



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:34 PM UTC

PDB ID : 9RTT / pdb_00009rtt
EMDB ID : EMD-54251
Title : Activated Elongation Complex with IWS1 and ELOF1
Authors : Walshe, J.L.; Cramer, P.
Deposited on : 2025-07-03
Resolution : 4.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

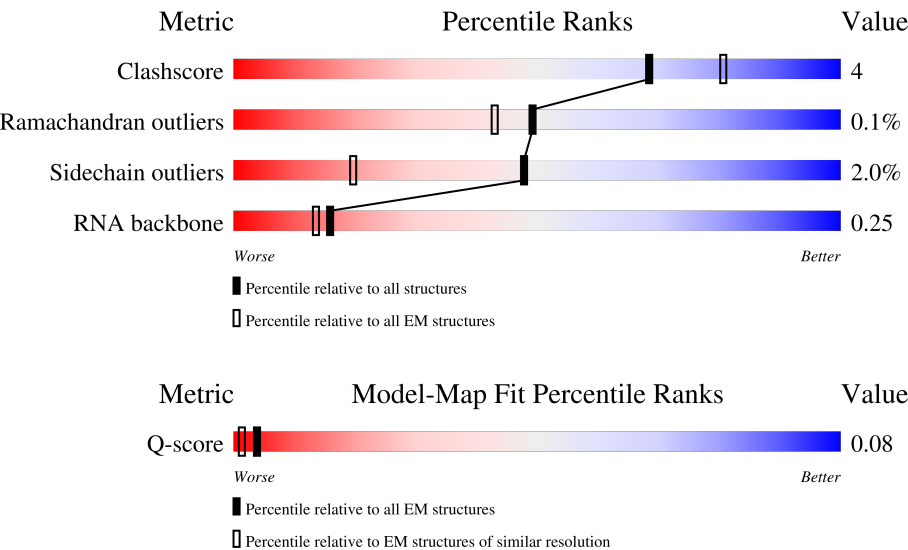
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.01 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	6765 (3.51 - 4.51)

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	D	142	
2	E	210	
3	F	127	

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Mol	Chain	Length	Quality of chain
4	G	172	
5	H	150	
6	I	125	
7	J	67	
8	K	117	
9	L	58	
10	P	21	
11	Q	1179	
12	T	257	
13	W	305	
14	Y	121	
15	b	85	
16	A	1970	
17	B	1174	
18	C	275	
19	M	1729	
20	N	247	
21	U	666	
22	V	531	
23	X	531	
24	Z	1087	
25	a	821	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 64867 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 RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	126	Total	C	N	O	S	0	0
			1014	634	170	206	4		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- 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
			1343	871	217	247	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	149	Total	C	N	O	S	0	0
			1198	759	195	239	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 9 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	21	Total	C	N	O	P	0	0
			439	196	68	154	21		

- Molecule 11 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	892	Total	C	N	O	S	0	0
			7240	4587	1266	1355	32		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 12 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	43	Total	C	N	O	P	0	0
			881	417	171	250	43		

- Molecule 13 is a protein called Superskiller complex protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	305	Total	C	N	O	S	0	0
			2374	1507	399	463	5		

- Molecule 14 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	116	Total	C	N	O	S	0	0
			912	570	159	174	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 15 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	67	Total	C	N	O	S	0	0
			523	322	84	110	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-1	SER	-	expression tag	UNP P60002
b	0	ASN	-	expression tag	UNP P60002
b	1	ALA	-	expression tag	UNP P60002

- Molecule 16 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	A	1473	Total	C	N	O	P	S	0	0
			11651	7315	2076	2183	2	75		

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	1136	Total	C	N	O	S	0	0
			9088	5745	1597	1682	64		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	258	Total	C	N	O	S	0	0
			2072	1300	356	410	6		

- Molecule 19 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	1074	Total	C	N	O	S	0	0
			8835	5613	1536	1644	42		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 20 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	31	Total	C	N	O	P	0	0
			633	302	106	194	31		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	179	Total	C	N	O	S	0	0
			1469	919	262	282	6		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	281	Total	C	N	O	S	0	0
			2310	1461	390	447	12		

- Molecule 23 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	227	Total	C	N	O	S	0	0
			1881	1207	340	329	5		

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	498	Total	C	N	O	S	0	0
			3976	2529	702	728	17		

- Molecule 25 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	232	Total	C	N	O	S	0	0
			1878	1183	340	340	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q96ST2
a	0	ASN	-	expression tag	UNP Q96ST2
a	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	I	2	Total	Zn	0
			2	2	
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	Y	1	Total	Zn	0
			1	1	
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	C	1	Total	Zn	0
			1	1	

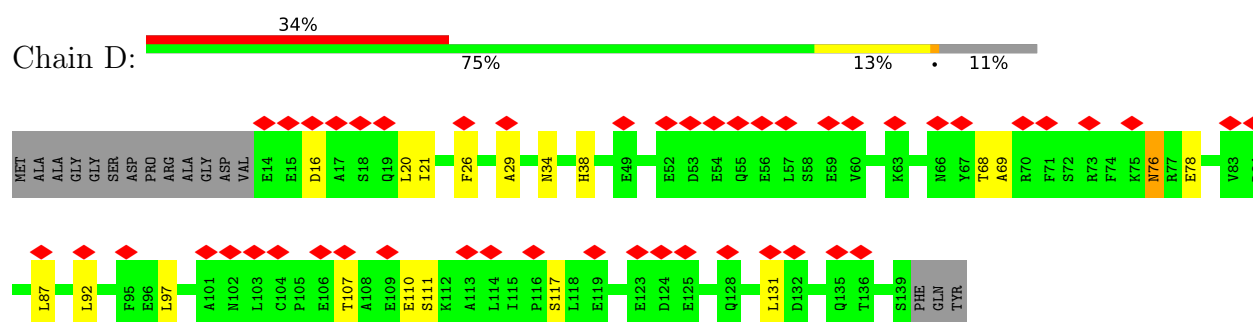
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

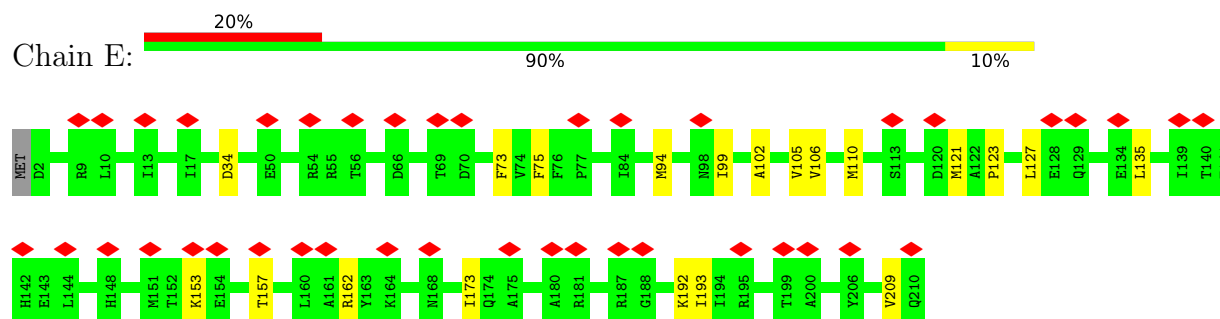
3 Residue-property plots [i](#)

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.

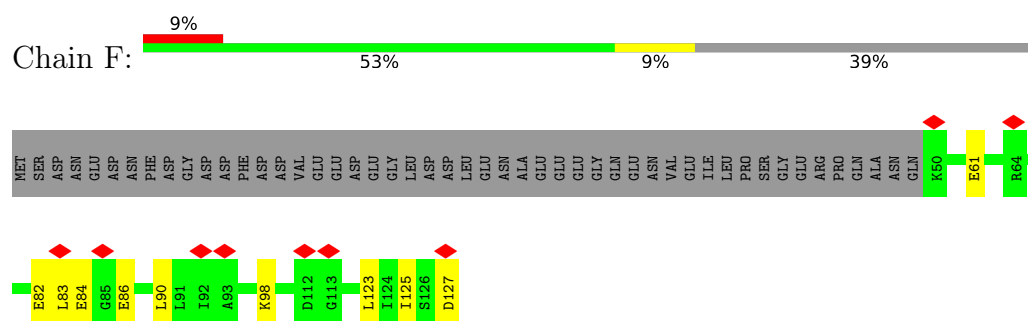
- Molecule 1: RNA polymerase II subunit D



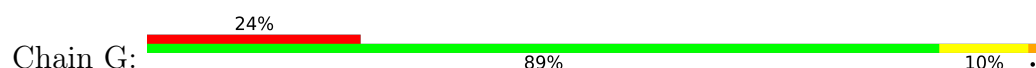
- Molecule 2: DNA-directed RNA polymerase II subunit E

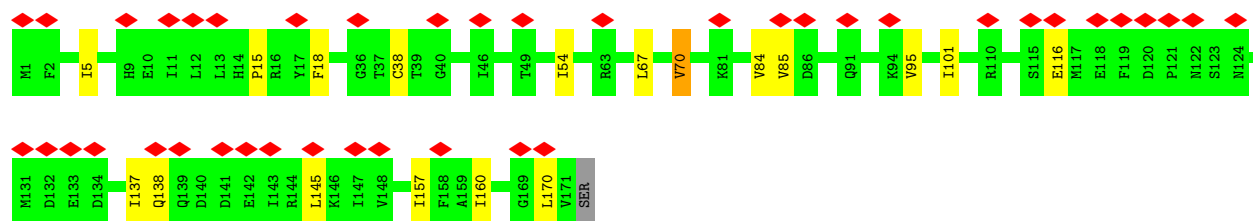


- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

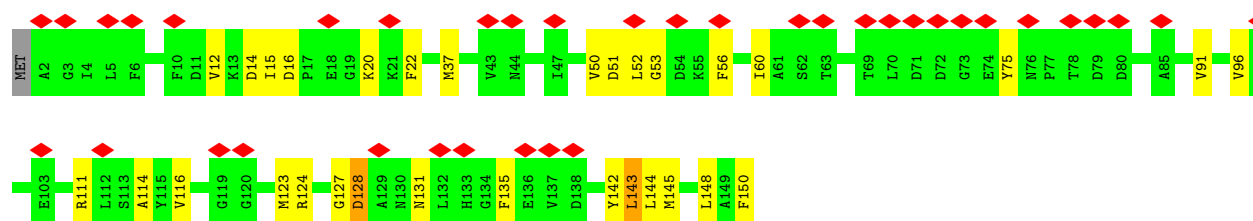
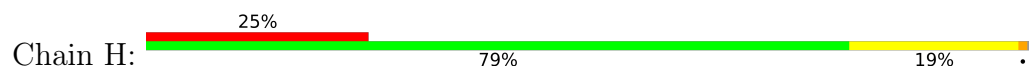


- Molecule 4: DNA-directed RNA polymerase II subunit RPB7

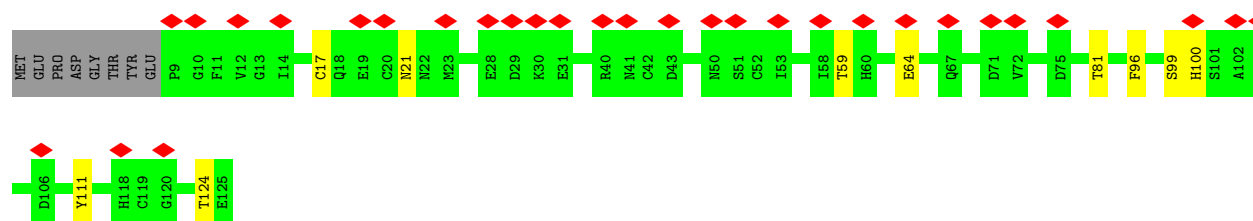
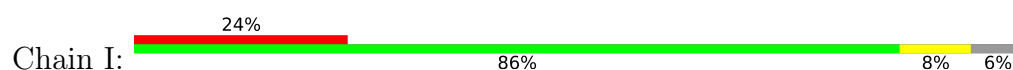




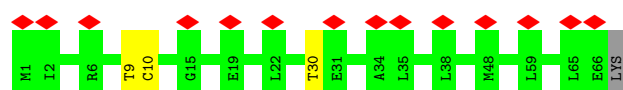
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3



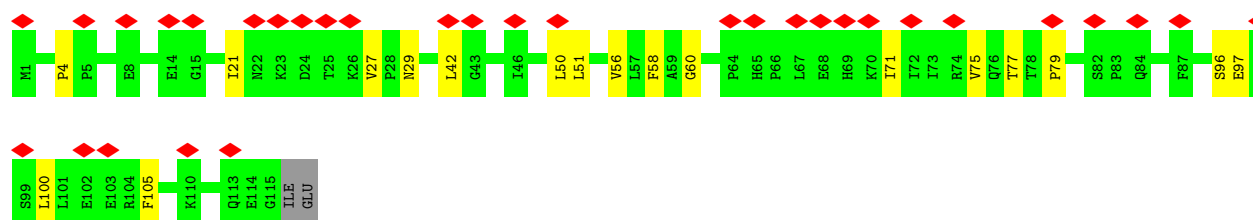
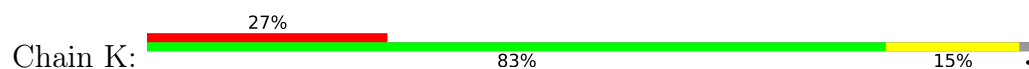
- Molecule 6: DNA-directed RNA polymerase II subunit RPB9



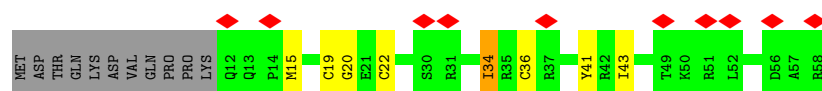
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5



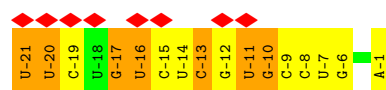
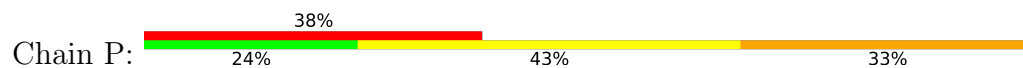
- Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a



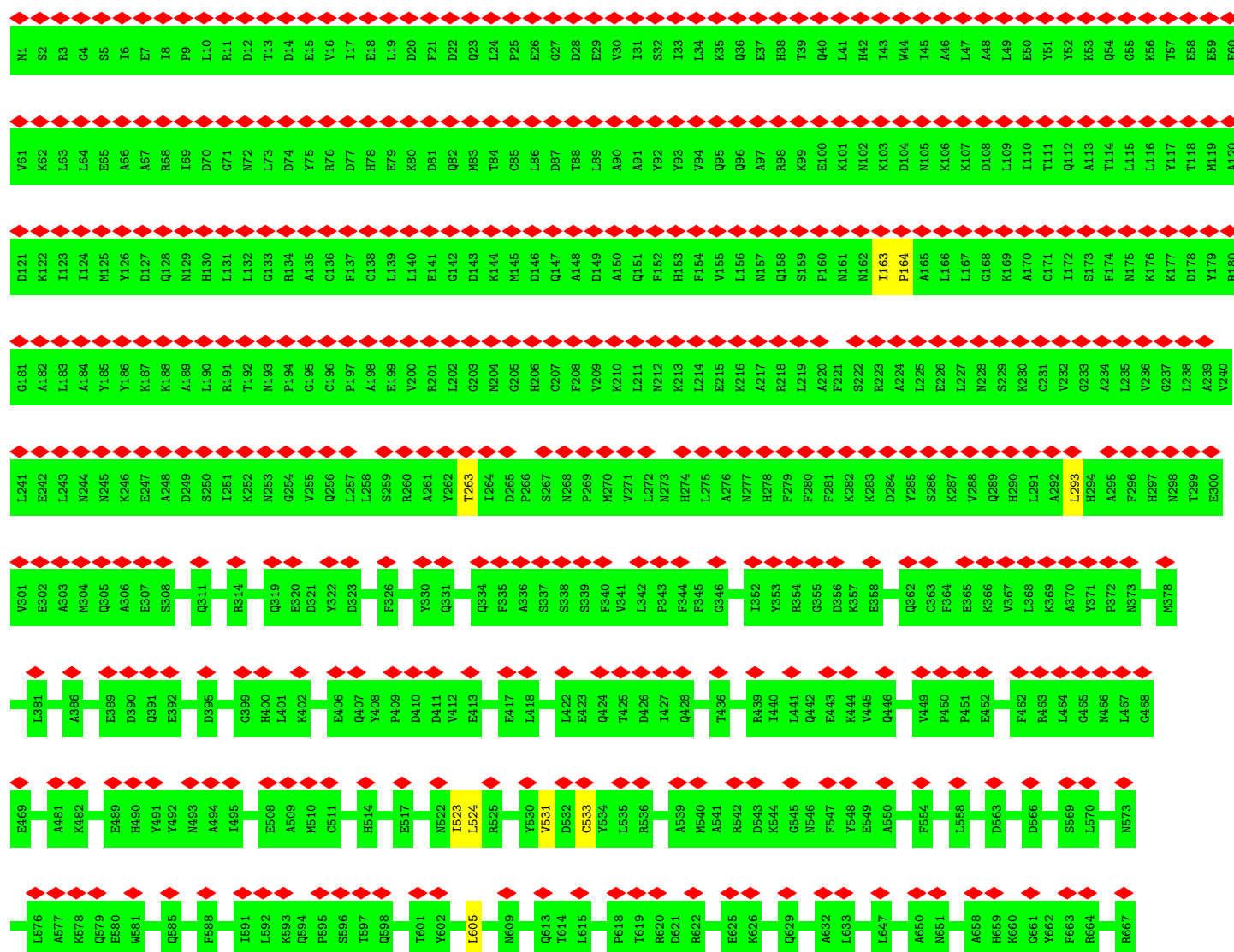
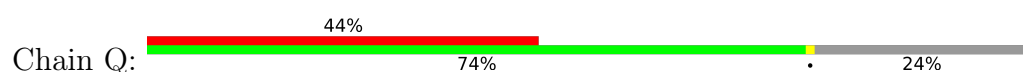
- Molecule 9: RNA polymerase II subunit K

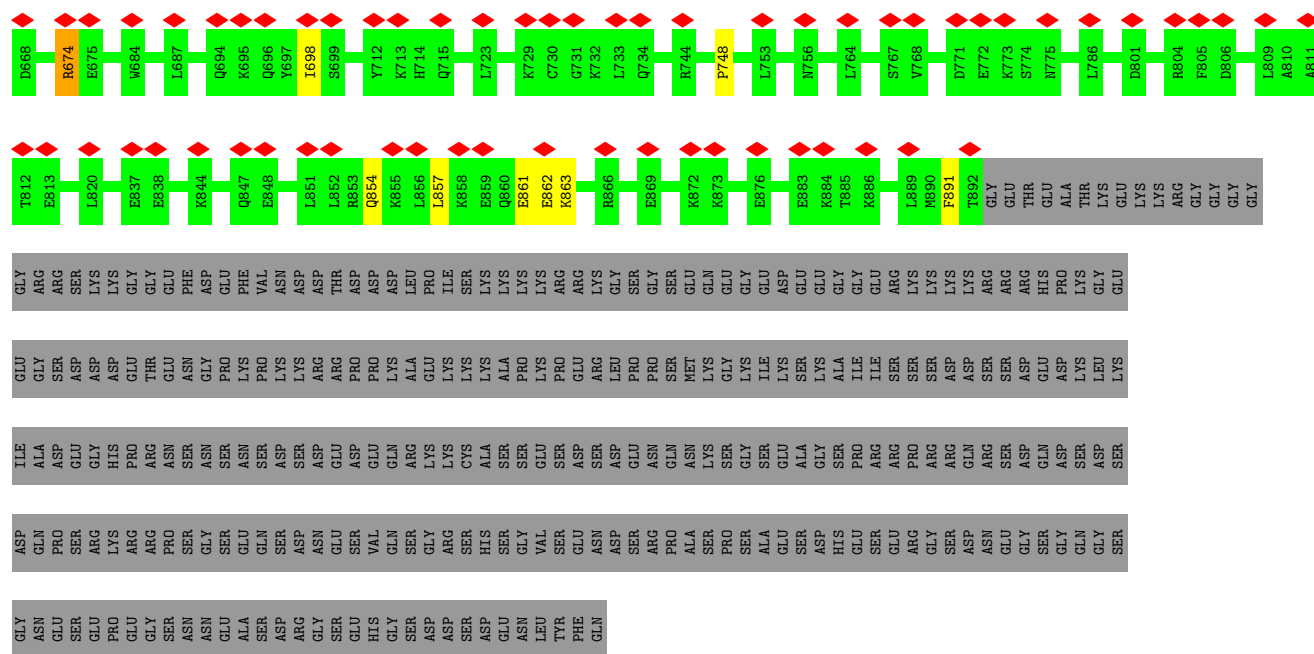


• Molecule 10: RNA

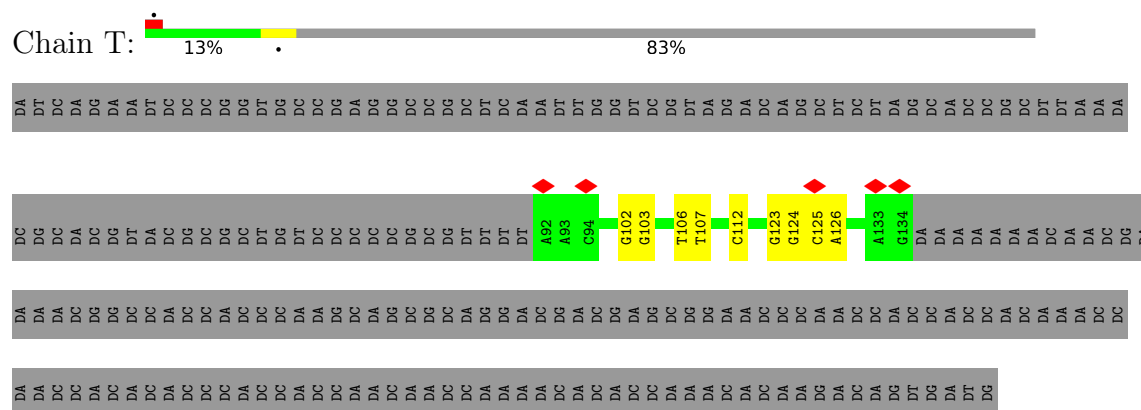


• Molecule 11: RNA polymerase-associated protein CTR9 homolog

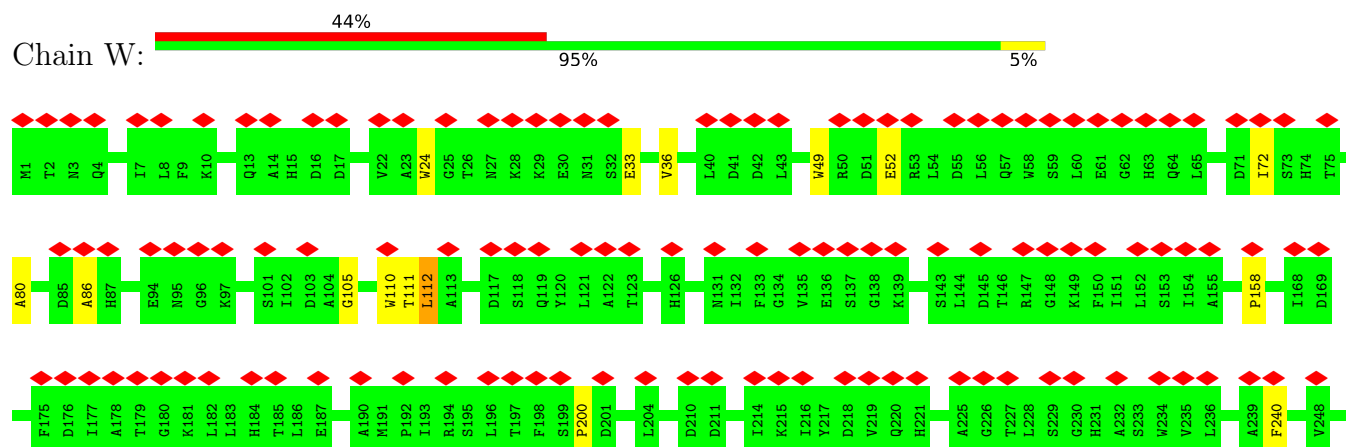


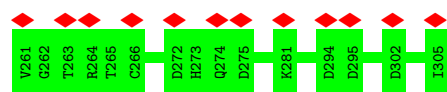


• Molecule 12: Template DNA

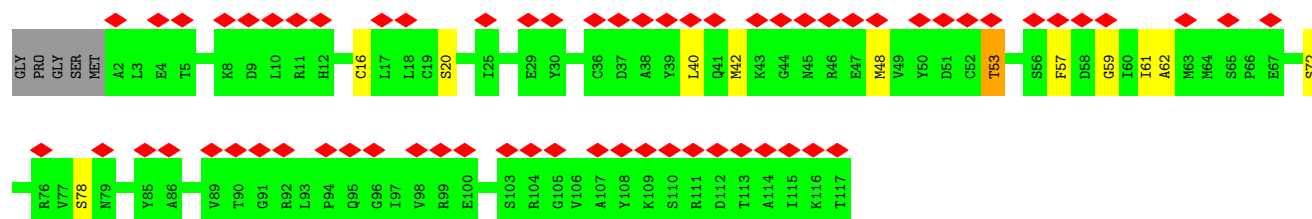
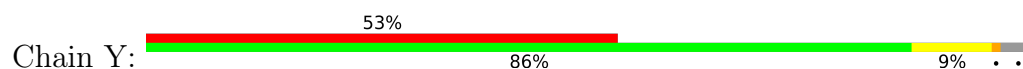


• Molecule 13: Supercollider complex protein 8

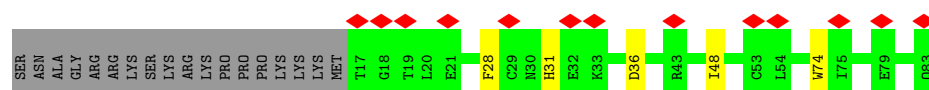




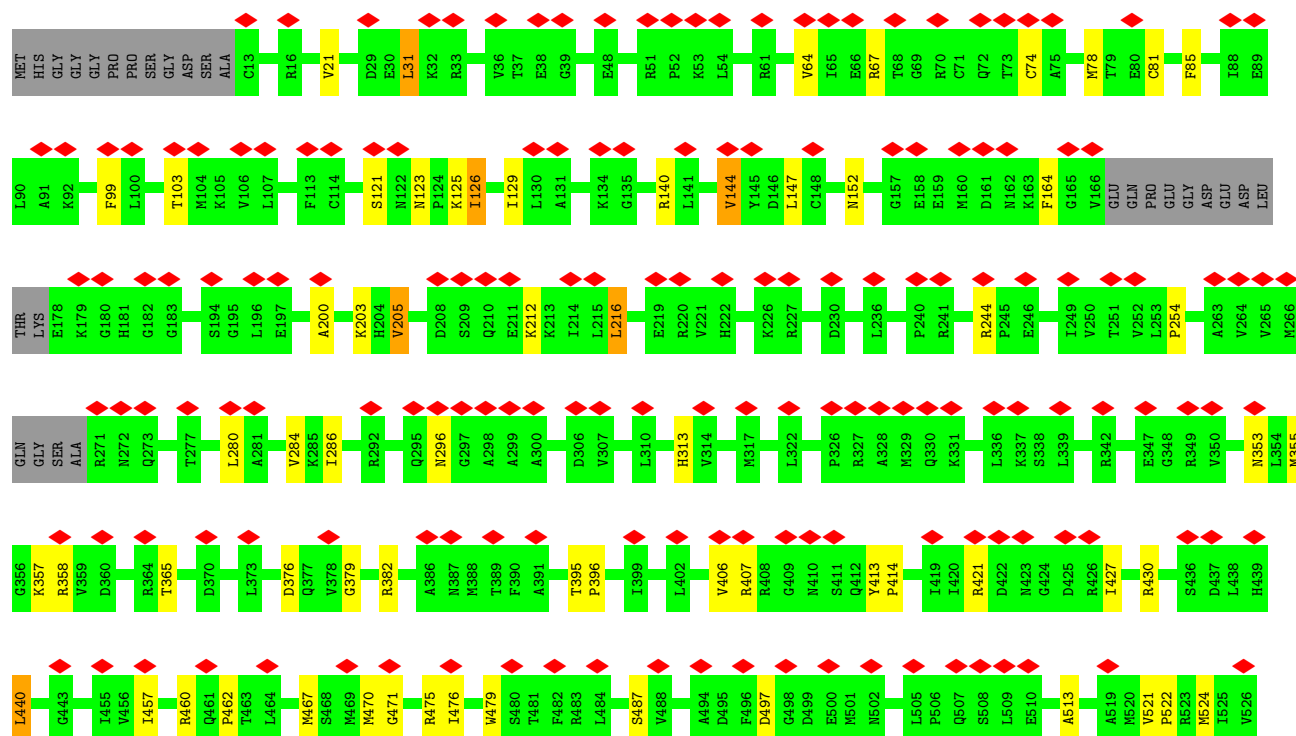
• Molecule 14: Transcription elongation factor SPT4

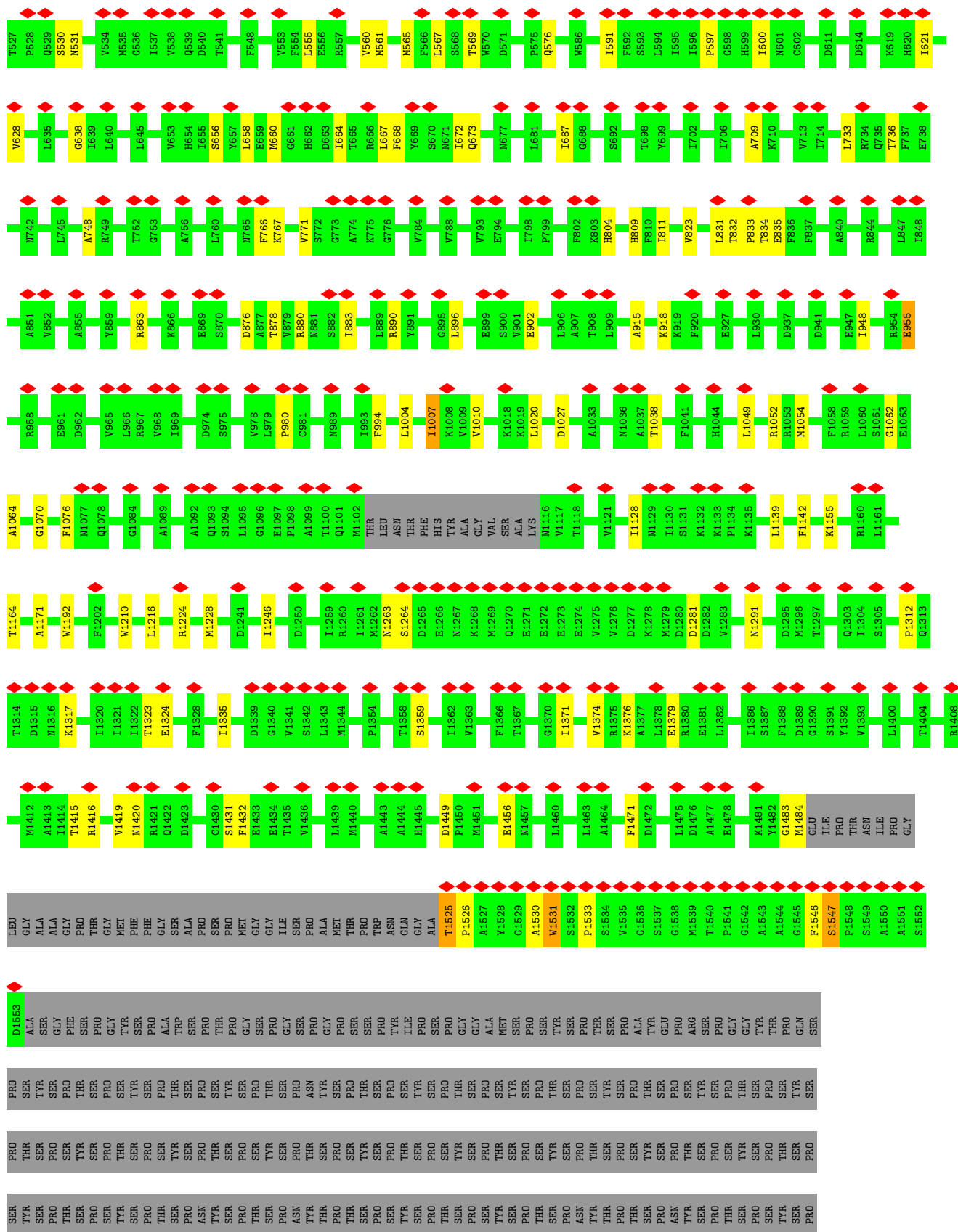


• Molecule 15: Transcription elongation factor 1 homolog

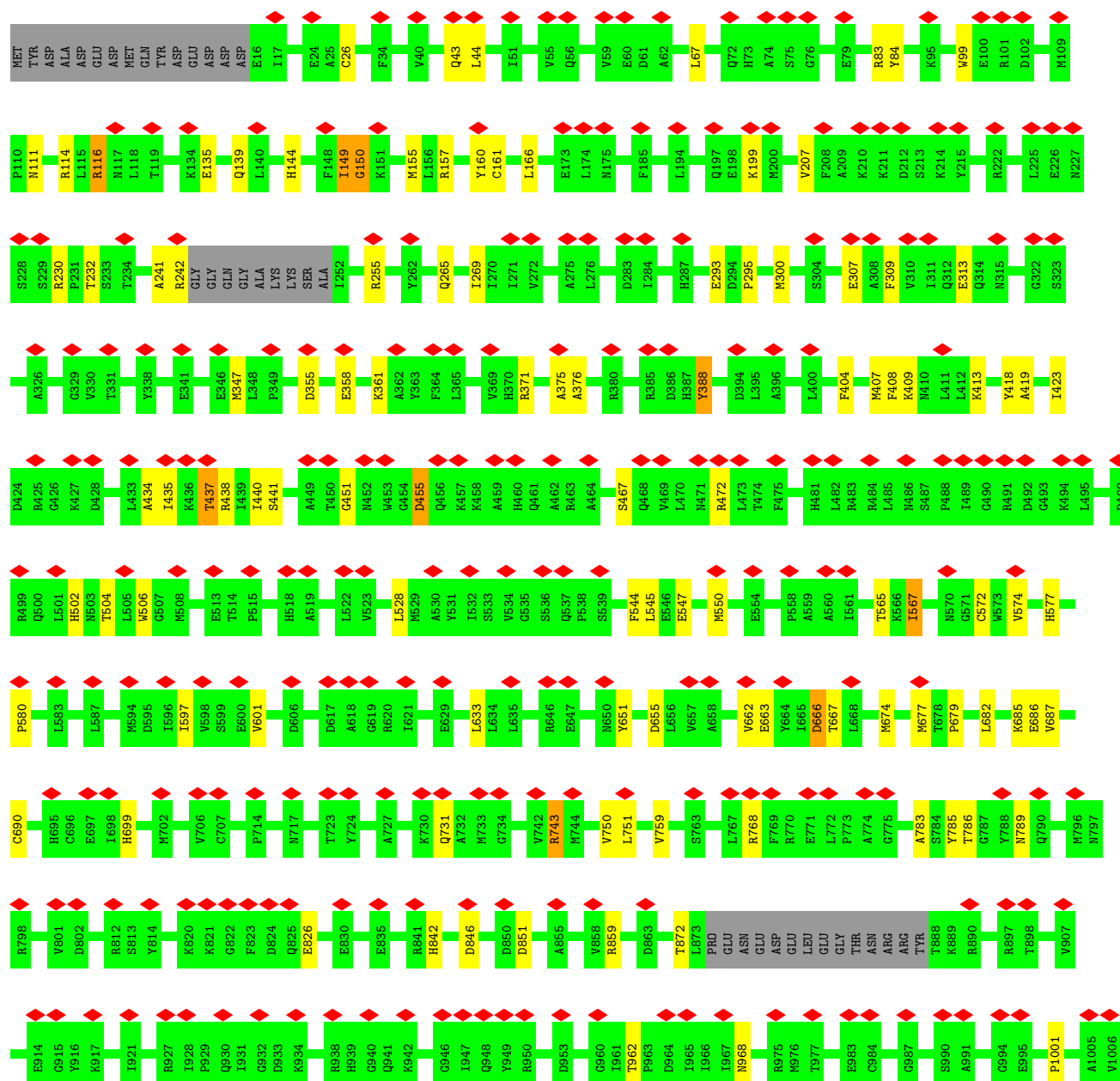
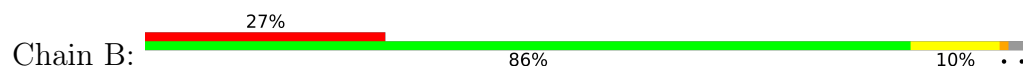


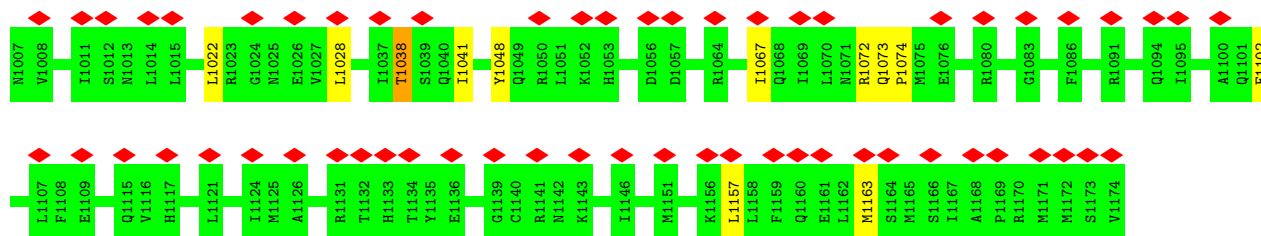
• Molecule 16: DNA-directed RNA polymerase subunit



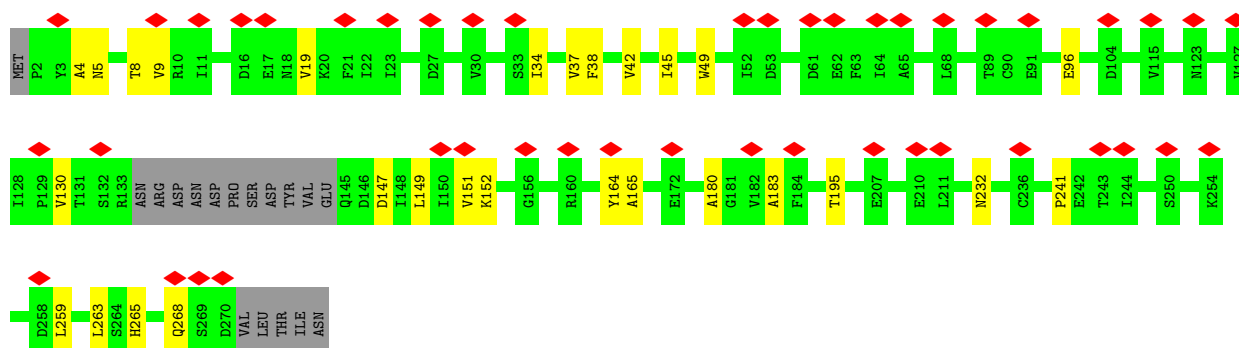
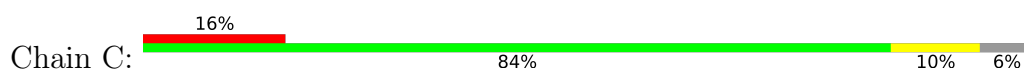


- Molecule 17: DNA-directed RNA polymerase subunit beta

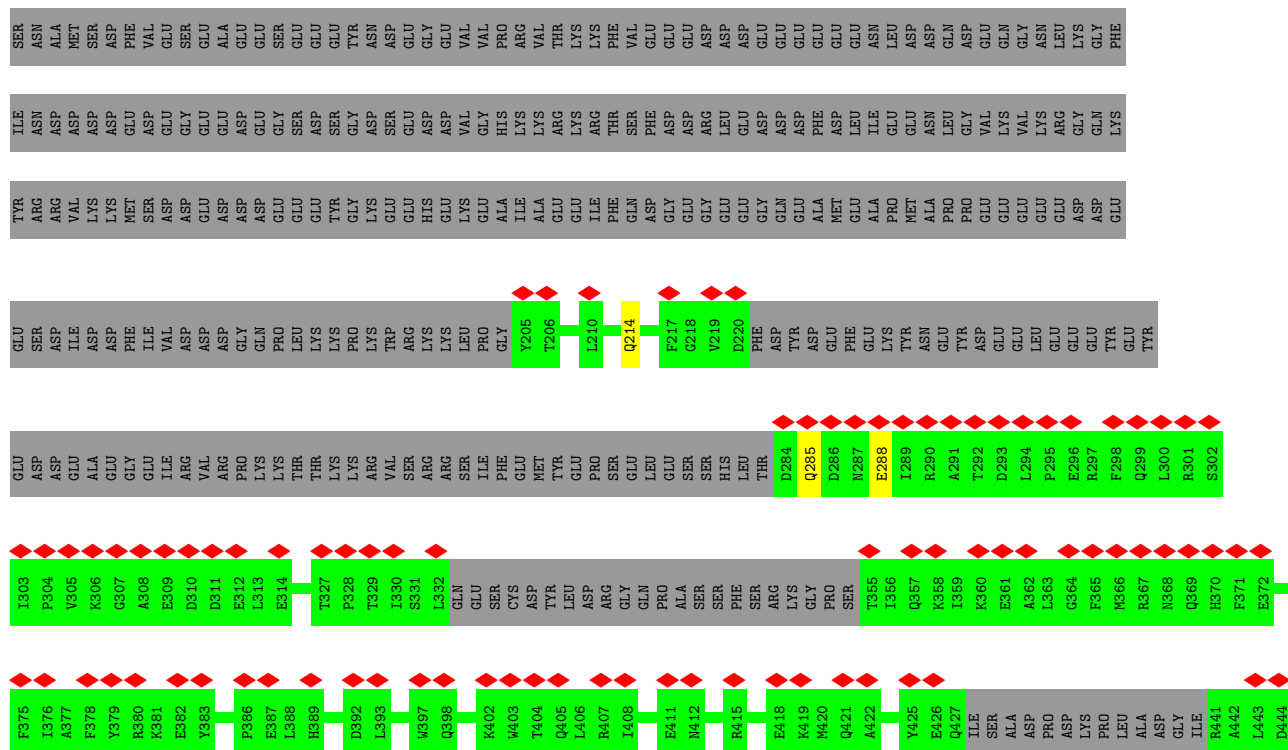


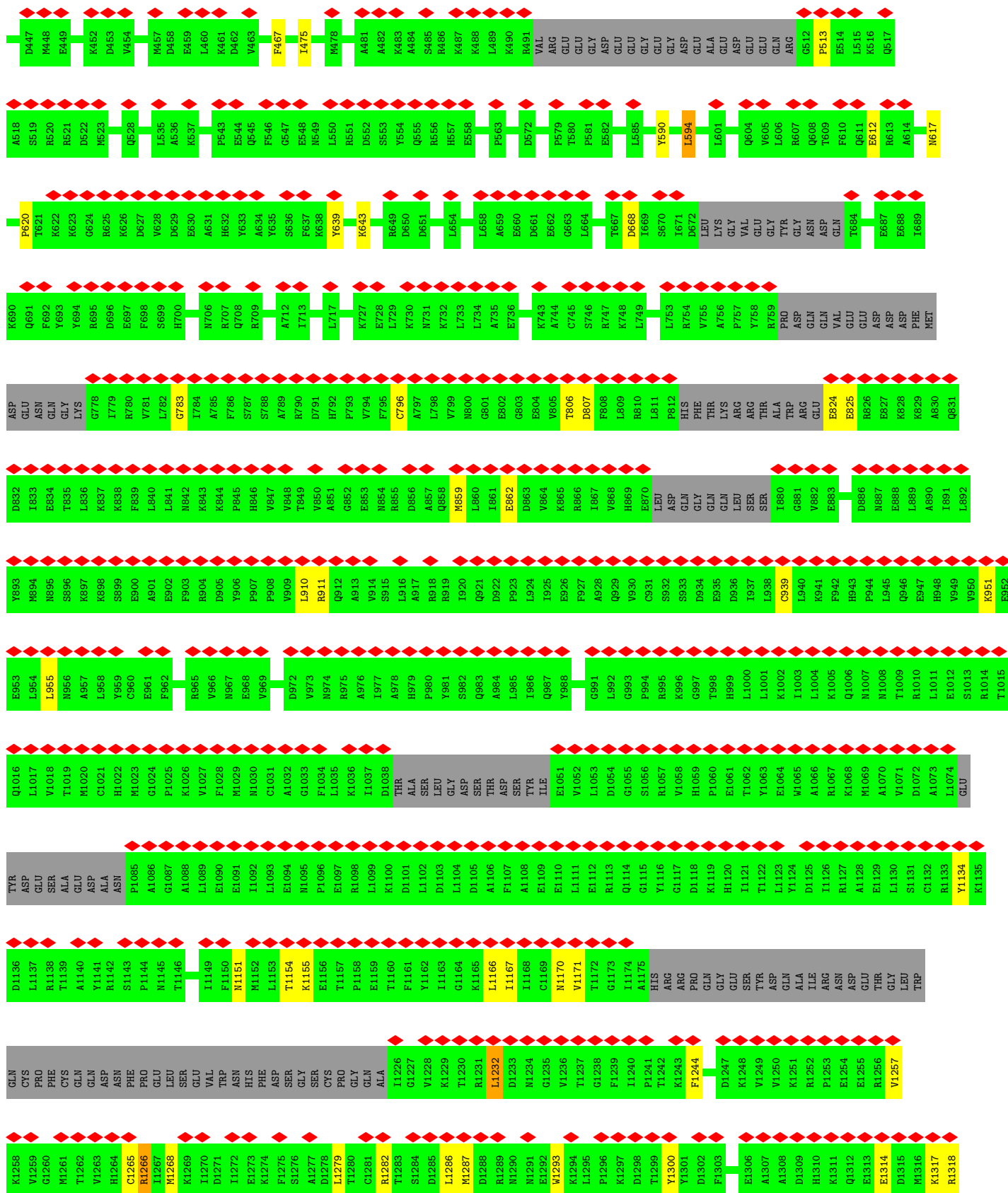


• Molecule 18: DNA-directed RNA polymerase II subunit RPB3



• Molecule 19: Transcription elongation factor SPT6









Chain a: 14% 28% 72%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1837	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 ($e^-/\text{\AA}^2$)	40.03	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.608	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	D	0.27	0/1027	0.74	0/1381
2	E	0.23	0/1752	0.77	0/2366
3	F	0.31	0/637	0.84	0/859
4	G	0.21	0/1374	0.77	0/1865
5	H	0.26	0/1220	0.77	1/1644 (0.1%)
6	I	0.28	0/973	0.82	0/1316
7	J	0.26	0/533	0.75	0/719
8	K	0.30	0/939	0.85	0/1271
9	L	0.62	0/404	0.92	0/536
10	P	0.89	8/487 (1.6%)	0.95	0/755
11	Q	0.26	0/7379	0.68	0/9945
12	T	0.50	1/990 (0.1%)	1.06	0/1524
13	W	0.22	0/2433	0.64	0/3311
14	Y	0.28	0/928	0.87	1/1250 (0.1%)
15	b	0.26	0/533	0.78	0/725
16	A	0.26	0/11844	0.76	0/15984
17	B	0.76	6/9269 (0.1%)	0.93	15/12512 (0.1%)
18	C	0.25	0/2115	0.71	0/2873
19	M	0.28	0/9010	0.81	0/12135
20	N	0.35	0/705	1.06	0/1084
21	U	0.40	0/1498	0.99	10/2018 (0.5%)
22	V	0.24	0/2360	0.78	0/3188
23	X	0.38	0/1926	1.04	4/2606 (0.2%)
24	Z	0.26	0/4045	0.84	0/5445
25	a	0.23	0/1907	0.69	0/2547
All	All	0.39	15/66288 (0.0%)	0.81	31/89859 (0.0%)

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
9	L	0	1
12	T	0	2
16	A	0	6
17	B	0	4
19	M	0	5
20	N	0	2
21	U	0	2
22	V	0	1
23	X	0	3
24	Z	0	2
All	All	0	28

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	-14	U	C1'-N1	6.62	1.58	1.48
10	P	-1	A	P-OP1	6.51	1.61	1.48
12	T	112	DC	P-OP1	6.49	1.61	1.48
10	P	-11	U	C1'-N1	6.41	1.57	1.47
10	P	-15	C	C1'-N1	6.38	1.58	1.48
10	P	-20	U	C1'-N1	6.08	1.57	1.48
10	P	-17	G	C1'-N9	-6.04	1.38	1.48
17	B	441	SER	CA-C	-5.71	1.45	1.52
10	P	-19	C	C1'-N1	5.71	1.56	1.47
10	P	-16	U	C1'-N1	5.67	1.55	1.47
17	B	408	PHE	CA-CB	-5.65	1.44	1.53
17	B	407	MET	CA-C	-5.64	1.45	1.52
17	B	404	PHE	N-CA	-5.49	1.39	1.46
17	B	408	PHE	N-CA	-5.34	1.39	1.46
17	B	472	ARG	NE-CZ	-5.27	1.27	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	111	ASN	CA-CB-CG	-8.84	103.76	112.60
17	B	743	ARG	NE-CZ-NH2	8.72	127.05	119.20
17	B	455	ASP	CA-CB-CG	7.44	120.04	112.60
17	B	114	ARG	NE-CZ-NH2	7.43	125.89	119.20
17	B	144	HIS	CA-CB-CG	-6.55	107.25	113.80
21	U	531	GLN	OE1-CD-NE2	-6.42	116.18	122.60
23	X	399	ARG	N-CA-C	6.19	120.35	109.96
17	B	149	ILE	O-C-N	-6.02	116.52	122.12
21	U	525	GLY	CA-C-N	5.91	135.36	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	U	525	GLY	C-N-CA	5.91	135.36	121.52
17	B	157	ARG	NE-CZ-NH2	5.77	124.39	119.20
21	U	527	ASP	CA-C-O	-5.75	112.28	120.16
21	U	531	GLN	CA-C-N	5.68	127.89	120.28
21	U	531	GLN	C-N-CA	5.68	127.89	120.28
17	B	144	HIS	CB-CG-CD2	-5.59	123.93	131.20
17	B	407	MET	CA-CB-CG	-5.53	103.05	114.10
17	B	408	PHE	CA-CB-CG	-5.42	108.38	113.80
21	U	527	ASP	CA-CB-CG	-5.35	107.25	112.60
17	B	161	CYS	N-CA-CB	-5.33	103.02	110.38
21	U	502	ARG	CA-C-N	5.32	128.39	120.31
21	U	502	ARG	C-N-CA	5.32	128.39	120.31
21	U	531	GLN	N-CA-C	-5.31	105.18	110.97
23	X	445	VAL	N-CA-C	5.29	120.34	109.34
5	H	96	VAL	N-CA-C	-5.27	100.99	108.58
17	B	43	GLN	CB-CA-C	-5.22	102.86	110.95
17	B	437	THR	CA-CB-CG2	5.21	119.35	110.50
17	B	157	ARG	NE-CZ-NH1	-5.09	116.41	121.50
17	B	438	ARG	NE-CZ-NH2	5.07	123.77	119.20
23	X	398	GLN	CA-C-N	5.04	129.55	122.09
23	X	398	GLN	C-N-CA	5.04	129.55	122.09
14	Y	53	THR	N-CA-C	5.02	117.79	109.46

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	A	1052	ARG	Sidechain
16	A	1263	ASN	Mainchain
16	A	152	ASN	Mainchain
16	A	203	LYS	Mainchain
16	A	244	ARG	Sidechain
16	A	890	ARG	Sidechain
17	B	116	ARG	Sidechain
17	B	160	TYR	Sidechain
17	B	743	ARG	Sidechain
17	B	859	ARG	Sidechain
9	L	41	TYR	Sidechain
19	M	1266	ARG	Sidechain
19	M	1287	MET	Mainchain
19	M	1318	ARG	Mainchain
19	M	1483	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	M	911	ARG	Sidechain
20	N	156	DC	Sidechain
20	N	157	DC	Sidechain
12	T	123	DG	Sidechain
12	T	124	DG	Sidechain
21	U	357	ARG	Sidechain
21	U	387	ARG	Sidechain
22	V	329	ARG	Sidechain
23	X	232	ARG	Sidechain
23	X	407	ARG	Sidechain
23	X	441	ARG	Sidechain
24	Z	516	ARG	Sidechain
24	Z	571	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	D	1014	0	988	12	0
2	E	1721	0	1737	10	0
3	F	627	0	657	9	0
4	G	1343	0	1340	9	0
5	H	1198	0	1156	22	0
6	I	950	0	879	7	0
7	J	524	0	540	2	0
8	K	920	0	942	16	0
9	L	398	0	402	6	0
10	P	439	0	222	4	0
11	Q	7240	0	7186	10	0
12	T	881	0	480	3	0
13	W	2374	0	2290	9	0
14	Y	912	0	904	10	0
15	b	523	0	484	3	0
16	A	11651	0	11722	114	0
17	B	9088	0	9112	61	0
18	C	2072	0	2019	17	0
19	M	8835	0	8777	72	0
20	N	633	0	354	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	1469	0	1441	9	0
22	V	2310	0	2247	15	0
23	X	1881	0	1919	66	0
24	Z	3976	0	4048	35	0
25	a	1878	0	1957	4	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	C	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	Y	1	0	0	0	0
27	A	1	0	0	0	0
All	All	64867	0	63803	471	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 4.

All (471) 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)
24:Z:181:THR:HG22	24:Z:226:TYR:CE2	2.14	0.82
23:X:364:ILE:HG23	23:X:427:VAL:HG12	1.63	0.80
16:A:834:THR:HG23	17:B:677:MET:HE3	1.63	0.78
19:M:1487:VAL:HG13	19:M:1495:ARG:O	1.89	0.73
23:X:364:ILE:CG2	23:X:427:VAL:HG12	2.20	0.71
23:X:444:ALA:HB1	23:X:476:PHE:CE2	2.26	0.71
16:A:126:ILE:CD1	16:A:147:LEU:HD12	2.24	0.68
20:N:149:DG:H2'	20:N:150:DT:H72	1.76	0.68
16:A:99:PHE:O	16:A:103:THR:HG23	1.95	0.67
17:B:677:MET:H	17:B:682:LEU:HD12	1.58	0.67
19:M:1470:GLY:C	19:M:1488:THR:HG23	2.20	0.66
16:A:767:LYS:O	16:A:771:VAL:HG22	1.96	0.65
16:A:471:GLY:O	16:A:521:VAL:HG23	1.97	0.65
3:F:90:LEU:HD21	16:A:513:ALA:HB2	1.79	0.65
5:H:37:MET:SD	5:H:127:GLY:HA3	2.36	0.65
19:M:1464:ALA:HB2	19:M:1472:PHE:CE2	2.31	0.65
19:M:1347:MET:HE3	19:M:1370:THR:HG22	1.79	0.64
17:B:44:LEU:HD23	17:B:155:MET:HE3	1.78	0.64
1:D:87:LEU:HD21	1:D:92:LEU:HD22	1.79	0.64
19:M:1355:VAL:HG22	19:M:1416:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:1357:ILE:HG12	19:M:1369:VAL:HG22	1.78	0.64
11:Q:674:ARG:HG2	11:Q:674:ARG:HH21	1.62	0.64
17:B:565:THR:HG21	17:B:580:PRO:HB3	1.79	0.64
8:K:58:PHE:CE1	16:A:565:MET:HE1	2.33	0.64
16:A:668:PHE:CE1	16:A:672:ILE:HD11	2.33	0.64
16:A:1415:THR:O	16:A:1419:VAL:HG22	1.98	0.63
23:X:362:ILE:HA	23:X:444:ALA:O	1.96	0.63
18:C:183:ALA:HB3	18:C:232:ASN:HB3	1.80	0.63
8:K:58:PHE:HE1	16:A:565:MET:HE1	1.64	0.63
17:B:550:MET:HE1	17:B:567:ILE:HG21	1.81	0.62
16:A:687:ILE:HD11	16:A:766:PHE:CZ	2.34	0.62
23:X:459:TRP:CZ3	23:X:473:ILE:HD11	2.34	0.62
18:C:19:VAL:HG23	18:C:241:PRO:HB2	1.80	0.62
19:M:1371:TRP:CH2	19:M:1373:VAL:HG22	2.35	0.62
16:A:31:LEU:HD21	16:A:254:PRO:HB3	1.83	0.61
14:Y:48:MET:HE3	14:Y:48:MET:HA	1.83	0.61
17:B:388:TYR:H	17:B:504:THR:HG21	1.65	0.61
16:A:1531:TRP:CG	19:M:1471:LYS:HZ3	2.19	0.61
17:B:44:LEU:HA	17:B:155:MET:HE1	1.83	0.61
23:X:444:ALA:HB1	23:X:476:PHE:HE2	1.63	0.60
18:C:45:ILE:HG22	18:C:165:ALA:HB1	1.83	0.60
23:X:362:ILE:O	23:X:427:VAL:HA	2.01	0.60
19:M:1470:GLY:O	19:M:1488:THR:HG23	2.02	0.60
8:K:60:GLY:C	16:A:565:MET:HE3	2.26	0.59
16:A:896:LEU:HD13	16:A:980:PRO:HG3	1.83	0.59
13:W:80:ALA:HB1	13:W:112:LEU:HD21	1.84	0.59
16:A:660:MET:HG2	16:A:664:ILE:HG21	1.83	0.59
20:N:147:DG:H2"	20:N:148:DT:H72	1.84	0.59
17:B:506:TRP:CH2	17:B:677:MET:HE1	2.38	0.59
23:X:364:ILE:HA	23:X:446:PHE:HB2	1.84	0.59
13:W:36:VAL:HG23	13:W:72:ILE:HD11	1.85	0.58
24:Z:485:PHE:CD2	24:Z:511:LEU:HD21	2.37	0.58
23:X:444:ALA:HA	23:X:474:LYS:O	2.03	0.58
16:A:878:THR:HG21	16:A:880:ARG:HE	1.69	0.58
23:X:374:MET:SD	23:X:429:ASP:HB2	2.44	0.58
6:I:59:THR:HG23	16:A:1171:ALA:HA	1.86	0.57
17:B:666:ASP:OD1	17:B:667:THR:N	2.37	0.57
19:M:806:THR:HG22	19:M:807:ASP:H	1.69	0.57
19:M:1429:HIS:CE1	19:M:1508:PHE:CZ	2.92	0.57
5:H:60:ILE:CD1	5:H:123:MET:HE1	2.34	0.57
23:X:380:LEU:HD22	23:X:511:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:1355:VAL:CG2	19:M:1416:VAL:HG11	2.35	0.57
17:B:565:THR:HG22	17:B:577:HIS:O	2.04	0.56
23:X:423:VAL:HB	23:X:531:PHE:HA	1.86	0.56
14:Y:42:MET:HE1	14:Y:53:THR:OG1	2.04	0.56
24:Z:225:ILE:HD11	24:Z:245:LEU:HD11	1.87	0.56
17:B:26:CYS:SG	17:B:699:HIS:HB2	2.46	0.56
19:M:467:PHE:HE2	19:M:475:ILE:HD11	1.70	0.56
23:X:387:VAL:HG11	23:X:392:LYS:HE2	1.87	0.56
16:A:809:HIS:CG	17:B:677:MET:HE2	2.41	0.56
19:M:1511:PHE:O	19:M:1515:TYR:HB3	2.06	0.56
16:A:413:TYR:OH	16:A:476:ILE:HG21	2.06	0.56
16:A:834:THR:CG2	17:B:677:MET:HE3	2.35	0.55
23:X:363:ILE:HA	23:X:428:VAL:HB	1.88	0.55
23:X:425:TYR:CE2	23:X:522:MET:HE1	2.42	0.55
23:X:443:VAL:C	23:X:473:ILE:HG23	2.31	0.55
24:Z:182:VAL:O	24:Z:224:TYR:HB3	2.06	0.55
24:Z:546:THR:HG22	24:Z:547:VAL:N	2.22	0.55
23:X:362:ILE:HD11	23:X:518:LEU:HD11	1.88	0.55
4:G:137:ILE:HG22	4:G:170:LEU:HD13	1.88	0.55
24:Z:182:VAL:HG22	24:Z:225:ILE:O	2.07	0.55
8:K:97:GLU:CG	18:C:4:ALA:HB1	2.37	0.54
5:H:60:ILE:HD11	5:H:123:MET:HE1	1.88	0.54
8:K:50:LEU:HD13	8:K:75:VAL:HG22	1.90	0.54
7:J:9:THR:HG23	17:B:962:THR:O	2.08	0.54
16:A:123:ASN:OD1	16:A:125:LYS:HG2	2.08	0.54
19:M:1468:LEU:HB3	19:M:1471:LYS:HD2	1.89	0.54
24:Z:171:LEU:CD2	24:Z:261:THR:HG21	2.38	0.54
1:D:16:ASP:H	1:D:21:ILE:HG23	1.73	0.53
16:A:955:GLU:OE1	16:A:1010:VAL:HG22	2.08	0.53
16:A:64:VAL:HG11	16:A:78:MET:HA	1.91	0.53
16:A:809:HIS:CD2	17:B:677:MET:HE2	2.44	0.53
2:E:94:MET:SD	2:E:102:ALA:HB2	2.48	0.53
23:X:445:VAL:HG13	23:X:475:ALA:HA	1.91	0.53
17:B:785:TYR:O	17:B:786:THR:HG22	2.09	0.52
16:A:1049:LEU:HG	16:A:1054:MET:HE3	1.91	0.52
23:X:429:ASP:OD1	23:X:429:ASP:N	2.41	0.52
19:M:643:LYS:HD3	19:M:1300:TYR:CD1	2.44	0.52
22:V:286:VAL:HG11	22:V:350:VAL:HG12	1.92	0.52
5:H:128:ASP:C	5:H:128:ASP:OD1	2.52	0.52
20:N:147:DG:H2''	20:N:148:DT:C7	2.38	0.52
17:B:1038:THR:HA	18:C:195:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M:1347:MET:HE3	19:M:1370:THR:CG2	2.38	0.52
23:X:454:PHE:CE2	23:X:470:PHE:HZ	2.28	0.52
8:K:56:VAL:HA	8:K:77:THR:HG22	1.92	0.52
23:X:362:ILE:CD1	23:X:518:LEU:HD11	2.39	0.52
8:K:42:LEU:HD21	18:C:259:LEU:HD22	1.91	0.52
2:E:153:LYS:O	2:E:157:THR:HG23	2.09	0.52
5:H:143:LEU:O	5:H:144:LEU:C	2.53	0.52
23:X:367:ALA:HB3	23:X:448:GLN:OE1	2.09	0.52
24:Z:215:VAL:CG1	24:Z:225:ILE:HD12	2.40	0.51
19:M:1266:ARG:CD	19:M:1286:LEU:HA	2.41	0.51
23:X:361:ILE:C	23:X:362:ILE:HG13	2.34	0.51
2:E:75:PHE:CE1	11:Q:891:PHE:CZ	2.99	0.51
4:G:54:ILE:HD13	4:G:70:VAL:HG23	1.92	0.51
16:A:948:ILE:HG23	16:A:1007:ILE:HD13	1.91	0.51
17:B:572:CYS:O	17:B:574:VAL:HG13	2.11	0.51
19:M:1494:PHE:CE1	19:M:1504:VAL:HG22	2.46	0.51
20:N:161:DG:H2'	20:N:162:DC:C5	2.45	0.51
23:X:361:ILE:HG13	23:X:441:ARG:NE	2.26	0.51
5:H:60:ILE:HA	5:H:142:TYR:O	2.11	0.51
14:Y:59:GLY:H	24:Z:219:GLU:HG3	1.74	0.51
16:A:1546:PHE:O	16:A:1547:SEP:C	2.58	0.51
23:X:459:TRP:CH2	23:X:473:ILE:HD11	2.45	0.51
17:B:241:ALA:O	17:B:242:ARG:C	2.54	0.51
23:X:442:VAL:HB	23:X:473:ILE:HD13	1.91	0.51
23:X:361:ILE:CG2	23:X:362:ILE:N	2.74	0.51
3:F:79:VAL:HG21	3:F:83:LEU:HD13	1.92	0.51
6:I:17:CYS:O	6:I:21:ASN:HA	2.10	0.51
16:A:121:SER:HA	16:A:126:ILE:HG21	1.93	0.51
19:M:1266:ARG:HD3	19:M:1286:LEU:HA	1.93	0.51
23:X:445:VAL:HG22	23:X:445:VAL:O	2.10	0.51
1:D:76:ASN:OD1	1:D:78:GLU:N	2.44	0.50
4:G:116:GLU:OE1	19:M:513:PRO:HG2	2.11	0.50
14:Y:62:ALA:HB1	24:Z:197:MET:HG2	1.91	0.50
16:A:395:THR:HG23	16:A:396:PRO:HD2	1.93	0.50
17:B:506:TRP:CZ2	17:B:677:MET:HE1	2.45	0.50
23:X:362:ILE:HG23	23:X:444:ALA:O	2.10	0.50
23:X:402:GLU:HA	23:X:429:ASP:OD2	2.12	0.50
24:Z:215:VAL:HG11	24:Z:225:ILE:HD12	1.93	0.50
15:b:31:HIS:CE1	25:a:696:TYR:CE2	3.00	0.50
16:A:1420:ASN:OD1	16:A:1432:PHE:CE1	2.64	0.50
16:A:1483:GLY:C	16:A:1484:MET:HG3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:363:ILE:HG22	23:X:446:PHE:O	2.12	0.50
16:A:668:PHE:CZ	16:A:672:ILE:HD11	2.46	0.50
16:A:915:ALA:HA	16:A:918:LYS:HG2	1.94	0.50
17:B:545:LEU:HD23	17:B:550:MET:HE1	1.92	0.50
22:V:250:MET:HG2	22:V:254:GLY:HA2	1.93	0.50
23:X:364:ILE:HG12	23:X:428:VAL:O	2.12	0.50
24:Z:540:VAL:HB	24:Z:575:VAL:CG2	2.42	0.50
5:H:75:TYR:HB2	16:A:576:GLN:HA	1.94	0.50
23:X:380:LEU:HD22	23:X:511:PHE:HZ	1.77	0.50
23:X:438:ASP:HA	23:X:441:ARG:HD3	1.92	0.50
8:K:21:ILE:HD11	18:C:263:LEU:CD1	2.42	0.49
23:X:359:THR:HG22	23:X:441:ARG:NH1	2.26	0.49
16:A:74:CYS:SG	16:A:81:CYS:HB2	2.52	0.49
14:Y:61:ILE:HG22	24:Z:216:VAL:HG13	1.93	0.49
8:K:97:GLU:HG2	18:C:4:ALA:HB1	1.94	0.49
16:A:140:ARG:O	16:A:144:VAL:HG13	2.13	0.49
1:D:20:LEU:HD13	1:D:117:SER:HB2	1.95	0.49
3:F:79:VAL:HG21	3:F:83:LEU:CD1	2.43	0.49
23:X:362:ILE:O	23:X:428:VAL:HG23	2.13	0.49
9:L:15:MET:HE3	17:B:851:ASP:H	1.75	0.49
19:M:1369:VAL:HG23	19:M:1383:VAL:CG2	2.43	0.49
24:Z:182:VAL:HG12	24:Z:252:GLN:HG2	1.93	0.49
4:G:95:VAL:HG13	4:G:95:VAL:O	2.13	0.49
17:B:783:ALA:O	17:B:789:ASN:ND2	2.45	0.49
12:T:102:DG:H2''	12:T:103:DG:C8	2.48	0.49
16:A:733:LEU:O	16:A:736:THR:HG22	2.12	0.49
16:A:1531:TRP:CD1	19:M:1471:LYS:HZ3	2.31	0.49
17:B:418:TYR:CD2	17:B:434:ALA:HB2	2.48	0.49
19:M:1151:ASN:O	19:M:1155:LYS:HA	2.13	0.49
14:Y:72:SER:OG	14:Y:78:SER:HA	2.13	0.48
16:A:413:TYR:HB3	16:A:414:PRO:HD3	1.95	0.48
16:A:1546:PHE:CD2	19:M:1458:ILE:HD11	2.48	0.48
23:X:425:TYR:CE1	23:X:531:PHE:HB2	2.48	0.48
17:B:293:GLU:O	17:B:295:PRO:HD3	2.14	0.48
21:U:365:VAL:HG11	21:U:473:ILE:HD13	1.95	0.48
17:B:506:TRP:CD1	17:B:506:TRP:C	2.92	0.48
24:Z:499:PHE:HA	24:Z:515:PRO:HD3	1.96	0.48
10:P:-13:C:H41	16:A:430:ARG:NH2	2.12	0.48
15:b:48:ILE:HD13	15:b:74:TRP:CE3	2.48	0.48
16:A:355:MET:HE3	16:A:1431:SER:OG	2.13	0.48
17:B:207:VAL:HG11	17:B:375:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:255:ARG:HE	17:B:307:GLU:CD	2.21	0.48
3:F:98:LYS:HE2	3:F:98:LYS:HA	1.96	0.48
19:M:467:PHE:CE2	19:M:475:ILE:HD11	2.49	0.48
1:D:87:LEU:C	1:D:87:LEU:HD23	2.38	0.48
16:A:597:PRO:HB2	16:A:664:ILE:CG2	2.43	0.48
23:X:475:ALA:HB3	23:X:494:VAL:HA	1.94	0.48
10:P:-10:G:C8	10:P:-10:G:H5''	2.49	0.48
17:B:44:LEU:HD23	17:B:155:MET:CE	2.44	0.48
23:X:358:ARG:O	23:X:529:LEU:HB3	2.14	0.48
5:H:114:ALA:HB1	5:H:135:PHE:CD2	2.48	0.47
16:A:125:LYS:O	16:A:129:ILE:HG12	2.13	0.47
16:A:1484:MET:HE3	19:M:1330:ILE:N	2.29	0.47
23:X:361:ILE:HG12	23:X:426:ARG:HB3	1.96	0.47
1:D:38:HIS:CE1	1:D:69:ALA:HB2	2.50	0.47
9:L:19:CYS:SG	9:L:20:GLY:N	2.88	0.47
17:B:67:LEU:O	17:B:83:ARG:HA	2.14	0.47
19:M:1265:CYS:SG	19:M:1279:LEU:HD13	2.54	0.47
20:N:158:DT:H2''	20:N:159:DT:H72	1.97	0.47
22:V:246:ILE:HG23	22:V:258:VAL:CG1	2.44	0.47
16:A:1484:MET:HE2	19:M:1329:VAL:HG13	1.95	0.47
23:X:458:PRO:O	23:X:459:TRP:HB2	2.14	0.47
18:C:265:HIS:HA	18:C:268:GLN:HG2	1.97	0.47
19:M:1154:THR:O	19:M:1155:LYS:HB2	2.14	0.47
4:G:145:LEU:HD12	4:G:145:LEU:C	2.40	0.47
16:A:1192:TRP:HZ3	16:A:1246:ILE:HG22	1.80	0.47
20:N:155:DC:H2''	20:N:156:DC:C6	2.49	0.47
16:A:457:ILE:HG21	17:B:1102:PHE:CZ	2.49	0.47
19:M:951:LYS:O	19:M:955:LEU:HD23	2.15	0.47
14:Y:59:GLY:H	24:Z:219:GLU:CG	2.27	0.47
23:X:442:VAL:HG12	23:X:473:ILE:HG21	1.97	0.47
24:Z:181:THR:HG22	24:Z:226:TYR:CD2	2.50	0.47
11:Q:674:ARG:HH21	11:Q:674:ARG:CG	2.26	0.47
16:A:1164:THR:HG21	16:A:1224:ARG:CD	2.45	0.47
16:A:823:VAL:CG1	16:A:831:LEU:HD22	2.45	0.46
19:M:1286:LEU:CD2	24:Z:664:PRO:HB2	2.45	0.46
24:Z:211:GLN:O	24:Z:234:HIS:HB3	2.15	0.46
16:A:658:LEU:HD13	16:A:902:GLU:CD	2.40	0.46
19:M:1166:LEU:HD23	19:M:1266:ARG:CG	2.45	0.46
20:N:125:DT:H1'	20:N:126:DG:H5''	1.97	0.46
23:X:423:VAL:HB	23:X:531:PHE:CA	2.45	0.46
16:A:467:MET:SD	16:A:524:MET:HE3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:85:VAL:HG11	4:G:101:ILE:HD13	1.98	0.46
15:b:28:PHE:O	24:Z:231:LYS:HE3	2.16	0.46
11:Q:163:ILE:HB	11:Q:164:PRO:HD3	1.98	0.46
12:T:106:DT:C2'	12:T:107:DT:H71	2.46	0.46
23:X:364:ILE:CG2	23:X:427:VAL:CG1	2.93	0.46
1:D:34:ASN:O	1:D:68:THR:CG2	2.63	0.46
23:X:434:LEU:C	23:X:439:TRP:HE1	2.24	0.46
14:Y:62:ALA:HB1	24:Z:197:MET:CG	2.46	0.46
5:H:114:ALA:HB1	5:H:135:PHE:HD2	1.82	0.45
16:A:709:ALA:CB	16:A:748:ALA:HB2	2.46	0.45
17:B:451:GLY:HA2	17:B:467:SER:HB3	1.98	0.45
18:C:149:LEU:HD21	18:C:152:LYS:HE3	1.97	0.45
19:M:1372:LYS:HE3	19:M:1375:ASP:HA	1.98	0.45
20:N:124:DC:H2''	20:N:125:DT:C6	2.51	0.45
21:U:394:TYR:CE2	22:V:176:ILE:HD11	2.51	0.45
23:X:362:ILE:HD13	23:X:518:LEU:HD21	1.98	0.45
24:Z:546:THR:CG2	24:Z:547:VAL:N	2.79	0.45
2:E:34:ASP:C	2:E:34:ASP:OD1	2.59	0.45
14:Y:16:CYS:O	14:Y:20:SER:HA	2.15	0.45
16:A:823:VAL:HG22	16:A:835:GLU:HB2	1.98	0.45
19:M:1512:LYS:HA	19:M:1515:TYR:CD1	2.51	0.45
8:K:56:VAL:HG22	8:K:77:THR:HG22	1.99	0.45
16:A:832:THR:HG23	16:A:833:PRO:HD2	1.97	0.45
16:A:1533:PRO:HG2	19:M:1497:ARG:HA	1.98	0.45
6:I:64:GLU:HG2	6:I:99:SER:CB	2.46	0.45
11:Q:523:ILE:HG21	11:Q:533:CYS:SG	2.56	0.45
16:A:376:ASP:HB3	16:A:522:PRO:HD3	1.99	0.45
16:A:569:THR:CG2	16:A:667:LEU:HD13	2.46	0.45
5:H:15:ILE:O	5:H:16:ASP:C	2.60	0.45
16:A:876:ASP:HB3	16:A:878:THR:HG22	1.98	0.45
19:M:590:TYR:CE1	19:M:594:LEU:HD23	2.51	0.45
19:M:1360:SER:HB3	19:M:1366:HIS:C	2.42	0.45
21:U:384:VAL:HG11	22:V:323:TYR:CE1	2.52	0.45
1:D:107:THR:HG23	1:D:110:GLU:CB	2.47	0.45
3:F:82:GLU:HB2	19:M:1331:ALA:HB3	1.98	0.45
13:W:24:TRP:HE1	13:W:33:GLU:HB3	1.82	0.45
16:A:560:VAL:CG1	16:A:591:ILE:HD11	2.47	0.45
8:K:105:PHE:CD2	18:C:9:VAL:HG11	2.52	0.45
16:A:1210:TRP:CD1	16:A:1281:ASP:HB2	2.52	0.45
16:A:1547:SEP:O3P	19:M:1512:LYS:NZ	2.50	0.45
19:M:1464:ALA:HB2	19:M:1472:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:409:LYS:C	23:X:420:SER:HB2	2.41	0.45
24:Z:274:LYS:HG3	24:Z:275:PRO:HD2	1.98	0.45
17:B:674:MET:HG2	17:B:690:CYS:SG	2.56	0.45
18:C:34:ILE:HG22	18:C:38:PHE:CZ	2.52	0.45
19:M:1330:ILE:HG21	19:M:1408:LEU:HD11	1.99	0.45
16:A:628:VAL:HA	16:A:638:GLY:HA3	1.99	0.45
22:V:282:ALA:HB3	22:V:285:ASP:HB2	1.99	0.45
5:H:111:ARG:HA	5:H:128:ASP:HA	1.98	0.44
16:A:1546:PHE:CD1	19:M:1458:ILE:HG13	2.52	0.44
11:Q:524:LEU:HD21	11:Q:533:CYS:HB2	1.98	0.44
16:A:560:VAL:HG13	16:A:591:ILE:HD11	1.99	0.44
23:X:359:THR:O	23:X:441:ARG:HG2	2.17	0.44
24:Z:479:LYS:HA	24:Z:489:THR:HG22	1.98	0.44
25:a:647:VAL:HG13	25:a:647:VAL:O	2.17	0.44
6:I:81:THR:HG23	6:I:96:PHE:CE1	2.52	0.44
16:A:497:ASP:OD1	16:A:497:ASP:C	2.60	0.44
13:W:49:TRP:CZ2	13:W:52:GLU:HA	2.52	0.44
16:A:1291:ASN:C	16:A:1291:ASN:OD1	2.59	0.44
16:A:1525:TPO:H2	16:A:1526:PRO:HD3	1.82	0.44
18:C:149:LEU:HD21	18:C:152:LYS:CE	2.47	0.44
23:X:522:MET:O	23:X:527:SER:N	2.50	0.44
6:I:100:HIS:CG	16:A:804:HIS:CE1	3.06	0.44
16:A:1027:ASP:C	16:A:1027:ASP:OD1	2.61	0.44
19:M:1326:ILE:HG23	19:M:1326:ILE:O	2.18	0.44
23:X:443:VAL:C	23:X:473:ILE:CG2	2.91	0.44
19:M:1369:VAL:HG23	19:M:1383:VAL:HG21	1.99	0.44
1:D:107:THR:HG23	1:D:110:GLU:HB3	1.98	0.44
17:B:826:GLU:H	17:B:872:THR:HG22	1.83	0.44
5:H:148:LEU:C	5:H:150:PHE:H	2.25	0.44
6:I:64:GLU:HG2	6:I:99:SER:HB2	1.99	0.44
16:A:487:SER:OG	16:A:673:GLN:NE2	2.50	0.44
3:F:61:GLU:HA	16:A:1471:PHE:CZ	2.53	0.44
10:P:-21:U:O2	10:P:-21:U:C2'	2.66	0.44
16:A:600:ILE:HD11	16:A:656:SER:HA	1.99	0.44
17:B:149:ILE:HG22	17:B:150:GLY:N	2.33	0.44
17:B:347:MET:O	17:B:361:LYS:CE	2.66	0.44
19:M:824:GLU:HG3	19:M:825:GLU:H	1.83	0.44
13:W:86:ALA:HB1	13:W:105:GLY:O	2.18	0.43
16:A:21:VAL:HG22	16:A:1449:ASP:HB3	2.00	0.43
17:B:651:TYR:HA	17:B:655:ASP:OD2	2.18	0.43
23:X:359:THR:CG2	23:X:441:ARG:CZ	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:200:ALA:HB2	16:A:216:LEU:HD23	1.98	0.43
16:A:1020:LEU:HD22	16:A:1076:PHE:CG	2.54	0.43
19:M:806:THR:HG22	19:M:807:ASP:N	2.33	0.43
19:M:859:MET:O	19:M:862:GLU:HG3	2.17	0.43
21:U:394:TYR:CD2	22:V:176:ILE:HD11	2.52	0.43
23:X:359:THR:HG22	23:X:441:ARG:CZ	2.48	0.43
23:X:374:MET:SD	23:X:429:ASP:CB	3.06	0.43
11:Q:854:GLN:OE1	11:Q:854:GLN:HA	2.19	0.43
19:M:214:GLN:HA	24:Z:165:ILE:HD13	1.99	0.43
19:M:620:PRO:HD2	19:M:639:TYR:CE2	2.54	0.43
24:Z:192:THR:HG21	24:Z:245:LEU:HG	1.99	0.43
24:Z:262:ASP:HA	24:Z:265:LYS:HB2	2.00	0.43
1:D:87:LEU:HD22	1:D:97:LEU:HG	2.00	0.43
17:B:544:PHE:O	17:B:547:GLU:HG2	2.19	0.43
17:B:1028:LEU:HD12	17:B:1041:ILE:HG13	1.99	0.43
23:X:515:TRP:CZ3	23:X:518:LEU:HD23	2.53	0.43
1:D:29:ALA:HB2	4:G:5:ILE:CG2	2.48	0.43
5:H:20:LYS:HG2	5:H:22:PHE:O	2.18	0.43
9:L:19:CYS:SG	9:L:36:CYS:SG	3.15	0.43
19:M:1244:PHE:HA	19:M:1282:ARG:HD2	1.99	0.43
19:M:1368:THR:HG23	19:M:1381:VAL:O	2.19	0.43
23:X:454:PHE:O	23:X:457:TRP:HB2	2.18	0.43
2:E:121:MET:C	2:E:123:PRO:HD2	2.43	0.43
2:E:192:LYS:HG2	2:E:193:ILE:N	2.34	0.43
16:A:1546:PHE:CG	19:M:1458:ILE:HG13	2.53	0.43
17:B:67:LEU:CD1	17:B:419:ALA:HB3	2.49	0.43
17:B:207:VAL:HG11	17:B:375:ALA:HB3	2.00	0.43
19:M:783:GLY:O	19:M:796:CYS:HA	2.18	0.43
19:M:939:CYS:SG	24:Z:573:GLN:HB2	2.59	0.43
19:M:1390:ASN:ND2	19:M:1392:PHE:H	2.16	0.43
22:V:309:GLU:CD	22:V:325:GLU:OE2	2.62	0.43
25:a:560:VAL:HG13	25:a:607:PHE:CD1	2.54	0.43
2:E:73:PHE:CE2	2:E:99:ILE:HD12	2.54	0.43
16:A:1419:VAL:HG23	16:A:1432:PHE:CE1	2.54	0.43
22:V:286:VAL:CG1	22:V:350:VAL:HG12	2.49	0.43
23:X:362:ILE:O	23:X:428:VAL:N	2.52	0.43
4:G:15:PRO:HA	4:G:18:PHE:CE1	2.54	0.43
16:A:621:ILE:HG23	16:A:621:ILE:O	2.18	0.43
18:C:49:TRP:CE3	18:C:164:TYR:HD1	2.37	0.43
2:E:173:ILE:O	2:E:209:VAL:HA	2.19	0.43
3:F:90:LEU:HD21	16:A:513:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:286:ILE:CD1	16:A:313:HIS:ND1	2.81	0.43
16:A:460:ARG:HG2	16:A:462:PRO:HD2	2.01	0.43
17:B:440:ILE:N	17:B:440:ILE:HD12	2.34	0.43
17:B:597:ILE:HG22	17:B:601:VAL:HB	2.01	0.43
17:B:789:ASN:OD1	17:B:968:ASN:N	2.52	0.43
19:M:1494:PHE:CE1	19:M:1504:VAL:CG2	3.02	0.43
11:Q:863:LYS:HA	11:Q:863:LYS:HE3	2.01	0.42
16:A:440:LEU:O	16:A:440:LEU:HD12	2.19	0.42
16:A:555:LEU:HB2	16:A:560:VAL:HG23	2.00	0.42
19:M:1314:GLU:O	19:M:1317:LYS:HB2	2.19	0.42
20:N:147:DG:C2'	20:N:148:DT:H72	2.48	0.42
22:V:312:PHE:CZ	22:V:324:ASN:HB3	2.54	0.42
1:D:111:SER:HB3	1:D:131:LEU:HD21	2.01	0.42
24:Z:255:VAL:CG2	24:Z:260:MET:HG2	2.50	0.42
19:M:1167:ILE:HD12	19:M:1232:LEU:CD1	2.49	0.42
3:F:98:LYS:NZ	3:F:125:ILE:HD12	2.34	0.42
2:E:106:VAL:HG11	2:E:110:MET:HE2	2.01	0.42
16:A:421:ARG:CZ	16:A:427:ILE:HD11	2.49	0.42
16:A:1216:LEU:HD12	16:A:1228:MET:SD	2.59	0.42
16:A:1323:THR:HG22	16:A:1324:GLU:N	2.34	0.42
18:C:37:VAL:O	18:C:42:VAL:HG23	2.20	0.42
24:Z:418:HIS:CD2	24:Z:465:ALA:CB	3.02	0.42
16:A:1164:THR:HG21	16:A:1224:ARG:HD3	2.01	0.42
19:M:1268:MET:SD	19:M:1293:TRP:CH2	3.12	0.42
19:M:1507:LEU:O	19:M:1508:PHE:C	2.63	0.42
24:Z:229:ALA:HB1	24:Z:234:HIS:HB2	2.00	0.42
6:I:99:SER:HB3	6:I:111:TYR:CE1	2.55	0.42
23:X:478:LEU:HD21	23:X:499:LEU:CD1	2.50	0.42
16:A:353:ASN:O	16:A:357:LYS:HE2	2.20	0.42
19:M:617:ASN:HB2	19:M:668:ASP:OD1	2.19	0.42
21:U:400:ASP:OD1	21:U:401:GLU:N	2.53	0.42
5:H:60:ILE:HG21	5:H:135:PHE:CZ	2.54	0.42
8:K:96:SER:O	8:K:100:LEU:HD13	2.20	0.42
16:A:407:ARG:NH2	16:A:407:ARG:HB2	2.35	0.42
17:B:633:LEU:HD11	17:B:679:PRO:HG3	2.00	0.42
23:X:444:ALA:C	23:X:445:VAL:HG12	2.44	0.42
24:Z:236:LYS:O	24:Z:237:GLN:C	2.62	0.42
13:W:110:TRP:CD1	13:W:111:THR:H	2.38	0.42
16:A:164:PHE:CZ	25:a:563:MET:HG3	2.55	0.42
16:A:358:ARG:O	17:B:1074:PRO:HD2	2.20	0.42
16:A:1139:LEU:HD23	16:A:1359:SER:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1376:LYS:O	16:A:1379:GLU:HG2	2.19	0.42
17:B:1067:ILE:HG13	17:B:1072:ARG:C	2.45	0.42
13:W:36:VAL:CG2	13:W:72:ILE:HD11	2.49	0.41
16:A:205:VAL:CG2	16:A:212:LYS:HE2	2.50	0.41
17:B:783:ALA:HB2	17:B:1041:ILE:HD12	2.02	0.41
19:M:1166:LEU:HD23	19:M:1266:ARG:HG3	2.02	0.41
19:M:1462:ILE:HD11	19:M:1508:PHE:CE1	2.55	0.41
8:K:51:LEU:HD22	16:A:561:MET:HE1	2.02	0.41
17:B:84:TYR:CE1	17:B:423:ILE:HB	2.55	0.41
19:M:285:GLN:H	19:M:285:GLN:CD	2.29	0.41
8:K:4:PRO:HD2	16:A:479:TRP:CZ2	2.56	0.41
11:Q:748:PRO:HB3	13:W:110:TRP:CH2	2.55	0.41
16:A:200:ALA:HB2	16:A:216:LEU:CD2	2.49	0.41
16:A:994:PHE:CD2	16:A:1064:ALA:HB2	2.55	0.41
16:A:1142:PHE:HE2	16:A:1317:LYS:O	2.03	0.41
7:J:10:CYS:HB2	18:C:180:ALA:O	2.21	0.41
8:K:29:ASN:CG	8:K:79:PRO:HA	2.45	0.41
16:A:832:THR:CG2	16:A:833:PRO:HD2	2.50	0.41
23:X:361:ILE:HG13	23:X:441:ARG:HB2	2.02	0.41
23:X:445:VAL:HG13	23:X:475:ALA:CA	2.50	0.41
24:Z:181:THR:HG22	24:Z:226:TYR:HE2	1.74	0.41
5:H:60:ILE:HD13	5:H:123:MET:HE1	2.01	0.41
17:B:300:MET:HE1	17:B:376:ALA:HB1	2.02	0.41
19:M:1286:LEU:HD21	24:Z:664:PRO:HB2	2.01	0.41
19:M:1350:MET:O	19:M:1372:LYS:HD3	2.20	0.41
24:Z:459:ASP:OD1	24:Z:459:ASP:N	2.53	0.41
14:Y:57:PHE:CD1	14:Y:57:PHE:C	2.99	0.41
17:B:502:HIS:ND1	17:B:504:THR:HG22	2.36	0.41
17:B:550:MET:CE	17:B:567:ILE:HG21	2.49	0.41
19:M:620:PRO:CD	19:M:639:TYR:CE2	3.04	0.41
19:M:1266:ARG:HH11	19:M:1293:TRP:HB2	1.85	0.41
21:U:442:LYS:HE3	22:V:205:MET:HE1	2.02	0.41
4:G:38:CYS:SG	4:G:157:ILE:HG13	2.61	0.41
5:H:91:VAL:HG22	5:H:144:LEU:HD23	2.00	0.41
5:H:116:VAL:CG2	5:H:123:MET:HE2	2.51	0.41
8:K:97:GLU:HG3	18:C:4:ALA:HB1	2.01	0.41
17:B:388:TYR:H	17:B:504:THR:CG2	2.32	0.41
17:B:686:GLU:N	17:B:686:GLU:OE1	2.54	0.41
2:E:105:VAL:HG13	2:E:135:LEU:HD12	2.03	0.41
3:F:98:LYS:NZ	3:F:127:ASP:O	2.54	0.41
12:T:125:DC:H3'	12:T:126:DA:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:379:GLY:HA2	16:A:475:ARG:O	2.20	0.41
5:H:12:VAL:HG11	5:H:15:ILE:HD11	2.03	0.41
5:H:52:LEU:HD23	5:H:53:GLY:N	2.35	0.41
5:H:56:PHE:CG	5:H:145:MET:HE3	2.56	0.41
16:A:687:ILE:HD11	16:A:766:PHE:CE2	2.56	0.41
16:A:1004:LEU:HD13	16:A:1062:GLY:HA2	2.03	0.41
16:A:1371:ILE:O	16:A:1374:VAL:HB	2.21	0.41
19:M:1326:ILE:O	19:M:1326:ILE:CG2	2.68	0.41
19:M:1330:ILE:CD1	19:M:1394:LEU:HD13	2.51	0.41
19:M:1470:GLY:O	19:M:1488:THR:HA	2.20	0.41
21:U:527:ASP:O	21:U:531:GLN:HG3	2.21	0.41
22:V:258:VAL:HG21	22:V:297:TRP:CD2	2.56	0.41
23:X:364:ILE:CG1	23:X:428:VAL:O	2.69	0.41
23:X:475:ALA:HB3	23:X:494:VAL:HG22	2.02	0.41
5:H:123:MET:HG2	5:H:124:ARG:N	2.36	0.41
9:L:19:CYS:SG	9:L:22:CYS:HB2	2.61	0.40
11:Q:605:LEU:HD12	23:X:238:LEU:HD13	2.03	0.40
16:A:296:ASN:OD1	16:A:296:ASN:C	2.64	0.40
21:U:443:TRP:CH2	22:V:193:HIS:HA	2.56	0.40
22:V:251:ASP:OD1	22:V:251:ASP:C	2.64	0.40
16:A:85:PHE:CZ	17:B:1163:MET:HB2	2.55	0.40
17:B:99:TRP:CE3	21:U:528:PRO:HD3	2.55	0.40
17:B:662:VAL:HG12	17:B:663:GLU:N	2.35	0.40
10:P:-7:U:H2'	10:P:-6:G:C8	2.56	0.40
16:A:470:MET:HB3	16:A:521:VAL:HG22	2.02	0.40
16:A:530:SER:O	16:A:531:ASN:CG	2.65	0.40
16:A:1070:GLY:HA3	23:X:505:HIS:CG	2.57	0.40
17:B:1022:LEU:H	17:B:1022:LEU:HD23	1.87	0.40
23:X:423:VAL:CG1	23:X:424:PRO:HD2	2.50	0.40
9:L:34:ILE:O	9:L:34:ILE:HG22	2.21	0.40
13:W:158:PRO:HG2	13:W:200:PRO:HA	2.03	0.40
16:A:280:LEU:O	16:A:284:VAL:HG23	2.21	0.40
16:A:1312:PRO:HG3	16:A:1335:ILE:HD13	2.03	0.40
17:B:1073:GLN:O	17:B:1074:PRO:C	2.63	0.40
20:N:152:DA:H2'	20:N:153:DT:C6	2.57	0.40
22:V:251:ASP:CB	22:V:335:ARG:HH12	2.34	0.40
23:X:423:VAL:HG13	23:X:424:PRO:HD2	2.02	0.40
5:H:37:MET:CE	5:H:131:ASN:ND2	2.84	0.40
9:L:43:ILE:HD11	17:B:116:ARG:HG3	2.04	0.40
16:A:1416:ARG:O	16:A:1420:ASN:HB2	2.22	0.40
17:B:409:LYS:O	17:B:413:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	124/142 (87%)	124 (100%)	0	0	100	100
2	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
3	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
4	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	H	147/150 (98%)	135 (92%)	12 (8%)	0	100	100
6	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
7	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
8	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
9	L	45/58 (78%)	39 (87%)	6 (13%)	0	100	100
11	Q	890/1179 (76%)	877 (98%)	13 (2%)	0	100	100
13	W	303/305 (99%)	296 (98%)	7 (2%)	0	100	100
14	Y	114/121 (94%)	108 (95%)	6 (5%)	0	100	100
15	b	65/85 (76%)	62 (95%)	3 (5%)	0	100	100
16	A	1462/1970 (74%)	1389 (95%)	72 (5%)	1 (0%)	48	81
17	B	1130/1174 (96%)	1063 (94%)	65 (6%)	2 (0%)	43	75
18	C	254/275 (92%)	240 (94%)	13 (5%)	1 (0%)	30	65
19	M	1050/1729 (61%)	1007 (96%)	42 (4%)	1 (0%)	48	81
21	U	175/666 (26%)	169 (97%)	6 (3%)	0	100	100
22	V	275/531 (52%)	266 (97%)	9 (3%)	0	100	100
23	X	223/531 (42%)	211 (95%)	10 (4%)	2 (1%)	14	48
24	Z	484/1087 (44%)	461 (95%)	23 (5%)	0	100	100
25	a	224/821 (27%)	218 (97%)	6 (3%)	0	100	100
All	All	7709/11642 (66%)	7385 (96%)	317 (4%)	7 (0%)	49	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	424	PRO
17	B	150	GLY
19	M	1515	TYR
16	A	1530	ALA
23	X	242	GLY
17	B	1001	PRO
18	C	130	VAL

5.3.2 Protein sidechains [i](#)

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	D	112/126 (89%)	110 (98%)	2 (2%)	51	68
2	E	191/192 (100%)	189 (99%)	2 (1%)	68	76
3	F	68/111 (61%)	65 (96%)	3 (4%)	25	48
4	G	149/153 (97%)	144 (97%)	5 (3%)	32	55
5	H	130/131 (99%)	125 (96%)	5 (4%)	29	51
6	I	105/112 (94%)	104 (99%)	1 (1%)	68	76
7	J	55/56 (98%)	54 (98%)	1 (2%)	51	68
8	K	104/106 (98%)	102 (98%)	2 (2%)	50	67
9	L	44/55 (80%)	43 (98%)	1 (2%)	44	64
11	Q	763/1011 (76%)	755 (99%)	8 (1%)	68	76
13	W	260/260 (100%)	258 (99%)	2 (1%)	73	78
14	Y	102/105 (97%)	101 (99%)	1 (1%)	68	76
15	b	61/77 (79%)	60 (98%)	1 (2%)	55	69
16	A	1290/1747 (74%)	1268 (98%)	22 (2%)	53	68
17	B	996/1027 (97%)	964 (97%)	32 (3%)	34	56
18	C	235/252 (93%)	230 (98%)	5 (2%)	47	65
19	M	954/1524 (63%)	943 (99%)	11 (1%)	63	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	163/590 (28%)	162 (99%)	1 (1%)	78	81
22	V	255/462 (55%)	247 (97%)	8 (3%)	35	57
23	X	208/467 (44%)	196 (94%)	12 (6%)	18	42
24	Z	438/940 (47%)	427 (98%)	11 (2%)	42	62
25	a	211/737 (29%)	211 (100%)	0	100	100
All	All	6894/10241 (67%)	6758 (98%)	136 (2%)	48	66

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	26	PHE
1	D	76	ASN
2	E	127	LEU
2	E	162	ARG
3	F	84	GLU
3	F	86	GLU
3	F	123	LEU
4	G	67	LEU
4	G	70	VAL
4	G	84	VAL
4	G	138	GLN
4	G	160	ILE
5	H	14	ASP
5	H	50	VAL
5	H	51	ASP
5	H	128	ASP
5	H	143	LEU
6	I	124	THR
7	J	30	THR
8	K	27	VAL
8	K	71	ILE
9	L	34	ILE
11	Q	263	THR
11	Q	293	LEU
11	Q	531	VAL
11	Q	674	ARG
11	Q	698	ILE
11	Q	857	LEU
11	Q	861	GLU
11	Q	862	GLU

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Mol	Chain	Res	Type
13	W	112	LEU
13	W	240	PHE
14	Y	40	LEU
15	b	36	ASP
16	A	31	LEU
16	A	67	ARG
16	A	126	ILE
16	A	144	VAL
16	A	205	VAL
16	A	216	LEU
16	A	365	THR
16	A	382	ARG
16	A	406	VAL
16	A	440	LEU
16	A	567	LEU
16	A	811	ILE
16	A	863	ARG
16	A	883	ILE
16	A	955	GLU
16	A	1007	ILE
16	A	1038	THR
16	A	1128	ILE
16	A	1155	LYS
16	A	1264	SER
16	A	1456	GLU
16	A	1531	TRP
17	B	135	GLU
17	B	139	GLN
17	B	166	LEU
17	B	199	LYS
17	B	230	ARG
17	B	232	THR
17	B	265	GLN
17	B	269	ILE
17	B	309	PHE
17	B	313	GLU
17	B	355	ASP
17	B	358	GLU
17	B	371	ARG
17	B	388	TYR
17	B	435	ILE
17	B	437	THR

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Mol	Chain	Res	Type
17	B	455	ASP
17	B	528	LEU
17	B	567	ILE
17	B	666	ASP
17	B	685	LYS
17	B	687	VAL
17	B	731	GLN
17	B	750	VAL
17	B	751	LEU
17	B	759	VAL
17	B	768	ARG
17	B	842	HIS
17	B	846	ASP
17	B	1038	THR
17	B	1048	TYR
17	B	1157	LEU
18	C	5	ASN
18	C	8	THR
18	C	96	GLU
18	C	147	ASP
18	C	151	VAL
19	M	288	GLU
19	M	594	LEU
19	M	612	GLU
19	M	910	LEU
19	M	1134	TYR
19	M	1170	ASN
19	M	1171	VAL
19	M	1232	LEU
19	M	1257	VAL
19	M	1390	ASN
19	M	1508	PHE
21	U	467	ASP
22	V	66	LEU
22	V	100	LEU
22	V	202	VAL
22	V	232	THR
22	V	238	LEU
22	V	285	ASP
22	V	286	VAL
22	V	296	ASN
23	X	213	PHE

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Mol	Chain	Res	Type
23	X	364	ILE
23	X	390	ASP
23	X	402	GLU
23	X	404	LEU
23	X	429	ASP
23	X	443	VAL
23	X	445	VAL
23	X	459	TRP
23	X	478	LEU
23	X	501	TYR
23	X	504	ARG
24	Z	224	TYR
24	Z	235	VAL
24	Z	259	GLU
24	Z	265	LYS
24	Z	390	LEU
24	Z	457	LEU
24	Z	459	ASP
24	Z	500	VAL
24	Z	502	LEU
24	Z	515	PRO
24	Z	599	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	GLN
1	D	38	HIS
1	D	47	GLN
2	E	35	GLN
2	E	71	GLN
2	E	133	GLN
4	G	24	ASN
4	G	138	GLN
4	G	155	ASN
5	H	29	HIS
5	H	131	ASN
6	I	46	GLN
6	I	100	HIS
7	J	52	HIS
8	K	2	ASN
11	Q	151	GLN

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Mol	Chain	Res	Type
11	Q	278	HIS
11	Q	324	GLN
11	Q	373	ASN
11	Q	564	HIS
11	Q	745	HIS
13	W	173	ASN
13	W	184	HIS
14	Y	12	HIS
15	b	31	HIS
16	A	62	GLN
16	A	72	GLN
16	A	96	HIS
16	A	372	ASN
16	A	403	GLN
16	A	410	ASN
16	A	439	HIS
16	A	742	ASN
16	A	804	HIS
16	A	995	HIS
16	A	1044	HIS
16	A	1417	HIS
16	A	1422	GLN
17	B	56	GLN
17	B	315	ASN
17	B	452	ASN
17	B	537	GLN
17	B	585	ASN
17	B	631	GLN
17	B	683	GLN
17	B	930	GLN
17	B	1030	ASN
17	B	1094	GLN
18	C	111	GLN
18	C	260	GLN
19	M	211	GLN
19	M	323	ASN
19	M	465	ASN
19	M	577	GLN
19	M	948	HIS
19	M	1007	ASN
19	M	1114	GLN
19	M	1151	ASN

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Mol	Chain	Res	Type
19	M	1264	HIS
19	M	1336	HIS
19	M	1342	GLN
23	X	525	HIS
24	Z	168	GLN
24	Z	169	GLN
24	Z	244	ASN
24	Z	300	GLN
24	Z	446	ASN
24	Z	534	HIS
24	Z	591	GLN
24	Z	593	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	20/21 (95%)	8 (40%)	5 (25%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	P	-20	U
10	P	-17	G
10	P	-16	U
10	P	-13	C
10	P	-12	G
10	P	-10	G
10	P	-9	C
10	P	-8	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	P	-21	U
10	P	-13	C
10	P	-11	U
10	P	-10	G
10	P	-9	C

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
16	TPO	A	1525	16	8,10,11	2.64	1 (12%)	10,14,16	1.29	1 (10%)
16	SEP	A	1547	16	8,9,10	1.54	1 (12%)	7,12,14	2.64	2 (28%)

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
16	TPO	A	1525	16	-	1/9/11/13	-
16	SEP	A	1547	16	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1525	TPO	P-OG1	7.29	1.72	1.59
16	A	1547	SEP	P-O1P	3.30	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1547	SEP	OG-CB-CA	6.22	114.20	108.14
16	A	1547	SEP	O3P-P-OG	2.56	113.33	106.67
16	A	1525	TPO	OG1-P-O1P	-2.27	101.23	109.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	1547	SEP	N-CA-CB-OG
16	A	1547	SEP	C-CA-CB-OG
16	A	1525	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1525	TPO	1	0
16	A	1547	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

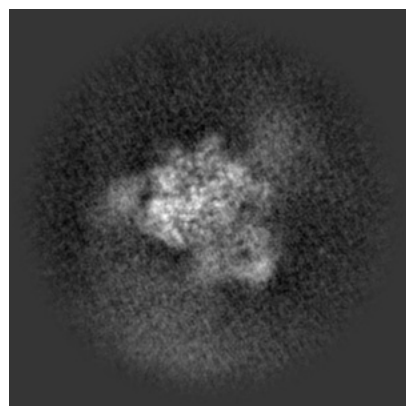
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54251. These allow visual inspection of the internal detail of the map and identification of artifacts.

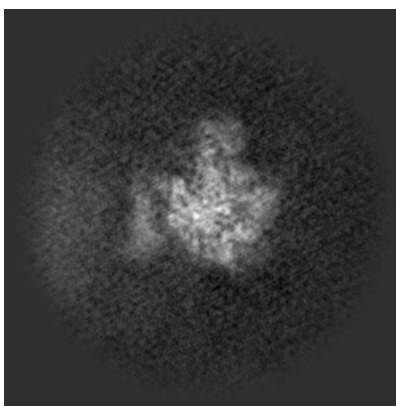
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

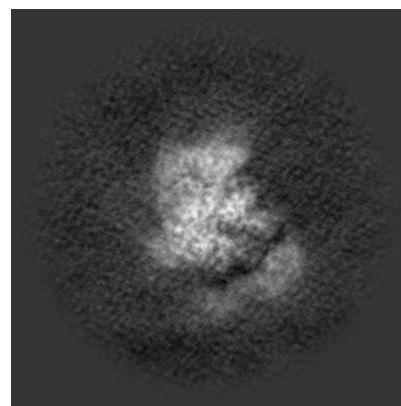
6.1.1 Primary map



X

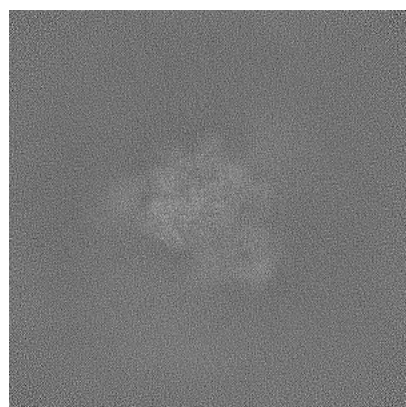


Y

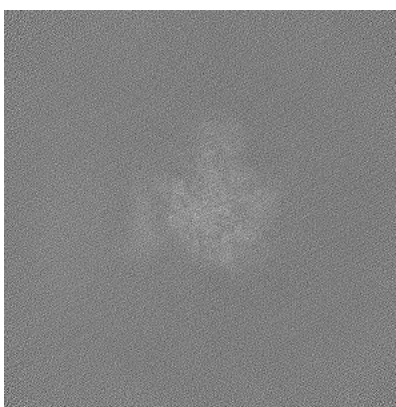


Z

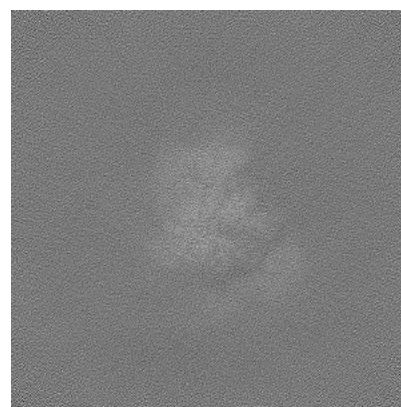
6.1.2 Raw map



X



Y

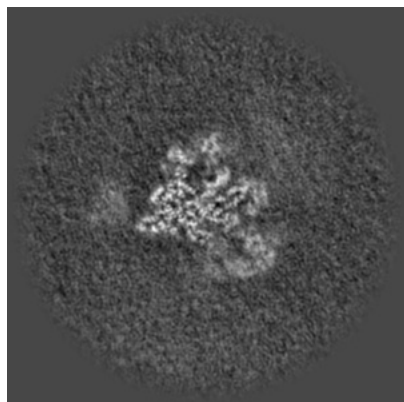


Z

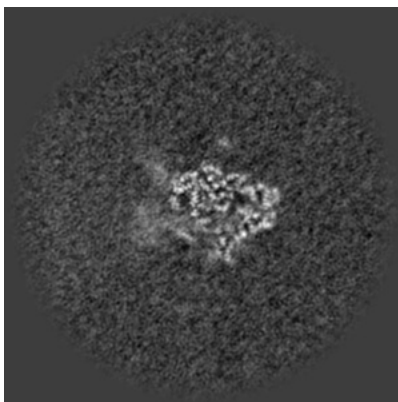
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

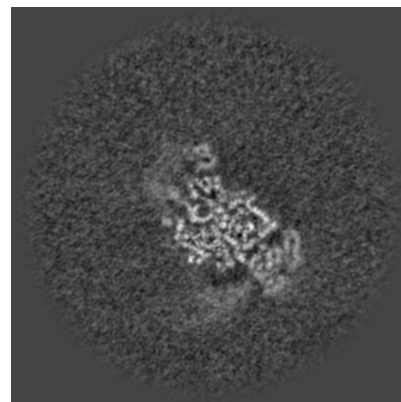
6.2.1 Primary map



X Index: 220

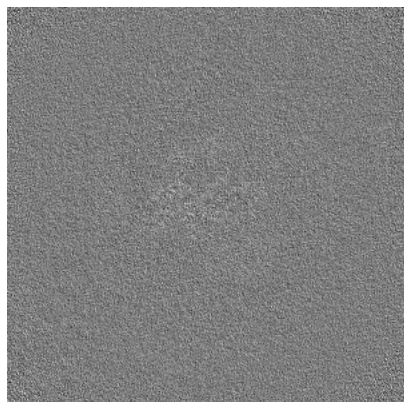


Y Index: 220

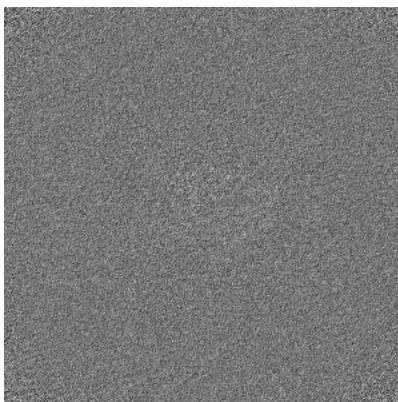


Z Index: 220

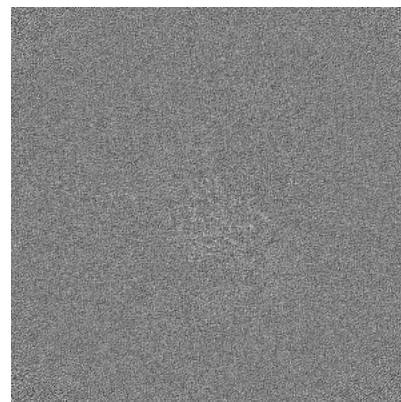
6.2.2 Raw map



X Index: 220



Y Index: 220

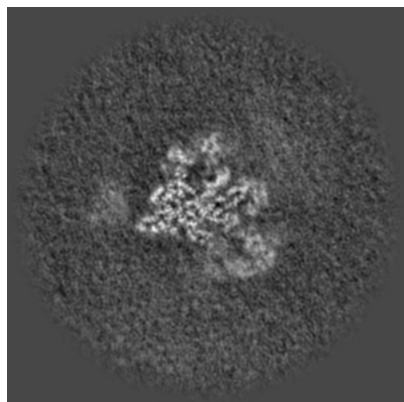


Z Index: 220

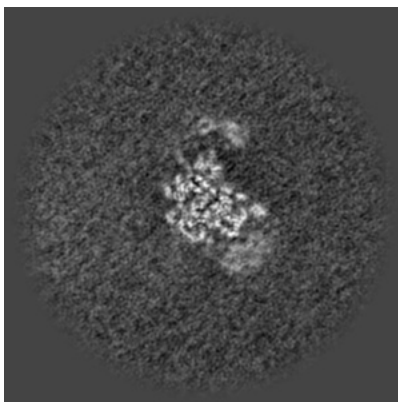
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

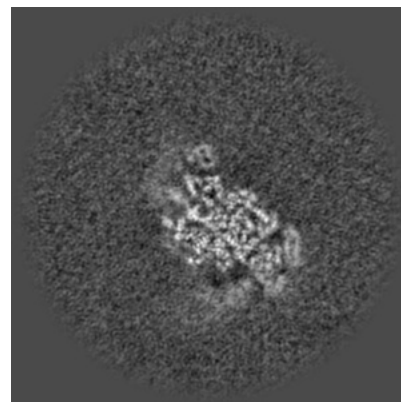
6.3.1 Primary map



X Index: 220

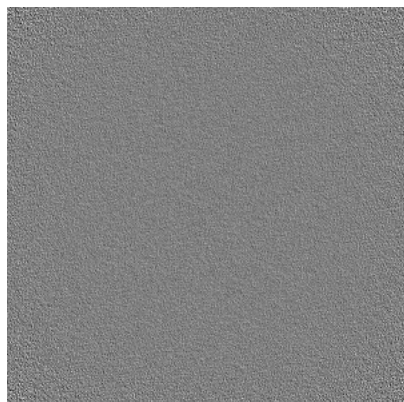


Y Index: 180

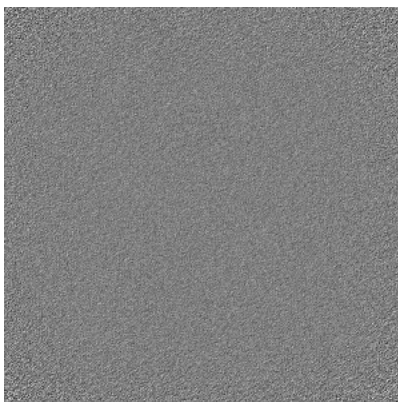


Z Index: 222

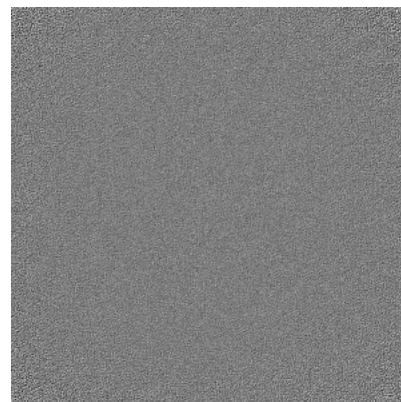
6.3.2 Raw map



X Index: 0



Y Index: 0

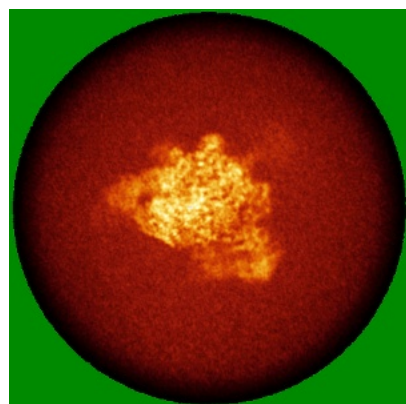


Z Index: 0

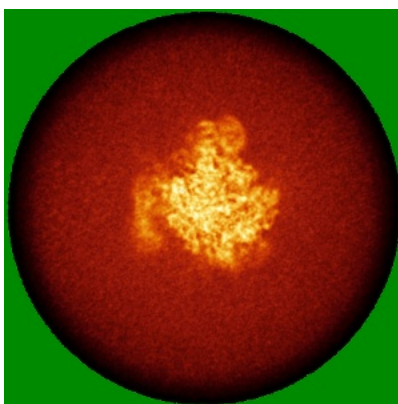
The images above show the largest variance slices of the map in three orthogonal directions.

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

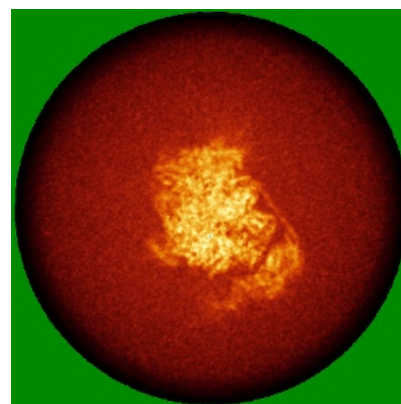
6.4.1 Primary map



X

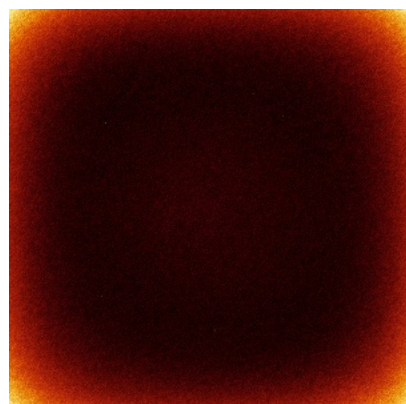


Y

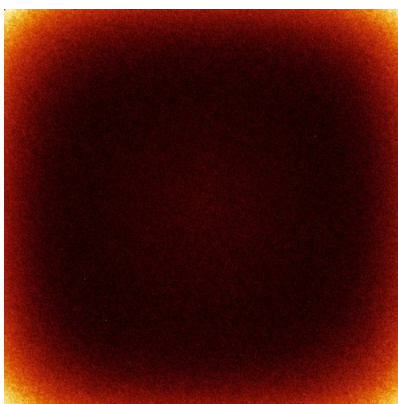


Z

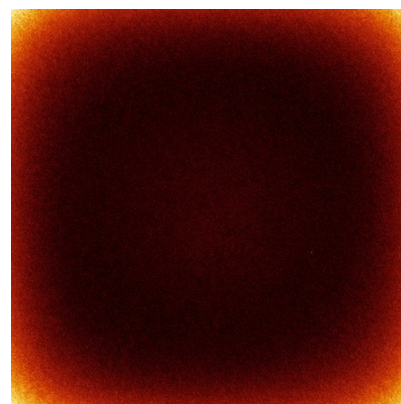
6.4.2 Raw map



X



Y

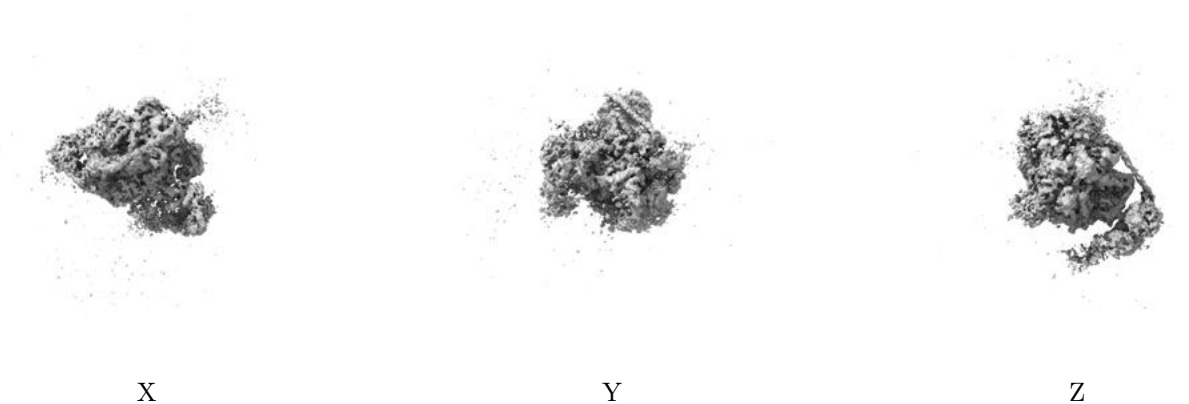


Z

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.

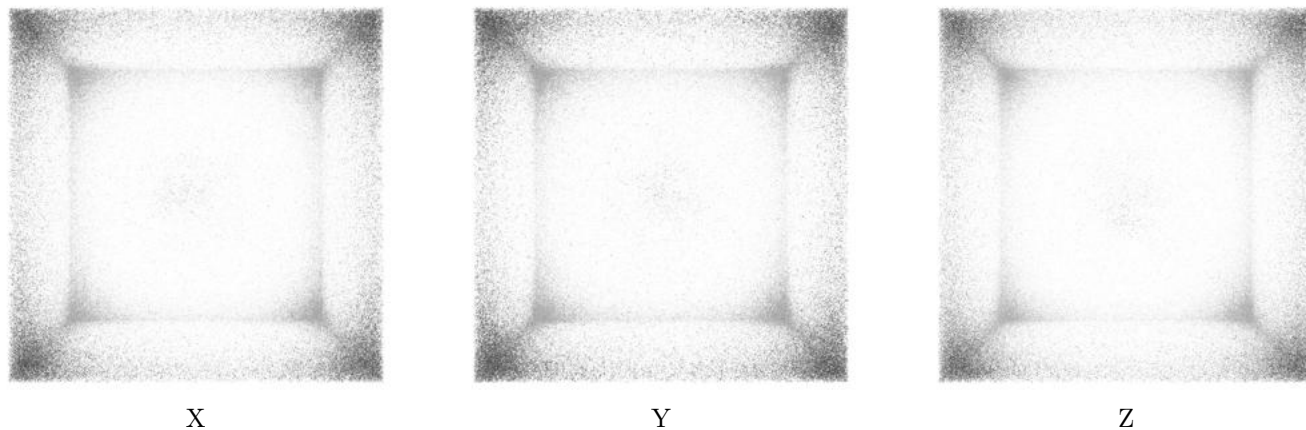
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

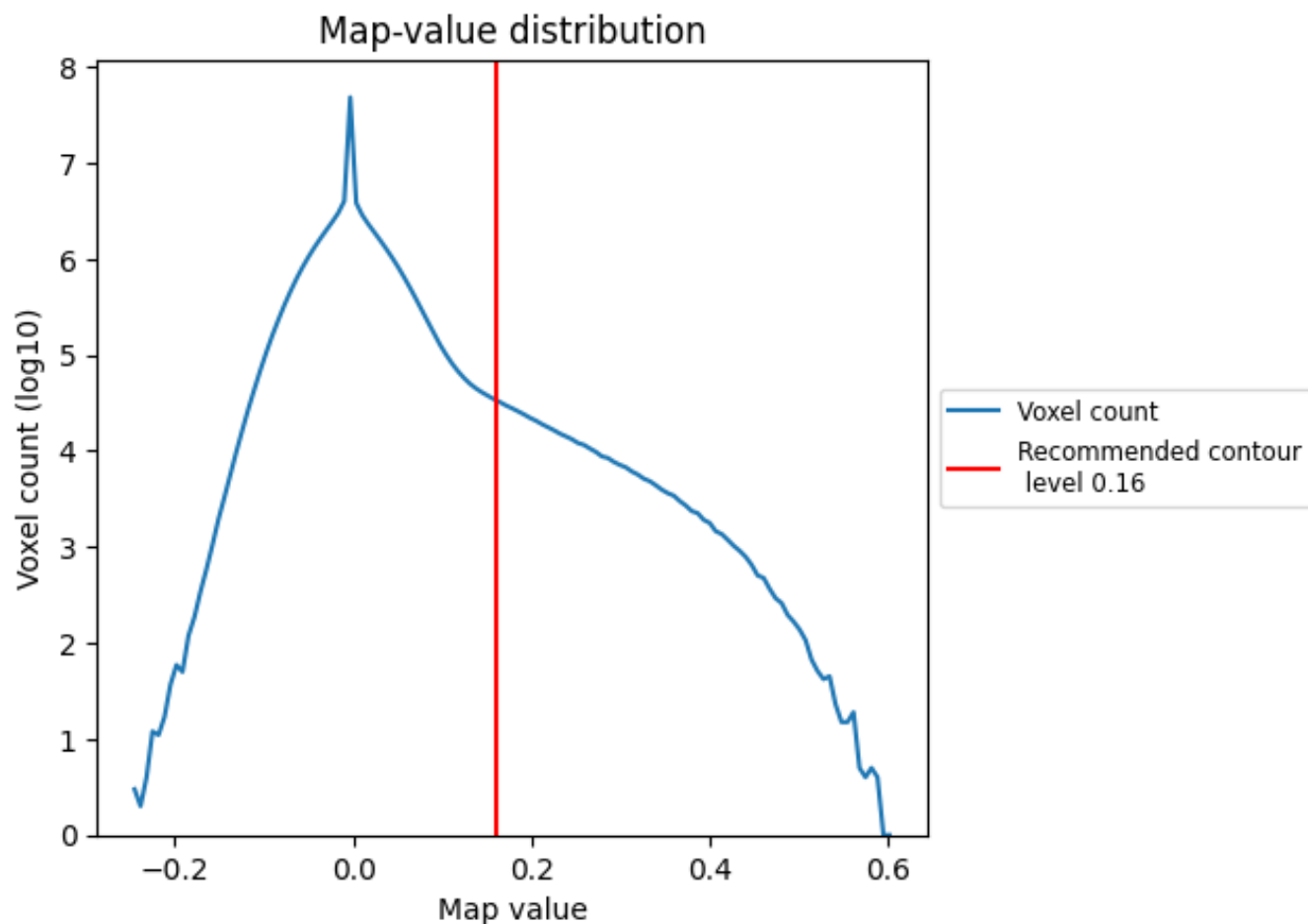
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

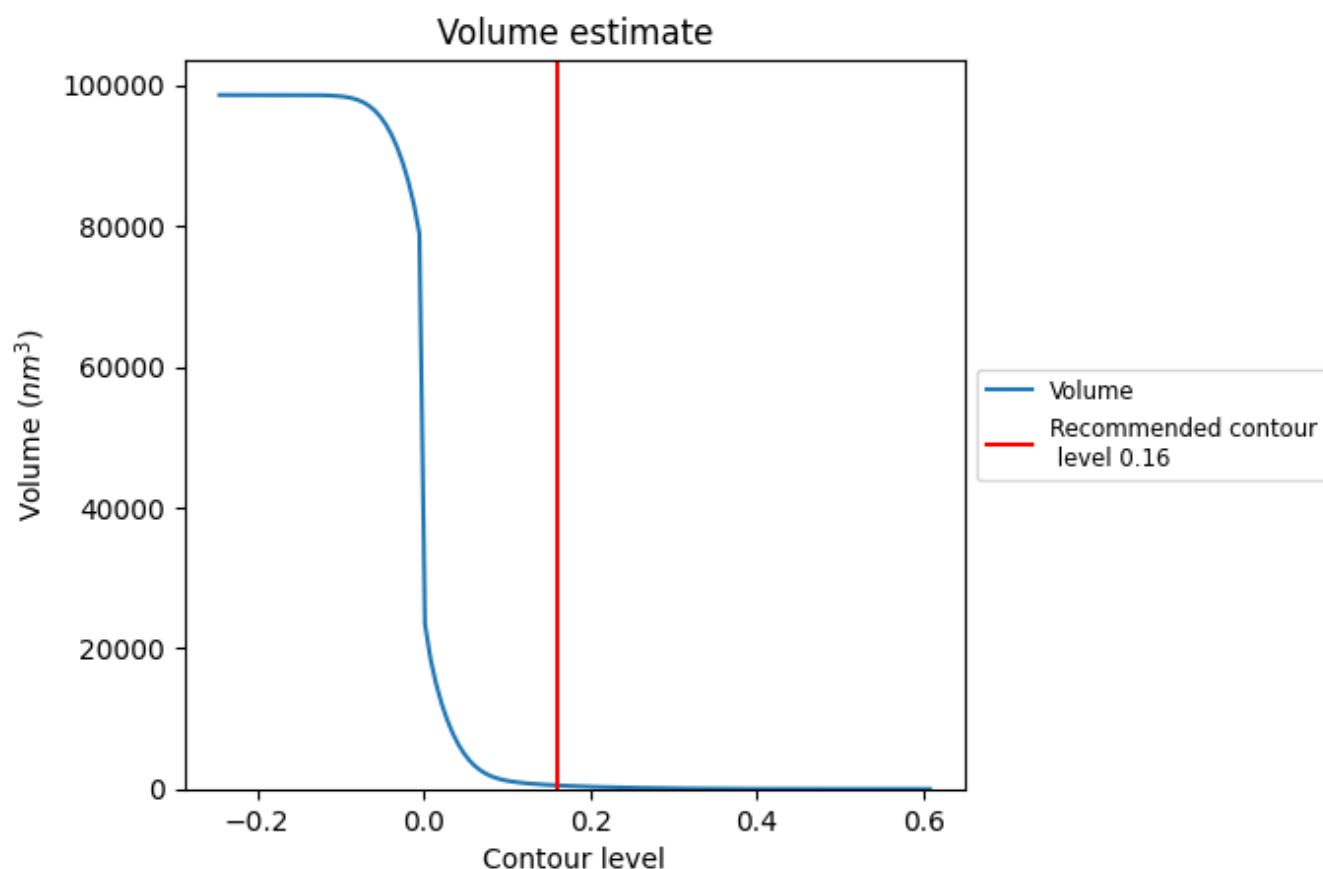
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

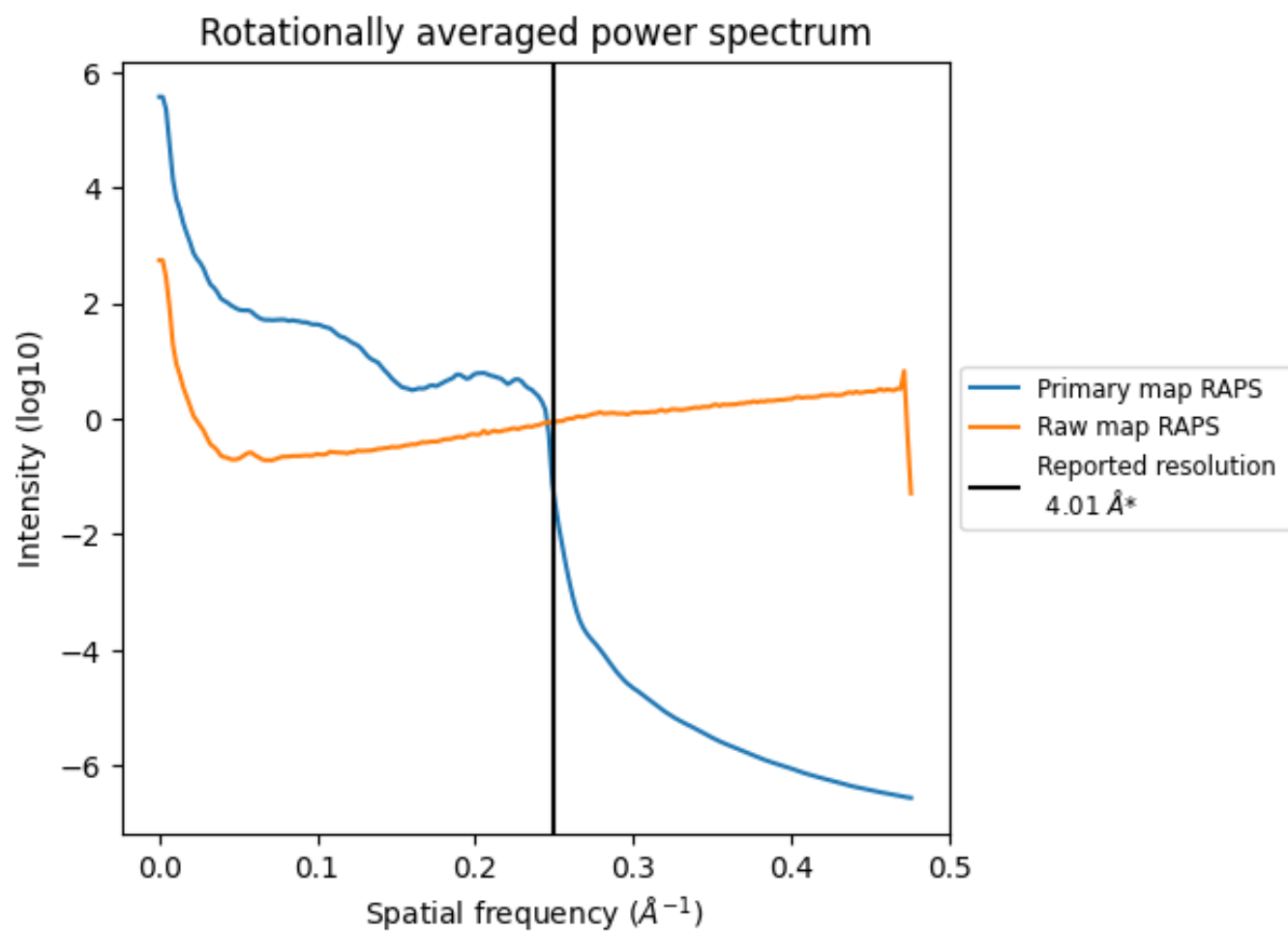
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm³; this corresponds to an approximate mass of 467 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 [i](#)

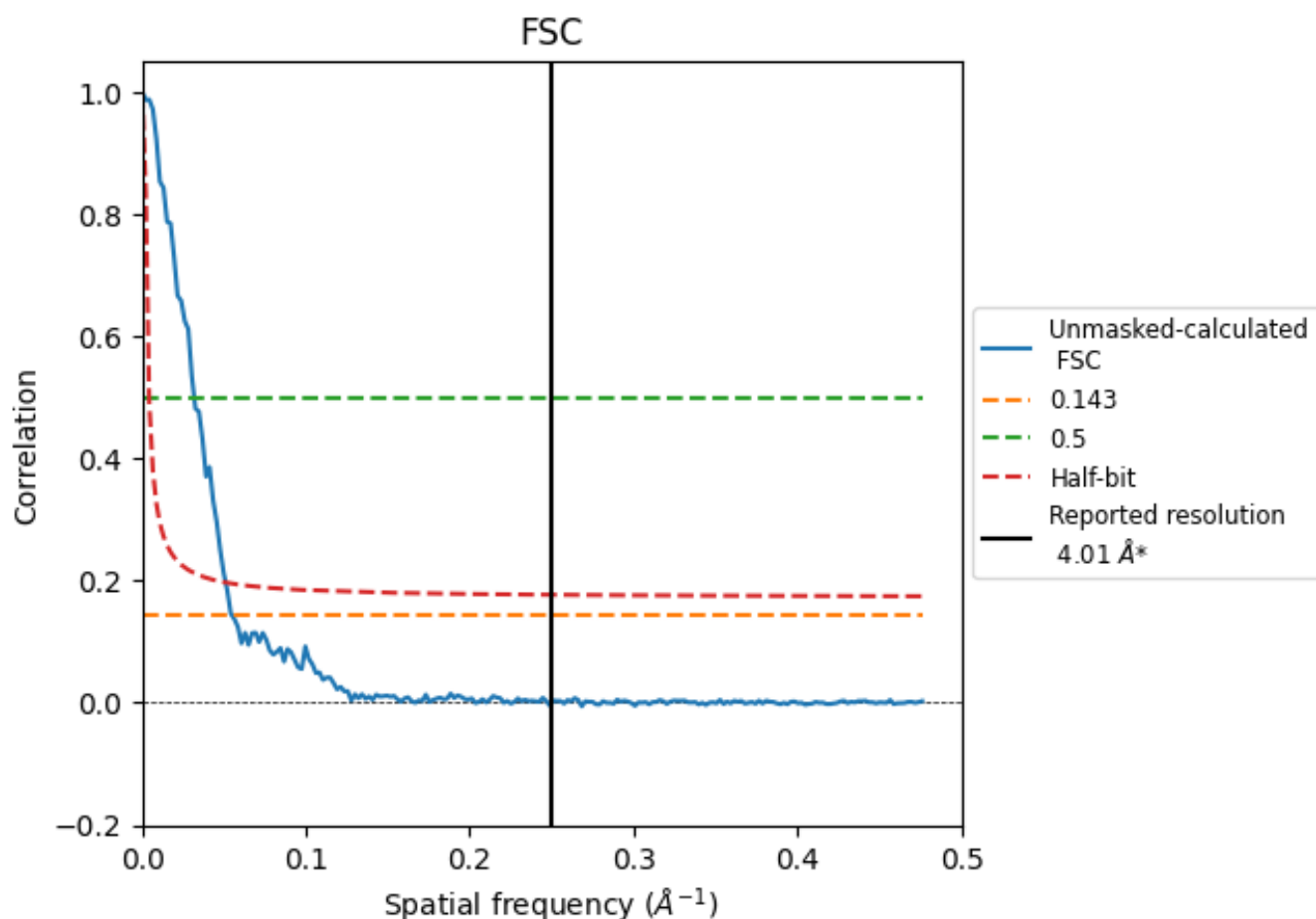


*Reported resolution corresponds to spatial frequency of 0.249 $\text{\AA}^{-1}$

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 0.249 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

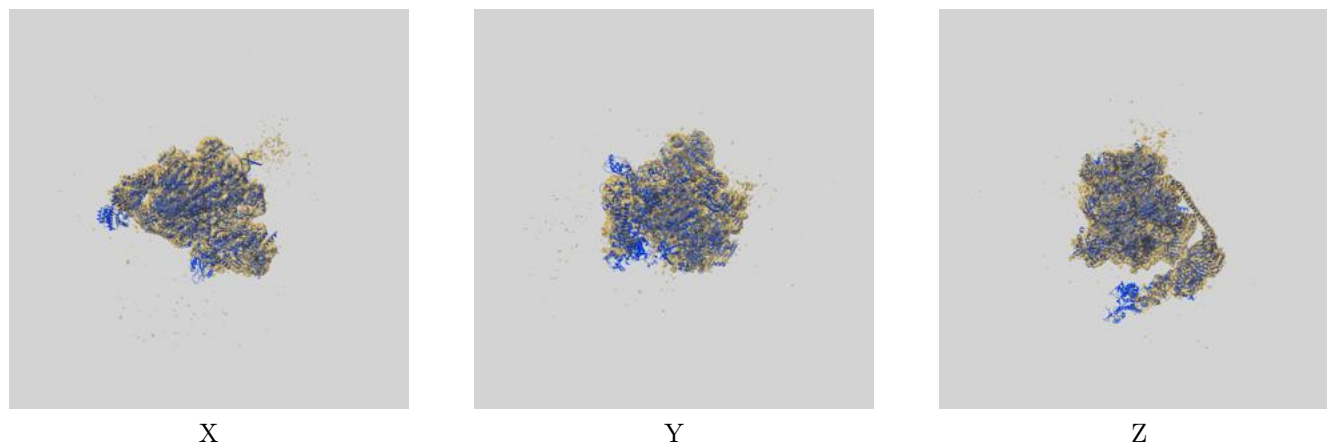
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	18.28	31.55	19.61

*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 18.28 differs from the reported value 4.01 by more than 10 %

9 Map-model fit [i](#)

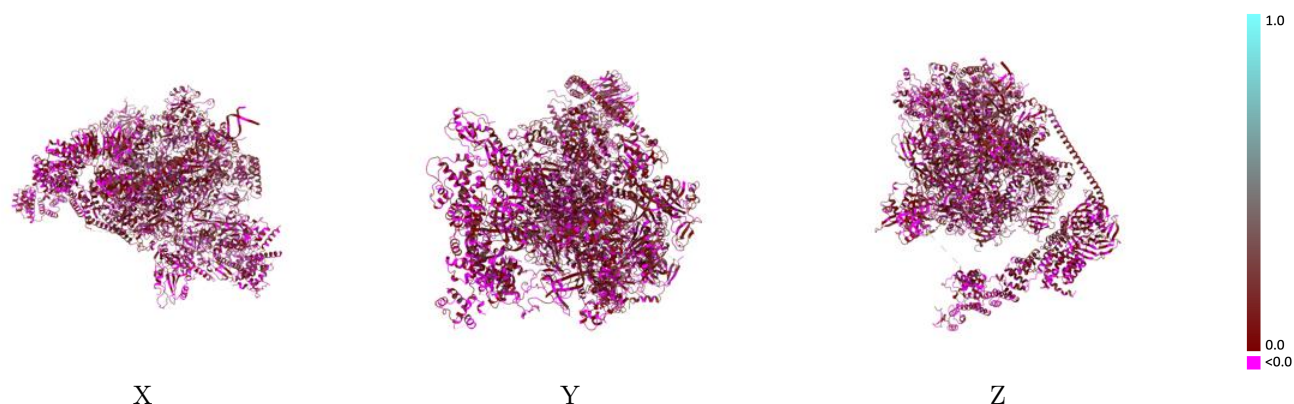
This section contains information regarding the fit between EMDB map EMD-54251 and PDB model 9RTT. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



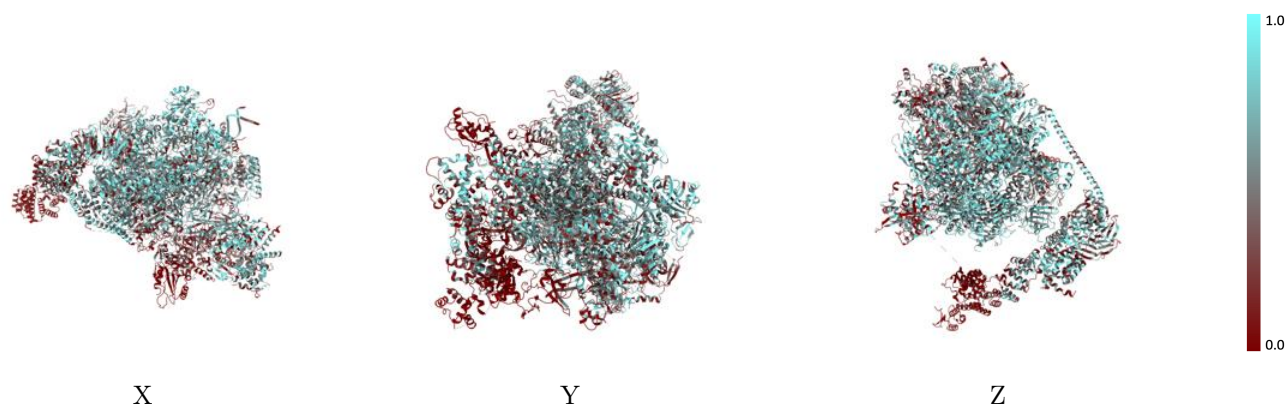
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



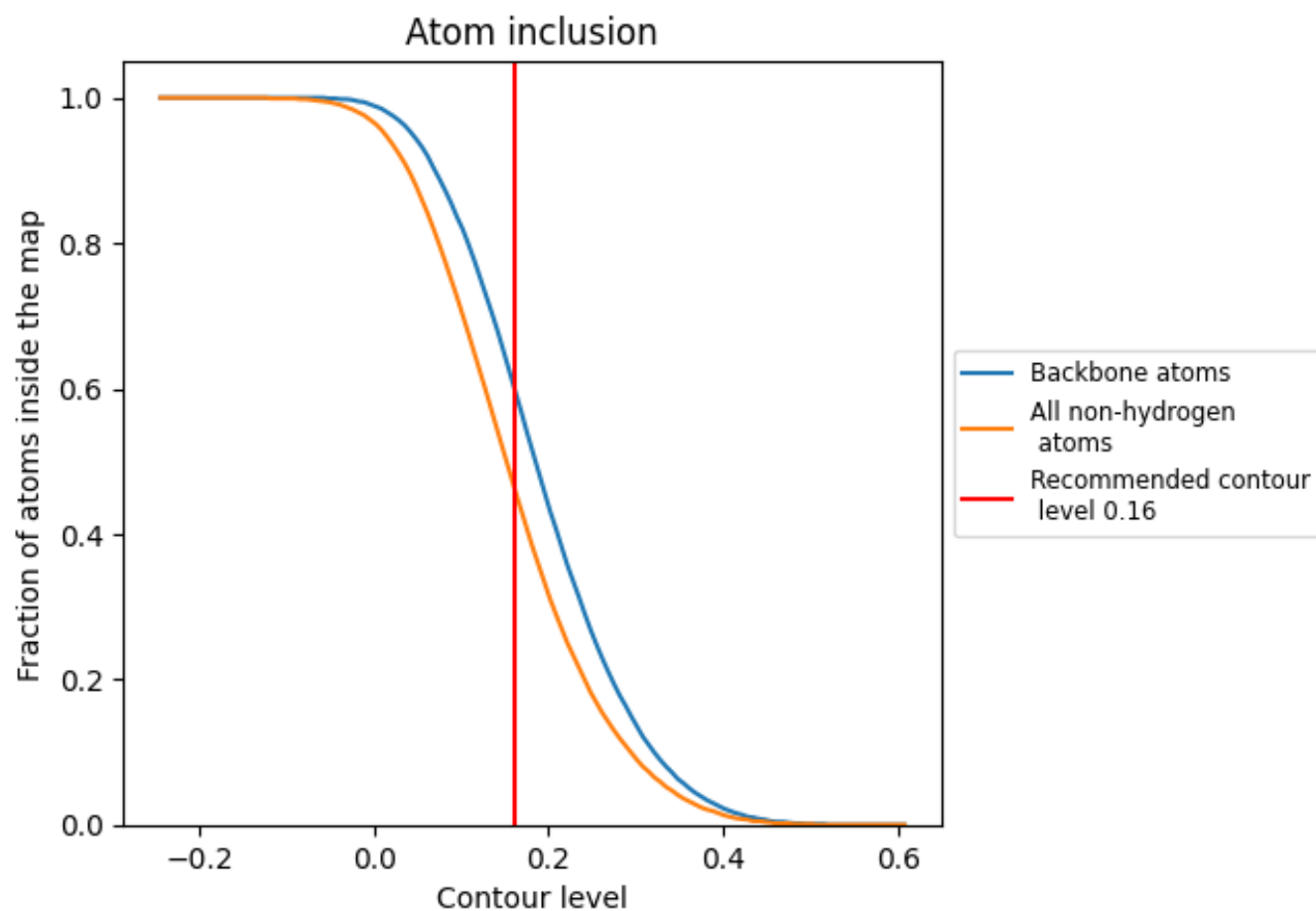
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 47% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4660	 0.0800
A	 0.5760	 0.0970
B	 0.5840	 0.0960
C	 0.6610	 0.1030
D	 0.5300	 0.0620
E	 0.6680	 0.1170
F	 0.6580	 0.1140
G	 0.5840	 0.0940
H	 0.5850	 0.0840
I	 0.6400	 0.0930
J	 0.6270	 0.0780
K	 0.5840	 0.1040
L	 0.6470	 0.1420
M	 0.2420	 0.0380
N	 0.5810	 0.1170
P	 0.5120	 0.1400
Q	 0.3480	 0.0560
T	 0.6530	 0.1400
U	 0.3590	 0.0770
V	 0.3030	 0.0640
W	 0.4860	 0.0650
X	 0.2900	 0.1100
Y	 0.3740	 0.0570
Z	 0.3230	 0.0530
a	 0.4290	 0.0860
b	 0.6800	 0.1110

