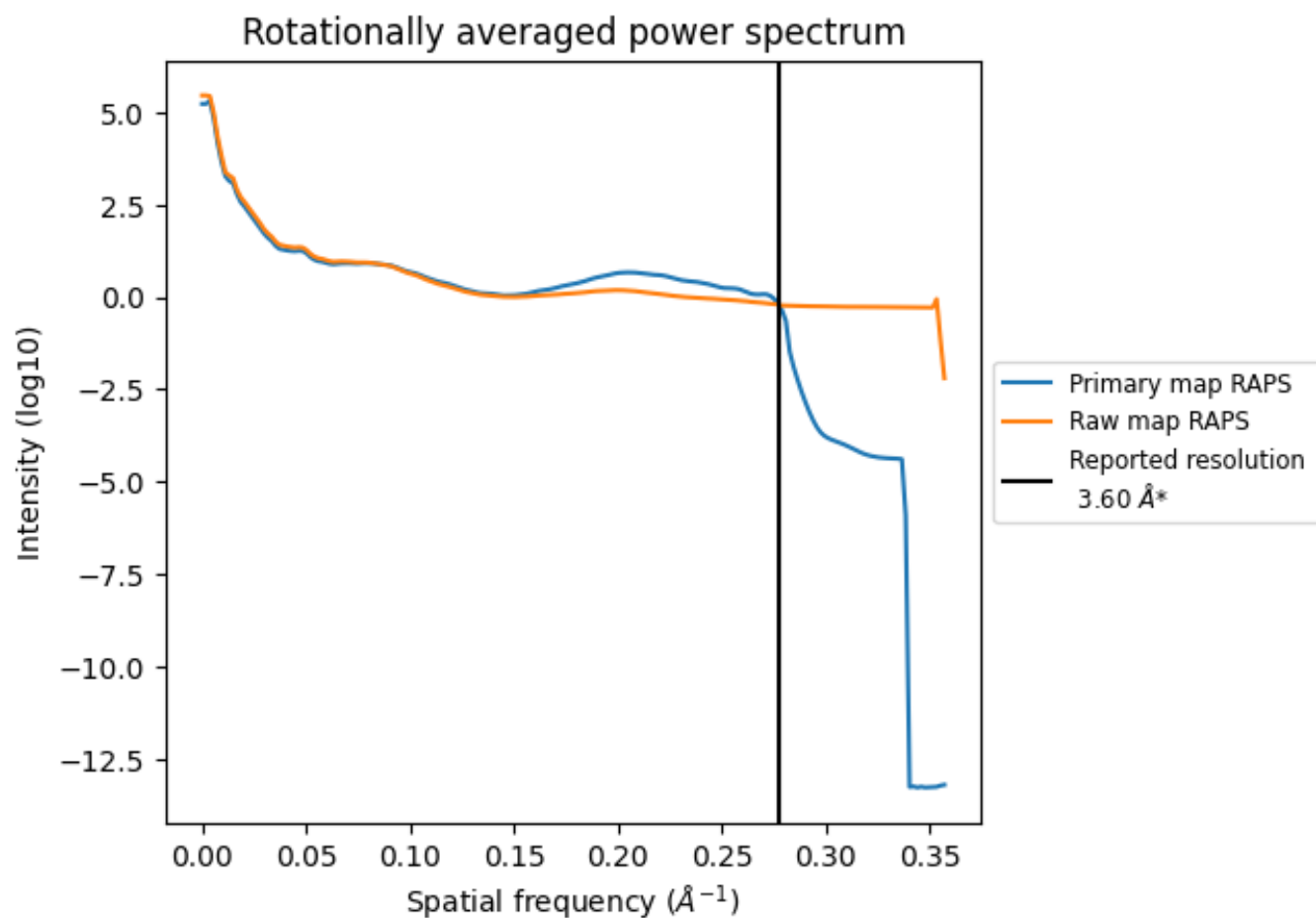
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334 nm^3 ; this corresponds to an approximate mass of 302 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 ⓘ

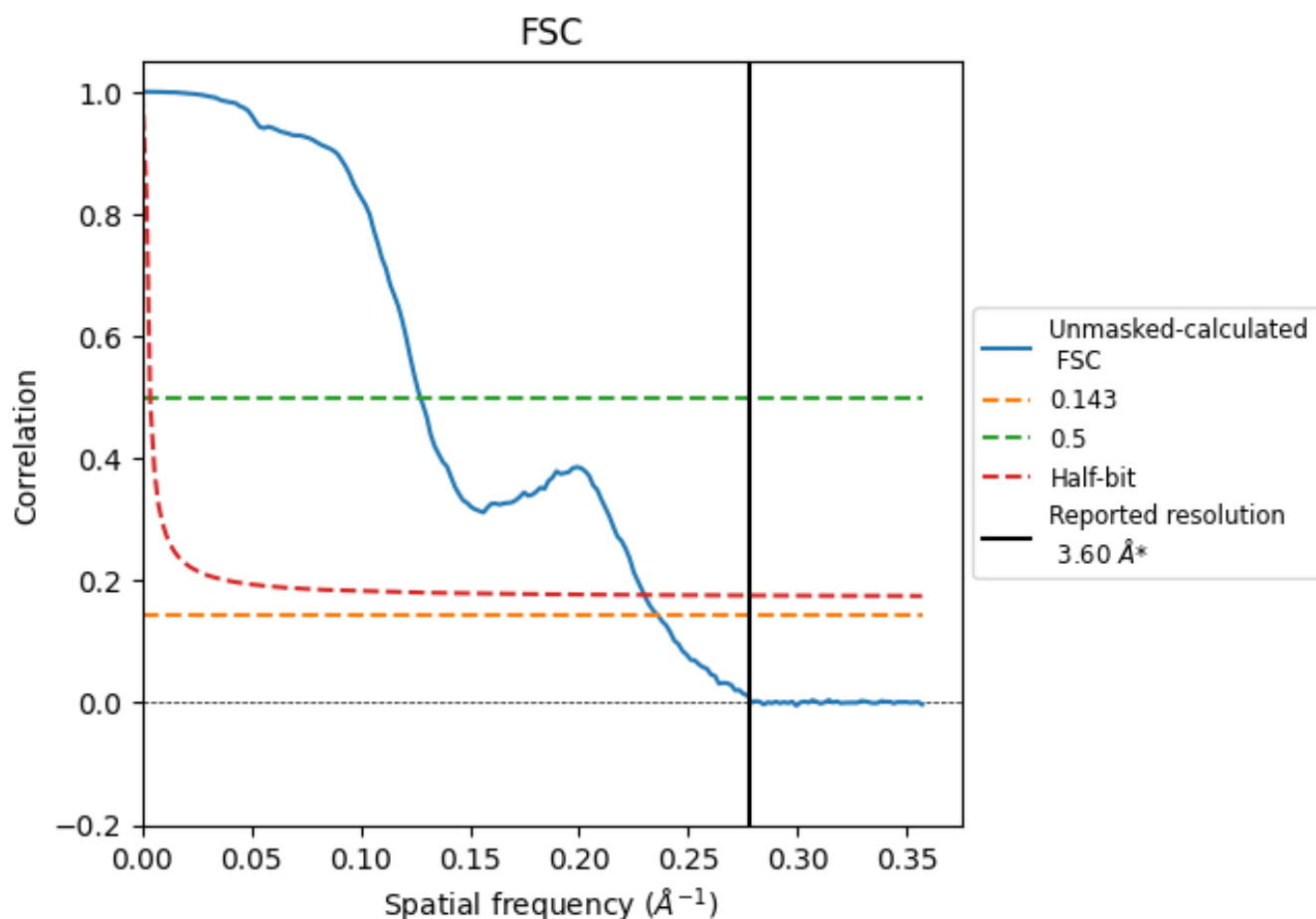


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

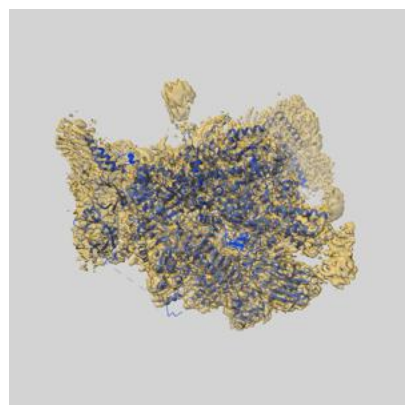
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.86	4.35

*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 4.24 differs from the reported value 3.6 by more than 10 %

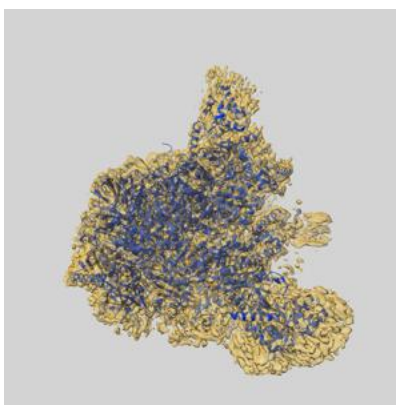
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71494 and PDB model 9PBZ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

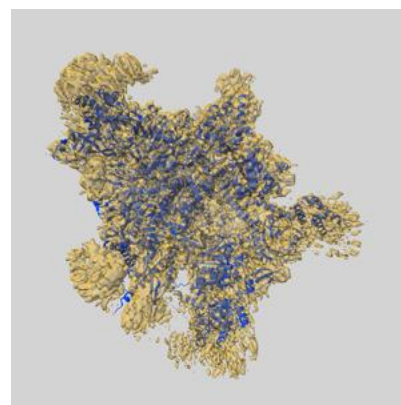
9.1 Map-model overlay [i](#)



X



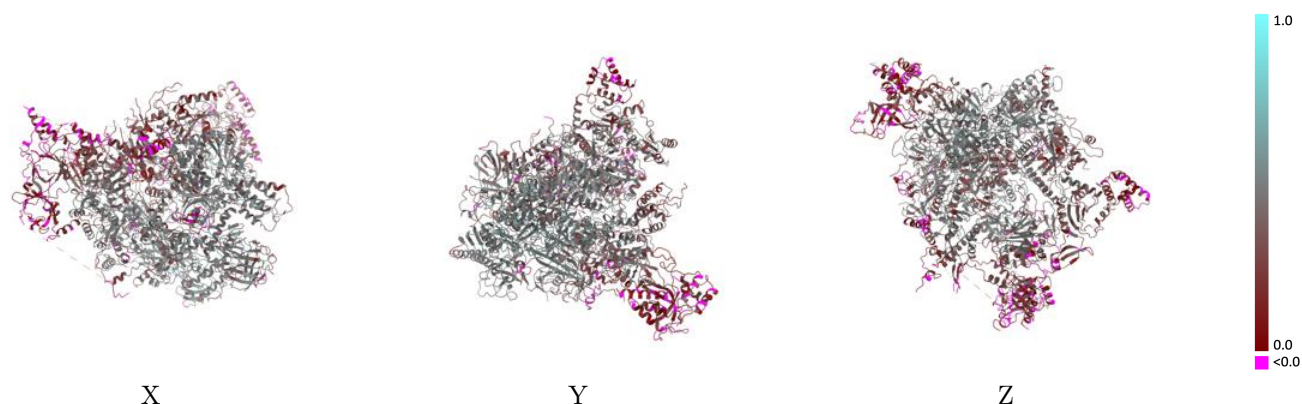
Y



Z

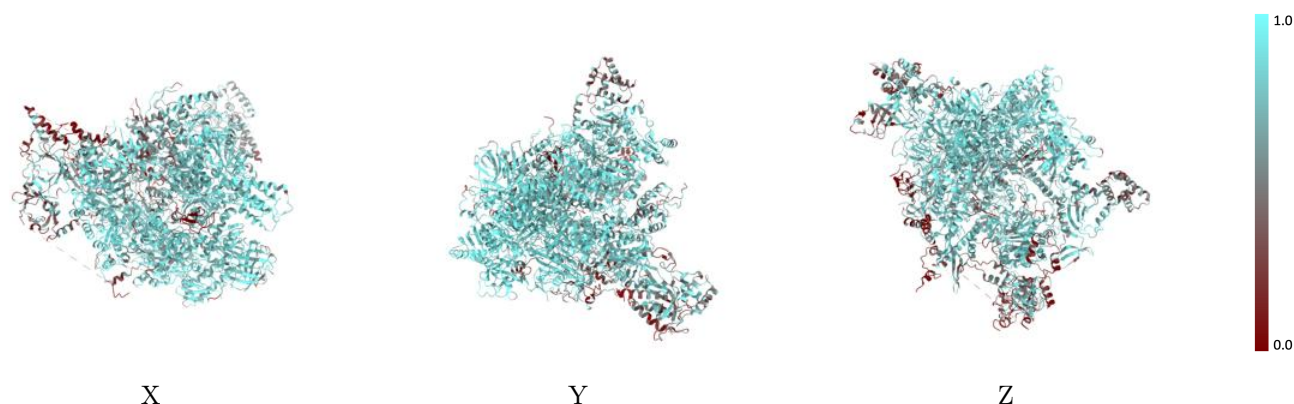
The images above show the 3D surface view of the map at the recommended contour level 0.419 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



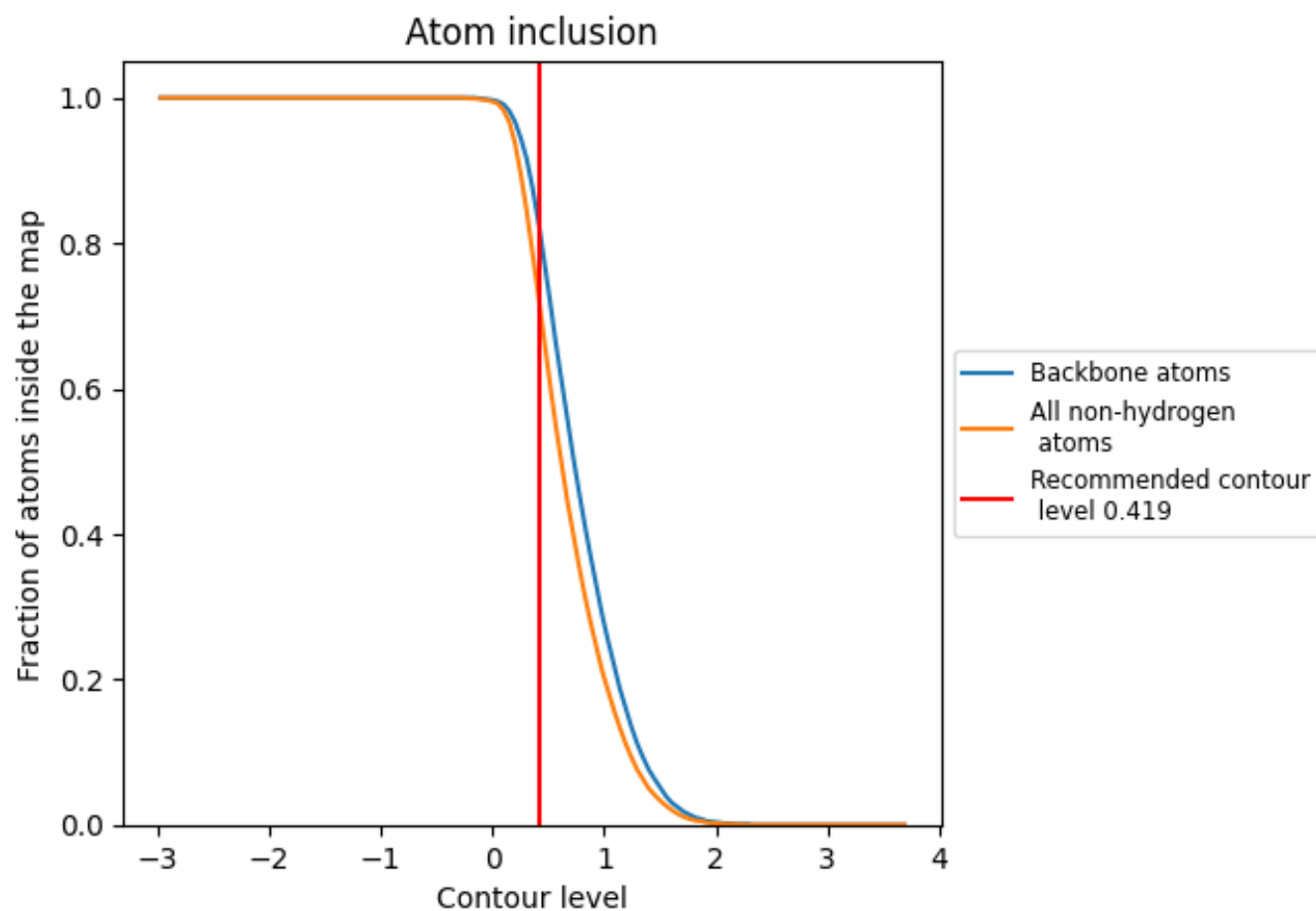
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.419).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.419) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.3680
A	 0.7910	 0.4220
B	 0.7850	 0.4260
C	 0.8820	 0.4850
D	 0.4880	 0.1270
E	 0.8140	 0.4080
F	 0.8480	 0.4620
G	 0.6150	 0.2400
H	 0.7760	 0.4010
I	 0.7220	 0.3200
J	 0.8500	 0.4450
K	 0.7840	 0.4280
L	 0.7920	 0.4390
M	 0.4790	 0.2510
Q	 0.4260	 0.1570
R	 0.3610	 0.1190
S	 0.3480	 0.1490

