



Full wwPDB EM Validation Report ⓘ

Sep 22, 2026 – 12:34 PM EDT

PDB ID : 9PB7 / pdb_00009pb7
EMDB ID : EMD-71456
Title : TFIIH of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-26
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

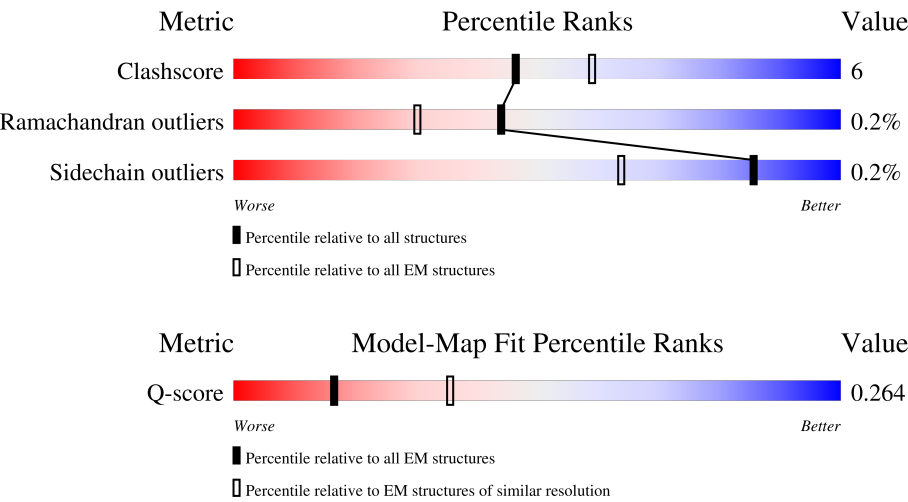
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.40 Å.

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



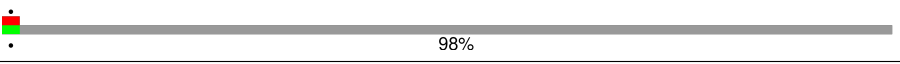
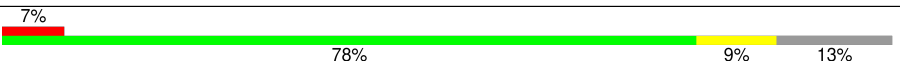
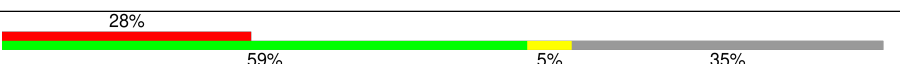
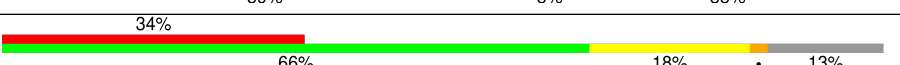
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	5	72	
2	0	778	
3	3	321	
4	7	843	

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Mol	Chain	Length	Quality of chain
5	8	905	
6	9	244	
7	N	26	
8	T	26	
9	4	338	
10	6	461	
11	1	642	
12	2	513	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26523 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 General transcription and DNA repair factor IIIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 3 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 4 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	607	Total	C	N	O	S	0	0
			4881	3104	846	905	26		

- Molecule 5 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	17	Total	C	N	O	S	0	0
			134	89	22	22	1		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	68	Total	C	N	O	S	0	0
			542	345	82	113	2		

- Molecule 7 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	26	Total	C	N	O	P	0	0
			534	257	91	160	26		

- Molecule 8 is a DNA chain called promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	26	Total	C	N	O	P	0	0
			532	255	99	152	26		

- Molecule 9 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4	293	Total	C	N	O	S	0	0
			2274	1454	377	429	14		

- Molecule 10 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	6	374	Total	C	N	O	S	0	0
			2946	1870	507	541	28		

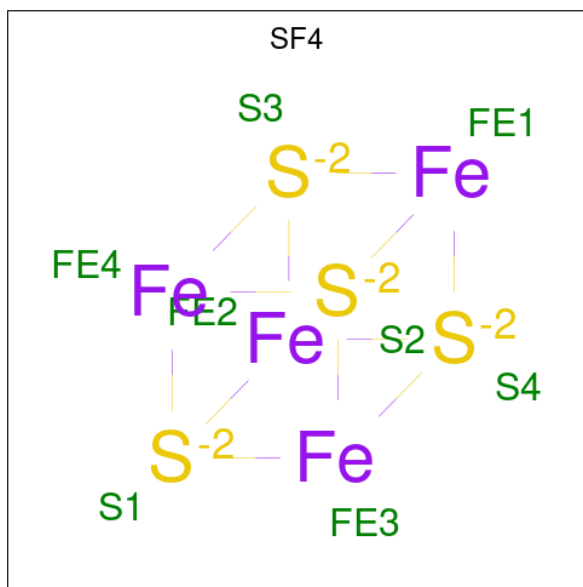
- Molecule 11 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	416	Total	C	N	O	S	0	0
			3374	2133	586	639	16		

- Molecule 12 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	445	Total	C	N	O	S	0	0
			3597	2327	591	663	16		

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
13	0	1	Total	Fe	S	0
			8	4	4	

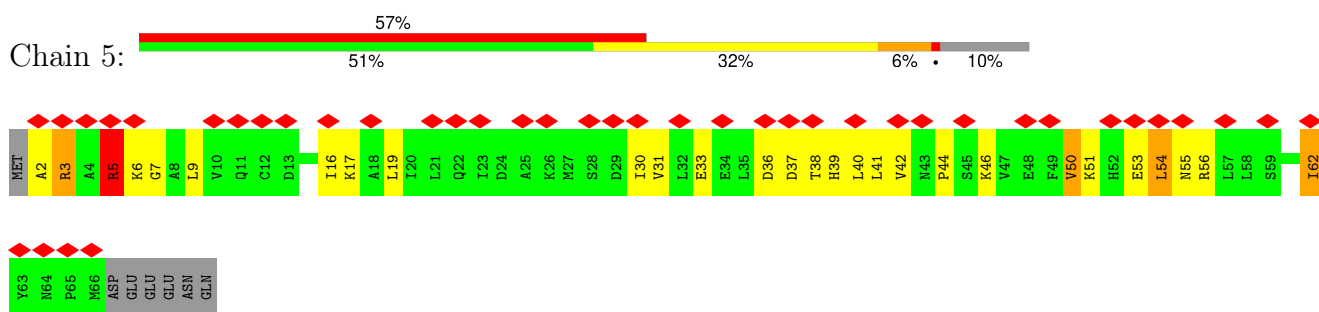
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	3	2	Total	Zn	0
			2	2	
14	4	1	Total	Zn	0
			1	1	
14	6	4	Total	Zn	0
			4	4	

3 Residue-property plots

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

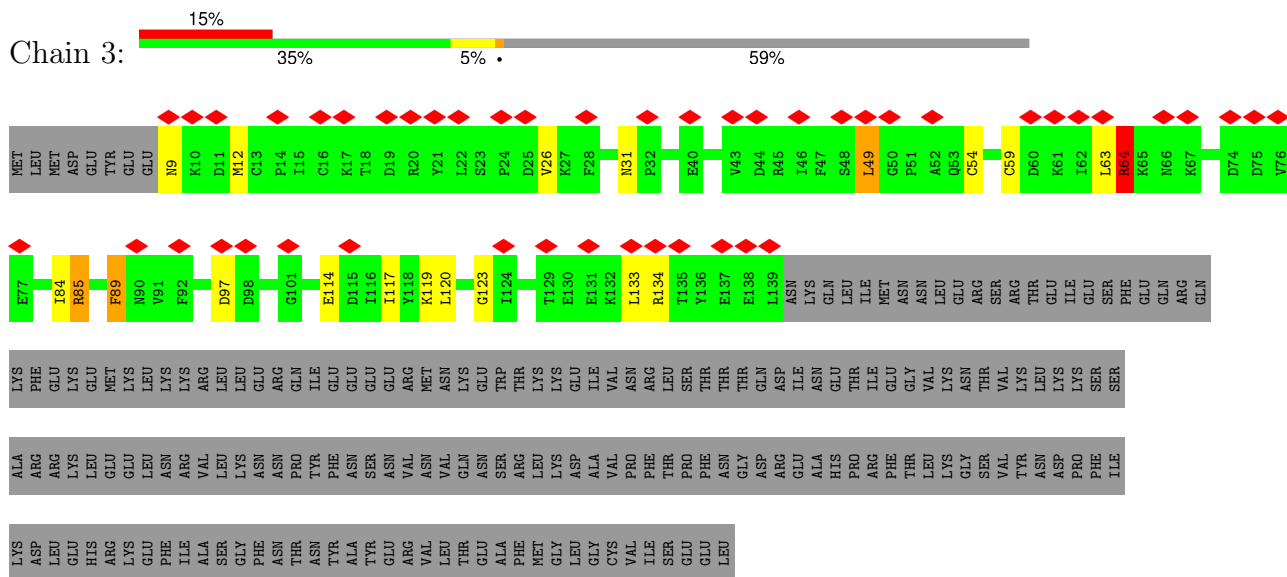
- Molecule 1: General transcription and DNA repair factor IIH subunit TFB5



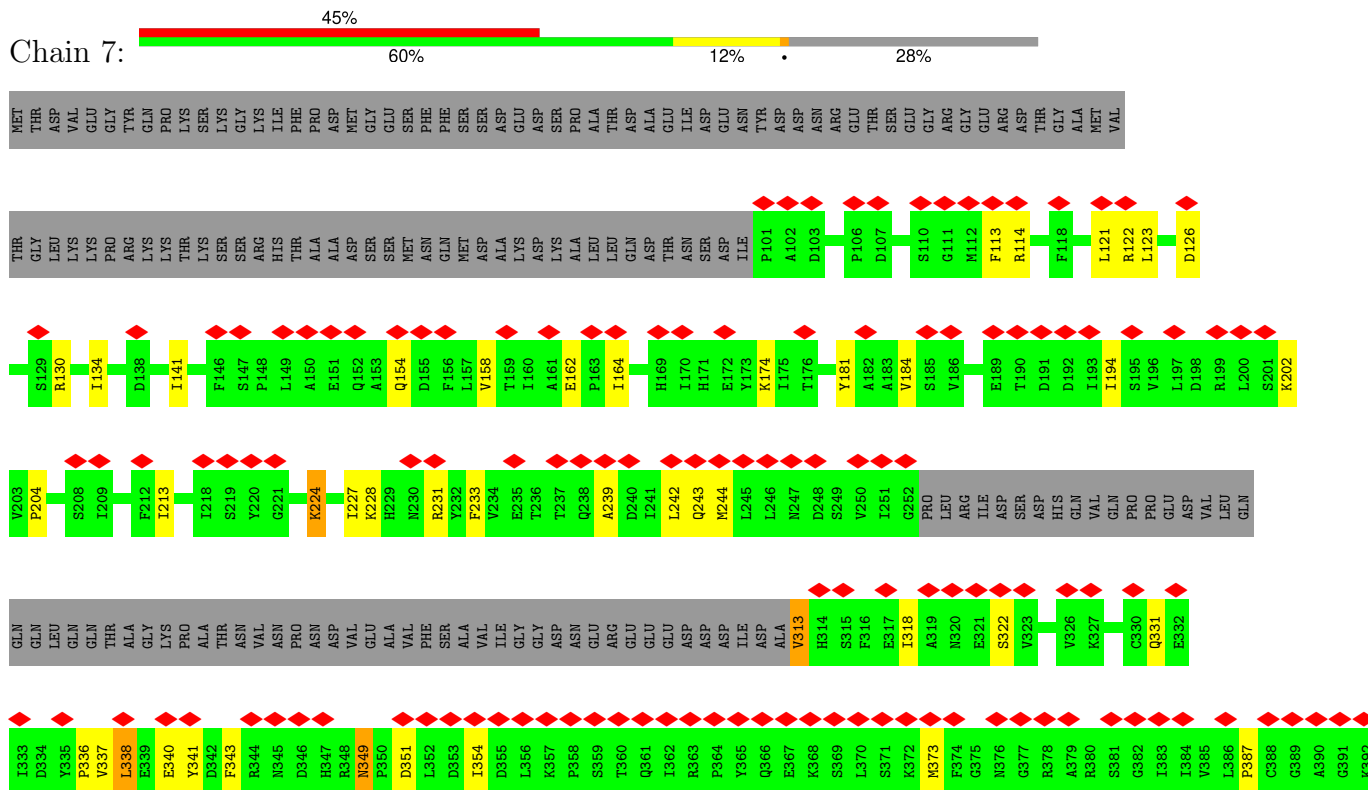
- Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3

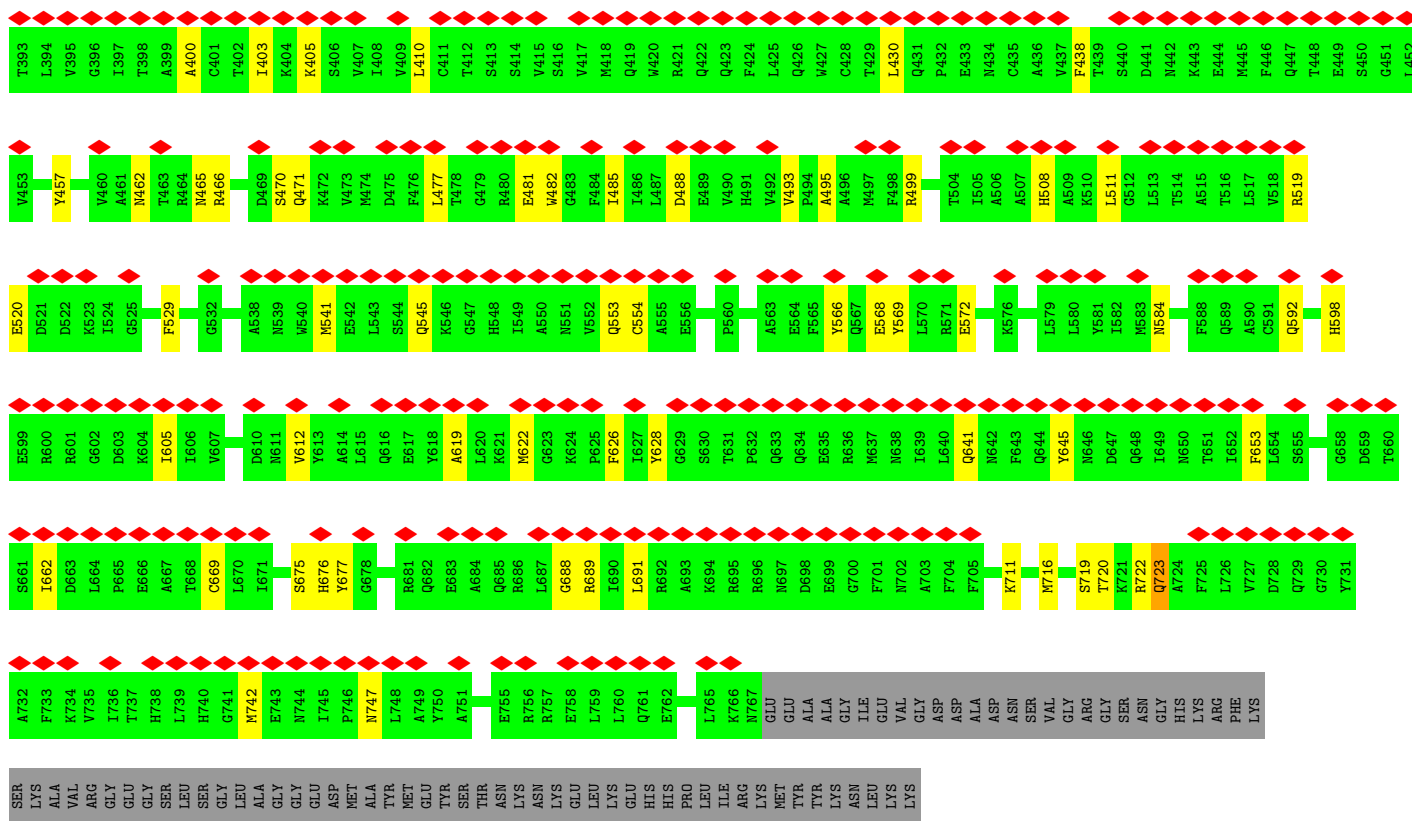


- Molecule 3: RNA polymerase II transcription factor B subunit 3

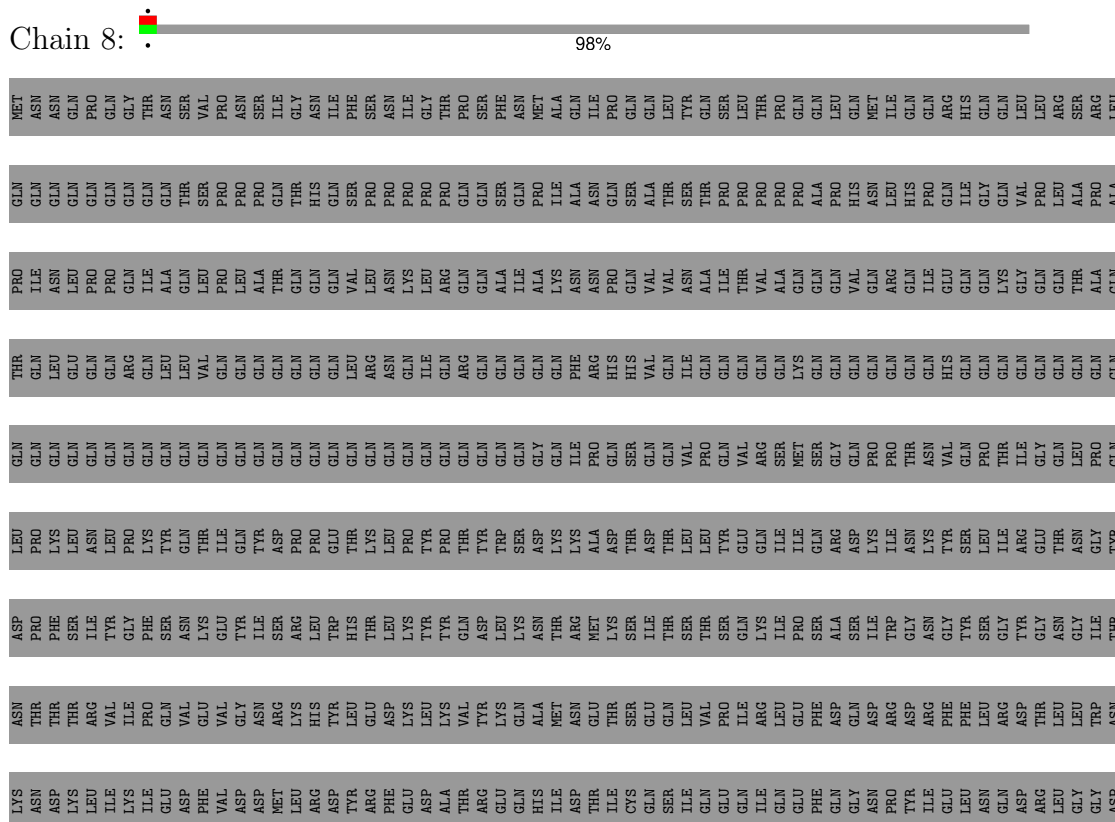


- Molecule 4: General transcription and DNA repair factor IIH helicase subunit XPB



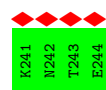
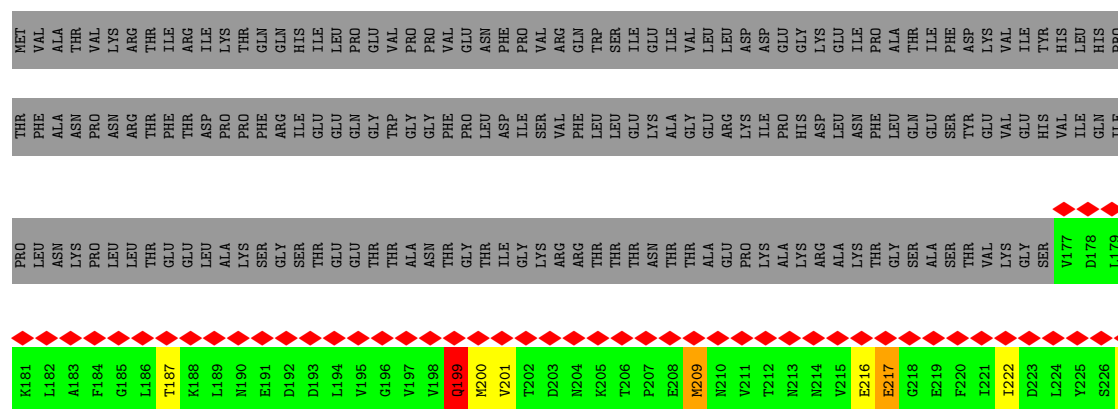


• Molecule 5: SWI/SNF chromatin-remodeling complex subunit SNF5





- Molecule 6: Transcription initiation factor TFIID subunit 14

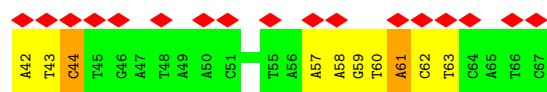


- Molecule 7: promoter DNA

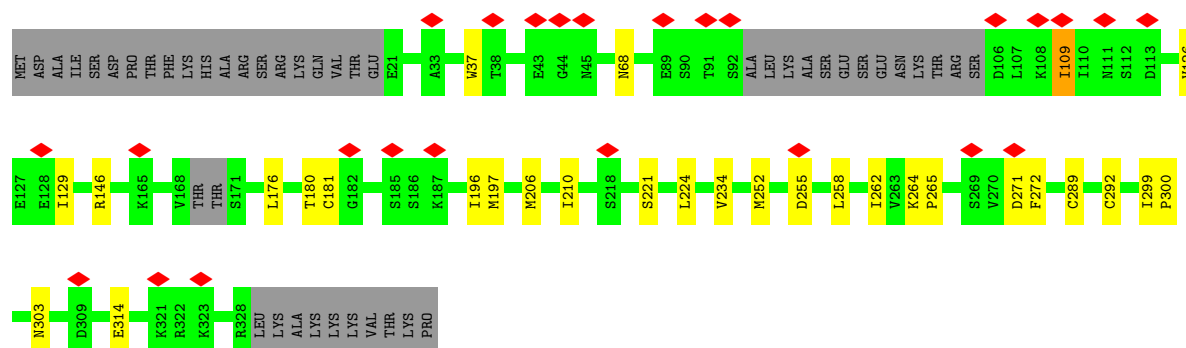
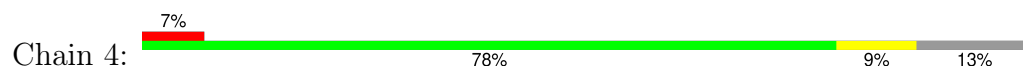


- Molecule 8: promoter DNA

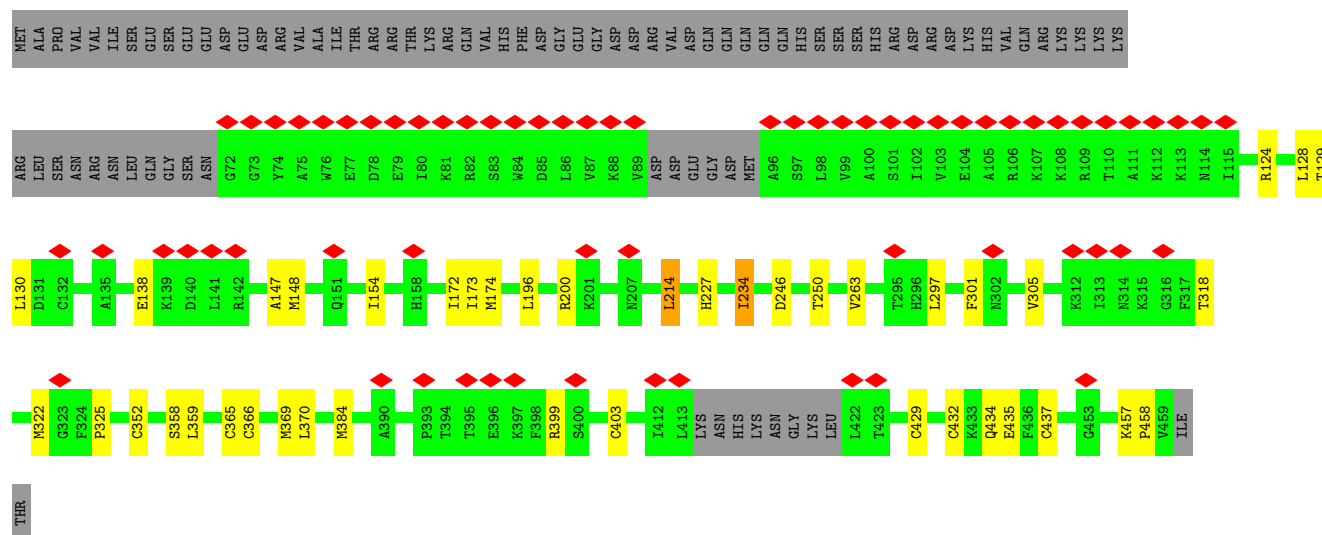




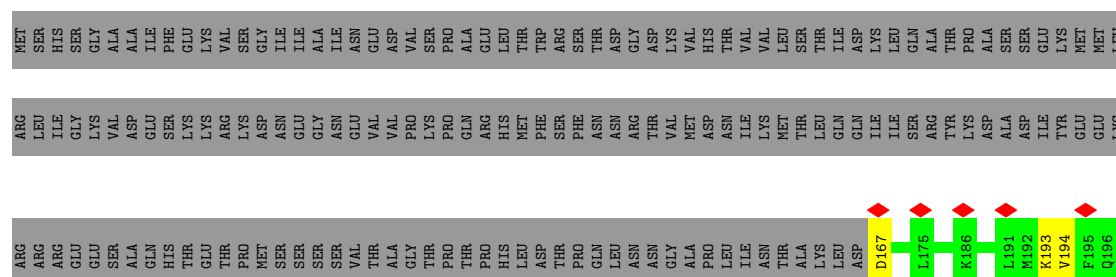
- Molecule 9: General transcription and DNA repair factor IIH subunit TFB4

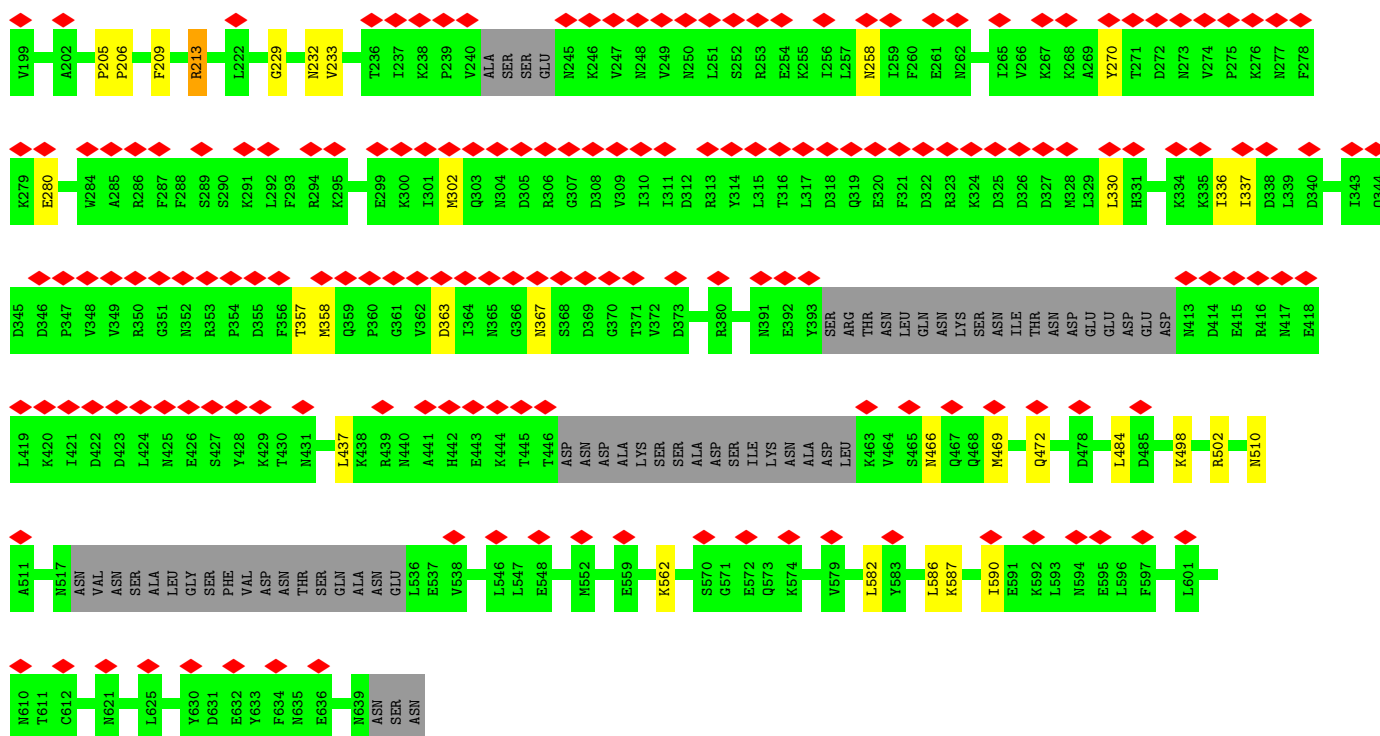


- Molecule 10: General transcription and DNA repair factor IIH subunit SSL1



- Molecule 11: General transcription and DNA repair factor IIH subunit TFB1





• Molecule 12: General transcription and DNA repair factor IIH subunit TFB2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SF4, ZN

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	5	1.29	10/520 (1.9%)	2.37	15/701 (2.1%)
2	0	0.52	10/6209 (0.2%)	0.63	6/8384 (0.1%)
3	3	0.86	6/1109 (0.5%)	1.30	13/1492 (0.9%)
4	7	0.43	5/4985 (0.1%)	0.67	1/6745 (0.0%)
5	8	0.72	0/137	1.19	0/185
6	9	1.65	8/549 (1.5%)	2.59	23/743 (3.1%)
7	N	0.61	1/597 (0.2%)	0.92	4/920 (0.4%)
8	T	0.64	2/597 (0.3%)	0.98	5/918 (0.5%)
9	4	0.31	1/2312 (0.0%)	0.58	0/3127
10	6	0.43	4/3007 (0.1%)	0.60	0/4066
11	1	0.35	2/3426 (0.1%)	0.63	5/4613 (0.1%)
12	2	0.76	20/3664 (0.5%)	1.51	37/4952 (0.7%)
All	All	0.60	69/27112 (0.3%)	0.98	109/36846 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	0	2
2	0	0	1
3	3	0	2
4	7	0	4
5	8	0	1
6	9	1	2
9	4	0	1
11	1	0	1
12	2	0	5
All	All	1	19

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	64	ARG	CG-CD	-16.11	1.04	1.52
2	0	553	MET	SD-CE	-16.02	1.39	1.79
6	9	199	GLN	CA-CB	-15.09	1.27	1.53
2	0	557	MET	CG-SD	-15.03	1.43	1.80
6	9	217	GLU	CD-OE2	14.69	1.53	1.25
3	3	49	LEU	CB-CG	-13.97	1.25	1.53
12	2	490	LYS	CB-CG	-13.36	1.12	1.52
6	9	200	MET	CB-CG	-12.51	1.15	1.52
6	9	209	MET	CB-CG	-12.10	1.16	1.52
1	5	5	ARG	CA-CB	-11.18	1.26	1.53
1	5	50	VAL	CB-CG1	-10.74	1.17	1.52
6	9	199	GLN	CD-NE2	10.71	1.55	1.33
1	5	3	ARG	CG-CD	-10.19	1.21	1.52
2	0	537	MET	CG-SD	-10.12	1.55	1.80
4	7	349	ASN	CG-ND2	-9.79	1.12	1.33
6	9	199	GLN	CD-OE1	-9.22	1.06	1.23
10	6	384	MET	SD-CE	-8.99	1.57	1.79
12	2	69	ASN	CG-OD1	-8.94	1.06	1.23
12	2	195	GLU	CD-OE1	-8.80	1.08	1.25
12	2	352	ASN	CG-OD1	-8.46	1.07	1.23
12	2	408	MET	SD-CE	-8.45	1.58	1.79
4	7	545	GLN	CD-OE1	-8.39	1.07	1.23
1	5	3	ARG	CB-CG	-8.35	1.27	1.52
2	0	251	ASP	CG-OD1	-8.19	1.09	1.25
12	2	97	MET	CG-SD	-8.06	1.60	1.80
6	9	199	GLN	CB-CG	-7.85	1.28	1.52
1	5	3	ARG	CD-NE	-7.62	1.35	1.46
12	2	506	LYS	CB-CG	-7.52	1.29	1.52
9	4	109	ILE	CB-CG2	-7.46	1.27	1.52
2	0	537	MET	SD-CE	-7.39	1.61	1.79
6	9	217	GLU	CD-OE1	-7.36	1.11	1.25
11	1	197	GLU	CD-OE1	-7.30	1.11	1.25
12	2	69	ASN	N-CA	-7.25	1.37	1.46
2	0	199	MET	SD-CE	-7.16	1.61	1.79
12	2	69	ASN	CB-CG	-7.09	1.34	1.52
4	7	338	LEU	C-O	-6.96	1.15	1.24
1	5	3	ARG	CZ-NH2	-6.85	1.24	1.33
2	0	557	MET	CB-CG	-6.83	1.31	1.52
2	0	495	MET	SD-CE	-6.71	1.62	1.79
3	3	64	ARG	CB-CG	-6.69	1.32	1.52
7	N	-43	DA	C3'-C2'	-6.64	1.39	1.52
10	6	214	LEU	CG-CD1	-6.59	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	64	ARG	CA-C	-6.44	1.44	1.52
3	3	85	ARG	CB-CG	-6.38	1.33	1.52
10	6	234	ILE	CG1-CD1	-6.37	1.26	1.51
8	T	61	DA	C3'-O3'	-6.34	1.23	1.42
12	2	506	LYS	CE-NZ	6.30	1.68	1.49
12	2	258	LEU	CG-CD2	-6.29	1.31	1.52
12	2	22	GLN	CB-CG	-6.27	1.33	1.52
3	3	49	LEU	CA-CB	-6.02	1.42	1.54
8	T	44	DC	O3'-P	5.97	1.70	1.61
4	7	723	GLN	CD-OE1	-5.93	1.12	1.23
12	2	464	THR	CB-CG2	5.83	1.71	1.52
2	0	167	VAL	CB-CG2	-5.81	1.33	1.52
12	2	463	GLU	CB-CG	-5.75	1.35	1.52
12	2	490	LYS	CD-CE	-5.70	1.35	1.52
1	5	62	ILE	CG1-CD1	-5.68	1.29	1.51
12	2	506	LYS	CA-C	5.66	1.60	1.52
10	6	128	LEU	CG-CD2	-5.62	1.34	1.52
12	2	253	MET	SD-CE	-5.61	1.65	1.79
12	2	490	LYS	CG-CD	-5.59	1.35	1.52
1	5	3	ARG	CZ-NH1	5.45	1.40	1.32
1	5	54	LEU	CG-CD1	-5.33	1.34	1.52
2	0	451	GLU	CD-OE1	-5.19	1.15	1.25
4	7	224	LYS	CD-CE	-5.10	1.37	1.52
12	2	195	GLU	CD-OE2	-5.09	1.15	1.25
12	2	506	LYS	CG-CD	-5.08	1.37	1.52
11	1	437	LEU	CG-CD2	-5.03	1.35	1.52
1	5	55	ASN	CG-OD1	-5.01	1.14	1.23

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	2	69	ASN	CA-CB-CG	54.91	167.51	112.60
6	9	199	GLN	CA-CB-CG	32.93	179.97	114.10
12	2	69	ASN	CB-CG-ND2	-32.14	68.19	116.40
3	3	64	ARG	CB-CG-CD	26.43	172.08	111.30
1	5	3	ARG	CA-CB-CG	25.28	164.66	114.10
1	5	3	ARG	CB-CG-CD	25.15	169.15	111.30
6	9	200	MET	CA-CB-CG	24.82	163.73	114.10
12	2	490	LYS	CB-CG-CD	23.49	165.32	111.30
12	2	69	ASN	CB-CG-OD1	22.97	166.74	120.80
1	5	5	ARG	CA-CB-CG	21.98	158.05	114.10
1	5	3	ARG	CG-CD-NE	20.45	156.99	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	5	ARG	NE-CZ-NH1	-19.32	102.18	121.50
12	2	506	LYS	CB-CG-CD	18.59	154.07	111.30
6	9	199	GLN	N-CA-CB	18.55	141.84	110.49
12	2	463	GLU	CG-CD-OE1	-16.97	79.37	118.40
12	2	97	MET	CB-CG-SD	16.85	163.26	112.70
6	9	200	MET	CB-CG-SD	15.25	158.46	112.70
12	2	490	LYS	CG-CD-CE	14.97	145.74	111.30
6	9	200	MET	N-CA-CB	14.08	132.10	110.28
6	9	209	MET	CA-CB-CG	14.04	142.18	114.10
3	3	49	LEU	N-CA-C	-13.38	96.57	113.43
12	2	69	ASN	N-CA-CB	13.29	129.82	110.16
3	3	49	LEU	N-CA-CB	-13.17	88.13	110.51
12	2	463	GLU	CG-CD-OE2	12.93	148.14	118.40
6	9	217	GLU	CG-CD-OE1	12.79	147.81	118.40
1	5	5	ARG	CG-CD-NE	-12.68	84.11	112.00
6	9	217	GLU	CA-CB-CG	12.52	139.13	114.10
6	9	217	GLU	OE1-CD-OE2	-12.50	92.91	122.90
6	9	209	MET	CB-CA-C	12.45	131.01	110.22
3	3	64	ARG	N-CA-C	12.37	128.43	110.24
3	3	49	LEU	CB-CA-C	12.32	130.34	109.65
3	3	64	ARG	CG-CD-NE	12.31	139.09	112.00
1	5	3	ARG	CD-NE-CZ	12.26	141.56	124.40
1	5	5	ARG	NE-CZ-NH2	12.06	130.05	119.20
12	2	97	MET	CA-CB-CG	-12.02	90.05	114.10
1	5	3	ARG	N-CA-CB	10.93	130.77	111.00
6	9	209	MET	N-CA-CB	-10.59	92.38	110.17
12	2	463	GLU	CB-CG-CD	10.46	130.38	112.60
6	9	199	GLN	OE1-CD-NE2	-9.79	112.81	122.60
6	9	217	GLU	N-CA-CB	9.62	127.24	111.27
12	2	490	LYS	N-CA-CB	-9.45	94.18	111.37
12	2	464	THR	OG1-CB-CG2	-8.96	91.39	109.30
6	9	217	GLU	CG-CD-OE2	-8.85	98.04	118.40
12	2	490	LYS	CA-CB-CG	8.80	131.70	114.10
12	2	506	LYS	N-CA-CB	-8.77	96.11	110.40
8	T	61	DA	OP2-P-O3'	8.61	133.84	108.00
8	T	61	DA	O3'-P-O5'	-8.41	91.38	104.00
1	5	5	ARG	CD-NE-CZ	7.97	135.56	124.40
1	5	5	ARG	CB-CG-CD	7.86	129.38	111.30
1	5	3	ARG	CB-CA-C	-7.69	94.12	109.35
8	T	44	DC	P-O3'-C3'	7.65	131.67	120.20
6	9	209	MET	CG-SD-CE	-7.62	84.13	100.90
6	9	199	GLN	CG-CD-NE2	-7.60	104.99	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	537	MET	CG-SD-CE	7.56	117.53	100.90
3	3	49	LEU	CD1-CG-CD2	-7.28	94.78	110.80
8	T	44	DC	O3'-P-O5'	7.27	114.90	104.00
12	2	506	LYS	CD-CE-NZ	-7.24	88.73	111.90
3	3	64	ARG	N-CA-CB	7.23	120.69	109.48
6	9	209	MET	CB-CG-SD	7.22	134.35	112.70
2	0	619	THR	CA-CB-CG2	7.12	122.60	110.50
11	1	197	GLU	CG-CD-OE1	-7.08	102.12	118.40
6	9	200	MET	CB-CA-C	-7.01	97.21	110.67
12	2	490	LYS	CD-CE-NZ	-6.94	89.69	111.90
6	9	216	GLU	CA-C-N	6.91	133.06	122.08
6	9	216	GLU	C-N-CA	6.91	133.06	122.08
3	3	85	ARG	CG-CD-NE	6.90	127.19	112.00
12	2	506	LYS	CA-CB-CG	6.75	127.60	114.10
7	N	-45	DA	O3'-P-O5'	6.73	114.10	104.00
12	2	69	ASN	CB-CA-C	-6.53	99.75	110.85
12	2	65	TRP	N-CA-C	6.53	120.98	112.89
11	1	213	ARG	CA-C-N	6.42	124.28	120.24
11	1	213	ARG	C-N-CA	6.42	124.28	120.24
2	0	447	LYS	CA-C-O	-6.33	112.20	118.34
12	2	506	LYS	CB-CA-C	-6.29	96.84	109.99
2	0	557	MET	CB-CG-SD	6.27	131.51	112.70
6	9	199	GLN	CB-CA-C	-6.26	97.97	110.42
1	5	5	ARG	N-CA-CB	-6.25	99.69	111.00
6	9	199	GLN	CG-CD-OE1	6.24	133.28	120.80
12	2	489	LYS	CA-C-N	6.12	132.16	122.62
12	2	489	LYS	C-N-CA	6.12	132.16	122.62
11	1	197	GLU	CG-CD-OE2	6.10	132.42	118.40
4	7	114	ARG	CA-CB-CG	6.05	126.19	114.10
12	2	97	MET	N-CA-CB	-6.02	101.17	110.56
3	3	64	ARG	CB-CA-C	-5.98	100.86	109.84
12	2	138	TYR	CZ-CE2-CD2	5.92	130.26	119.60
7	N	-45	DA	OP1-P-O3'	-5.88	90.35	108.00
3	3	64	ARG	CA-CB-CG	5.88	125.85	114.10
12	2	96	LEU	CA-C-N	5.85	133.39	122.74
12	2	96	LEU	C-N-CA	5.85	133.39	122.74
12	2	66	VAL	N-CA-C	5.82	117.08	108.65
2	0	451	GLU	CG-CD-OE1	-5.78	105.10	118.40
12	2	463	GLU	CA-C-N	-5.78	112.43	122.37
12	2	463	GLU	C-N-CA	-5.78	112.43	122.37
7	N	-43	DA	O4'-C1'-C2'	-5.77	97.75	106.40
8	T	61	DA	OP1-P-O3'	-5.66	91.03	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2	ALA	CA-C-N	-5.64	113.59	122.73
1	5	2	ALA	C-N-CA	-5.64	113.59	122.73
11	1	229	GLY	N-CA-C	5.59	123.74	112.34
6	9	217	GLU	CB-CG-CD	-5.41	103.41	112.60
3	3	49	LEU	CB-CG-CD1	-5.35	94.64	110.70
2	0	619	THR	OG1-CB-CG2	-5.21	98.89	109.30
3	3	26	VAL	N-CA-C	-5.19	107.29	111.91
12	2	62	LEU	CA-C-N	-5.11	113.14	122.38
12	2	62	LEU	C-N-CA	-5.11	113.14	122.38
12	2	66	VAL	CA-CB-CG2	5.10	119.07	110.40
12	2	463	GLU	N-CA-C	5.09	121.64	110.80
7	N	-42	DT	C4-C5-C7	-5.07	114.80	122.40
12	2	97	MET	CB-CA-C	5.02	118.08	109.80
12	2	253	MET	CB-CG-SD	-5.01	97.68	112.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	9	199	GLN	CA

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	553	MET	Mainchain
11	1	193	LYS	Mainchain
12	2	182	PHE	Peptide
12	2	257	GLY	Peptide
12	2	449	ASP	Peptide
12	2	463	GLU	Sidechain
12	2	507	ARG	Sidechain
3	3	64	ARG	Sidechain
3	3	89	PHE	Sidechain
9	4	68	ASN	Peptide
1	5	3	ARG	Sidechain
1	5	5	ARG	Sidechain
4	7	231	ARG	Peptide
4	7	387	PRO	Peptide
4	7	541	MET	Mainchain
4	7	584	ASN	Peptide
5	8	775	TYR	Sidechain
6	9	199	GLN	Sidechain
6	9	217	GLU	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	5	514	0	541	20	0
2	0	6091	0	6155	78	0
3	3	1089	0	1069	10	0
4	7	4881	0	4868	63	0
5	8	134	0	141	2	0
6	9	542	0	537	6	0
7	N	534	0	298	11	0
8	T	532	0	294	10	0
9	4	2274	0	2332	20	0
10	6	2946	0	2958	30	0
11	1	3374	0	3425	25	0
12	2	3597	0	3687	67	0
13	0	8	0	0	0	0
14	3	2	0	0	0	0
14	4	1	0	0	0	0
14	6	4	0	0	0	0
All	All	26523	0	26305	321	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (321) 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)
12:2:506:LYS:NZ	12:2:506:LYS:CE	1.68	1.57
1:5:7:GLY:HA3	1:5:41:LEU:HD11	1.42	1.02
12:2:506:LYS:NZ	12:2:506:LYS:CD	2.24	0.98
2:0:544:TYR:H	11:1:358:MET:HE1	1.32	0.92
7:N:-62:DG:N2	8:T:62:DC:O2	2.06	0.87
12:2:261:GLN:HG2	12:2:263:HIS:H	1.41	0.85
12:2:253:MET:HE2	12:2:258:LEU:HD23	1.58	0.83
2:0:104:ARG:NH2	2:0:202:LEU:O	2.14	0.80
1:5:9:LEU:HB3	12:2:454:TYR:HB2	1.63	0.78
4:7:239:ALA:HA	4:7:313:VAL:HG21	1.65	0.78
4:7:349:ASN:HD22	4:7:481:GLU:HG2	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:6:352:CYS:HB3	10:6:366:CYS:SG	2.24	0.77
2:0:536:GLY:O	2:0:537:MET:HE2	1.86	0.76
10:6:399:ARG:NH2	10:6:435:GLU:OE1	2.20	0.75
8:T:61:DA:H1'	8:T:62:DC:H5'	1.68	0.75
12:2:506:LYS:NZ	12:2:506:LYS:HG3	2.00	0.74
4:7:224:LYS:HD3	4:7:338:LEU:O	1.90	0.72
2:0:125:LYS:NZ	2:0:127:THR:OG1	2.21	0.71
1:5:30:ILE:HD11	1:5:50:VAL:HG12	1.72	0.71
1:5:5:ARG:NH2	1:5:33:GLU:OE2	2.26	0.69
12:2:506:LYS:CD	12:2:506:LYS:HZ2	2.06	0.68
4:7:619:ALA:HA	4:7:622:MET:HE2	1.75	0.68
2:0:533:THR:HG21	2:0:537:MET:HE3	1.76	0.67
2:0:554:TRP:HA	2:0:557:MET:SD	2.34	0.67
3:3:31:ASN:HD22	3:3:63:LEU:HD12	1.60	0.67
4:7:711:LYS:HA	4:7:716:MET:HE3	1.76	0.67
3:3:54:CYS:HB3	3:3:59:CYS:SG	2.34	0.67
12:2:155:LEU:HD12	12:2:157:LYS:H	1.60	0.66
2:0:537:MET:HE1	2:0:619:THR:N	2.10	0.66
10:6:399:ARG:NH2	10:6:434:GLN:HA	2.10	0.66
4:7:719:SER:O	4:7:722:ARG:N	2.29	0.65
6:9:236:TRP:CE2	6:9:240:LYS:HE3	2.32	0.65
2:0:418:LEU:HD13	2:0:435:MET:HE1	1.78	0.65
2:0:676:TYR:HB3	2:0:724:MET:HE3	1.79	0.65
10:6:352:CYS:CB	10:6:366:CYS:SG	2.84	0.65
2:0:550:ILE:HA	2:0:553:MET:HE3	1.80	0.64
12:2:480:VAL:HG11	12:2:497:GLY:HA3	1.78	0.64
4:7:181:TYR:CZ	4:7:336:PRO:HB2	2.33	0.63
2:0:507:SER:OG	2:0:685:ARG:NH2	2.32	0.63
2:0:494:PRO:O	2:0:495:MET:HE2	1.97	0.62
9:4:262:ILE:HA	12:2:66:VAL:HG12	1.81	0.62
2:0:537:MET:HE1	2:0:619:THR:H	1.64	0.62
4:7:242:LEU:HB2	4:7:313:VAL:HB	1.82	0.62
11:1:209:PHE:O	11:1:213:ARG:NH2	2.33	0.62
1:5:36:ASP:HB2	1:5:39:HIS:HB2	1.81	0.61
9:4:271:ASP:OD1	9:4:272:PHE:N	2.34	0.61
12:2:443:LEU:O	12:2:447:GLU:HG2	2.00	0.61
4:7:243:GLN:HE21	4:7:244:MET:HE3	1.66	0.61
2:0:539:VAL:HG12	2:0:621:LEU:HB2	1.82	0.61
7:N:-58:DT:O2	8:T:59:DG:N2	2.34	0.60
4:7:742:MET:HE3	4:7:742:MET:O	2.01	0.60
9:4:255:ASP:HB3	9:4:258:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:172:LEU:HD13	12:2:188:GLY:HA2	1.84	0.60
12:2:444:TRP:HA	12:2:448:LEU:HD23	1.84	0.60
4:7:126:ASP:O	4:7:130:ARG:NH1	2.35	0.60
2:0:464:SER:OG	2:0:659:MET:HE1	2.02	0.60
4:7:181:TYR:O	4:7:184:VAL:HG12	2.01	0.60
9:4:264:LYS:O	11:1:510:ASN:ND2	2.35	0.60
12:2:506:LYS:NZ	12:2:506:LYS:CG	2.64	0.60
7:N:-60:DA:N6	8:T:59:DG:O6	2.36	0.59
9:4:109:ILE:HG21	11:1:484:LEU:HD13	1.84	0.59
2:0:135:ARG:NH1	2:0:391:THR:O	2.35	0.59
12:2:32:CYS:SG	12:2:107:SER:OG	2.47	0.59
12:2:51:VAL:O	12:2:109:ARG:NH2	2.36	0.59
12:2:503:ASP:O	12:2:506:LYS:HB3	2.03	0.59
2:0:577:GLN:HE21	11:1:330:LEU:HD11	1.68	0.59
12:2:117:VAL:HG12	12:2:120:SER:H	1.68	0.58
12:2:195:GLU:OE2	12:2:196:ILE:HG22	2.02	0.58
10:6:403:CYS:SG	10:6:437:CYS:HB3	2.43	0.58
2:0:252:LEU:HB2	2:0:435:MET:HB3	1.85	0.58
4:7:134:ILE:HG22	4:7:141:ILE:HG12	1.85	0.58
12:2:36:TYR:HA	12:2:39:LEU:HD13	1.86	0.57
1:5:38:THR:HG23	1:5:39:HIS:CD2	2.39	0.57
12:2:51:VAL:HG21	12:2:108:LEU:HD22	1.85	0.57
3:3:85:ARG:HD2	3:3:89:PHE:CZ	2.40	0.57
4:7:227:ILE:O	4:7:508:HIS:NE2	2.37	0.57
2:0:541:PHE:HB2	2:0:547:MET:HE2	1.86	0.57
11:1:466:ASN:HA	11:1:469:MET:HE3	1.86	0.57
1:5:9:LEU:HD23	12:2:454:TYR:HD2	1.70	0.57
10:6:124:ARG:NH1	10:6:305:VAL:O	2.38	0.56
2:0:334:PHE:O	2:0:338:LEU:HD23	2.04	0.56
2:0:642:MET:HE1	2:0:646:TYR:CD2	2.41	0.56
7:N:-44:DG:H2"	7:N:-43:DA:C8	2.40	0.56
2:0:509:ARG:NH1	2:0:511:GLU:OE2	2.39	0.56
4:7:466:ARG:NH2	4:7:471:GLN:OE1	2.34	0.56
9:4:196:ILE:HG22	9:4:197:MET:HE2	1.87	0.56
3:3:114:GLU:HA	3:3:117:ILE:HG22	1.88	0.56
10:6:234:ILE:HG23	10:6:263:VAL:HG23	1.87	0.55
4:7:641:GLN:NE2	4:7:645:TYR:HE2	2.04	0.55
10:6:322:MET:HE1	10:6:369:MET:HG3	1.88	0.55
2:0:167:VAL:CG2	2:0:199:MET:HE1	2.36	0.55
3:3:84:ILE:HG23	3:3:120:LEU:HD23	1.88	0.55
2:0:493:LEU:HG	2:0:495:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:603:ARG:NH2	2:0:657:ASP:OD2	2.38	0.55
12:2:22:GLN:HE21	12:2:26:TYR:HE1	1.54	0.55
12:2:372:ASN:HB3	12:2:373:MET:HE2	1.88	0.55
12:2:506:LYS:NZ	12:2:506:LYS:HD2	2.19	0.55
4:7:154:GLN:O	4:7:158:VAL:HG23	2.07	0.55
4:7:626:PHE:HE2	4:7:628:TYR:HE1	1.54	0.55
8:T:62:DC:H2"	8:T:63:DT:C5	2.42	0.55
2:0:550:ILE:HD13	2:0:553:MET:HE1	1.89	0.54
12:2:405:HIS:HD1	12:2:407:GLN:H	1.54	0.54
12:2:138:TYR:HE2	12:2:260:PHE:CD1	2.24	0.54
11:1:363:ASP:OD1	11:1:367:ASN:N	2.40	0.54
9:4:221:SER:OG	9:4:224:LEU:HD23	2.07	0.54
1:5:16:ILE:HA	1:5:19:LEU:HD12	1.90	0.54
1:5:31:VAL:HG22	1:5:42:VAL:HG12	1.89	0.54
1:5:46:LYS:O	1:5:50:VAL:HG13	2.08	0.54
10:6:129:THR:HG22	10:6:174:MET:HE1	1.90	0.53
9:4:303:ASN:ND2	9:4:314:GLU:OE2	2.38	0.53
12:2:22:GLN:HG3	12:2:26:TYR:CZ	2.44	0.53
2:0:210:TYR:OH	2:0:235:ASP:O	2.27	0.53
9:4:299:ILE:HD12	9:4:300:PRO:HD2	1.90	0.53
2:0:676:TYR:HB3	2:0:724:MET:CE	2.37	0.53
10:6:325:PRO:HG3	10:6:359:LEU:HD21	1.90	0.53
2:0:577:GLN:NE2	11:1:330:LEU:HD11	2.23	0.53
4:7:462:ASN:ND2	4:7:465:ASN:OD1	2.34	0.52
7:N:-43:DA:H2"	7:N:-42:DT:C7	2.38	0.52
10:6:322:MET:HE1	10:6:369:MET:HB3	1.91	0.52
4:7:598:HIS:CD2	4:7:605:ILE:HD11	2.44	0.52
12:2:488:LYS:HD2	12:2:490:LYS:HE3	1.91	0.52
2:0:132:LYS:O	2:0:136:MET:HE3	2.10	0.52
4:7:122:ARG:NH1	4:7:123:LEU:O	2.42	0.52
4:7:224:LYS:HG2	4:7:337:VAL:HG23	1.92	0.52
6:9:209:MET:HE3	6:9:227:LEU:CD2	2.40	0.52
2:0:141:ALA:HB1	2:0:153:VAL:HG21	1.92	0.51
12:2:62:LEU:HA	12:2:65:TRP:HD1	1.75	0.51
7:N:-66:DA:C8	7:N:-65:DT:H72	2.45	0.51
10:6:214:LEU:CD1	10:6:250:THR:HG21	2.40	0.51
11:1:587:LYS:HA	11:1:590:ILE:HG22	1.91	0.51
9:4:176:LEU:HB2	9:4:210:ILE:HG22	1.92	0.51
4:7:553:GLN:NE2	4:7:554:CYS:O	2.44	0.51
11:1:357:THR:O	11:1:358:MET:HE2	2.10	0.51
2:0:625:ILE:HD12	2:0:627:PHE:CE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:519:ARG:HG2	4:7:520:GLU:H	1.76	0.51
4:7:400:ALA:HA	4:7:403:ILE:HG22	1.92	0.51
10:6:322:MET:HE2	10:6:322:MET:HA	1.93	0.51
5:8:775:TYR:HA	6:9:187:THR:HG22	1.92	0.50
9:4:289:CYS:HB3	9:4:292:CYS:SG	2.51	0.50
11:1:336:ILE:HG23	11:1:337:ILE:HG23	1.93	0.50
2:0:399:LEU:HD13	2:0:402:ILE:HD11	1.92	0.50
11:1:498:LYS:O	11:1:502:ARG:NE	2.40	0.50
1:5:17:LYS:HG3	1:5:40:LEU:HD21	1.94	0.50
2:0:102:ASP:OD1	2:0:173:LYS:HE2	2.10	0.50
10:6:129:THR:HG23	10:6:172:ILE:HG23	1.93	0.50
12:2:354:PRO:HA	12:2:357:ILE:HB	1.94	0.50
3:3:85:ARG:HE	3:3:117:ILE:HD13	1.77	0.50
2:0:198:ARG:C	2:0:199:MET:HE2	2.36	0.50
4:7:113:PHE:CE1	12:2:368:ALA:HA	2.46	0.50
4:7:224:LYS:HE3	4:7:340:GLU:O	2.11	0.50
12:2:138:TYR:CE2	12:2:260:PHE:CD1	2.99	0.50
4:7:331:GLN:HG3	4:7:529:PHE:HA	1.94	0.50
6:9:236:TRP:CZ2	6:9:240:LYS:HE3	2.47	0.50
12:2:204:LEU:O	12:2:208:LEU:HD23	2.12	0.50
2:0:220:GLU:O	2:0:224:ASN:ND2	2.45	0.49
7:N:-57:DT:H2''	7:N:-56:DT:H5''	1.93	0.49
2:0:27:ASP:OD2	2:0:483:TYR:OH	2.30	0.49
10:6:147:ALA:HA	10:6:200:ARG:HH12	1.77	0.49
12:2:124:VAL:HG22	12:2:126:GLU:H	1.77	0.49
1:5:7:GLY:HA3	1:5:41:LEU:CD1	2.30	0.49
2:0:108:LEU:HB2	2:0:208:TYR:HB3	1.95	0.49
2:0:711:ASP:N	2:0:711:ASP:OD1	2.45	0.49
2:0:570:LEU:HB2	2:0:598:LEU:HD23	1.95	0.48
7:N:-58:DT:H1'	7:N:-57:DT:H5'	1.95	0.48
9:4:206:MET:HE3	9:4:206:MET:HA	1.96	0.48
4:7:121:LEU:HD13	4:7:204:PRO:HG2	1.96	0.48
2:0:244:CYS:SG	2:0:245:ILE:N	2.87	0.48
2:0:104:ARG:NE	2:0:203:CYS:HA	2.29	0.48
4:7:341:TYR:CZ	4:7:343:PHE:HB2	2.47	0.48
4:7:493:VAL:O	4:7:495:ALA:N	2.46	0.48
12:2:43:ALA:O	12:2:47:ILE:HG12	2.14	0.48
12:2:493:ILE:HD13	12:2:501:VAL:HG21	1.96	0.47
12:2:423:ASP:N	12:2:423:ASP:OD1	2.47	0.47
9:4:37:TRP:HB3	11:1:472:GLN:HE22	1.79	0.47
12:2:39:LEU:O	12:2:44:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:251:ASP:OD1	2:0:436:ARG:HG3	2.14	0.47
4:7:605:ILE:HG12	4:7:669:CYS:HB3	1.97	0.47
12:2:50:MET:HG3	12:2:100:LEU:HD13	1.95	0.47
12:2:62:LEU:O	12:2:65:TRP:HB2	2.15	0.47
2:0:1:MET:SD	2:0:15:PRO:HA	2.54	0.47
4:7:622:MET:HE1	4:7:653:PHE:CG	2.50	0.47
4:7:720:THR:HA	4:7:723:GLN:NE2	2.29	0.47
9:4:109:ILE:CG2	11:1:484:LEU:HD13	2.45	0.47
12:2:368:ALA:HB3	12:2:375:LEU:HD21	1.97	0.47
2:0:68:LYS:HD2	2:0:204:ASN:HA	1.96	0.47
4:7:566:TYR:HA	4:7:569:TYR:HB3	1.96	0.47
2:0:277:VAL:HG23	2:0:278:ASP:OD1	2.15	0.47
4:7:438:PHE:HZ	4:7:470:SER:HB3	1.80	0.46
11:1:302:MET:SD	11:1:302:MET:N	2.88	0.46
12:2:123:VAL:HG13	12:2:238:LYS:HB3	1.97	0.46
2:0:544:TYR:N	11:1:358:MET:HE1	2.14	0.46
8:T:43:DT:H2"	8:T:44:DC:C6	2.50	0.46
12:2:506:LYS:HZ2	12:2:506:LYS:HD2	1.74	0.46
4:7:130:ARG:HD3	4:7:202:LYS:HA	1.97	0.46
4:7:626:PHE:HE2	4:7:628:TYR:CE1	2.31	0.46
9:4:146:ARG:NH1	10:6:457:LYS:O	2.48	0.46
1:5:30:ILE:HG23	1:5:31:VAL:HG23	1.96	0.46
8:T:42:DA:H2"	8:T:43:DT:C6	2.51	0.46
10:6:358:SER:C	10:6:359:LEU:HD12	2.41	0.46
2:0:550:ILE:HA	2:0:553:MET:CE	2.44	0.46
4:7:349:ASN:O	4:7:405:LYS:NZ	2.40	0.46
1:5:6:LYS:HB3	1:5:44:PRO:HG2	1.98	0.46
1:5:53:GLU:HB2	1:5:56:ARG:CZ	2.46	0.46
3:3:9:ASN:HB2	3:3:12:MET:HE3	1.98	0.46
4:7:612:VAL:HG11	4:7:628:TYR:CZ	2.51	0.46
2:0:523:GLY:O	2:0:527:VAL:HG23	2.16	0.45
7:N:-43:DA:H2"	7:N:-42:DT:C6	2.51	0.45
12:2:56:GLU:OE2	12:2:99:ASN:HB2	2.16	0.45
4:7:164:ILE:HD11	4:7:174:LYS:HE3	1.98	0.45
12:2:253:MET:HE3	12:2:256:TYR:HB2	1.98	0.45
12:2:338:SER:HB2	12:2:405:HIS:HB2	1.98	0.45
2:0:199:MET:HE2	2:0:199:MET:N	2.31	0.45
4:7:349:ASN:HD22	4:7:481:GLU:CG	2.22	0.45
8:T:60:DT:H2"	8:T:61:DA:H8	1.81	0.45
11:1:582:LEU:O	11:1:586:LEU:HD23	2.16	0.45
12:2:174:GLU:HG3	12:2:183:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:261:GLN:HG2	12:2:263:HIS:N	2.22	0.45
2:0:25:MET:HE1	2:0:51:SER:O	2.17	0.45
2:0:86:LEU:O	2:0:90:MET:HG2	2.16	0.45
2:0:553:MET:HB3	2:0:557:MET:HE1	1.98	0.45
4:7:457:TYR:OH	4:7:488:ASP:O	2.32	0.45
12:2:213:THR:O	12:2:216:MET:N	2.50	0.45
9:4:180:THR:OG1	9:4:181:CYS:N	2.48	0.45
12:2:455:GLU:C	12:2:495:LYS:HG3	2.41	0.45
4:7:121:LEU:HD13	4:7:204:PRO:HD2	1.99	0.44
4:7:162:GLU:N	4:7:174:LYS:O	2.49	0.44
3:3:119:LYS:O	3:3:123:GLY:N	2.51	0.44
4:7:228:LYS:HG3	4:7:233:PHE:H	1.81	0.44
4:7:410:LEU:HD11	4:7:485:ILE:HD11	1.98	0.44
4:7:711:LYS:HA	4:7:716:MET:CE	2.46	0.44
10:6:429:CYS:HB3	10:6:432:CYS:SG	2.56	0.44
11:1:270:TYR:OH	11:1:280:GLU:OE1	2.31	0.44
12:2:197:ASN:OD1	12:2:198:SER:N	2.50	0.44
12:2:125:VAL:HG22	12:2:238:LYS:HB2	2.00	0.44
2:0:195:ILE:O	2:0:199:MET:HE3	2.18	0.44
12:2:448:LEU:HD13	12:2:448:LEU:HA	1.89	0.44
12:2:90:ASN:OD1	12:2:97:MET:HB2	2.17	0.44
3:3:133:LEU:HD12	3:3:134:ARG:HG3	1.99	0.44
11:1:167:ASP:OD1	11:1:167:ASP:N	2.50	0.44
2:0:465:PRO:HG2	2:0:468:MET:HB2	1.99	0.44
7:N:-44:DG:H2"	7:N:-43:DA:H8	1.83	0.44
10:6:130:LEU:HB2	10:6:173:ILE:HG22	2.00	0.44
10:6:246:ASP:N	10:6:246:ASP:OD1	2.49	0.44
4:7:688:GLY:HA2	4:7:691:LEU:HG	2.00	0.44
2:0:260:ALA:HB2	2:0:398:ALA:HB3	2.00	0.43
4:7:477:LEU:HA	4:7:482:TRP:HE1	1.83	0.43
4:7:592:GLN:NE2	4:7:747:ASN:O	2.47	0.43
9:4:126:VAL:HA	9:4:129:ILE:HG22	2.00	0.43
2:0:564:TRP:HE1	11:1:232:ASN:HB2	1.84	0.43
4:7:373:MET:HE1	4:7:511:LEU:HD11	2.00	0.43
1:5:30:ILE:HD13	1:5:30:ILE:HG21	1.79	0.43
1:5:62:ILE:HG21	1:5:62:ILE:HD13	1.81	0.43
2:0:106:LEU:O	2:0:206:ILE:HD12	2.19	0.43
2:0:233:ILE:HG22	2:0:457:ILE:HB	2.01	0.43
12:2:408:MET:HG3	12:2:409:ARG:HD3	1.99	0.43
2:0:493:LEU:HB3	2:0:678:VAL:HG12	2.00	0.43
12:2:101:ASN:HD21	12:2:104:PHE:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:368:ALA:O	12:2:375:LEU:HD23	2.18	0.43
2:0:136:MET:HE2	2:0:136:MET:HB3	1.80	0.43
2:0:280:GLN:HA	2:0:283:GLN:HB3	2.01	0.43
2:0:4:TYR:CZ	2:0:9:PRO:HB3	2.54	0.42
2:0:549:SER:O	2:0:553:MET:HG3	2.19	0.42
4:7:677:TYR:O	4:7:722:ARG:NH2	2.52	0.42
12:2:30:ALA:O	12:2:33:LEU:HG	2.18	0.42
1:5:37:ASP:OD1	1:5:37:ASP:N	2.52	0.42
2:0:179:GLU:HA	2:0:182:LEU:HG	2.01	0.42
2:0:495:MET:N	2:0:679:MET:O	2.51	0.42
10:6:214:LEU:HD13	10:6:250:THR:HG21	2.00	0.42
12:2:30:ALA:HA	12:2:33:LEU:HD21	2.02	0.42
4:7:194:ILE:HD11	4:7:213:ILE:HG21	2.01	0.42
8:T:57:DA:H2''	8:T:58:DA:H2'	1.99	0.42
9:4:146:ARG:HD3	10:6:458:PRO:HA	2.01	0.42
11:1:205:PRO:HA	11:1:206:PRO:HD3	1.82	0.42
6:9:201:VAL:HG21	6:9:222:ILE:HD12	2.01	0.42
12:2:134:LEU:HD12	12:2:134:LEU:HA	1.69	0.42
12:2:184:ILE:HG22	12:2:185:THR:O	2.19	0.42
2:0:571:VAL:HG12	2:0:599:LEU:HB2	2.02	0.42
10:6:154:ILE:HD11	10:6:196:LEU:HD22	2.02	0.42
2:0:681:LEU:HD12	2:0:686:PHE:CE2	2.54	0.42
5:8:780:ILE:CG1	12:2:63:ASP:HB3	2.49	0.42
1:5:41:LEU:HA	1:5:41:LEU:HD12	1.55	0.41
2:0:5:ILE:HG22	2:0:6:ASP:H	1.85	0.41
2:0:521:ASN:O	2:0:525:MET:HG2	2.20	0.41
2:0:695:LYS:HA	2:0:698:ALA:HB3	2.01	0.41
2:0:538:VAL:HG12	2:0:598:LEU:HD12	2.02	0.41
10:6:297:LEU:HG	10:6:301:PHE:HE2	1.85	0.41
4:7:318:ILE:HD12	4:7:322:SER:HB3	2.02	0.41
2:0:533:THR:HA	2:0:534:PRO:HD3	1.96	0.41
4:7:495:ALA:O	4:7:499:ARG:N	2.53	0.41
9:4:264:LYS:HA	9:4:265:PRO:HD3	1.93	0.41
10:6:227:HIS:CD2	10:6:318:THR:HG21	2.56	0.41
3:3:97:ASP:OD1	3:3:97:ASP:N	2.53	0.41
10:6:365:CYS:HA	11:1:562:LYS:HD3	2.03	0.41
12:2:229:GLY:O	12:2:279:THR:OG1	2.27	0.41
2:0:642:MET:HE2	2:0:642:MET:HA	2.02	0.41
4:7:568:GLU:O	4:7:572:GLU:N	2.51	0.41
10:6:370:LEU:HD23	10:6:370:LEU:HA	1.93	0.41
11:1:233:VAL:HG12	11:1:258:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2:24:ARG:NH2	12:2:217:ASP:OD2	2.52	0.41
12:2:394:ASP:HA	12:2:397:ILE:HG12	2.03	0.41
1:5:51:LYS:O	1:5:54:LEU:HG	2.21	0.41
6:9:209:MET:HE3	6:9:227:LEU:HD22	2.02	0.41
8:T:58:DA:H4'	8:T:59:DG:H5'	2.03	0.41
2:0:550:ILE:HD13	2:0:553:MET:CE	2.51	0.40
4:7:676:HIS:O	4:7:722:ARG:NH2	2.48	0.40
9:4:234:VAL:HB	9:4:252:MET:HE1	2.03	0.40
4:7:622:MET:HE1	4:7:653:PHE:CD1	2.57	0.40
10:6:148:MET:HB2	10:6:148:MET:HE2	1.83	0.40
10:6:148:MET:N	10:6:148:MET:SD	2.94	0.40
11:1:587:LYS:O	11:1:590:ILE:HG22	2.21	0.40
2:0:18:TYR:HA	2:0:19:PRO:HD3	1.94	0.40
2:0:533:THR:HG21	2:0:537:MET:CE	2.47	0.40
4:7:354:ILE:HG22	4:7:430:LEU:HB2	2.03	0.40
7:N:-43:DA:H2''	7:N:-42:DT:C5	2.56	0.40
11:1:194:VAL:O	11:1:198:THR:OG1	2.35	0.40
12:2:438:VAL:HA	12:2:441:ILE:HG22	2.04	0.40
4:7:351:ASP:OD1	4:7:405:LYS:NZ	2.50	0.40
2:0:611:ASP:OD1	2:0:611:ASP:N	2.55	0.40
4:7:662:ILE:HG13	4:7:689:ARG:HH12	1.87	0.40
4:7:675:SER:OG	4:7:676:HIS:N	2.52	0.40
10:6:138:GLU:OE1	10:6:138:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	63/72 (88%)	62 (98%)	1 (2%)	0	100	100
2	0	750/778 (96%)	731 (98%)	19 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	129/321 (40%)	126 (98%)	3 (2%)	0	100	100
4	7	605/843 (72%)	572 (94%)	32 (5%)	1 (0%)	43	77
5	8	15/905 (2%)	12 (80%)	3 (20%)	0	100	100
6	9	66/244 (27%)	65 (98%)	1 (2%)	0	100	100
9	4	287/338 (85%)	281 (98%)	6 (2%)	0	100	100
10	6	368/461 (80%)	354 (96%)	14 (4%)	0	100	100
11	1	406/642 (63%)	389 (96%)	17 (4%)	0	100	100
12	2	435/513 (85%)	418 (96%)	13 (3%)	4 (1%)	14	49
All	All	3124/5117 (61%)	3010 (96%)	109 (4%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	7	313	VAL
12	2	68	SER
12	2	173	MET
12	2	463	GLU
12	2	235	LYS

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	5	59/66 (89%)	59 (100%)	0	100	100
2	0	684/707 (97%)	684 (100%)	0	100	100
3	3	125/303 (41%)	123 (98%)	2 (2%)	55	69
4	7	539/737 (73%)	539 (100%)	0	100	100
5	8	16/823 (2%)	16 (100%)	0	100	100
6	9	63/219 (29%)	62 (98%)	1 (2%)	55	69
9	4	260/300 (87%)	260 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	6	338/418 (81%)	338 (100%)	0	100	100
11	1	388/589 (66%)	388 (100%)	0	100	100
12	2	408/468 (87%)	406 (100%)	2 (0%)	81	81
All	All	2880/4630 (62%)	2875 (100%)	5 (0%)	85	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	49	LEU
3	3	64	ARG
6	9	199	GLN
12	2	464	THR
12	2	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	22	GLN
1	5	43	ASN
2	0	280	GLN
2	0	283	GLN
2	0	350	HIS
2	0	577	GLN
3	3	9	ASN
3	3	100	ASN
3	3	107	ASN
4	7	116	HIS
4	7	243	GLN
4	7	247	ASN
4	7	331	GLN
4	7	349	ASN
4	7	434	ASN
4	7	539	ASN
4	7	598	HIS
4	7	633	GLN
4	7	641	GLN
4	7	644	GLN
6	9	210	ASN
6	9	213	ASN
9	4	62	ASN

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Mol	Chain	Res	Type
9	4	145	GLN
10	6	114	ASN
10	6	146	HIS
10	6	339	HIS
11	1	258	ASN
11	1	273	ASN
11	1	277	ASN
11	1	417	ASN
11	1	425	ASN
11	1	500	ASN
11	1	513	GLN
11	1	567	HIS
11	1	621	ASN
11	1	638	ASN
12	2	8	HIS
12	2	69	ASN
12	2	251	GLN
12	2	261	GLN
12	2	352	ASN
12	2	356	GLN
12	2	500	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	SF4	0	801	2	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	0	801	2	-	-	0/6/5/5

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](#)

There are no chain breaks in this entry.

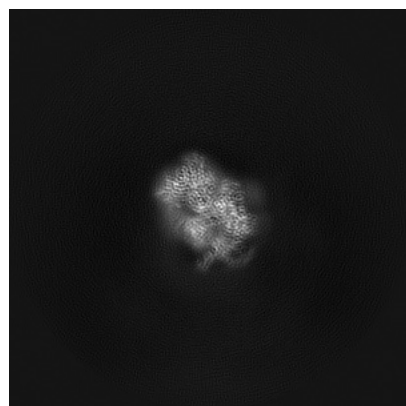
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71456. These allow visual inspection of the internal detail of the map and identification of artifacts.

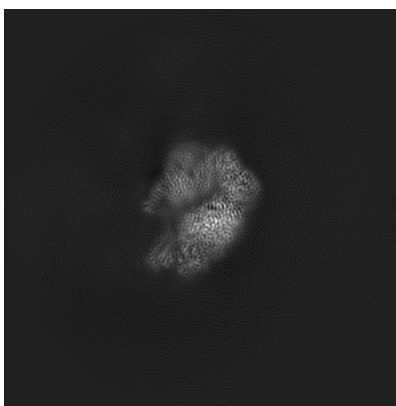
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

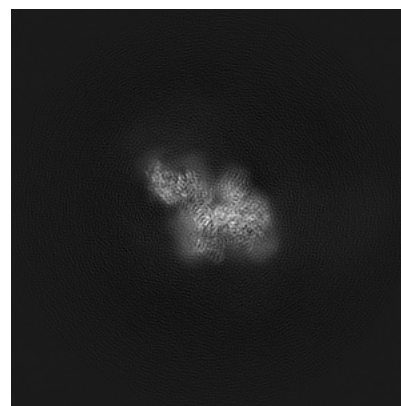
6.1.1 Primary map



X

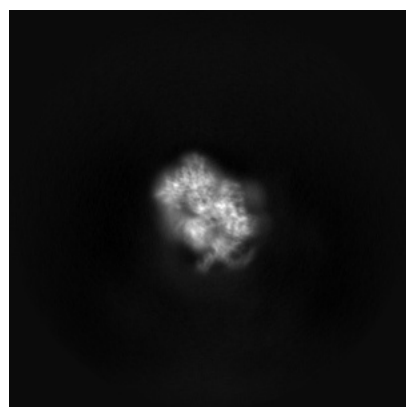


Y

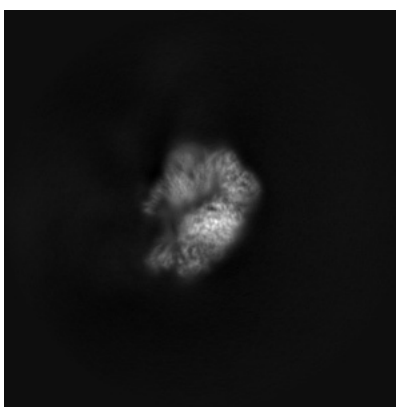


Z

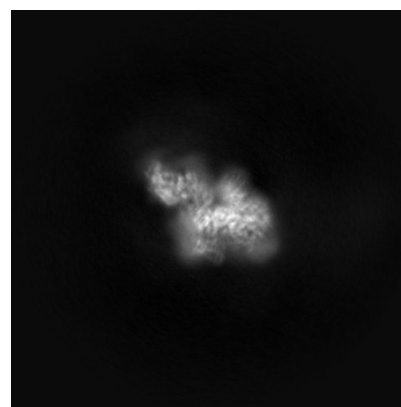
6.1.2 Raw map



X



Y

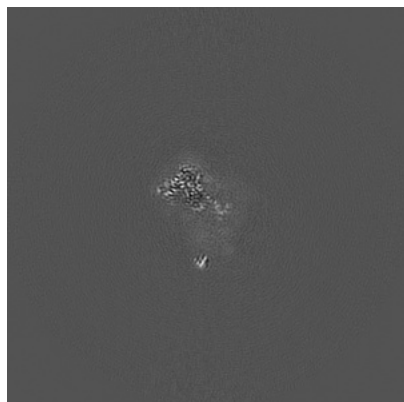


Z

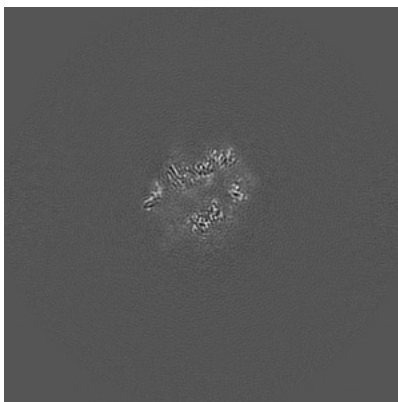
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

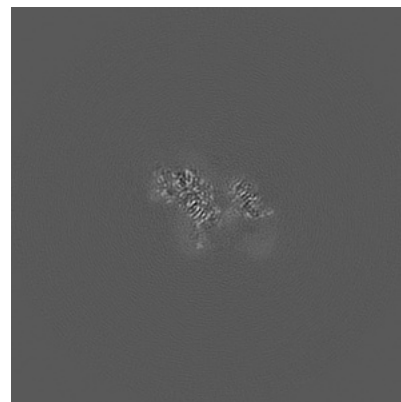
6.2.1 Primary map



X Index: 192

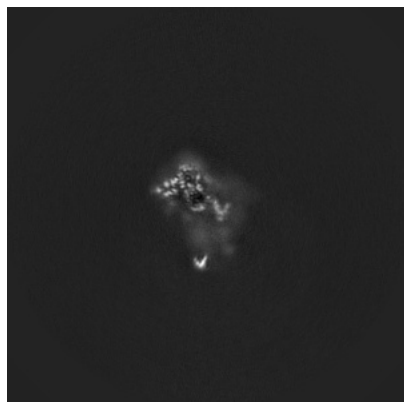


Y Index: 192

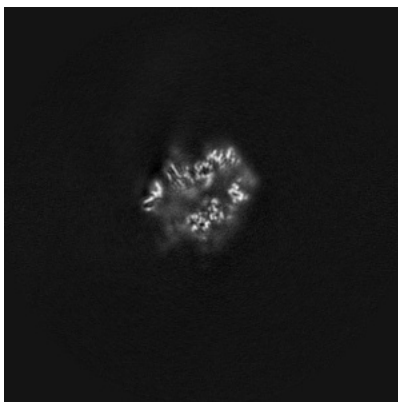


Z Index: 192

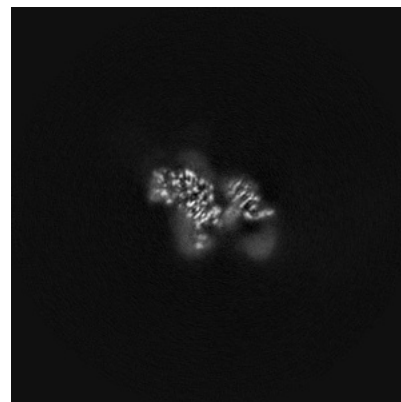
6.2.2 Raw map



X Index: 192



Y Index: 192

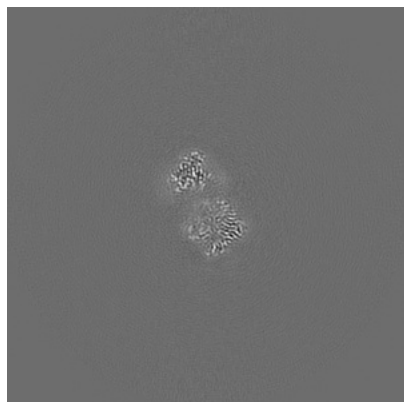


Z Index: 192

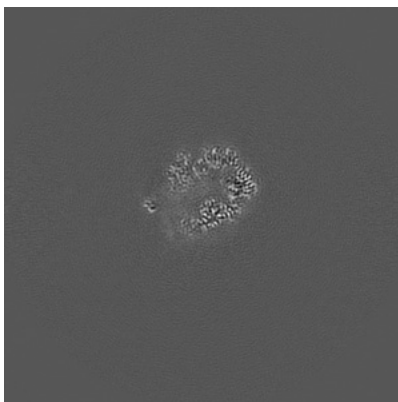
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

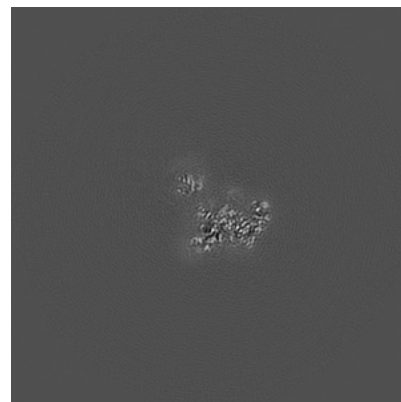
6.3.1 Primary map



X Index: 214

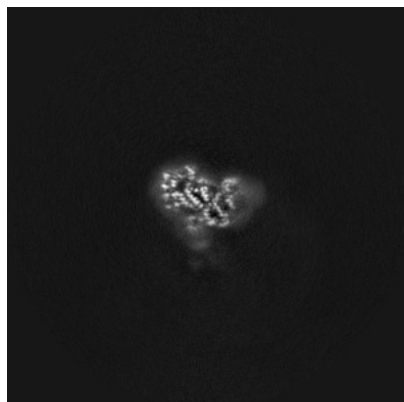


Y Index: 184

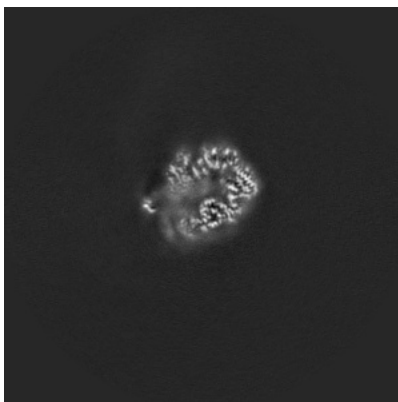


Z Index: 216

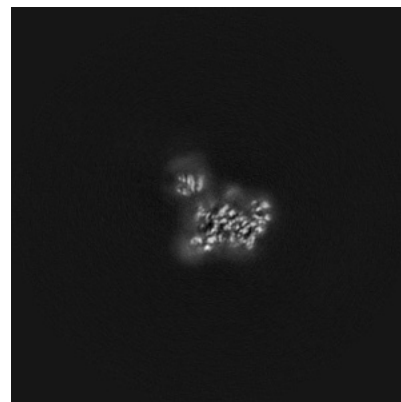
6.3.2 Raw map



X Index: 181



Y Index: 184

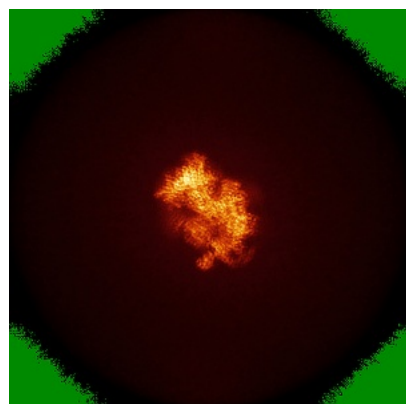


Z Index: 216

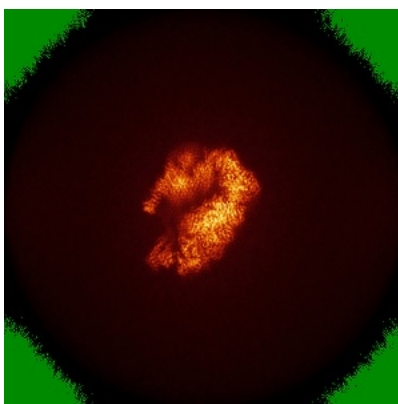
The images above show the largest variance slices of the map in three orthogonal directions.

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

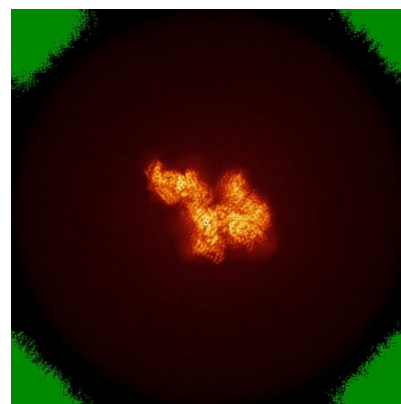
6.4.1 Primary map



X

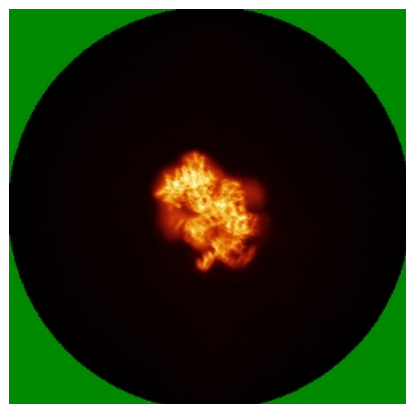


Y



Z

6.4.2 Raw map



X



Y

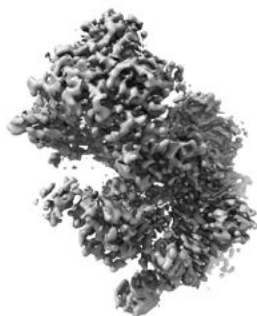


Z

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

6.5 Orthogonal surface views [i](#)

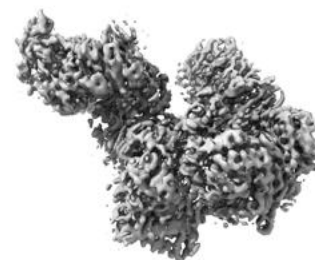
6.5.1 Primary map



X



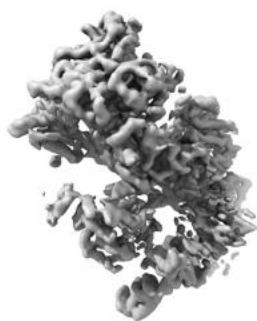
Y



Z

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

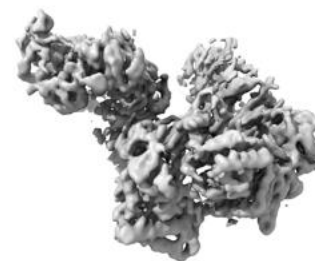
6.5.2 Raw map



X



Y



Z

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

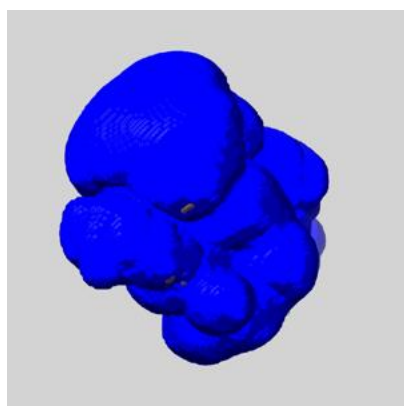
6.6 Mask visualisation [i](#)

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

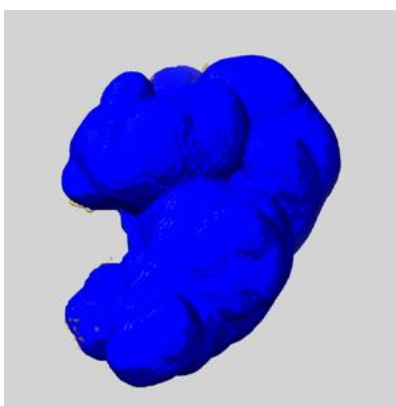
A mask typically either:

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

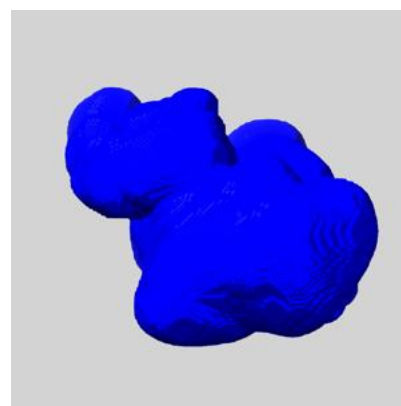
6.6.1 emd_71456_msk_1.map [i](#)



X



Y

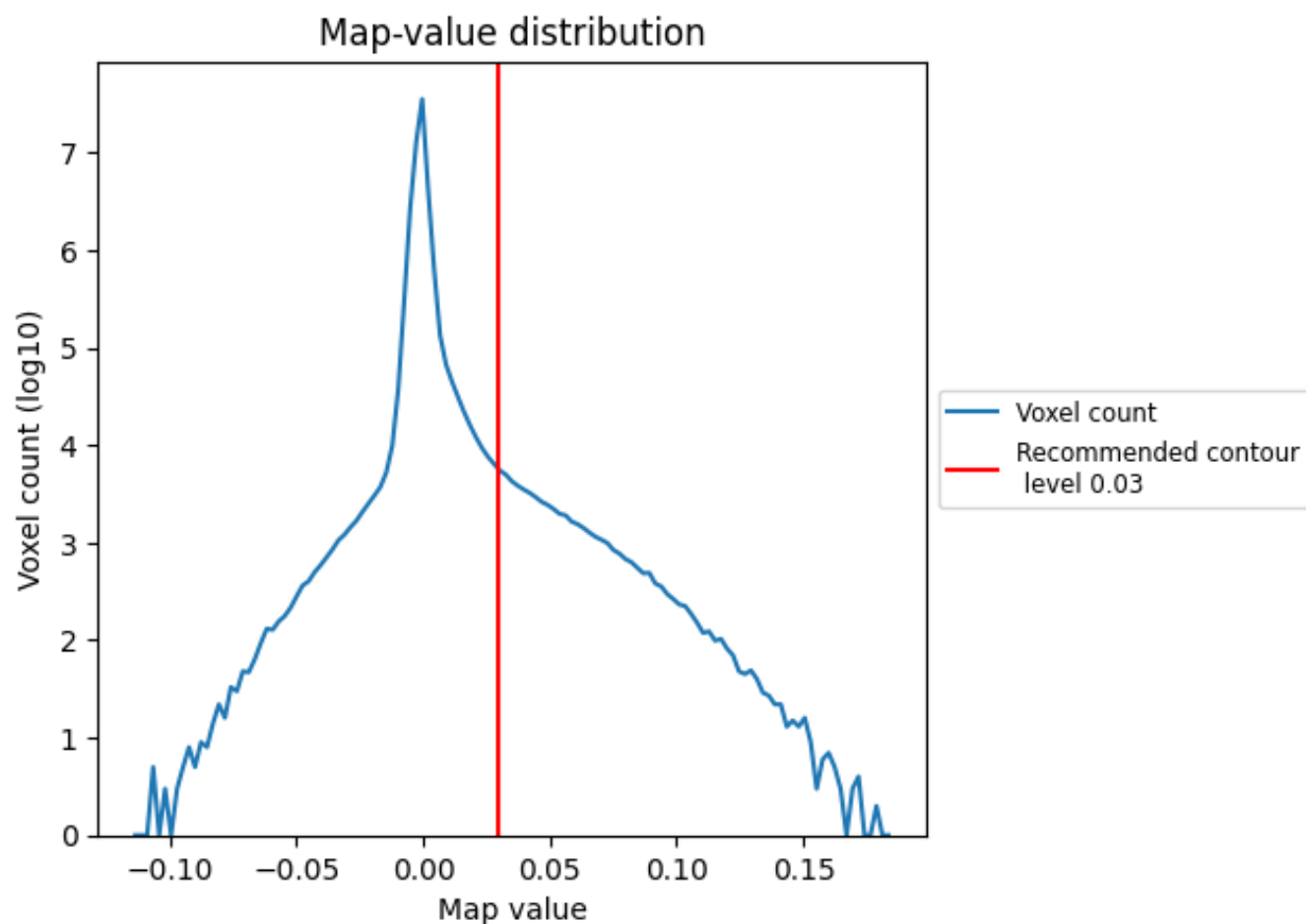


Z

7 Map analysis [i](#)

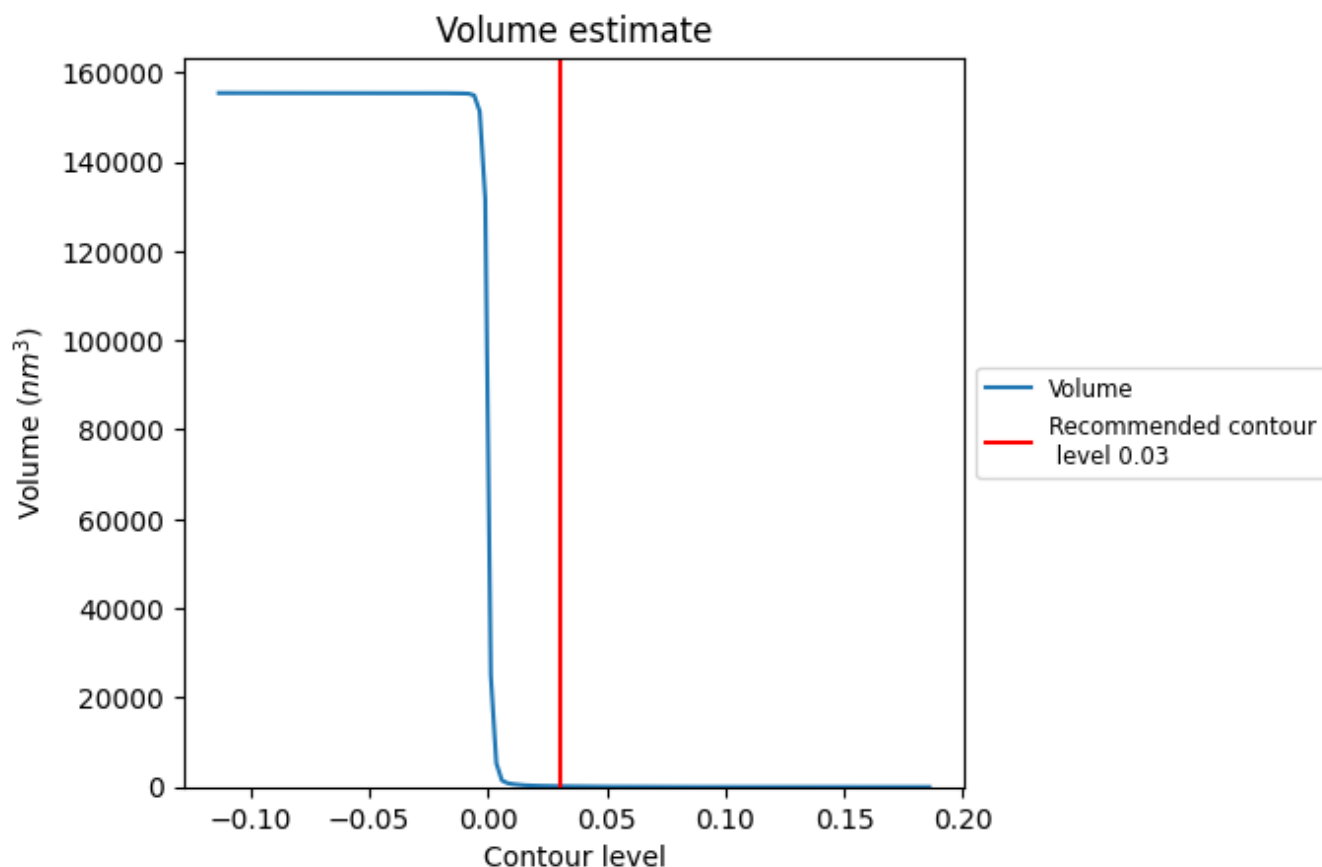
This section contains the results of statistical analysis of the map.

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.

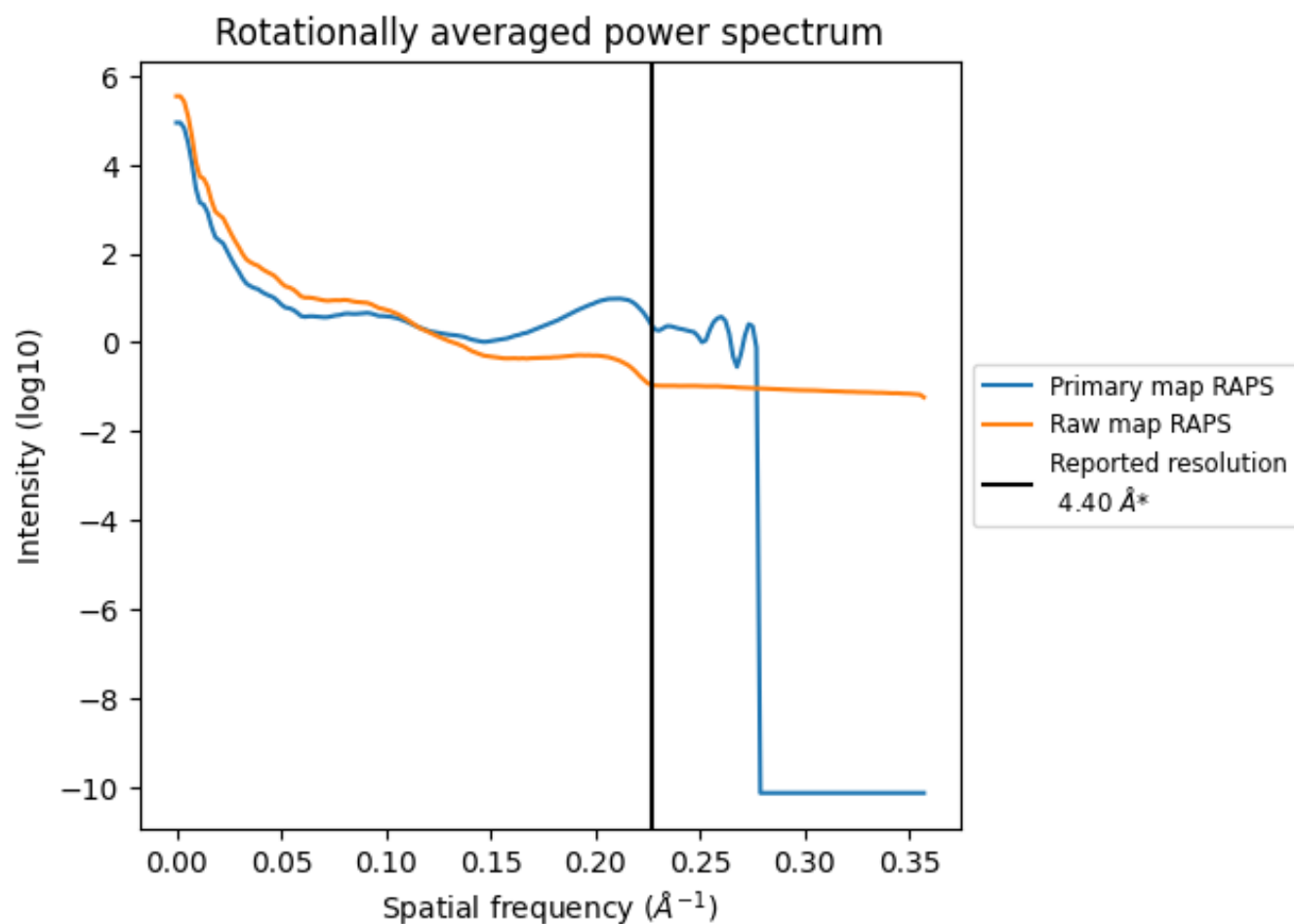
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm^3 ; this corresponds to an approximate mass of 141 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 ⓘ

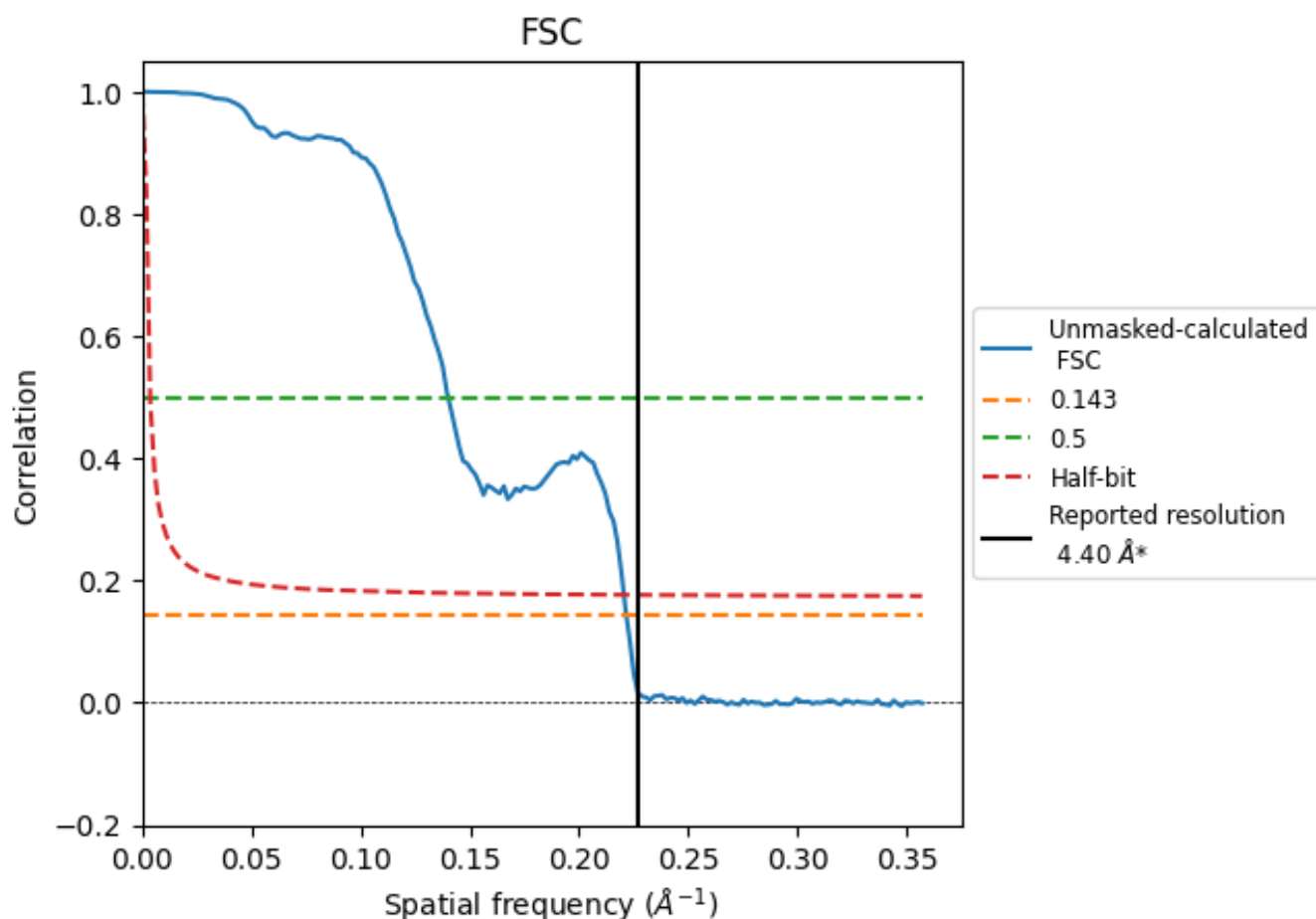


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

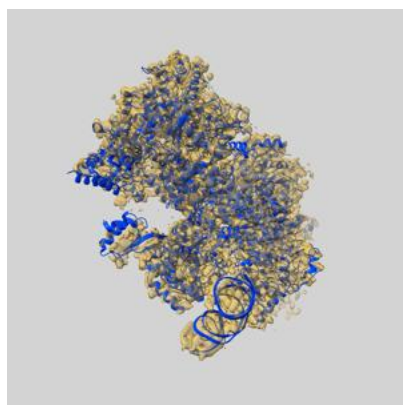
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.51	7.14	4.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

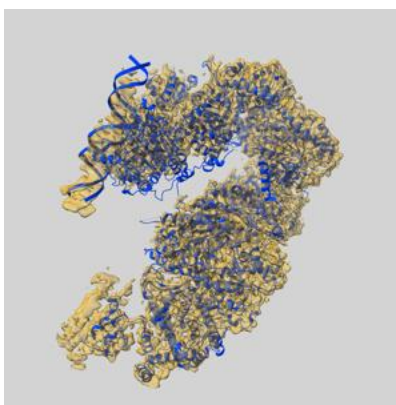
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71456 and PDB model 9PB7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

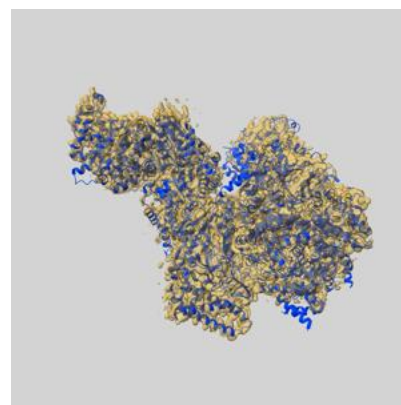
9.1 Map-model overlay [i](#)



X



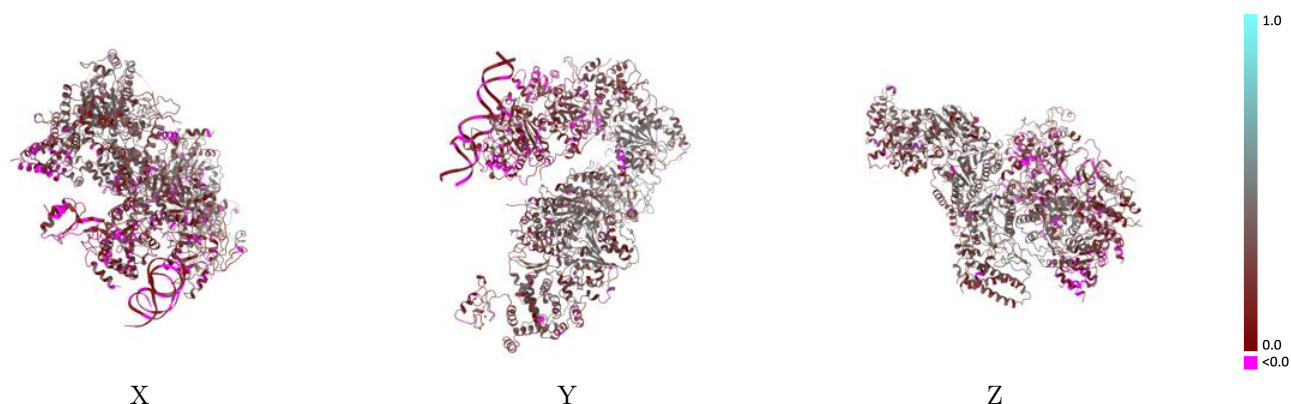
Y



Z

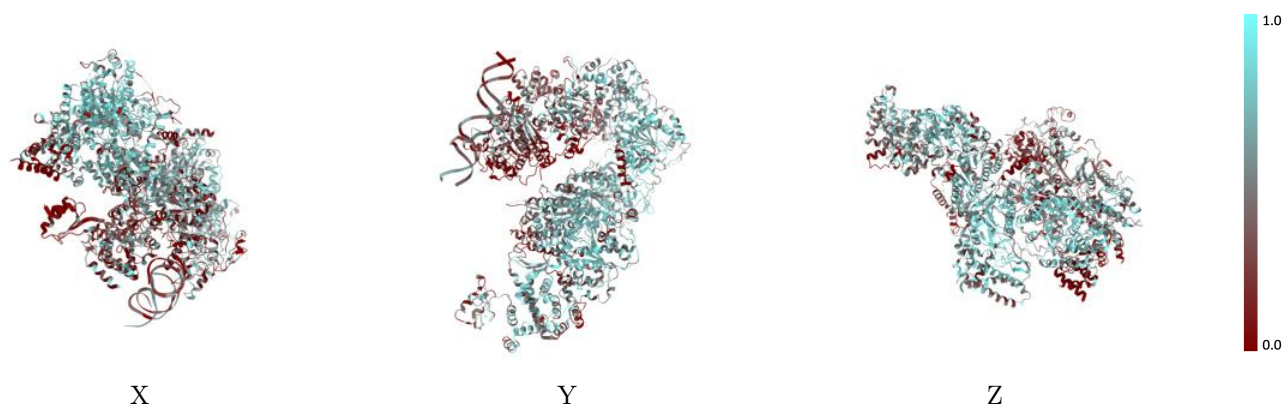
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



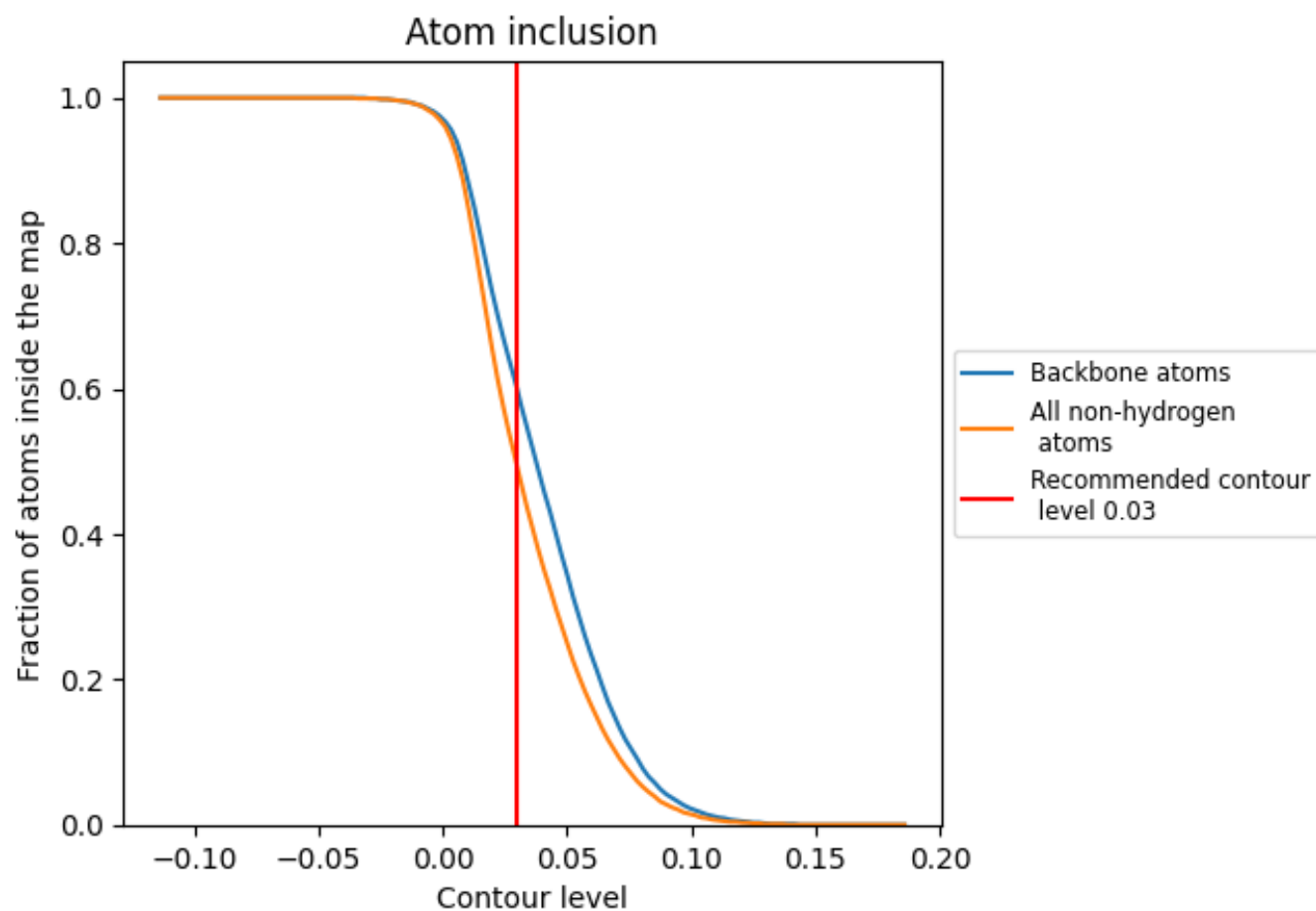
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4930	0.2640
0	0.6030	0.3340
1	0.4450	0.2850
2	0.4720	0.2140
3	0.5050	0.2440
4	0.7280	0.3970
5	0.3310	0.0700
6	0.6500	0.3600
7	0.3140	0.1860
8	0.0150	0.0170
9	0.0060	-0.0200
N	0.3670	0.0760
T	0.3290	0.0640

1.0

0.0

<0.0