



Full wwPDB EM Validation Report ⓘ

Sep 28, 2026 – 11:29 AM EDT

PDB ID : 9PBD / pdb_00009pbd
EMDB ID : EMD-71476
Title : PolII/TFIIF of PIC-Med-SWI/SNF
Authors : Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on : 2025-06-26
Resolution : 2.90 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:

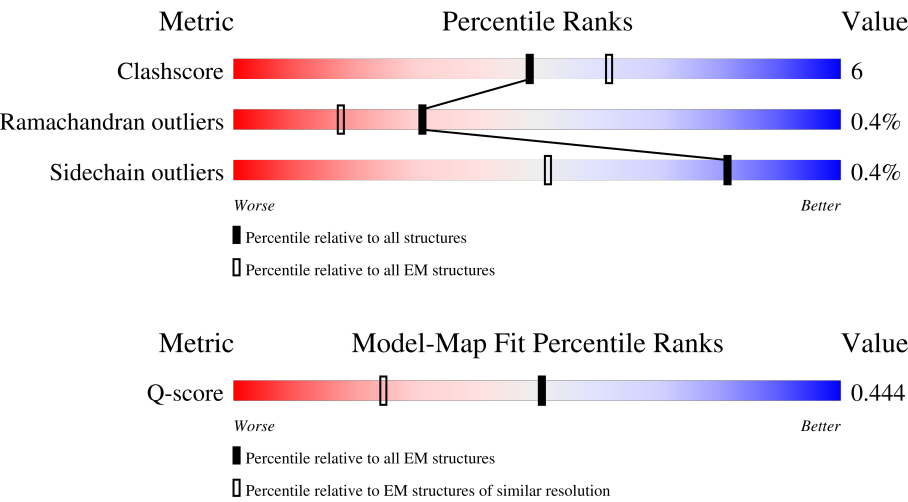
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	Q	735	
11	A	1733	
12	B	1224	
13	D	221	
14	R	400	
15	M	345	
16	H	146	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36670 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
			1301	812	230	251	8		

- Molecule 10 is a protein called Transcription initiation factor IIF subunit alpha.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB1.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	1161	Total	C	N	O	S	0	0
			9249	5848	1619	1726	56		

- 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 Transcription initiation factor IIF subunit beta.

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

- Molecule 15 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	96	Total	C	N	O	S	0	0
			714	447	122	136	9		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- 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	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	M	1	Total	Zn	0
			1	1	

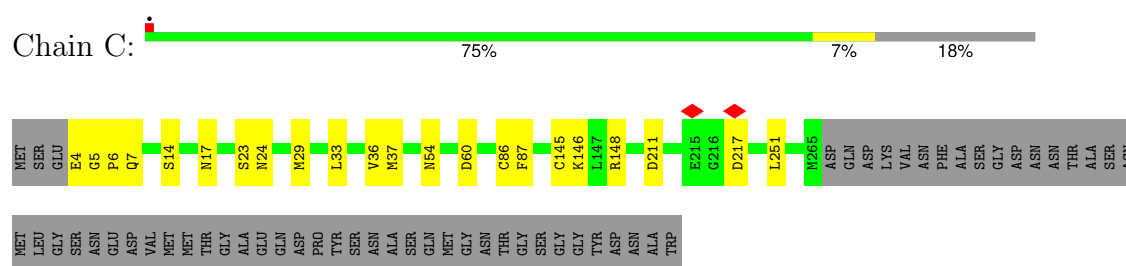
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

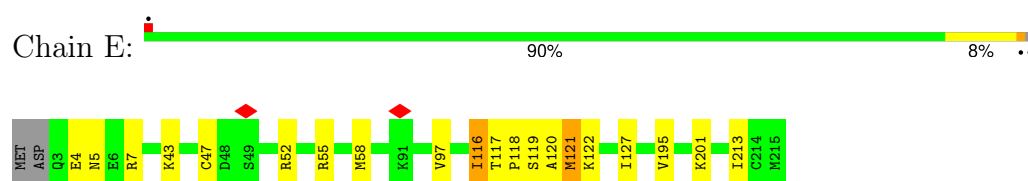
3 Residue-property plots [i](#)

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.

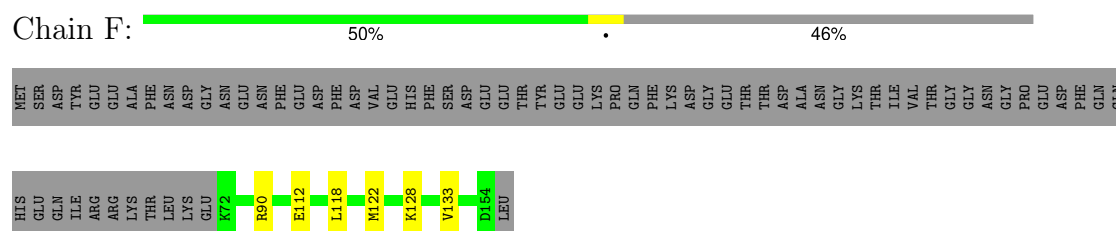
- Molecule 1: DNA-directed RNA polymerase II subunit RPB3



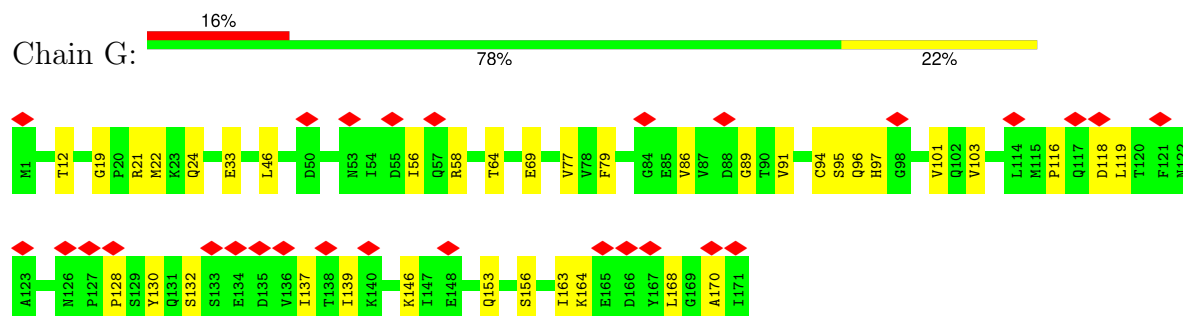
- Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1



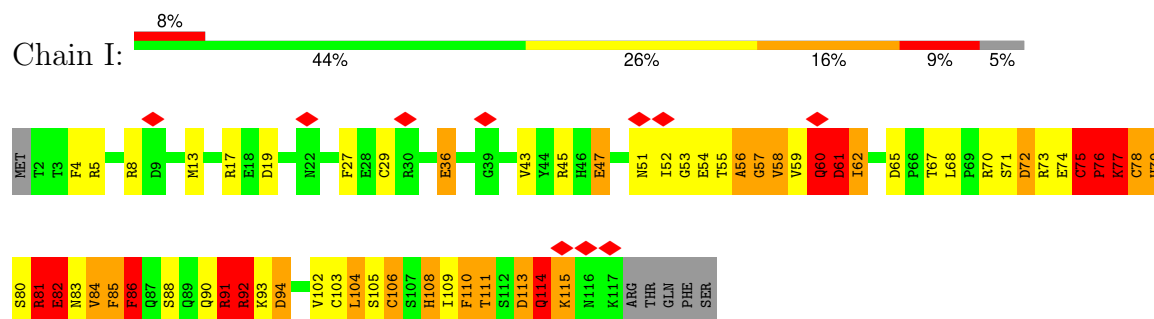
- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2



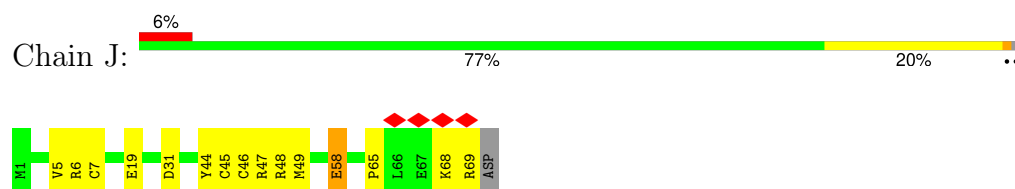
- Molecule 4: DNA-directed RNA polymerase II subunit RPB7



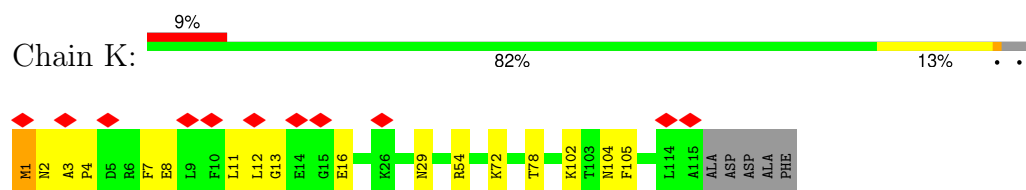
- Molecule 5: DNA-directed RNA polymerase II subunit RPB9



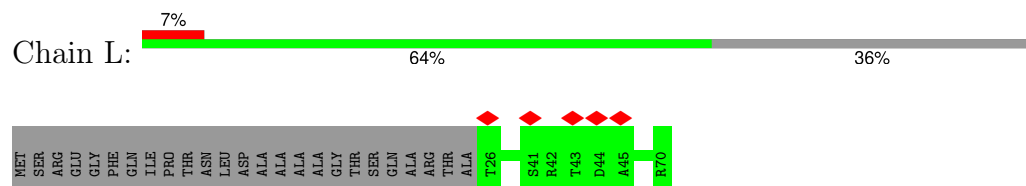
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC5



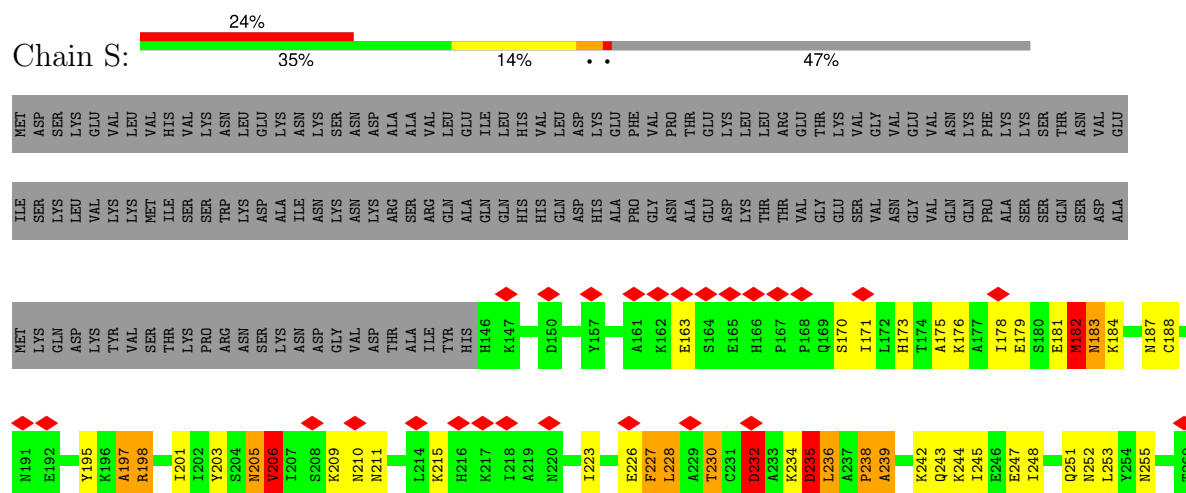
- Molecule 7: DNA-directed RNA polymerase II subunit RPB11

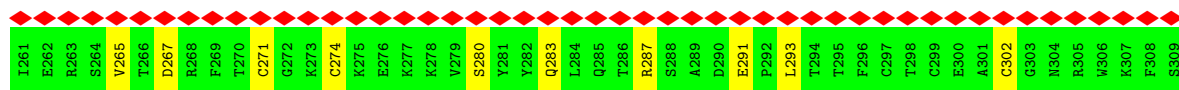


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC4

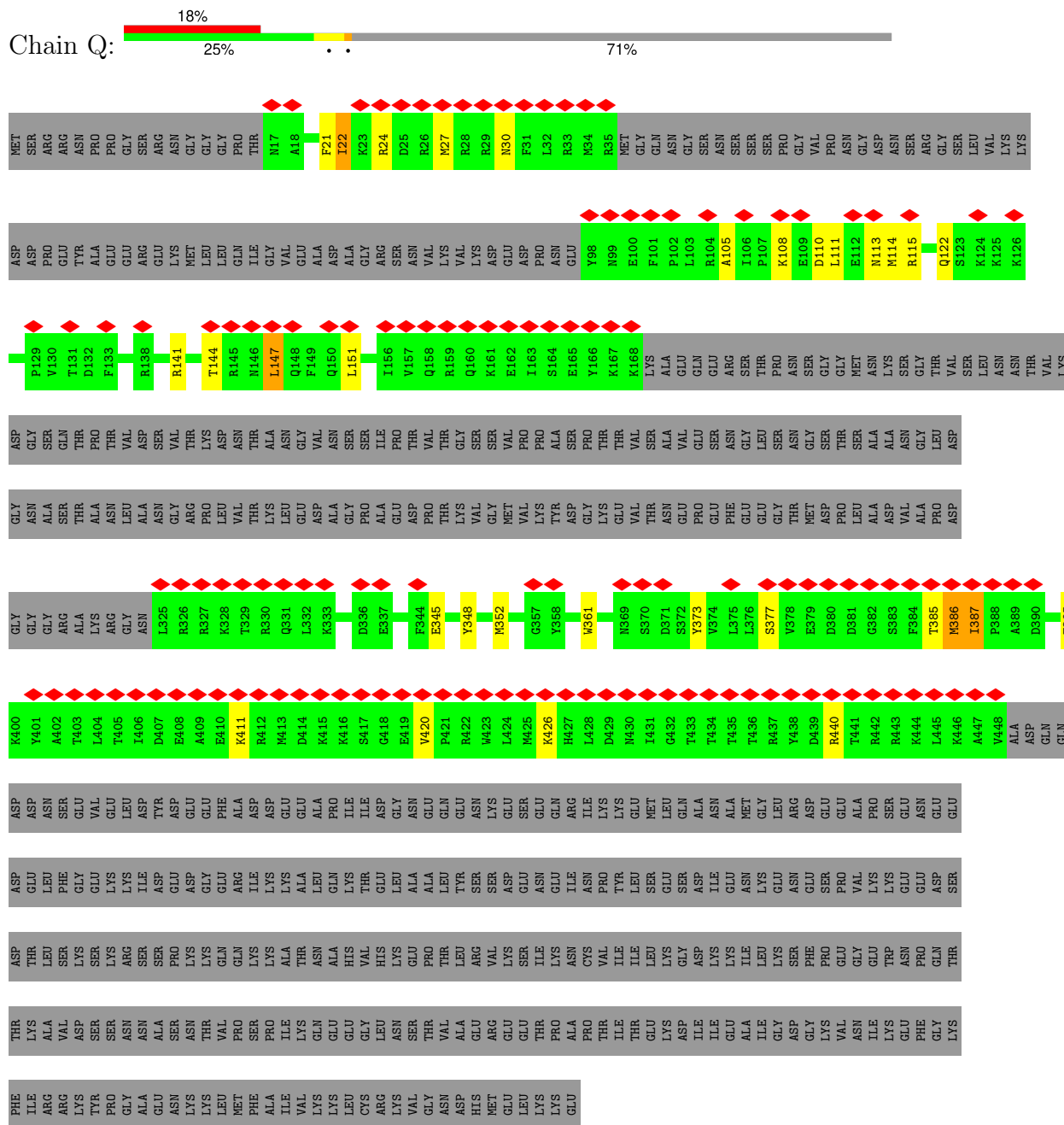


- Molecule 9: Transcription elongation factor S-II

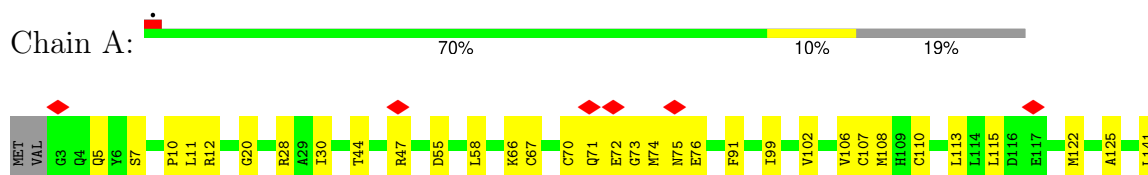


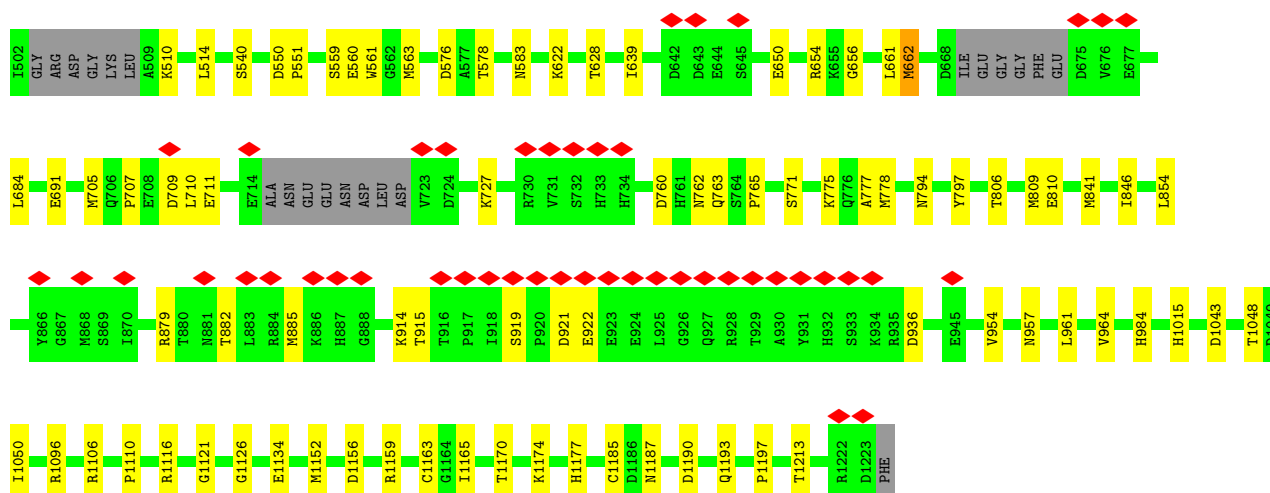


• Molecule 10: Transcription initiation factor IIF subunit alpha

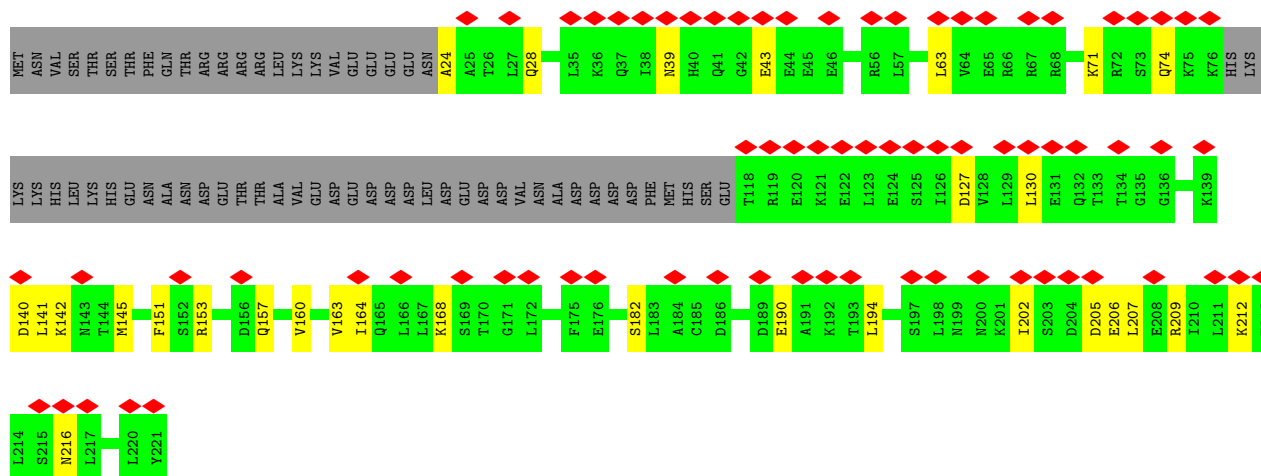


• Molecule 11: DNA-directed RNA polymerase II subunit RPB1

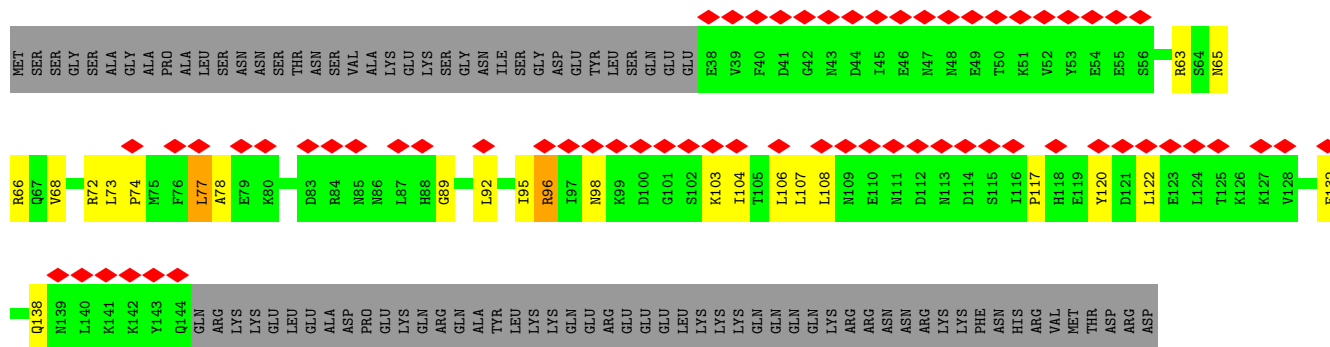
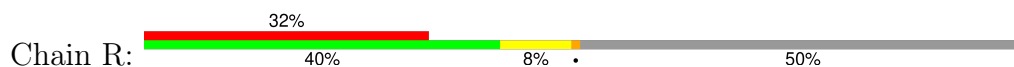


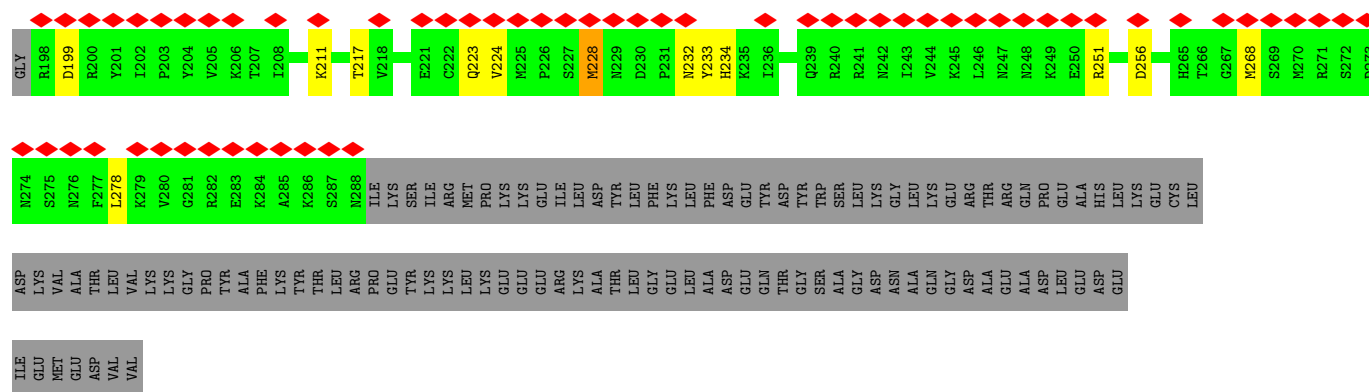


• Molecule 13: DNA-directed RNA polymerase II subunit RPB4

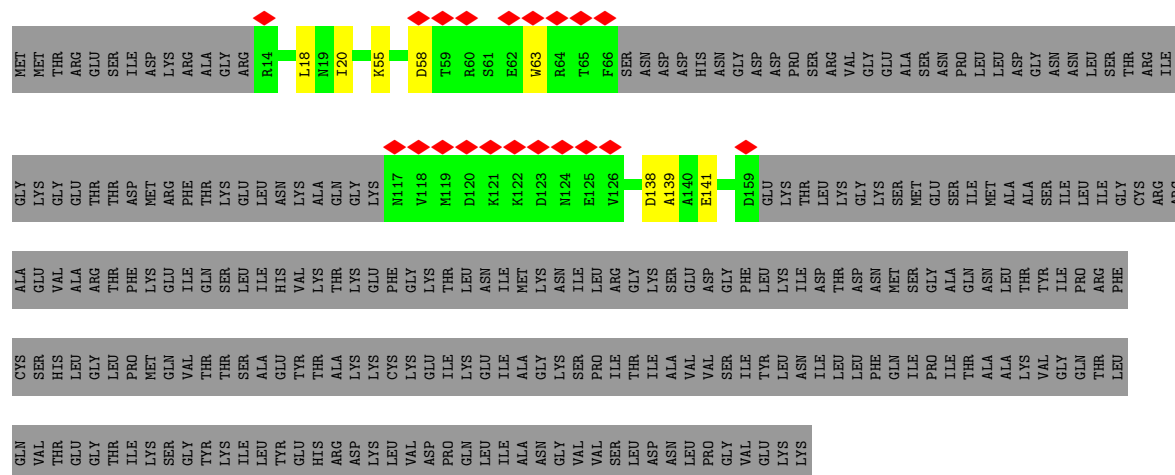


• Molecule 14: Transcription initiation factor IIF subunit beta

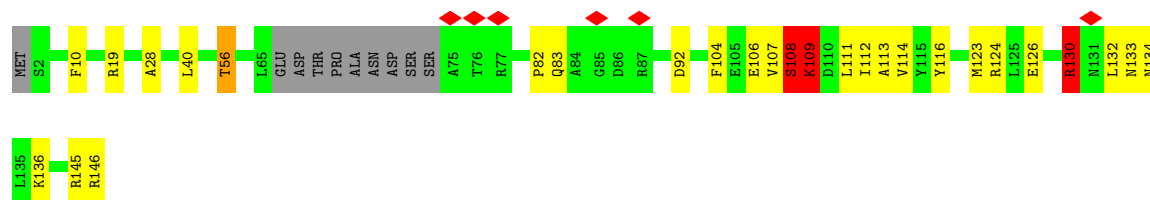




- Molecule 15: Transcription initiation factor IIB



- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	2985639	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	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.917	Depositor
Minimum map value	-3.956	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.652	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: MG, 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	C	0.19	0/2099	0.40	0/2845
2	E	0.29	1/1780 (0.1%)	0.45	1/2395 (0.0%)
3	F	0.31	0/682	0.61	1/922 (0.1%)
4	G	0.36	0/1368	0.74	4/1844 (0.2%)
5	I	2.04	31/962 (3.2%)	3.30	102/1295 (7.9%)
6	J	0.70	3/578 (0.5%)	0.93	3/775 (0.4%)
7	K	0.29	0/942	0.58	1/1272 (0.1%)
8	L	0.29	0/361	0.51	0/478
9	S	1.15	14/1324 (1.1%)	1.69	35/1787 (2.0%)
10	Q	0.42	4/1852 (0.2%)	0.55	1/2480 (0.0%)
11	A	0.43	13/11191 (0.1%)	0.76	34/15127 (0.2%)
12	B	0.34	4/9431 (0.0%)	0.58	18/12718 (0.1%)
13	D	0.23	0/1262	0.51	0/1693
14	R	0.55	2/1651 (0.1%)	0.76	8/2219 (0.4%)
15	M	0.41	0/721	0.81	4/968 (0.4%)
16	H	0.80	3/1107 (0.3%)	1.15	12/1499 (0.8%)
All	All	0.55	75/37311 (0.2%)	0.90	224/50317 (0.4%)

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
4	G	0	1
5	I	0	13
6	J	0	1
9	S	1	4
11	A	0	7
12	B	0	3
16	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	32

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	86	PHE	CG-CD2	21.72	1.84	1.38
9	S	206	VAL	CA-C	16.09	1.73	1.52
16	H	109	LYS	CA-C	15.75	1.73	1.52
11	A	688	LYS	CB-CG	-14.96	1.07	1.52
5	I	61	ASP	CA-C	14.80	1.73	1.52
9	S	198	ARG	CG-CD	-13.61	1.11	1.52
9	S	206	VAL	CA-CB	-13.14	1.36	1.54
6	J	58	GLU	CB-CG	-12.19	1.15	1.52
5	I	86	PHE	CG-CD1	-11.63	1.14	1.38
12	B	22	SER	C-N	11.60	1.50	1.33
11	A	688	LYS	CA-C	11.42	1.68	1.52
16	H	109	LYS	N-CA	-11.34	1.31	1.46
14	R	228	MET	SD-CE	-11.32	1.51	1.79
5	I	82	GLU	CG-CD	-11.07	1.24	1.52
12	B	23	ALA	N-CA	10.97	1.63	1.45
5	I	92	ARG	CG-CD	-10.58	1.20	1.52
11	A	688	LYS	CA-CB	10.27	1.72	1.53
5	I	92	ARG	CD-NE	-10.06	1.32	1.46
11	A	688	LYS	CD-CE	-9.98	1.22	1.52
5	I	93	LYS	CE-NZ	-9.71	1.20	1.49
10	Q	386	MET	SD-CE	-9.63	1.55	1.79
12	B	662	MET	CG-SD	-9.54	1.56	1.80
5	I	61	ASP	N-CA	-9.45	1.35	1.46
5	I	82	GLU	CD-OE1	-9.30	1.07	1.25
5	I	104	LEU	CG-CD2	8.96	1.82	1.52
5	I	62	ILE	CA-C	8.95	1.66	1.52
9	S	198	ARG	CB-CG	-8.84	1.25	1.52
9	S	183	ASN	C-O	-8.60	1.13	1.24
5	I	84	VAL	CA-CB	-8.51	1.44	1.54
11	A	455	MET	SD-CE	-8.44	1.58	1.79
5	I	62	ILE	CG1-CD1	-8.38	1.19	1.51
5	I	82	GLU	CD-OE2	8.12	1.40	1.25
5	I	94	ASP	CG-OD2	8.11	1.40	1.25
14	R	268	MET	SD-CE	-8.01	1.59	1.79
5	I	77	LYS	CE-NZ	-7.97	1.25	1.49
11	A	683	ILE	C-N	7.94	1.45	1.33
5	I	75	CYS	CB-SG	7.90	2.07	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	93	LYS	CB-CG	-7.82	1.28	1.52
5	I	78	CYS	CA-C	-7.62	1.42	1.52
5	I	91	ARG	CG-CD	-7.53	1.29	1.52
9	S	205	ASN	C-N	-7.34	1.23	1.33
11	A	684	ALA	N-CA	7.27	1.55	1.46
5	I	104	LEU	CG-CD1	-7.23	1.28	1.52
5	I	82	GLU	N-CA	-7.07	1.38	1.46
16	H	109	LYS	CA-CB	-6.95	1.43	1.53
2	E	121	MET	SD-CE	-6.79	1.62	1.79
11	A	683	ILE	CA-C	6.59	1.62	1.52
5	I	78	CYS	CB-SG	-6.49	1.59	1.81
9	S	182	MET	SD-CE	-6.39	1.63	1.79
9	S	206	VAL	N-CA	-6.28	1.38	1.46
10	Q	147	LEU	CG-CD2	-6.25	1.31	1.52
9	S	209	LYS	CG-CD	-6.21	1.33	1.52
5	I	84	VAL	CB-CG2	-6.13	1.32	1.52
6	J	58	GLU	CD-OE1	-6.03	1.14	1.25
11	A	542	GLU	CD-OE1	-5.99	1.14	1.25
9	S	182	MET	N-CA	5.94	1.53	1.46
12	B	22	SER	CA-C	5.93	1.60	1.52
11	A	688	LYS	N-CA	-5.84	1.38	1.46
9	S	209	LYS	CD-CE	-5.83	1.34	1.52
5	I	60	GLN	CD-OE1	-5.74	1.12	1.23
5	I	111	THR	CB-CG2	5.64	1.71	1.52
5	I	60	GLN	CD-NE2	5.61	1.45	1.33
5	I	111	THR	CA-C	5.60	1.60	1.53
10	Q	387	ILE	CG1-CD1	-5.58	1.29	1.51
9	S	228	LEU	CG-CD2	-5.58	1.34	1.52
9	S	182	MET	CA-C	-5.48	1.45	1.52
5	I	115	LYS	CG-CD	-5.48	1.36	1.52
11	A	1444	MET	SD-CE	-5.42	1.66	1.79
9	S	232	ASP	CG-OD2	5.36	1.35	1.25
11	A	692	ASP	CG-OD1	-5.33	1.15	1.25
6	J	58	GLU	CD-OE2	5.19	1.35	1.25
5	I	114	GLN	CD-OE1	-5.12	1.13	1.23
11	A	692	ASP	CA-C	5.05	1.59	1.52
5	I	85	PHE	N-CA	5.03	1.51	1.45
10	Q	22	ILE	CG1-CD1	-5.01	1.32	1.51

All (224) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	109	LYS	N-CA-C	-26.63	81.13	113.88
5	I	86	PHE	CD1-CG-CD2	-26.25	79.23	118.60
11	A	688	LYS	CB-CG-CD	21.29	160.26	111.30
5	I	77	LYS	CD-CE-NZ	21.26	179.93	111.90
9	S	205	ASN	CA-C-N	20.87	159.54	121.97
9	S	205	ASN	C-N-CA	20.87	159.54	121.97
5	I	82	GLU	CB-CG-CD	20.38	147.25	112.60
5	I	92	ARG	CG-CD-NE	20.28	156.62	112.00
5	I	93	LYS	CD-CE-NZ	19.88	175.53	111.90
5	I	92	ARG	CD-NE-CZ	-19.65	96.90	124.40
6	J	58	GLU	CA-CB-CG	19.34	152.77	114.10
11	A	692	ASP	N-CA-C	-19.28	90.17	113.88
5	I	91	ARG	CD-NE-CZ	19.15	151.21	124.40
11	A	688	LYS	CA-CB-CG	-18.77	76.56	114.10
9	S	206	VAL	CG1-CB-CG2	-18.74	69.57	110.80
5	I	93	LYS	CB-CG-CD	18.65	154.20	111.30
11	A	676	MET	CB-CG-SD	18.32	167.68	112.70
5	I	78	CYS	CB-CA-C	-18.19	73.27	110.38
11	A	688	LYS	N-CA-C	-17.30	92.17	113.28
5	I	75	CYS	CB-CA-C	-16.80	84.19	109.56
5	I	61	ASP	N-CA-C	-16.64	92.29	112.59
9	S	206	VAL	N-CA-CB	16.47	138.41	111.23
5	I	86	PHE	CG-CD1-CE1	16.21	148.25	120.70
5	I	62	ILE	CB-CG1-CD1	16.06	147.53	113.80
5	I	86	PHE	CB-CG-CD2	-15.79	93.86	120.70
11	A	676	MET	N-CA-CB	-15.60	84.13	110.49
5	I	84	VAL	CA-CB-CG2	15.53	136.80	110.40
5	I	84	VAL	N-CA-CB	14.57	131.07	111.25
5	I	82	GLU	CA-CB-CG	14.47	143.04	114.10
11	A	692	ASP	OD1-CG-OD2	-13.89	89.56	122.90
5	I	75	CYS	CA-CB-SG	13.84	146.24	114.40
5	I	82	GLU	N-CA-CB	13.46	132.79	110.59
5	I	86	PHE	CB-CG-CD1	13.38	143.45	120.70
12	B	19	GLU	CG-CD-OE1	12.86	147.98	118.40
5	I	113	ASP	CA-CB-CG	12.77	125.37	112.60
9	S	198	ARG	CD-NE-CZ	-12.58	106.78	124.40
5	I	62	ILE	CA-CB-CG1	12.24	131.21	110.40
5	I	60	GLN	CA-C-N	-11.86	103.82	122.67
5	I	60	GLN	C-N-CA	-11.86	103.82	122.67
12	B	19	GLU	CB-CG-CD	11.51	132.16	112.60
5	I	115	LYS	CG-CD-CE	11.31	137.31	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	60	GLN	OE1-CD-NE2	-11.27	111.33	122.60
14	R	228	MET	CA-CB-CG	-11.24	91.62	114.10
12	B	19	GLU	CG-CD-OE2	-11.08	92.92	118.40
6	J	58	GLU	CB-CA-C	-11.04	93.55	110.88
12	B	22	SER	CA-C-O	-10.93	104.89	120.51
9	S	232	ASP	CB-CA-C	10.87	128.28	110.88
9	S	182	MET	CG-SD-CE	10.80	124.67	100.90
5	I	104	LEU	CD1-CG-CD2	-10.77	87.10	110.80
5	I	93	LYS	CA-CB-CG	-10.73	92.63	114.10
9	S	206	VAL	CB-CA-C	-10.56	93.98	111.29
11	A	692	ASP	CA-CB-CG	10.47	123.07	112.60
12	B	22	SER	CA-C-N	10.46	140.99	122.48
12	B	22	SER	C-N-CA	10.46	140.99	122.48
9	S	182	MET	CB-CA-C	10.45	128.18	110.84
5	I	111	THR	OG1-CB-CG2	-10.40	88.50	109.30
9	S	209	LYS	CD-CE-NZ	-10.29	78.96	111.90
5	I	62	ILE	CA-CB-CG2	10.25	127.93	110.50
12	B	662	MET	CB-CG-SD	10.23	143.40	112.70
5	I	91	ARG	CA-CB-CG	-10.06	93.97	114.10
9	S	209	LYS	CG-CD-CE	10.02	134.35	111.30
5	I	78	CYS	N-CA-CB	9.92	125.58	110.30
9	S	182	MET	N-CA-CB	-9.87	92.95	109.72
5	I	113	ASP	N-CA-CB	9.70	126.89	110.49
14	R	228	MET	CG-SD-CE	9.67	122.17	100.90
5	I	62	ILE	CB-CA-C	-9.44	93.77	111.79
5	I	77	LYS	CB-CG-CD	9.38	132.89	111.30
5	I	91	ARG	CG-CD-NE	9.18	132.19	112.00
9	S	206	VAL	CA-CB-CG1	-9.18	94.80	110.40
11	A	676	MET	CB-CA-C	8.96	128.25	110.42
11	A	1444	MET	CG-SD-CE	-8.93	81.25	100.90
9	S	198	ARG	CA-CB-CG	8.91	131.92	114.10
16	H	130	ARG	NE-CZ-NH2	-8.85	111.23	119.20
9	S	232	ASP	OD1-CG-OD2	-8.82	101.74	122.90
5	I	78	CYS	CA-CB-SG	8.78	134.59	114.40
12	B	662	MET	CA-CB-CG	8.76	131.62	114.10
5	I	94	ASP	OD1-CG-OD2	-8.68	102.06	122.90
16	H	109	LYS	N-CA-CB	8.63	122.07	110.59
5	I	76	PRO	N-CA-C	8.56	130.10	112.47
5	I	94	ASP	CB-CG-OD2	-8.56	98.72	118.40
5	I	94	ASP	CA-CB-CG	8.51	121.11	112.60
5	I	60	GLN	CG-CD-NE2	-8.47	103.70	116.40
5	I	114	GLN	CG-CD-NE2	-8.43	103.76	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	111	THR	N-CA-C	-8.39	97.87	109.95
5	I	86	PHE	N-CA-CB	8.38	124.80	111.56
12	B	21	GLU	CA-C-O	-8.31	108.63	120.51
5	I	68	LEU	N-CA-C	8.20	119.03	109.60
5	I	83	ASN	CA-C-N	8.06	133.18	123.19
5	I	83	ASN	C-N-CA	8.06	133.18	123.19
5	I	77	LYS	CG-CD-CE	-8.05	92.78	111.30
11	A	1277	GLU	O-C-N	-8.03	111.92	122.59
5	I	94	ASP	CB-CG-OD1	8.00	136.80	118.40
9	S	227	PHE	N-CA-C	7.99	121.15	111.40
5	I	114	GLN	OE1-CD-NE2	-7.97	114.63	122.60
11	A	683	ILE	CA-C-N	7.91	133.91	120.71
11	A	683	ILE	C-N-CA	7.91	133.91	120.71
5	I	88	SER	CB-CA-C	7.87	122.05	109.61
9	S	230	THR	OG1-CB-CG2	7.81	124.92	109.30
5	I	92	ARG	N-CA-CB	7.80	122.76	111.05
9	S	206	VAL	N-CA-C	-7.75	93.22	109.34
5	I	115	LYS	CD-CE-NZ	-7.75	87.12	111.90
5	I	60	GLN	CG-CD-OE1	7.67	136.14	120.80
7	K	1	MET	CG-SD-CE	-7.67	84.04	100.90
5	I	104	LEU	CB-CG-CD1	7.62	133.56	110.70
9	S	171	ILE	CA-CB-CG1	7.56	123.26	110.40
12	B	18	PHE	N-CA-C	-7.53	101.16	112.54
9	S	235	ASP	CB-CA-C	-7.48	95.53	110.42
5	I	88	SER	N-CA-C	7.48	120.82	110.35
5	I	62	ILE	CG1-CB-CG2	-7.46	88.33	110.70
5	I	86	PHE	CD1-CE1-CZ	-7.43	106.62	120.00
5	I	77	LYS	CA-CB-CG	-7.32	99.45	114.10
5	I	94	ASP	N-CA-CB	-7.25	99.24	111.20
5	I	68	LEU	CB-CG-CD1	7.22	132.36	110.70
10	Q	22	ILE	CA-CB-CG1	-7.20	98.15	110.40
16	H	109	LYS	CA-C-O	7.18	127.36	119.24
5	I	67	THR	N-CA-C	7.13	122.24	112.90
9	S	183	ASN	CA-C-O	-7.11	111.80	119.97
9	S	198	ARG	N-CA-CB	7.01	121.14	110.28
5	I	81	ARG	CA-C-N	-7.00	110.80	121.86
5	I	81	ARG	C-N-CA	-7.00	110.80	121.86
11	A	691	LEU	CA-C-N	-6.96	110.39	122.36
11	A	691	LEU	C-N-CA	-6.96	110.39	122.36
5	I	104	LEU	CB-CA-C	6.93	121.89	110.81
15	M	63	TRP	N-CA-C	6.83	118.91	110.91
9	S	223	ILE	CA-CB-CG1	6.80	121.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	94	ASP	CB-CA-C	6.76	121.98	111.02
5	I	78	CYS	N-CA-C	6.74	120.72	112.23
16	H	109	LYS	CB-CA-C	-6.69	98.19	109.03
9	S	206	VAL	CA-C-O	6.68	129.14	120.78
16	H	56	THR	N-CA-CB	6.63	120.97	110.57
11	A	692	ASP	CB-CG-OD1	6.62	133.64	118.40
5	I	84	VAL	CB-CA-C	-6.62	100.96	110.83
11	A	1277	GLU	CA-C-O	-6.62	111.04	120.51
12	B	19	GLU	CB-CA-C	6.62	122.88	110.63
14	R	228	MET	CB-CA-C	6.56	122.57	110.10
16	H	108	SER	CA-C-N	-6.52	111.15	122.36
16	H	108	SER	C-N-CA	-6.52	111.15	122.36
9	S	209	LYS	CB-CG-CD	-6.49	96.38	111.30
5	I	61	ASP	CA-CB-CG	-6.45	106.15	112.60
5	I	61	ASP	CB-CA-C	-6.44	100.64	111.02
5	I	67	THR	CA-CB-CG2	6.42	121.41	110.50
5	I	108	HIS	CB-CG-CD2	6.39	139.51	131.20
5	I	110	PHE	CA-C-N	-6.38	111.46	123.27
5	I	110	PHE	C-N-CA	-6.38	111.46	123.27
9	S	243	GLN	N-CA-C	-6.37	104.96	114.64
5	I	114	GLN	CG-CD-OE1	6.37	133.53	120.80
15	M	58	ASP	CA-C-N	6.35	133.67	121.54
15	M	58	ASP	C-N-CA	6.35	133.67	121.54
5	I	104	LEU	CB-CG-CD2	-6.32	91.73	110.70
11	A	688	LYS	CA-C-O	6.22	126.58	119.18
11	A	1275	GLY	CA-C-N	-6.20	110.80	121.97
11	A	1275	GLY	C-N-CA	-6.20	110.80	121.97
12	B	19	GLU	N-CA-CB	-6.16	100.73	110.22
14	R	278	LEU	N-CA-C	6.13	118.08	110.91
5	I	67	THR	N-CA-CB	-6.09	101.20	110.33
12	B	662	MET	N-CA-C	-6.02	105.01	112.90
16	H	130	ARG	CD-NE-CZ	6.02	132.83	124.40
5	I	62	ILE	N-CA-CB	6.01	122.68	110.78
5	I	114	GLN	N-CA-CB	-5.94	100.46	110.49
5	I	114	GLN	CB-CG-CD	5.93	122.67	112.60
5	I	105	SER	CA-C-N	-5.91	112.94	121.98
5	I	105	SER	C-N-CA	-5.91	112.94	121.98
5	I	91	ARG	CB-CG-CD	5.91	124.89	111.30
11	A	1221	LYS	CA-C-N	5.87	130.80	121.18
11	A	1221	LYS	C-N-CA	5.87	130.80	121.18
2	E	116	ILE	CG1-CB-CG2	-5.82	93.25	110.70
5	I	67	THR	OG1-CB-CG2	5.76	120.82	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	96	ARG	CA-CB-CG	5.76	125.61	114.10
12	B	18	PHE	CB-CG-CD1	5.74	130.45	120.70
5	I	92	ARG	CA-CB-CG	5.72	125.54	114.10
5	I	75	CYS	N-CA-C	5.72	119.24	109.06
5	I	92	ARG	CB-CG-CD	-5.72	98.15	111.30
11	A	464	PRO	CA-C-N	5.71	132.44	121.54
11	A	464	PRO	C-N-CA	5.71	132.44	121.54
5	I	82	GLU	OE1-CD-OE2	-5.66	109.31	122.90
16	H	130	ARG	NE-CZ-NH1	5.65	127.15	121.50
5	I	72	ASP	CB-CA-C	-5.58	100.01	109.38
9	S	197	ALA	CA-C-N	-5.56	111.86	120.31
9	S	197	ALA	C-N-CA	-5.56	111.86	120.31
15	M	141	GLU	CA-CB-CG	5.54	125.19	114.10
5	I	8	ARG	CA-C-N	5.54	132.13	121.54
5	I	8	ARG	C-N-CA	5.54	132.13	121.54
14	R	77	LEU	CA-CB-CG	5.54	135.69	116.30
11	A	683	ILE	CA-C-O	-5.51	113.36	120.03
14	R	96	ARG	CG-CD-NE	5.51	124.13	112.00
14	R	228	MET	N-CA-CB	-5.47	101.20	110.50
11	A	1221	LYS	CA-CB-CG	5.46	125.03	114.10
5	I	84	VAL	CA-C-O	-5.42	114.74	120.48
3	F	128	LYS	N-CA-C	5.41	117.24	110.91
12	B	18	PHE	CB-CG-CD2	-5.41	111.50	120.70
4	G	33	GLU	CA-C-N	-5.37	113.79	121.52
4	G	33	GLU	C-N-CA	-5.37	113.79	121.52
11	A	688	LYS	CD-CE-NZ	-5.35	94.77	111.90
16	H	145	ARG	CA-C-N	5.32	131.27	121.70
16	H	145	ARG	C-N-CA	5.32	131.27	121.70
5	I	108	HIS	CB-CG-ND1	-5.30	114.75	122.70
9	S	227	PHE	CG-CD1-CE1	5.30	129.70	120.70
11	A	299	HIS	CA-C-N	-5.28	112.47	121.97
11	A	299	HIS	C-N-CA	-5.28	112.47	121.97
11	A	204	THR	OG1-CB-CG2	-5.27	98.77	109.30
4	G	64	THR	CA-C-N	5.23	131.52	121.54
4	G	64	THR	C-N-CA	5.23	131.52	121.54
5	I	106	CYS	N-CA-CB	5.22	117.87	110.98
9	S	232	ASP	CB-CG-OD2	-5.22	106.40	118.40
9	S	253	LEU	CA-C-N	5.21	127.52	120.38
9	S	253	LEU	C-N-CA	5.21	127.52	120.38
5	I	111	THR	N-CA-CB	-5.20	102.69	110.60
12	B	473	MET	CA-C-N	5.20	131.46	121.54
12	B	473	MET	C-N-CA	5.20	131.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	21	GLU	O-C-N	-5.19	115.69	122.59
9	S	228	LEU	CB-CG-CD2	5.18	126.23	110.70
5	I	77	LYS	N-CA-C	-5.17	107.14	113.50
11	A	601	LYS	CA-C-N	5.17	131.41	121.54
11	A	601	LYS	C-N-CA	5.17	131.41	121.54
5	I	36	GLU	CA-C-N	5.12	132.33	122.03
5	I	36	GLU	C-N-CA	5.12	132.33	122.03
9	S	205	ASN	O-C-N	-5.12	116.32	122.15
6	J	58	GLU	OE1-CD-OE2	-5.09	110.68	122.90
11	A	1160	SER	N-CA-C	5.08	117.83	110.42
5	I	86	PHE	CA-C-O	-5.07	116.03	121.45
5	I	53	GLY	N-CA-C	5.03	125.10	113.18
5	I	65	ASP	CB-CA-C	5.03	115.75	110.17
9	S	198	ARG	CB-CG-CD	-5.02	99.75	111.30
11	A	330	LYS	N-CA-C	5.02	116.44	110.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	S	206	VAL	CA

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	A	1277	GLU	Peptide,Mainchain
11	A	1278	ASN	Peptide
11	A	300	VAL	Peptide
11	A	464	PRO	Peptide
11	A	692	ASP	Sidechain
11	A	71	GLN	Peptide
12	B	21	GLU	Mainchain
12	B	22	SER	Mainchain
12	B	474	SER	Peptide
4	G	56	ILE	Peptide
16	H	107	VAL	Peptide
16	H	108	SER	Peptide
16	H	130	ARG	Sidechain
5	I	114	GLN	Sidechain
5	I	60	GLN	Sidechain,Peptide
5	I	61	ASP	Sidechain
5	I	70	ARG	Sidechain
5	I	72	ASP	Sidechain

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Mol	Chain	Res	Type	Group
5	I	75	CYS	Mainchain
5	I	81	ARG	Sidechain
5	I	82	GLU	Sidechain
5	I	86	PHE	Sidechain
5	I	91	ARG	Sidechain
5	I	92	ARG	Sidechain
5	I	94	ASP	Sidechain
6	J	58	GLU	Sidechain
9	S	198	ARG	Sidechain
9	S	210	ASN	Peptide
9	S	232	ASP	Sidechain
9	S	236	LEU	Mainchain

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	15	0
2	E	1744	0	1772	14	0
3	F	670	0	690	4	0
4	G	1340	0	1357	21	0
5	I	944	0	901	42	0
6	J	569	0	585	11	0
7	K	924	0	934	15	0
8	L	359	0	381	0	0
9	S	1301	0	1294	46	0
10	Q	1817	0	1843	25	0
11	A	10996	0	11079	118	0
12	B	9249	0	9248	86	0
13	D	1253	0	1275	18	0
14	R	1629	0	1618	30	0
15	M	714	0	712	6	0
16	H	1089	0	1062	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	36670	0	36780	429	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 (429) 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:86:PHE:CG	5:I:86:PHE:CD2	1.84	1.64
5:I:104:LEU:CG	5:I:104:LEU:CD2	1.82	1.56
5:I:75:CYS:SG	5:I:75:CYS:CB	2.07	1.43
5:I:86:PHE:CD2	5:I:86:PHE:CD1	1.98	1.26
5:I:104:LEU:CD2	5:I:104:LEU:CD1	2.17	1.23
5:I:104:LEU:CD2	5:I:104:LEU:CB	2.37	1.03
5:I:104:LEU:CD2	5:I:104:LEU:HD13	1.88	0.99
5:I:86:PHE:CD2	5:I:86:PHE:CB	2.45	0.99
9:S:274:CYS:HB3	9:S:302:CYS:SG	2.03	0.98
11:A:110:CYS:HB3	11:A:167:CYS:SG	2.11	0.90
9:S:187:ASN:HB2	9:S:228:LEU:HD21	1.56	0.86
5:I:78:CYS:SG	5:I:106:CYS:HB3	2.16	0.86
9:S:271:CYS:HB3	9:S:274:CYS:SG	2.17	0.85
11:A:1278:ASN:H	11:A:1279:ILE:HD12	1.42	0.83
9:S:183:ASN:O	9:S:228:LEU:HD22	1.78	0.82
9:S:184:LYS:HD2	9:S:228:LEU:HD13	1.64	0.80
9:S:184:LYS:HA	9:S:228:LEU:HD13	1.64	0.78
13:D:151:PHE:O	13:D:153:ARG:NH1	2.17	0.77
9:S:211:ASN:HB3	9:S:238:PRO:HG3	1.69	0.74
5:I:5:ARG:NH2	5:I:36:GLU:OE1	2.21	0.73
11:A:73:GLY:HA3	11:A:76:GLU:HG2	1.71	0.73
7:K:3:ALA:HA	11:A:465:TYR:HE1	1.55	0.71
5:I:59:VAL:HG13	5:I:61:ASP:H	1.55	0.71
14:R:73:LEU:HD12	14:R:74:PRO:HD2	1.72	0.70
12:B:705:MET:H	12:B:710:LEU:HD22	1.57	0.69
11:A:72:GLU:HG2	15:M:20:ILE:HD11	1.74	0.69
5:I:86:PHE:CD2	5:I:86:PHE:HB3	2.25	0.69
11:A:107:CYS:HB3	11:A:110:CYS:SG	2.34	0.68
10:Q:377:SER:OG	14:R:66:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:21:GLU:O	12:B:23:ALA:N	2.28	0.67
10:Q:24:ARG:NH1	12:B:810:GLU:OE1	2.27	0.67
6:J:7:CYS:HA	6:J:49:MET:HE2	1.76	0.66
12:B:806:THR:H	12:B:809:MET:HE3	1.62	0.65
16:H:114:VAL:HG13	16:H:132:LEU:HD12	1.79	0.65
11:A:10:PRO:HG2	11:A:12:ARG:HH12	1.63	0.64
5:I:104:LEU:CD2	5:I:104:LEU:HB2	2.25	0.64
11:A:150:THR:HA	11:A:166:GLY:HA2	1.78	0.64
10:Q:27:MET:SD	10:Q:27:MET:N	2.67	0.64
5:I:17:ARG:HH21	5:I:19:ASP:HB2	1.62	0.63
12:B:1106:ARG:NH2	12:B:1110:PRO:O	2.32	0.63
10:Q:144:THR:HA	10:Q:147:LEU:HD21	1.81	0.63
11:A:326:ARG:HG3	11:A:1406:VAL:HG21	1.81	0.63
12:B:486:TYR:HB3	12:B:1096:ARG:HH22	1.64	0.62
16:H:146:ARG:HH11	16:H:146:ARG:HG2	1.64	0.62
10:Q:352:MET:HB3	10:Q:361:TRP:HB2	1.80	0.62
10:Q:115:ARG:NH2	10:Q:345:GLU:OE2	2.32	0.62
11:A:44:THR:OG1	11:A:47:ARG:NH1	2.32	0.62
11:A:91:PHE:CE1	11:A:204:THR:HG22	2.35	0.62
13:D:153:ARG:NH2	13:D:182:SER:O	2.34	0.60
16:H:56:THR:N	16:H:146:ARG:HH12	1.99	0.60
7:K:4:PRO:HD2	11:A:465:TYR:CE1	2.37	0.60
12:B:21:GLU:OE1	12:B:22:SER:N	2.33	0.60
4:G:153:GLN:HB3	4:G:156:SER:HB2	1.83	0.60
13:D:206:GLU:HA	13:D:209:ARG:HG2	1.82	0.60
14:R:117:PRO:HA	14:R:232:ASN:HB2	1.82	0.60
16:H:56:THR:OG1	16:H:146:ARG:NH1	2.34	0.60
10:Q:151:LEU:HD23	10:Q:440:ARG:HH22	1.67	0.60
12:B:451:LYS:NZ	15:M:139:ALA:HA	2.17	0.60
14:R:233:TYR:O	14:R:234:HIS:ND1	2.34	0.60
11:A:894:GLU:O	11:A:898:ARG:HB2	2.02	0.59
11:A:1277:GLU:HB3	11:A:1312:ASN:HD22	1.67	0.59
7:K:8:GLU:OE2	7:K:8:GLU:N	2.35	0.59
11:A:30:ILE:HD12	12:B:1170:THR:HG21	1.84	0.59
2:E:97:VAL:HG13	2:E:127:ILE:HD11	1.84	0.59
11:A:74:MET:O	12:B:1116:ARG:NH1	2.30	0.58
11:A:1278:ASN:N	11:A:1279:ILE:HD12	2.15	0.58
12:B:919:SER:HB2	12:B:922:GLU:HB2	1.84	0.58
5:I:13:MET:HG2	12:B:294:ASP:OD2	2.03	0.58
5:I:104:LEU:CD1	5:I:104:LEU:HD21	2.27	0.58
11:A:687:LYS:NZ	11:A:795:GLU:OE2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:58:VAL:HG21	5:I:109:ILE:HD11	1.86	0.58
11:A:668:ASP:HA	11:A:741:ASN:HD21	1.67	0.57
12:B:451:LYS:HE3	15:M:138:ASP:HB3	1.85	0.57
12:B:957:ASN:HD21	12:B:961:LEU:HB2	1.69	0.57
16:H:106:GLU:OE1	16:H:112:ILE:HG22	2.04	0.57
11:A:1158:PRO:HB3	11:A:1188:GLN:HB2	1.86	0.57
2:E:195:VAL:HG22	2:E:213:ILE:HG22	1.86	0.57
1:C:148:ARG:HD3	6:J:65:PRO:HG3	1.86	0.57
9:S:232:ASP:CG	9:S:235:ASP:HB2	2.30	0.57
2:E:5:ASN:OD1	2:E:52:ARG:NH2	2.37	0.57
14:R:108:LEU:HD12	14:R:117:PRO:O	2.05	0.57
11:A:1140:HIS:HA	11:A:1275:GLY:HA3	1.86	0.57
12:B:762:ASN:HD21	12:B:984:HIS:HD2	1.52	0.57
4:G:46:LEU:HB2	4:G:77:VAL:HG23	1.87	0.56
9:S:283:GLN:HB3	9:S:293:LEU:HD13	1.87	0.56
14:R:63:ARG:NH2	14:R:65:ASN:O	2.37	0.56
12:B:63:ILE:HG13	12:B:95:ILE:HD12	1.86	0.56
1:C:145:CYS:SG	1:C:146:LYS:N	2.79	0.56
9:S:265:VAL:HG12	9:S:280:SER:HB3	1.88	0.56
7:K:3:ALA:HA	11:A:465:TYR:CE1	2.38	0.56
2:E:116:ILE:HG13	2:E:121:MET:CE	2.36	0.56
9:S:227:PHE:C	9:S:230:THR:H	2.14	0.56
11:A:1221:LYS:HD2	11:A:1222:ASN:H	1.70	0.56
12:B:496:ARG:NH2	12:B:540:SER:O	2.39	0.55
9:S:227:PHE:HA	9:S:230:THR:HG23	1.88	0.55
1:C:86:CYS:SG	1:C:87:PHE:N	2.79	0.55
4:G:116:PRO:HD3	4:G:164:LYS:HA	1.89	0.55
14:R:132:GLU:O	14:R:217:THR:OG1	2.25	0.55
9:S:226:GLU:O	9:S:230:THR:N	2.39	0.55
9:S:227:PHE:CD1	9:S:230:THR:HG21	2.41	0.54
11:A:66:LYS:HA	11:A:72:GLU:HG3	1.88	0.54
12:B:560:GLU:HG3	12:B:561:TRP:HD1	1.71	0.54
14:R:73:LEU:HD11	14:R:77:LEU:HB2	1.89	0.54
9:S:248:ILE:HG13	9:S:252:ASN:HD21	1.73	0.54
11:A:66:LYS:HB3	15:M:18:LEU:HD22	1.90	0.54
11:A:1279:ILE:HG23	11:A:1308:THR:HG23	1.90	0.54
12:B:1187:ASN:HD21	12:B:1190:ASP:HB3	1.71	0.54
1:C:5:GLY:O	1:C:7:GLN:NE2	2.41	0.54
11:A:590:ARG:NH2	11:A:618:GLU:OE2	2.41	0.54
12:B:882:THR:OG1	12:B:885:MET:SD	2.66	0.54
10:Q:141:ARG:NH1	10:Q:348:TYR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:24:ALA:N	13:D:28:GLN:O	2.40	0.54
9:S:230:THR:C	9:S:232:ASP:H	2.15	0.53
11:A:381:THR:HG23	11:A:383:TYR:H	1.73	0.53
12:B:248:SER:H	12:B:418:LYS:HE3	1.73	0.53
3:F:118:LEU:HG	3:F:122:MET:HE2	1.90	0.53
6:J:65:PRO:HD2	6:J:68:LYS:HE2	1.90	0.53
12:B:342:GLY:O	12:B:348:ARG:NH1	2.41	0.53
10:Q:108:LYS:HA	10:Q:111:LEU:HD13	1.89	0.53
11:A:1280:GLU:OE1	11:A:1309:ASP:HB2	2.08	0.53
12:B:583:ASN:HD21	12:B:628:THR:H	1.56	0.53
12:B:661:LEU:HD11	12:B:684:LEU:HD11	1.88	0.53
12:B:420:LEU:HD13	12:B:453:ILE:HA	1.90	0.53
12:B:309:GLN:O	12:B:313:MET:HG3	2.08	0.53
13:D:157:GLN:HA	13:D:160:VAL:HG22	1.90	0.53
5:I:104:LEU:HD13	5:I:104:LEU:HD22	1.87	0.53
11:A:28:ARG:NH2	11:A:238:CYS:SG	2.82	0.52
16:H:113:ALA:HB2	16:H:126:GLU:HG3	1.90	0.52
11:A:313:GLN:NE2	11:A:314:ALA:O	2.37	0.52
11:A:172:PRO:HB3	11:A:185:TRP:HD1	1.73	0.52
11:A:532:ARG:HE	11:A:749:ALA:HB2	1.74	0.52
11:A:818:MET:HA	12:B:514:LEU:HD21	1.91	0.52
3:F:112:GLU:OE1	3:F:112:GLU:N	2.42	0.52
11:A:66:LYS:HG2	11:A:72:GLU:HG3	1.92	0.52
16:H:10:PHE:HB3	16:H:28:ALA:HB1	1.91	0.52
10:Q:386:MET:HE1	14:R:92:LEU:HD23	1.91	0.52
3:F:90:ARG:NH1	11:A:503:GLN:OE1	2.41	0.52
9:S:302:CYS:HA	11:A:1300:LYS:HE2	1.91	0.52
11:A:186:LYS:NZ	11:A:187:LYS:O	2.43	0.52
12:B:1174:LYS:HB3	12:B:1177:HIS:HD2	1.75	0.52
11:A:881:GLN:NE2	11:A:957:PRO:O	2.43	0.52
2:E:116:ILE:HD12	2:E:121:MET:HB3	1.90	0.52
11:A:455:MET:HE1	12:B:1134:GLU:HA	1.92	0.52
11:A:543:LEU:HA	11:A:546:VAL:HG22	1.91	0.52
9:S:184:LYS:HD2	9:S:228:LEU:CD1	2.37	0.51
9:S:251:GLN:O	9:S:255:ASN:ND2	2.43	0.51
12:B:230:ALA:O	12:B:261:ARG:NH1	2.44	0.51
11:A:956:LEU:HD13	11:A:1021:LEU:HD22	1.92	0.51
12:B:559:SER:HA	12:B:563:MET:HE3	1.93	0.51
13:D:160:VAL:HA	13:D:163:VAL:HG12	1.93	0.51
5:I:57:GLY:C	5:I:59:VAL:N	2.68	0.51
12:B:199:MET:SD	12:B:199:MET:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:709:ASP:HB3	12:B:710:LEU:HD12	1.93	0.51
9:S:188:CYS:HB2	9:S:195:TYR:HB2	1.91	0.51
11:A:5:GLN:O	12:B:1159:ARG:NH1	2.43	0.51
13:D:202:ILE:HG23	13:D:207:LEU:HD21	1.93	0.51
2:E:116:ILE:HG13	2:E:121:MET:HE3	1.93	0.51
9:S:170:SER:HA	9:S:173:HIS:CE1	2.45	0.51
12:B:777:ALA:O	12:B:1096:ARG:NH2	2.43	0.51
7:K:54:ARG:HH21	16:H:83:GLN:HA	1.76	0.51
11:A:806:ARG:NH2	12:B:727:LYS:O	2.43	0.51
11:A:1221:LYS:HD2	11:A:1222:ASN:HB2	1.93	0.51
13:D:63:LEU:HB3	13:D:130:LEU:HD22	1.91	0.51
11:A:760:GLN:HE22	11:A:765:VAL:HA	1.75	0.50
2:E:119:SER:HA	2:E:122:LYS:HE3	1.94	0.50
5:I:71:SER:HB3	5:I:85:PHE:CE1	2.47	0.50
7:K:7:PHE:HB2	7:K:11:LEU:HD12	1.93	0.50
11:A:635:ARG:NH2	11:A:876:ALA:O	2.38	0.50
1:C:6:PRO:HA	1:C:24:ASN:HB3	1.93	0.50
1:C:211:ASP:N	1:C:211:ASP:OD1	2.44	0.50
7:K:54:ARG:NH2	16:H:82:PRO:O	2.45	0.50
10:Q:377:SER:HA	14:R:68:VAL:HG22	1.93	0.50
5:I:108:HIS:HE1	5:I:110:PHE:HB3	1.76	0.50
11:A:261:ASP:OD2	11:A:320:ARG:NH1	2.33	0.50
5:I:4:PHE:CD2	5:I:13:MET:HE1	2.46	0.50
5:I:45:ARG:NH2	5:I:47:GLU:OE1	2.41	0.50
2:E:118:PRO:HA	2:E:121:MET:SD	2.52	0.50
7:K:72:LYS:NZ	11:A:551:TYR:OH	2.37	0.50
11:A:1195:LEU:HB2	11:A:1238:ILE:HB	1.94	0.50
9:S:175:ALA:HA	9:S:178:ILE:HG12	1.94	0.50
4:G:119:LEU:HD21	4:G:130:TYR:HB3	1.93	0.50
12:B:763:GLN:HG2	12:B:765:PRO:HD2	1.93	0.50
12:B:771:SER:O	12:B:775:LYS:NZ	2.44	0.50
2:E:4:GLU:OE1	2:E:7:ARG:NH1	2.45	0.49
9:S:181:GLU:HG3	9:S:182:MET:HE2	1.94	0.49
5:I:108:HIS:CE1	5:I:110:PHE:HB3	2.47	0.49
12:B:21:GLU:CD	12:B:22:SER:H	2.19	0.49
11:A:506:ALA:O	11:A:510:GLN:NE2	2.45	0.49
12:B:451:LYS:HZ2	15:M:139:ALA:HA	1.77	0.49
6:J:48:ARG:NH1	6:J:49:MET:SD	2.86	0.49
11:A:451:HIS:HD2	11:A:453:MET:HE2	1.78	0.49
16:H:146:ARG:HG2	16:H:146:ARG:NH1	2.28	0.49
11:A:1280:GLU:OE1	11:A:1281:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:797:TYR:HE1	12:B:854:LEU:HG	1.77	0.49
10:Q:110:ASP:O	10:Q:114:MET:HG2	2.13	0.49
10:Q:386:MET:O	10:Q:387:ILE:HD13	2.11	0.49
12:B:576:ASP:OD1	12:B:576:ASP:N	2.46	0.49
12:B:467:GLY:HA2	12:B:473:MET:SD	2.52	0.48
11:A:849:MET:HE3	11:A:1061:GLY:HA2	1.95	0.48
4:G:95:SER:OG	4:G:96:GLN:N	2.43	0.48
7:K:2:ASN:OD1	11:A:465:TYR:HA	2.14	0.48
7:K:29:ASN:ND2	7:K:78:THR:O	2.47	0.48
11:A:1221:LYS:HD2	11:A:1222:ASN:N	2.27	0.48
5:I:43:VAL:HG21	11:A:1191:TRP:HZ3	1.79	0.48
11:A:901:LEU:HD22	11:A:919:ILE:HG13	1.94	0.48
12:B:957:ASN:OD1	12:B:961:LEU:N	2.45	0.48
14:R:73:LEU:HD11	14:R:77:LEU:CB	2.44	0.48
10:Q:420:VAL:HG11	12:B:322:PHE:HB2	1.94	0.48
12:B:21:GLU:OE2	12:B:656:GLY:N	2.34	0.48
4:G:58:ARG:HD2	11:A:1444:MET:CE	2.44	0.48
7:K:12:LEU:HD23	7:K:13:GLY:O	2.14	0.48
11:A:11:LEU:C	11:A:12:ARG:HD3	2.38	0.48
11:A:122:MET:HE3	11:A:141:LEU:HD21	1.96	0.48
13:D:190:GLU:HG2	13:D:194:LEU:HD23	1.95	0.48
10:Q:122:GLN:NE2	10:Q:395:PHE:O	2.46	0.48
14:R:104:ILE:HG13	14:R:122:LEU:HB3	1.95	0.48
5:I:54:GLU:HG3	5:I:55:THR:O	2.13	0.47
5:I:114:GLN:H	5:I:115:LYS:HZ3	1.62	0.47
1:C:36:VAL:HG21	1:C:251:LEU:HD13	1.97	0.47
12:B:954:VAL:HG12	12:B:964:VAL:HG12	1.95	0.47
9:S:163:GLU:HG2	9:S:215:LYS:CE	2.44	0.47
14:R:106:LEU:C	14:R:107:LEU:HD12	2.39	0.47
10:Q:113:ASN:O	10:Q:114:MET:HE2	2.13	0.47
12:B:21:GLU:CD	12:B:22:SER:N	2.73	0.47
4:G:86:VAL:HA	4:G:146:LYS:HA	1.97	0.47
6:J:69:ARG:HE	6:J:69:ARG:HA	1.80	0.47
9:S:230:THR:C	9:S:232:ASP:N	2.72	0.47
10:Q:377:SER:O	10:Q:385:THR:N	2.48	0.47
7:K:13:GLY:N	7:K:16:GLU:OE2	2.48	0.47
9:S:239:ALA:O	9:S:242:LYS:N	2.48	0.47
11:A:208:LEU:HD13	11:A:235:ILE:HG21	1.96	0.47
14:R:98:ASN:OD1	14:R:103:LYS:HB3	2.15	0.47
5:I:56:ALA:O	5:I:57:GLY:C	2.58	0.47
9:S:227:PHE:HD1	9:S:230:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:271:CYS:CB	9:S:274:CYS:SG	2.90	0.47
5:I:80:SER:O	5:I:81:ARG:HG3	2.15	0.46
11:A:1148:ILE:HD12	11:A:1196:GLU:HG3	1.97	0.46
1:C:6:PRO:O	7:K:104:ASN:ND2	2.38	0.46
13:D:141:LEU:O	13:D:145:MET:HE3	2.15	0.46
10:Q:373:TYR:OH	14:R:72:ARG:NH2	2.44	0.46
12:B:1163:CYS:HB2	12:B:1187:ASN:HD22	1.80	0.46
13:D:141:LEU:C	13:D:145:MET:HE3	2.40	0.46
4:G:46:LEU:HD11	4:G:79:PHE:HB2	1.96	0.46
11:A:99:ILE:HA	11:A:102:VAL:HG12	1.96	0.46
11:A:1144:LYS:HZ3	11:A:1268:LEU:HB3	1.79	0.46
9:S:163:GLU:HG2	9:S:215:LYS:CD	2.45	0.46
11:A:1143:LEU:HD11	11:A:1216:ILE:HD11	1.98	0.46
12:B:510:LYS:HD2	12:B:510:LYS:HA	1.84	0.46
11:A:148:CYS:HB3	11:A:169:ASN:H	1.79	0.46
9:S:163:GLU:HG2	9:S:215:LYS:HD3	1.98	0.46
12:B:879:ARG:HA	12:B:885:MET:HE1	1.98	0.46
11:A:900:ASP:N	11:A:900:ASP:OD1	2.49	0.46
12:B:182:SER:OG	12:B:183:GLU:OE1	2.33	0.46
14:R:256:ASP:OD1	14:R:256:ASP:N	2.47	0.46
5:I:103:CYS:HB2	5:I:106:CYS:SG	2.56	0.46
14:R:66:ARG:HG3	14:R:68:VAL:HG23	1.98	0.46
6:J:45:CYS:SG	6:J:46:CYS:N	2.89	0.45
14:R:95:ILE:HD13	14:R:106:LEU:HD13	1.98	0.45
4:G:12:THR:HA	4:G:69:GLU:HA	1.97	0.45
12:B:21:GLU:O	12:B:22:SER:C	2.59	0.45
12:B:100:PRO:HA	12:B:126:SER:HB3	1.97	0.45
9:S:248:ILE:HD12	9:S:248:ILE:HA	1.79	0.45
11:A:20:GLY:O	12:B:1213:THR:OG1	2.27	0.45
11:A:1423:GLY:O	11:A:1427:ASN:ND2	2.48	0.45
12:B:650:GLU:OE2	12:B:654:ARG:NH2	2.49	0.45
16:H:40:LEU:HD13	16:H:123:MET:HG3	1.99	0.45
4:G:137:ILE:HG12	4:G:170:ALA:HB2	1.99	0.45
9:S:201:ILE:O	9:S:205:ASN:ND2	2.49	0.45
9:S:227:PHE:HA	9:S:230:THR:CG2	2.47	0.45
9:S:227:PHE:HD1	9:S:230:THR:CG2	2.29	0.45
13:D:140:ASP:OD1	13:D:140:ASP:N	2.49	0.45
14:R:228:MET:HE2	14:R:228:MET:HA	1.97	0.45
1:C:217:ASP:OD1	1:C:217:ASP:N	2.49	0.45
14:R:63:ARG:HE	14:R:66:ARG:HB2	1.81	0.45
11:A:219:PHE:HA	11:A:222:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:890:ASP:OD1	11:A:940:ARG:NH2	2.50	0.45
14:R:73:LEU:HG	14:R:74:PRO:O	2.17	0.45
10:Q:105:ALA:H	14:R:89:GLY:HA2	1.80	0.45
11:A:7:SER:OG	12:B:1193:GLN:OE1	2.34	0.45
12:B:227:LYS:H	12:B:395:GLN:HE21	1.65	0.45
12:B:474:SER:O	12:B:476:ARG:N	2.51	0.44
9:S:244:LYS:HA	9:S:247:GLU:HG2	1.99	0.44
12:B:102:VAL:HG21	12:B:122:LEU:HD13	1.99	0.44
16:H:108:SER:OG	16:H:111:LEU:N	2.50	0.44
12:B:1165:ILE:HD12	12:B:1185:CYS:HB3	1.99	0.44
1:C:4:GLU:HG3	1:C:7:GLN:HE22	1.83	0.44
9:S:184:LYS:HA	9:S:228:LEU:CD1	2.42	0.44
11:A:1196:GLU:OE1	11:A:1235:LYS:NZ	2.40	0.44
11:A:1267:MET:HA	11:A:1271:ILE:HG12	1.99	0.44
12:B:1156:ASP:OD1	12:B:1156:ASP:N	2.48	0.44
10:Q:105:ALA:HB2	10:Q:386:MET:HE3	2.00	0.44
10:Q:440:ARG:NH1	14:R:199:ASP:OD1	2.51	0.44
12:B:185:THR:OG1	12:B:186:GLU:N	2.51	0.44
12:B:1121:GLY:O	12:B:1126:GLY:N	2.48	0.44
2:E:58:MET:HA	2:E:58:MET:HE2	2.00	0.44
4:G:118:ASP:OD1	4:G:118:ASP:N	2.50	0.44
12:B:451:LYS:HB2	12:B:451:LYS:HE2	1.71	0.44
4:G:163:ILE:HA	4:G:168:LEU:HD23	1.99	0.44
9:S:267:ASP:N	9:S:267:ASP:OD1	2.50	0.44
12:B:293:PRO:HG2	12:B:296:GLU:HB2	1.99	0.44
13:D:71:LYS:HA	13:D:74:GLN:HG2	2.00	0.44
11:A:663:SER:OG	11:A:664:THR:N	2.51	0.44
11:A:880:LYS:HA	11:A:955:PRO:HA	2.00	0.44
12:B:177:LYS:HE3	14:R:251:ARG:HH21	1.83	0.44
14:R:63:ARG:NE	14:R:66:ARG:HB2	2.32	0.44
11:A:252:PHE:CE2	11:A:256:GLN:HG3	2.53	0.43
12:B:130:VAL:HB	12:B:167:ILE:HD11	1.99	0.43
4:G:58:ARG:HD2	11:A:1444:MET:HE2	2.00	0.43
6:J:31:ASP:OD1	6:J:31:ASP:N	2.50	0.43
9:S:242:LYS:HB3	9:S:242:LYS:HE2	1.90	0.43
11:A:74:MET:N	11:A:74:MET:HE2	2.34	0.43
11:A:212:LYS:HB2	11:A:212:LYS:HE3	1.84	0.43
11:A:408:ASP:OD1	11:A:408:ASP:N	2.51	0.43
4:G:89:GLY:HA3	4:G:103:VAL:HG22	1.99	0.43
9:S:176:LYS:O	9:S:179:GLU:HG3	2.18	0.43
11:A:894:GLU:OE1	11:A:906:HIS:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:138:GLN:N	14:R:211:LYS:O	2.44	0.43
4:G:91:VAL:HB	4:G:139:ILE:HA	2.00	0.43
5:I:51:ASN:OD1	5:I:52:ILE:N	2.41	0.43
11:A:67:CYS:O	11:A:70:CYS:N	2.42	0.43
11:A:532:ARG:HH22	11:A:745:GLN:HB3	1.84	0.43
13:D:205:ASP:OD1	13:D:205:ASP:N	2.52	0.43
1:C:23:SER:OG	1:C:24:ASN:N	2.51	0.43
5:I:78:CYS:C	5:I:79:HIS:CG	2.96	0.43
12:B:215:GLN:HG3	12:B:476:ARG:NH2	2.34	0.43
12:B:1048:THR:HG22	12:B:1050:ILE:HG12	2.00	0.43
12:B:1152:MET:HE1	12:B:1197:PRO:HD3	1.99	0.43
9:S:203:TYR:HE2	11:A:1172:LEU:HA	1.83	0.43
1:C:29:MET:HE2	1:C:29:MET:HB3	1.97	0.43
1:C:33:LEU:O	1:C:37:MET:HG3	2.17	0.43
4:G:94:CYS:HB3	4:G:128:PRO:HB2	2.00	0.43
11:A:91:PHE:CZ	11:A:204:THR:HG22	2.54	0.43
11:A:1120:LEU:HD11	11:A:1306:LEU:HG	1.99	0.43
12:B:409:ALA:O	12:B:413:LEU:HD13	2.19	0.43
16:H:109:LYS:HD2	16:H:109:LYS:HA	1.68	0.43
5:I:76:PRO:HB2	5:I:77:LYS:HZ1	1.84	0.43
14:R:73:LEU:HD21	14:R:78:ALA:HA	2.01	0.43
11:A:75:ASN:HB3	15:M:55:LYS:HE3	2.01	0.43
11:A:1301:GLU:HA	11:A:1302:PRO:HD3	1.83	0.43
4:G:21:ARG:HH21	4:G:24:GLN:HG3	1.84	0.42
4:G:91:VAL:HG22	4:G:101:VAL:HG12	2.01	0.42
9:S:287:ARG:CG	9:S:291:GLU:HG3	2.49	0.42
13:D:212:LYS:O	13:D:216:ASN:ND2	2.51	0.42
16:H:130:ARG:HA	16:H:130:ARG:HD2	1.39	0.42
11:A:739:ASP:OD2	16:H:19:ARG:NH2	2.51	0.42
12:B:639:ILE:HD11	12:B:691:GLU:HG3	2.00	0.42
2:E:43:LYS:O	2:E:47:CYS:HB2	2.18	0.42
9:S:178:ILE:O	9:S:182:MET:HB2	2.20	0.42
11:A:115:LEU:HG	11:A:122:MET:HE2	2.01	0.42
11:A:122:MET:HA	11:A:125:ALA:HB3	2.00	0.42
5:I:74:GLU:HB2	5:I:81:ARG:HH21	1.85	0.42
6:J:5:VAL:HG12	6:J:6:ARG:HG2	2.01	0.42
12:B:1043:ASP:OD1	12:B:1043:ASP:N	2.45	0.42
13:D:127:ASP:HB3	13:D:142:LYS:HE3	2.02	0.42
4:G:96:GLN:HE21	4:G:97:HIS:HD2	1.67	0.42
16:H:133:ASN:OD1	16:H:134:ASN:ND2	2.52	0.42
2:E:117:THR:O	2:E:120:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:27:PHE:N	5:I:36:GLU:O	2.49	0.42
11:A:1039:LYS:HB2	11:A:1039:LYS:HE3	1.86	0.42
3:F:133:VAL:HG13	11:A:1444:MET:HB3	2.01	0.42
5:I:59:VAL:HG22	5:I:60:GLN:H	1.84	0.42
9:S:234:LYS:O	9:S:235:ASP:C	2.62	0.42
11:A:968:GLN:HA	11:A:973:ILE:HD13	2.01	0.42
12:B:276:ILE:HG22	12:B:278:GLN:H	1.85	0.42
12:B:760:ASP:OD1	12:B:760:ASP:N	2.52	0.42
1:C:54:ASN:ND2	1:C:60:ASP:OD1	2.47	0.42
11:A:106:VAL:HG23	11:A:113:LEU:HA	2.02	0.42
11:A:174:ILE:HG22	11:A:183:GLY:HA2	2.02	0.42
11:A:1116:LEU:HB3	11:A:1308:THR:HB	2.01	0.42
10:Q:21:PHE:C	10:Q:22:ILE:HG13	2.44	0.42
13:D:39:ASN:OD1	13:D:43:GLU:N	2.48	0.42
13:D:164:ILE:O	13:D:168:LYS:HB3	2.20	0.42
1:C:14:SER:HB2	1:C:17:ASN:HB2	2.01	0.41
11:A:108:MET:SD	11:A:108:MET:N	2.82	0.41
11:A:618:GLU:HG2	11:A:620:LYS:H	1.84	0.41
12:B:915:THR:HA	12:B:936:ASP:HA	2.02	0.41
11:A:746:MET:HE2	12:B:1015:HIS:CD2	2.55	0.41
11:A:958:VAL:HG11	11:A:1052:GLN:HB3	2.03	0.41
5:I:29:CYS:O	10:Q:426:LYS:NZ	2.50	0.41
7:K:102:LYS:O	7:K:105:PHE:N	2.49	0.41
11:A:55:ASP:OD1	11:A:58:LEU:HG	2.20	0.41
12:B:550:ASP:HA	12:B:551:PRO:HD3	1.92	0.41
14:R:108:LEU:HD11	14:R:120:TYR:HE2	1.85	0.41
4:G:119:LEU:HB2	4:G:132:SER:HB3	2.03	0.41
5:I:57:GLY:O	5:I:59:VAL:N	2.53	0.41
6:J:19:GLU:OE1	6:J:19:GLU:N	2.51	0.41
11:A:420:ARG:HE	11:A:420:ARG:HB2	1.64	0.41
11:A:549:MET:HE1	11:A:656:TRP:HD1	1.84	0.41
12:B:841:MET:HG2	12:B:846:ILE:HD11	2.02	0.41
5:I:90:GLN:O	5:I:92:ARG:N	2.53	0.41
14:R:223:GLN:NE2	14:R:224:VAL:O	2.53	0.41
6:J:44:TYR:HA	6:J:47:ARG:HD3	2.02	0.41
11:A:110:CYS:CB	11:A:167:CYS:SG	2.88	0.41
11:A:368:LYS:HE3	11:A:368:LYS:HB2	1.92	0.41
11:A:1197:LEU:HD12	11:A:1209:MET:HE1	2.03	0.41
2:E:55:ARG:HA	2:E:58:MET:HG2	2.01	0.41
5:I:73:ARG:HE	5:I:73:ARG:HB3	1.52	0.41
10:Q:27:MET:HA	10:Q:30:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:579:SER:HA	11:A:582:ILE:HG12	2.03	0.41
12:B:707:PRO:O	12:B:711:GLU:HB2	2.21	0.41
5:I:45:ARG:NH1	11:A:1151:GLU:OE2	2.53	0.41
6:J:65:PRO:HB2	6:J:68:LYS:HG2	2.03	0.41
9:S:197:ALA:O	9:S:201:ILE:HG13	2.21	0.41
9:S:242:LYS:HA	9:S:245:ILE:HG12	2.02	0.41
10:Q:411:LYS:HA	10:Q:411:LYS:HD3	1.85	0.41
12:B:344:LYS:HB2	12:B:347:LYS:HB2	2.02	0.41
16:H:92:ASP:OD1	16:H:92:ASP:N	2.44	0.41
16:H:116:TYR:HB2	16:H:123:MET:HE2	2.01	0.41
16:H:124:ARG:NH1	16:H:126:GLU:OE2	2.54	0.41
4:G:19:GLY:O	4:G:22:MET:HG3	2.21	0.41
12:B:578:THR:HG22	12:B:622:LYS:HB3	2.03	0.41
12:B:921:ASP:OD1	12:B:921:ASP:N	2.54	0.41
16:H:108:SER:OG	16:H:109:LYS:N	2.51	0.41
5:I:76:PRO:HB2	5:I:77:LYS:NZ	2.36	0.40
11:A:261:ASP:CG	11:A:320:ARG:HH22	2.28	0.40
11:A:353:ILE:HG22	11:A:468:PHE:HB2	2.03	0.40
14:R:96:ARG:NH2	14:R:107:LEU:HD22	2.36	0.40
16:H:112:ILE:HD13	16:H:112:ILE:HG21	1.85	0.40
7:K:1:MET:HB2	7:K:1:MET:HE2	1.54	0.40
9:S:245:ILE:O	9:S:248:ILE:HG22	2.21	0.40
11:A:847:ASP:OD1	11:A:847:ASP:N	2.51	0.40
11:A:1204:ASP:OD1	11:A:1204:ASP:N	2.53	0.40
11:A:481:ASP:OD1	11:A:481:ASP:N	2.53	0.40
11:A:1002:GLY:O	11:A:1008:GLN:NE2	2.55	0.40
12:B:778:MET:HE2	12:B:794:ASN:HD22	1.86	0.40
16:H:123:MET:HE2	16:H:123:MET:HB3	1.98	0.40
2:E:201:LYS:HD3	11:A:946:VAL:HA	2.02	0.40
12:B:914:LYS:HB3	12:B:914:LYS:HE2	1.84	0.40
16:H:104:PHE:CE2	16:H:136:LYS:HA	2.57	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	C	260/318 (82%)	252 (97%)	8 (3%)	0	100	100
2	E	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
3	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
4	G	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
5	I	114/122 (93%)	88 (77%)	18 (16%)	8 (7%)	1	2
6	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
7	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
8	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
9	S	162/309 (52%)	139 (86%)	19 (12%)	4 (2%)	4	17
10	Q	208/735 (28%)	200 (96%)	8 (4%)	0	100	100
11	A	1386/1733 (80%)	1315 (95%)	69 (5%)	2 (0%)	48	77
12	B	1147/1224 (94%)	1103 (96%)	42 (4%)	2 (0%)	43	72
13	D	153/221 (69%)	148 (97%)	5 (3%)	0	100	100
14	R	190/400 (48%)	183 (96%)	7 (4%)	0	100	100
15	M	91/345 (26%)	87 (96%)	4 (4%)	0	100	100
16	H	132/146 (90%)	122 (92%)	10 (8%)	0	100	100
All	All	4527/6354 (71%)	4302 (95%)	209 (5%)	16 (0%)	31	59

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	76	PRO
5	I	113	ASP
9	S	238	PRO
12	B	22	SER
12	B	474	SER
5	I	57	GLY
5	I	91	ARG
9	S	239	ALA
5	I	47	GLU
5	I	79	HIS
9	S	235	ASP
11	A	569	LYS
5	I	56	ALA
9	S	206	VAL

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Mol	Chain	Res	Type
5	I	58	VAL
11	A	464	PRO

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%)	101 (92%)	9 (8%)	10	32
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	77
10	Q	198/641 (31%)	198 (100%)	0	100	100
11	A	1221/1520 (80%)	1218 (100%)	3 (0%)	87	96
12	B	1007/1061 (95%)	1006 (100%)	1 (0%)	88	97
13	D	139/200 (70%)	139 (100%)	0	100	100
14	R	187/363 (52%)	187 (100%)	0	100	100
15	M	79/299 (26%)	79 (100%)	0	100	100
16	H	119/128 (93%)	117 (98%)	2 (2%)	53	82
All	All	4056/5586 (73%)	4038 (100%)	18 (0%)	81	94

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	60	GLN
5	I	61	ASP

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Mol	Chain	Res	Type
5	I	62	ILE
5	I	77	LYS
5	I	82	GLU
5	I	84	VAL
5	I	86	PHE
5	I	102	VAL
5	I	111	THR
9	S	182	MET
9	S	206	VAL
9	S	236	LEU
11	A	676	MET
11	A	688	LYS
11	A	692	ASP
12	B	662	MET
16	H	109	LYS
16	H	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	7	GLN
1	C	73	GLN
2	E	101	GLN
2	E	113	GLN
4	G	10	ASN
4	G	97	HIS
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
7	K	76	GLN
7	K	89	ASN
8	L	53	HIS
9	S	220	ASN
9	S	252	ASN
9	S	255	ASN
9	S	304	ASN
10	Q	122	GLN
10	Q	140	HIS

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Mol	Chain	Res	Type
10	Q	331	GLN
10	Q	369	ASN
10	Q	399	ASN
11	A	71	GLN
11	A	109	HIS
11	A	209	ASN
11	A	213	HIS
11	A	287	HIS
11	A	299	HIS
11	A	306	ASN
11	A	311	GLN
11	A	339	ASN
11	A	445	ASN
11	A	451	HIS
11	A	490	HIS
11	A	510	GLN
11	A	517	ASN
11	A	525	GLN
11	A	587	HIS
11	A	650	GLN
11	A	660	ASN
11	A	736	ASN
11	A	741	ASN
11	A	742	ASN
11	A	757	ASN
11	A	802	ASN
11	A	854	ASN
11	A	935	GLN
11	A	975	HIS
11	A	1008	GLN
11	A	1048	ASN
11	A	1312	ASN
11	A	1378	GLN
12	B	73	GLN
12	B	350	GLN
12	B	357	GLN
12	B	395	GLN
12	B	465	ASN
12	B	572	HIS
12	B	583	ASN
12	B	770	GLN
12	B	958	GLN

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Mol	Chain	Res	Type
12	B	984	HIS
12	B	1015	HIS
12	B	1025	HIS
12	B	1065	GLN
12	B	1161	HIS
12	B	1177	HIS
13	D	216	ASN
14	R	88	HIS
14	R	265	HIS
16	H	134	ASN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	R	2
15	M	1
12	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	65:THR	C	66:PHE	N	4.70
1	R	56:SER	C	57:LEU	N	3.73
1	B	1155:SER	C	1156:ASP	N	3.25
1	R	227:SER	C	228:MET	N	3.02

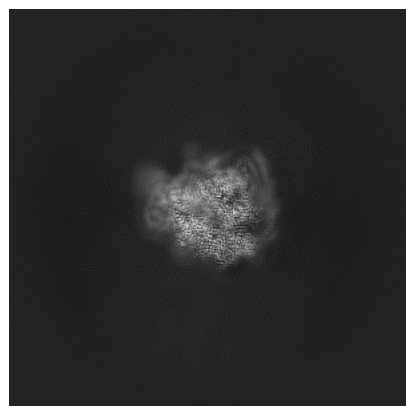
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71476. These allow visual inspection of the internal detail of the map and identification of artifacts.

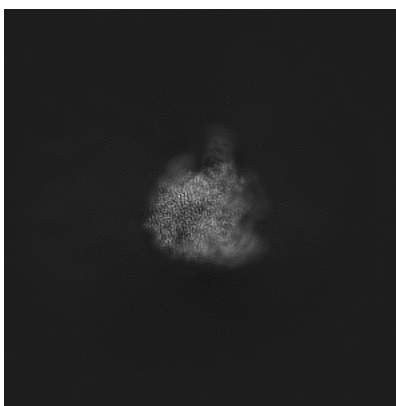
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

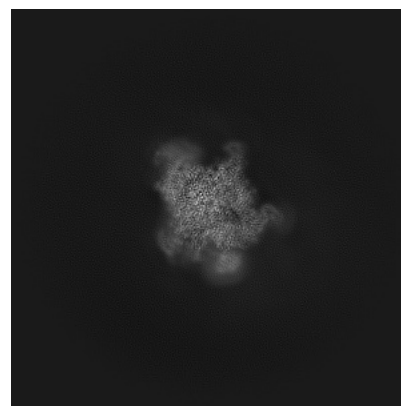
6.1.1 Primary map



X

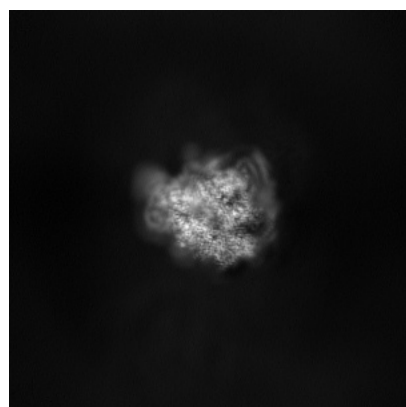


Y

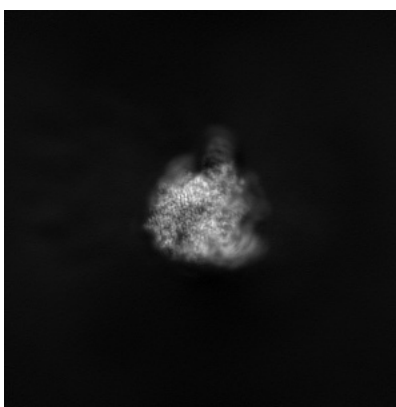


Z

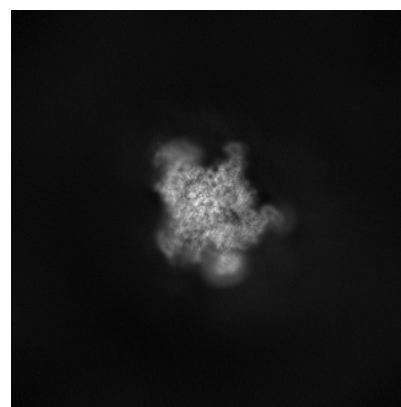
6.1.2 Raw map



X



Y

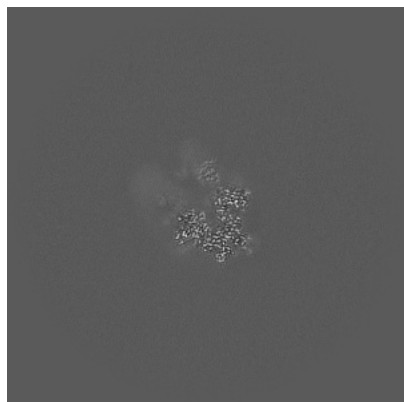


Z

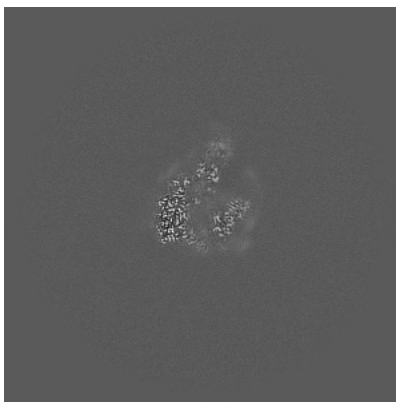
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

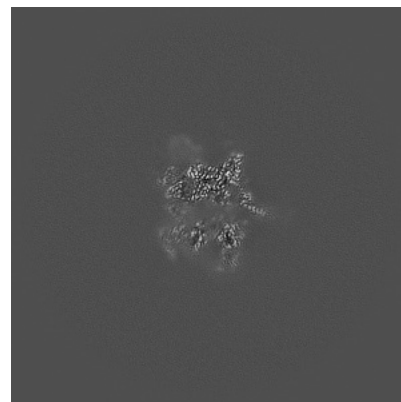
6.2.1 Primary map



X Index: 192

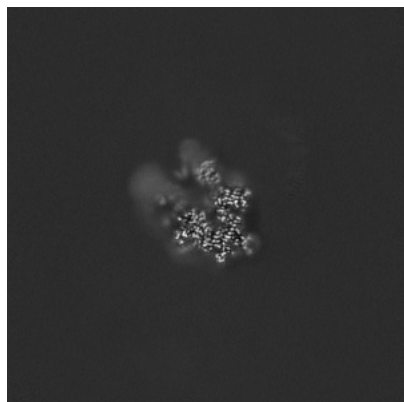


Y Index: 192

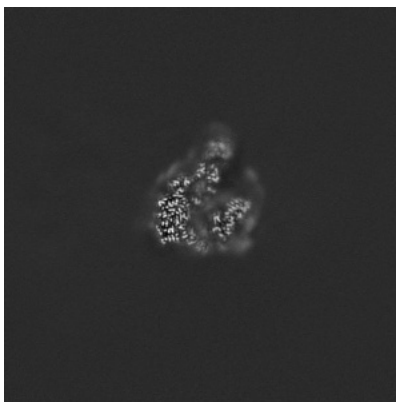


Z Index: 192

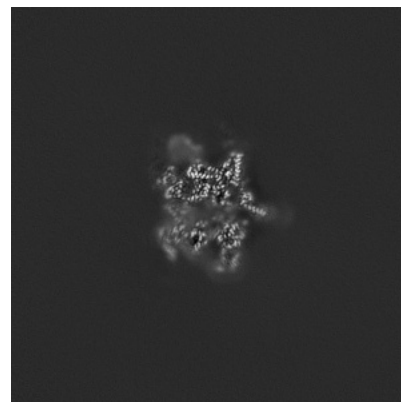
6.2.2 Raw map



X Index: 192



Y Index: 192

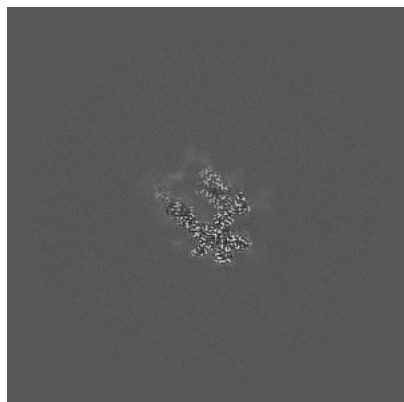


Z Index: 192

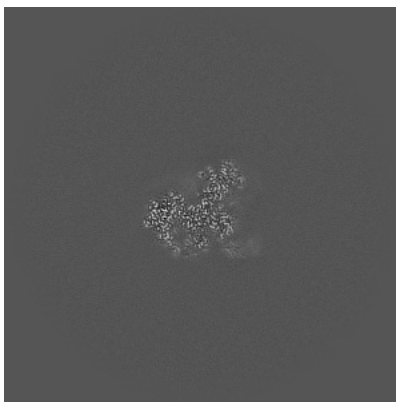
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

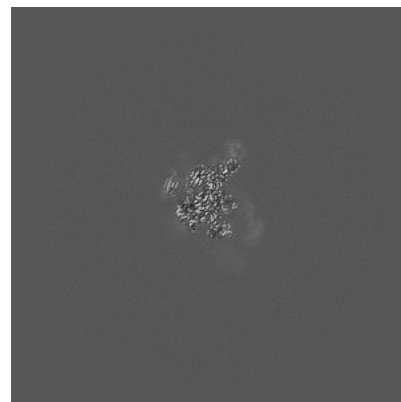
6.3.1 Primary map



X Index: 182

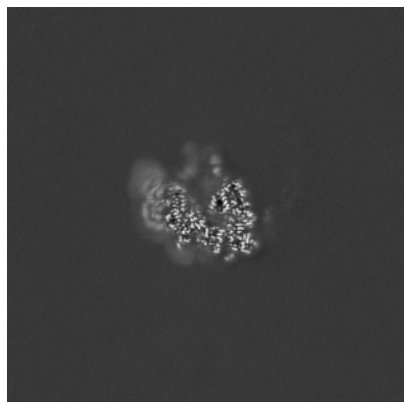


Y Index: 206

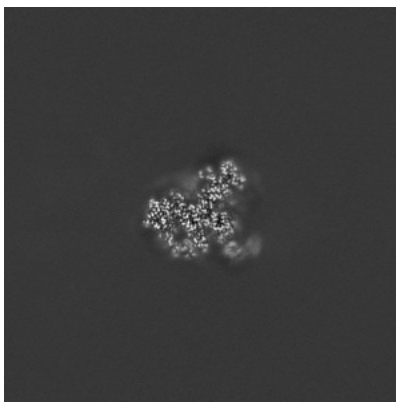


Z Index: 163

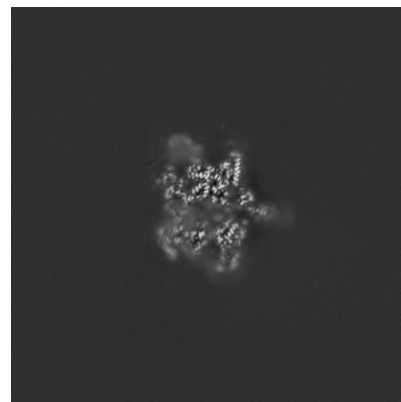
6.3.2 Raw map



X Index: 202



Y Index: 207

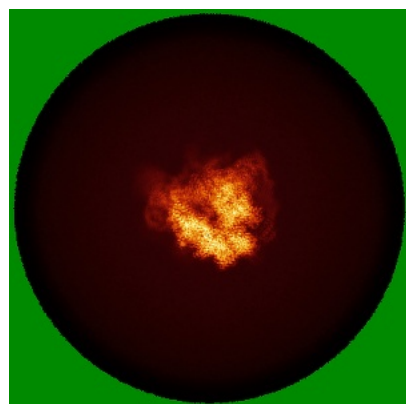


Z Index: 193

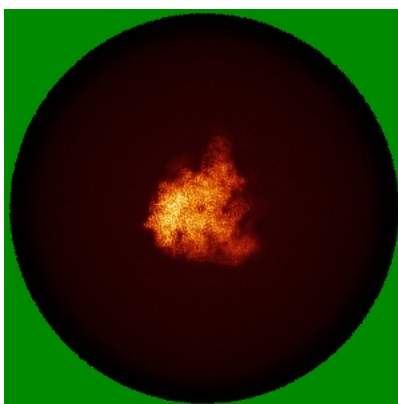
The images above show the largest variance slices of the map in three orthogonal directions.

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

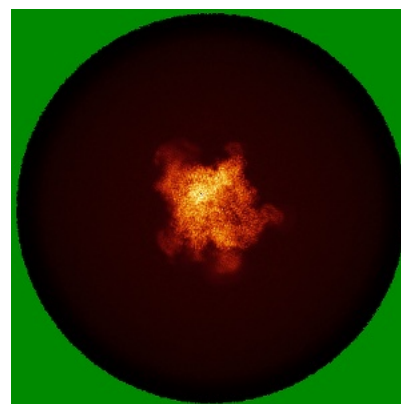
6.4.1 Primary map



X

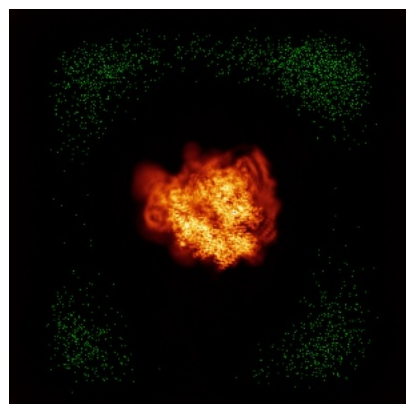


Y

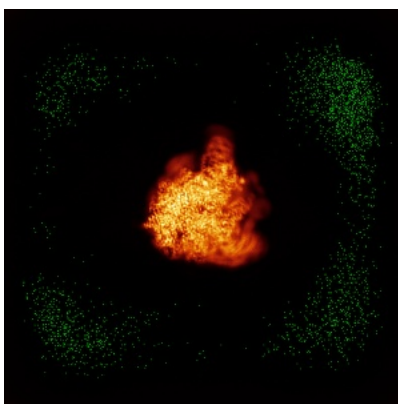


Z

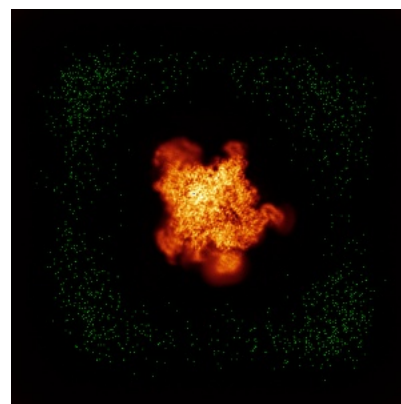
6.4.2 Raw map



X



Y

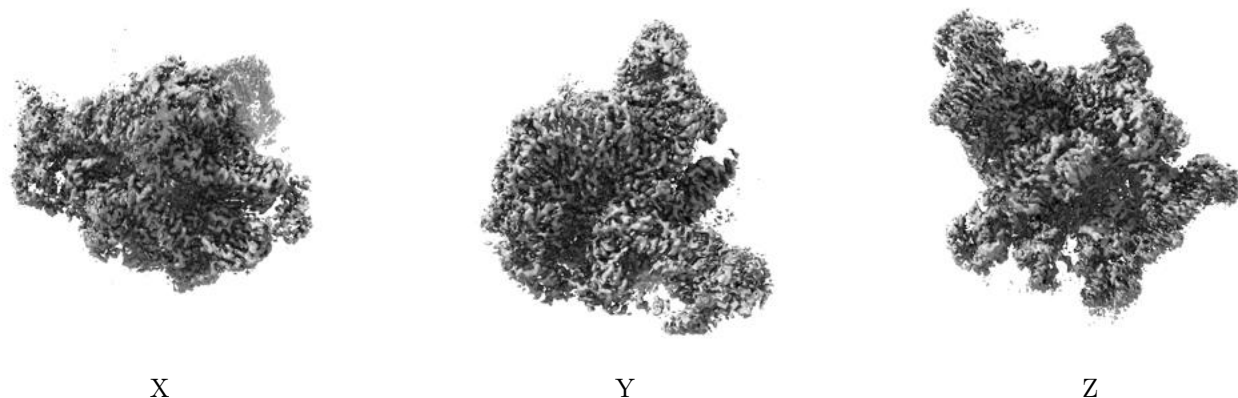


Z

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 0.652. 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.

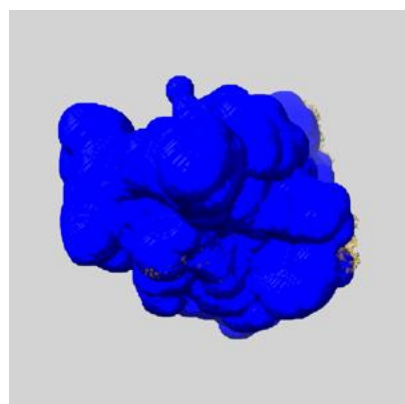
6.6 Mask visualisation [i](#)

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

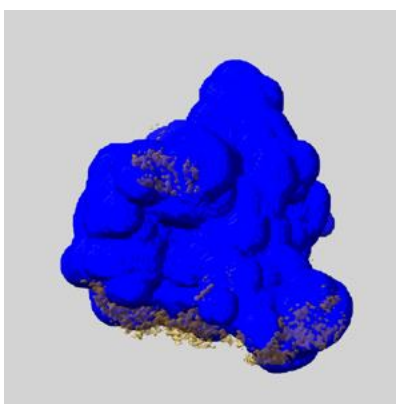
A mask typically either:

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

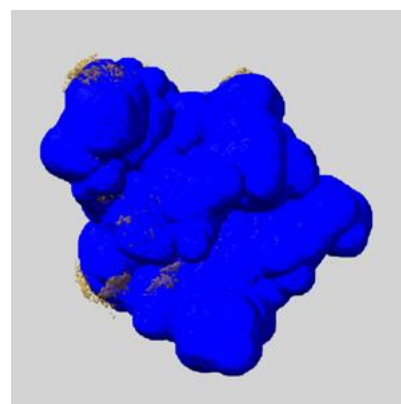
6.6.1 emd_71476_msk_1.map [i](#)



X



Y

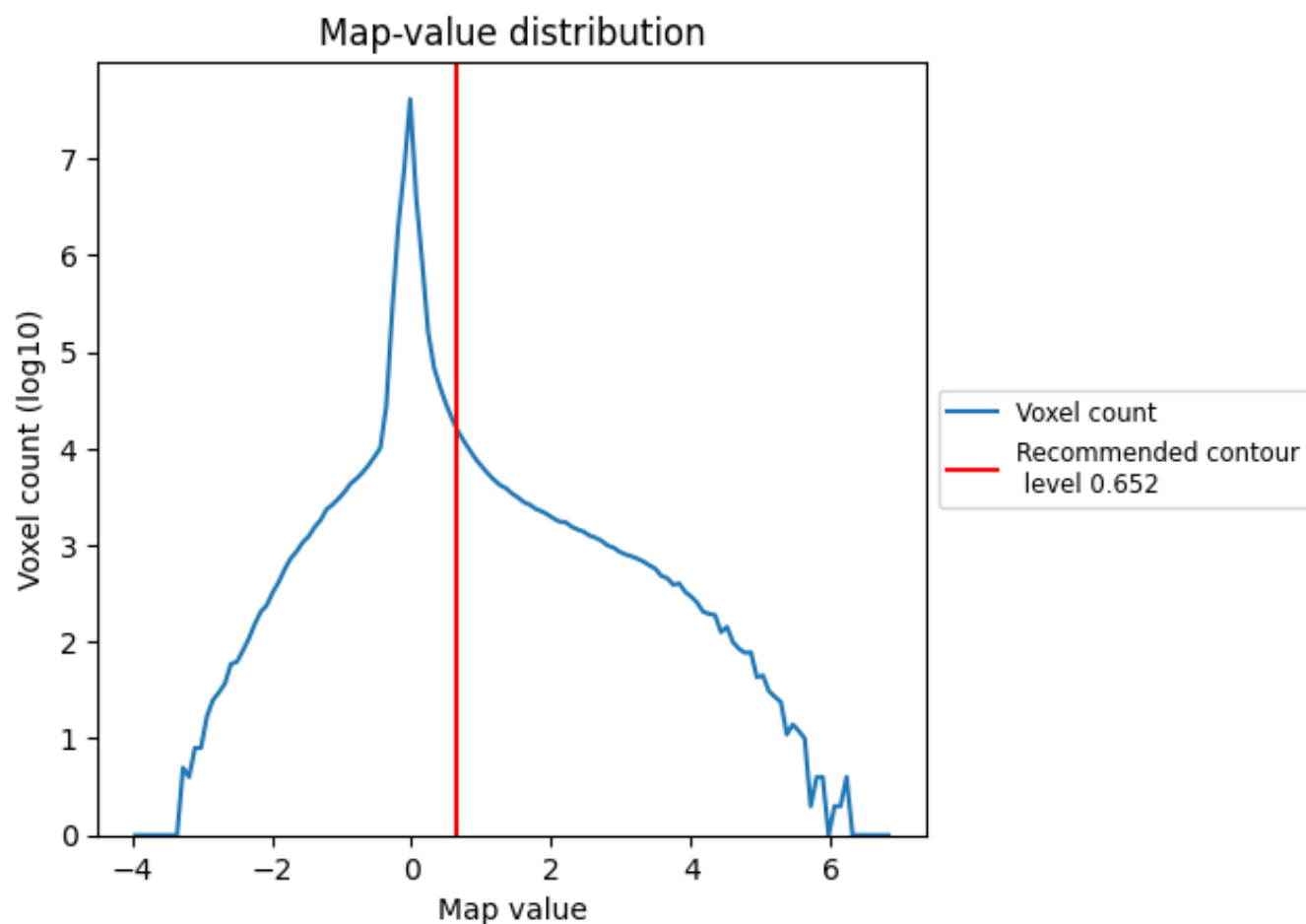


Z

7 Map analysis [i](#)

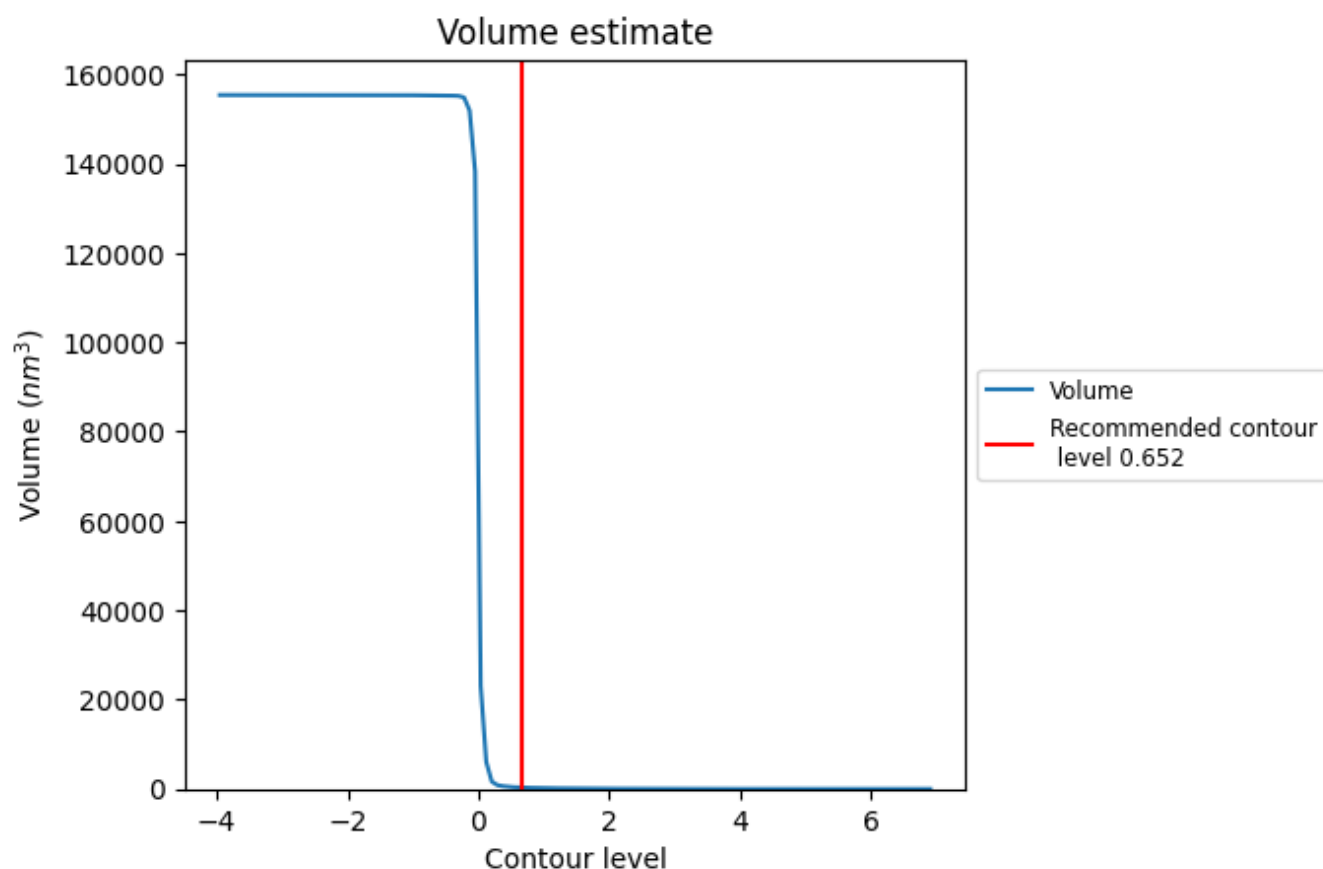
This section contains the results of statistical analysis of the map.

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.

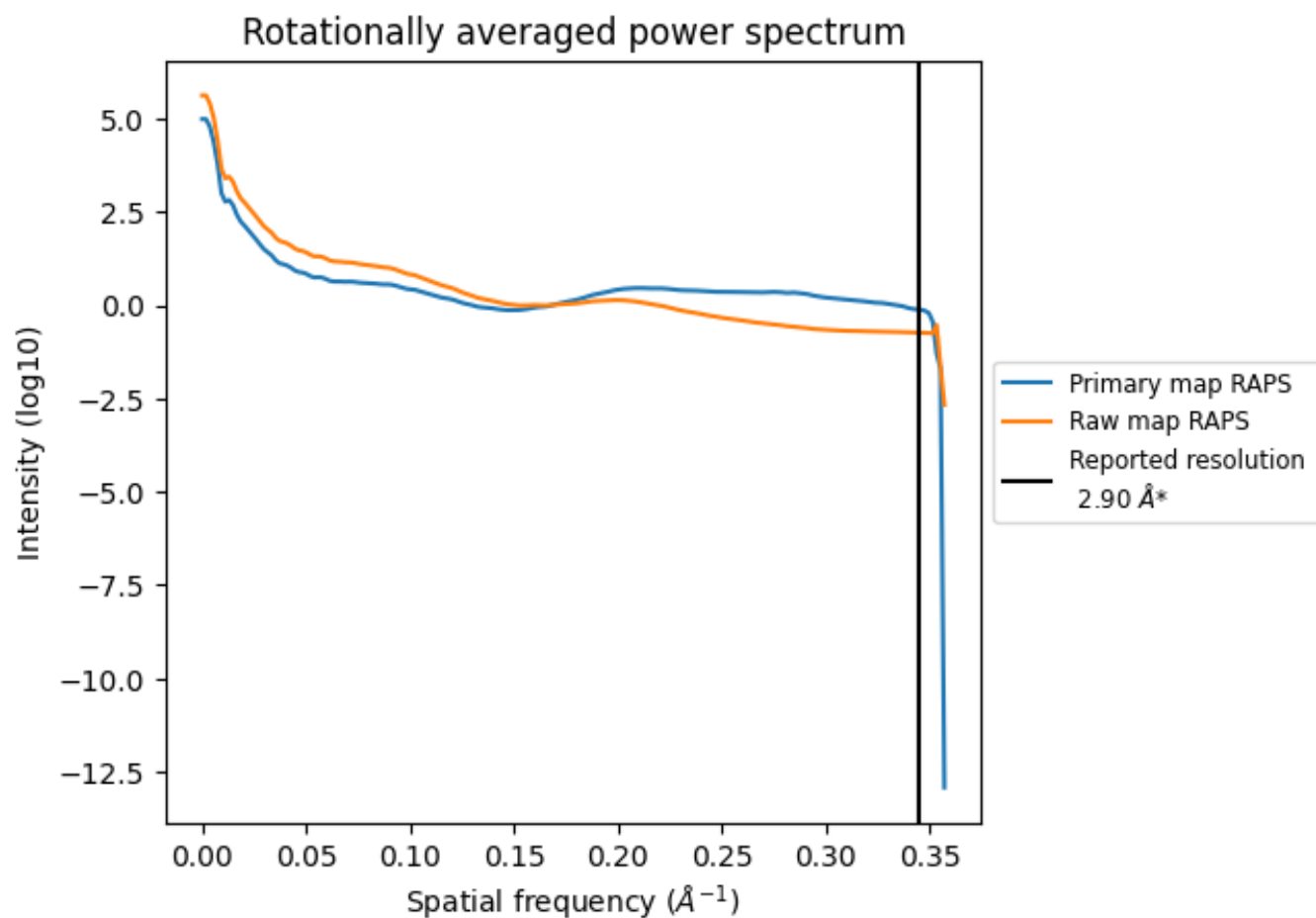
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 318 nm³; this corresponds to an approximate mass of 287 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 ⓘ

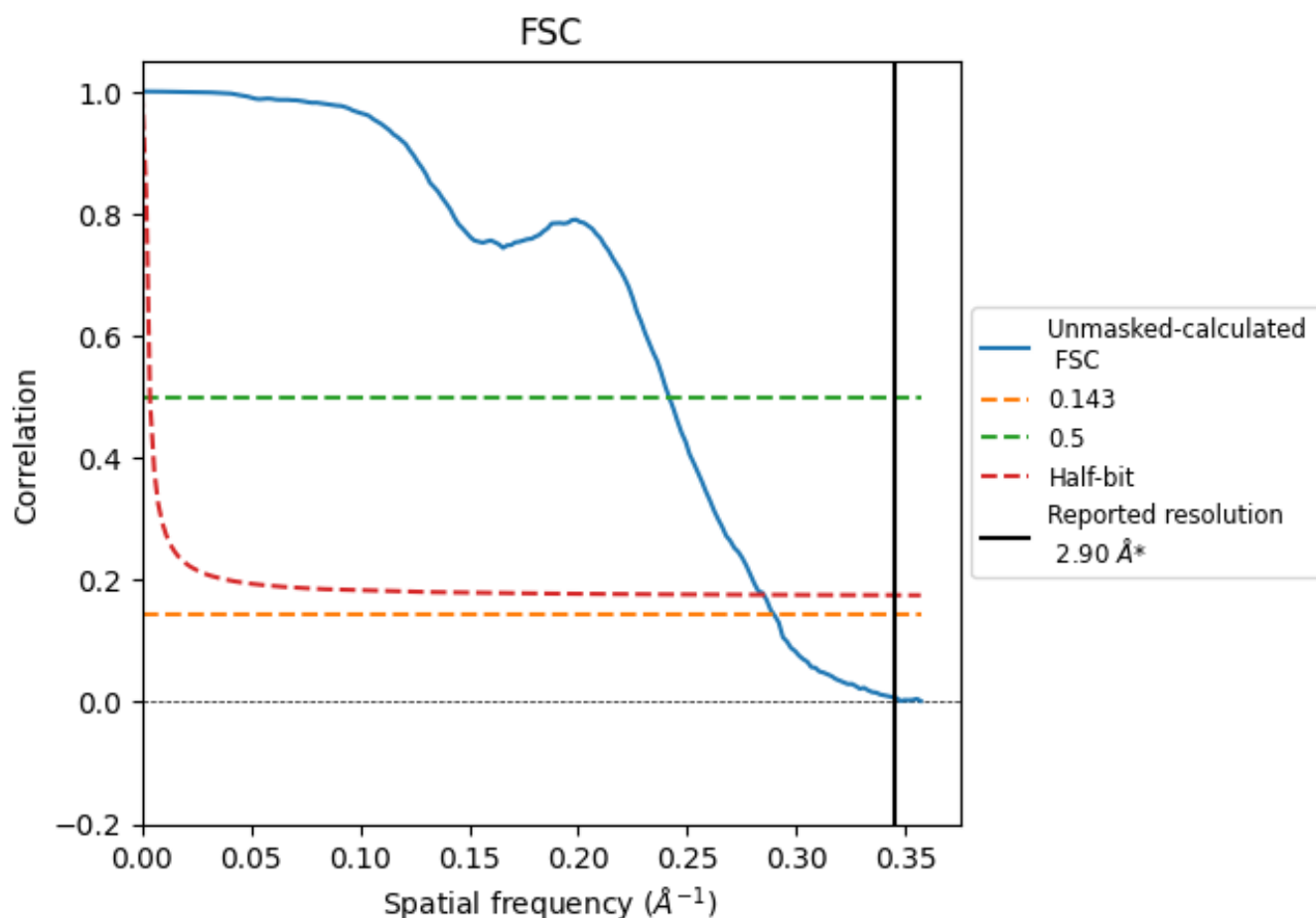


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

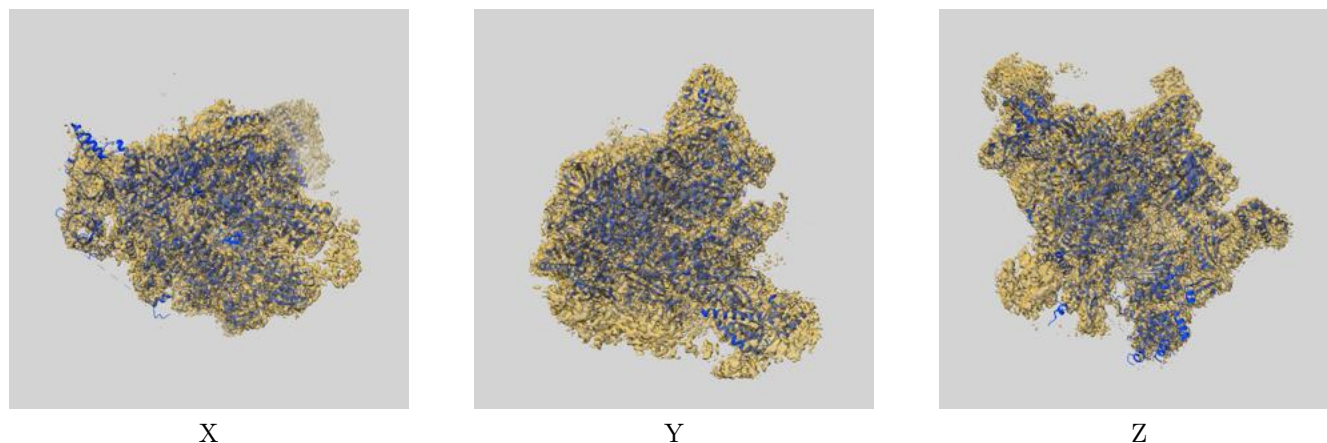
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.45	4.14	3.51

*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 3.45 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

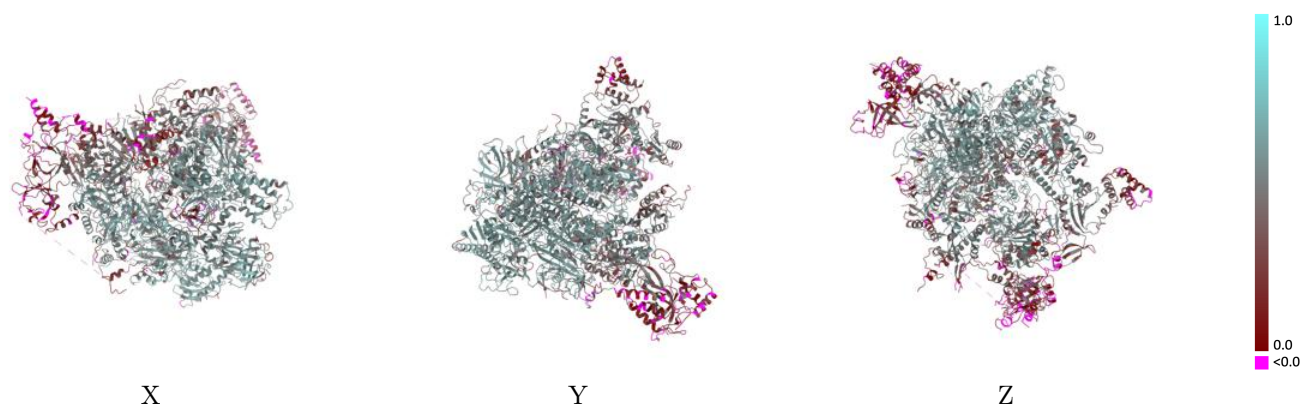
This section contains information regarding the fit between EMDB map EMD-71476 and PDB model 9PBD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



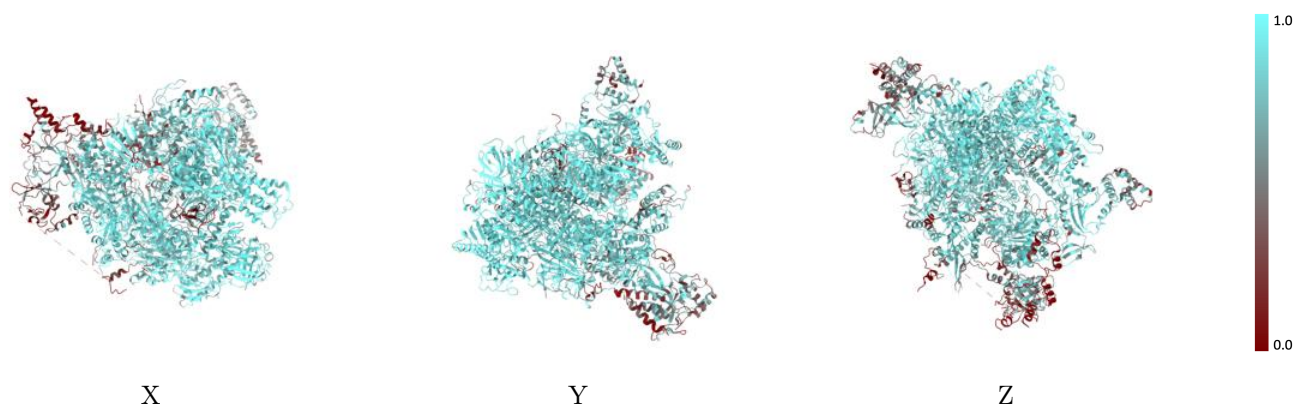
The images above show the 3D surface view of the map at the recommended contour level 0.652 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



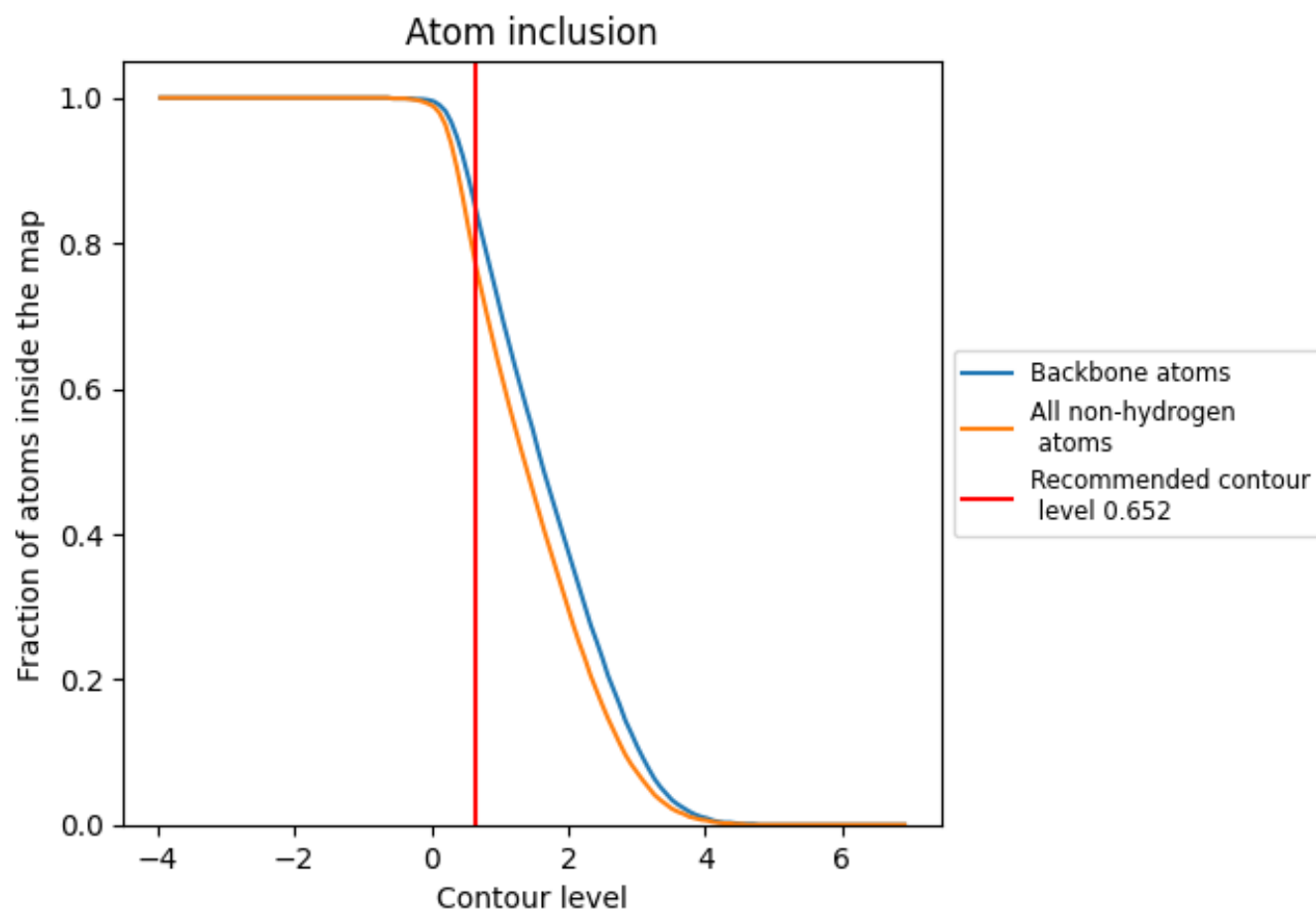
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.652).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.652) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.4440
A	0.8720	0.5150
B	0.8420	0.5010
C	0.9360	0.5740
D	0.4120	0.1400
E	0.8800	0.4940
F	0.9090	0.5450
G	0.6720	0.2830
H	0.8660	0.4970
I	0.7700	0.4050
J	0.8790	0.5370
K	0.8430	0.5220
L	0.8180	0.4470
M	0.6310	0.3830
Q	0.3480	0.1930
R	0.2800	0.1410
S	0.4240	0.2210

1.0

0.0

<0.0