



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:10 PM UTC

PDB ID : 8UHD / pdb_00008uhd
EMDB ID : EMD-42270
Title : Structure of paused transcription complex Pol II-DSIF-NELF - post-translocated
Authors : Su, B.G.; Vos, S.M.
Deposited on : 2023-10-08
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

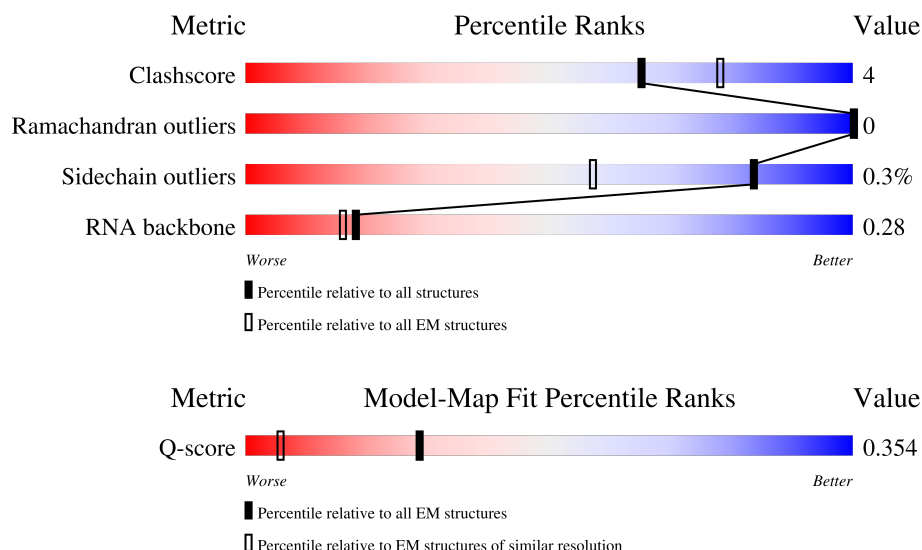
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	X	380	
2	Z	1087	
3	W	590	

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Mol	Chain	Length	Quality of chain
4	V	580	
5	A	1970	
6	B	1174	
7	C	271	
8	D	142	
9	E	210	
10	F	127	
11	G	172	
12	H	150	
13	I	125	
14	J	67	
15	K	117	
16	L	58	
17	N	50	
18	P	22	
19	T	50	
20	U	527	
21	Y	117	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 94662 atoms, of which 47102 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 Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	12	Total	C	H	N	O	0	0
			219	68	116	19	16		

- Molecule 2 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	471	Total	C	H	N	O	0	0
			7618	2404	3840	664	693	17	

- Molecule 3 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	530	Total	C	H	N	O	0	0
			8438	2699	4221	704	790	24	

- Molecule 4 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	550	Total	C	H	N	O	0	0
			8909	2825	4499	751	810	24	

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1416	Total	C	H	N	O	0	0
			22558	7055	11342	2006	2084	71	

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1136	Total	C	H	N	O	0	0
			18189	5739	9113	1597	1676	64	

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	C	254	Total	C	H	N	O	S	0	0
			4027	1282	1989	348	402	6		

- Molecule 8 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	D	124	Total	C	H	N	O	S	0	0
			2016	632	1004	173	203	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	E	207	Total	C	H	N	O	S	0	0
			3438	1083	1729	298	320	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	F	77	Total	C	H	N	O	S	0	0
			1271	397	653	105	111	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	G	171	Total	C	H	N	O	S	0	0
			2709	875	1358	219	249	8		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	H	148	Total	C	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	I	114	Total	C	H	N	O	S	0	0
			1787	571	859	166	180	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	J	65	Total	C	H	N	O	S	0	0
			1049	334	534	87	88	6		

- Molecule 15 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K	115	Total	C	H	N	O	S	0	0
			1862	593	942	152	173	2		

- Molecule 16 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L	44	Total	C	H	N	O	S	0	0
			751	231	378	72	64	6		

- Molecule 17 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N	28	Total	C	H	N	O	P	0	0
			886	272	316	100	170	28		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	P	15	Total	C	H	N	O	P	0	0
			474	141	158	50	110	15		

- Molecule 19 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	38	Total	C	H	N	O	P	0	0
			1208	371	426	148	225	38		

- Molecule 20 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	U	199	Total	C	H	N	O	S	0	0
			3092	965	1571	256	292	8		

- Molecule 21 is a protein called Transcription elongation factor SPT4.

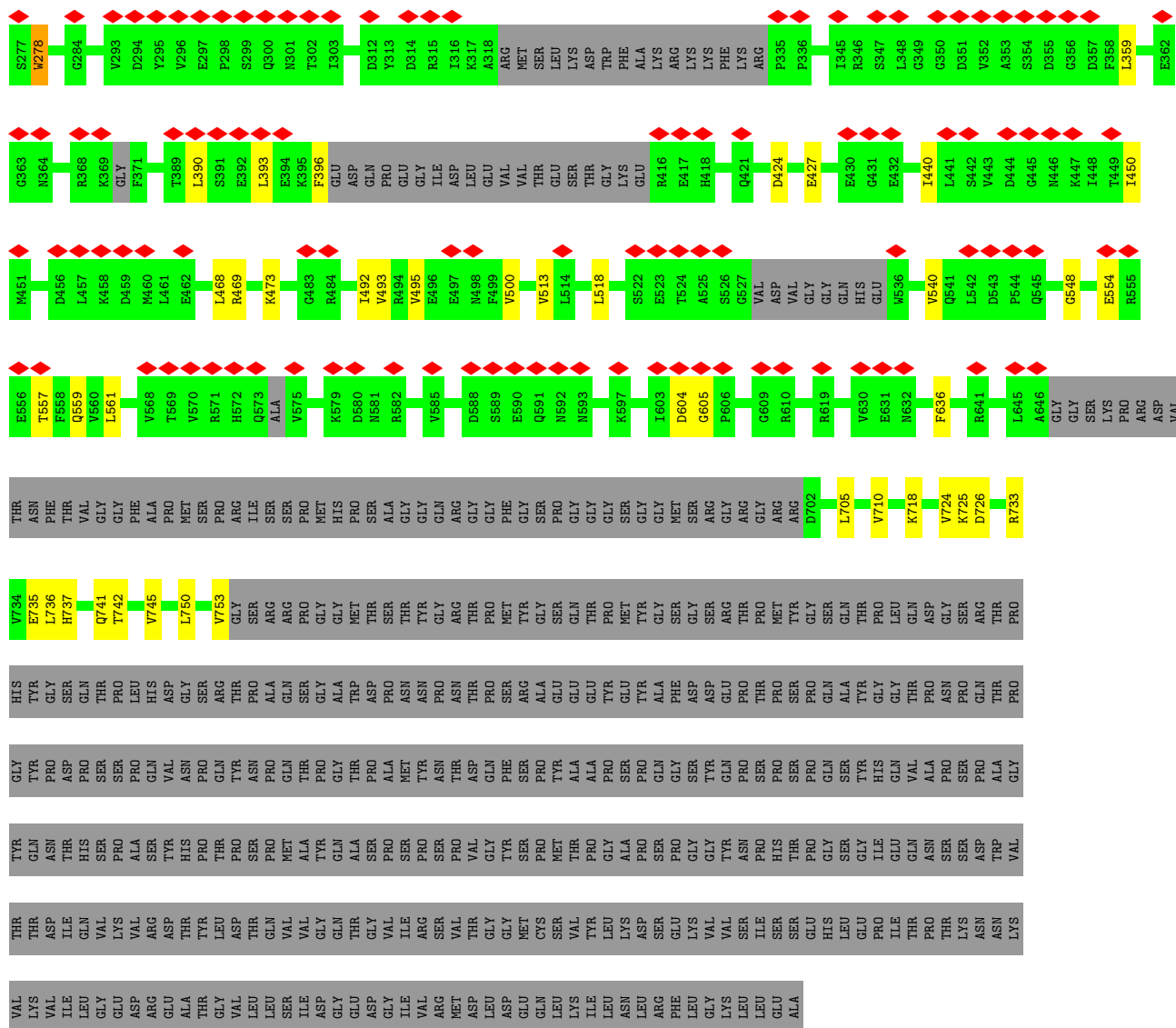
Mol	Chain	Residues	Atoms						AltConf	Trace
21	Y	116	Total	C	H	N	O	S	0	0
			1818	570	907	159	173	9		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

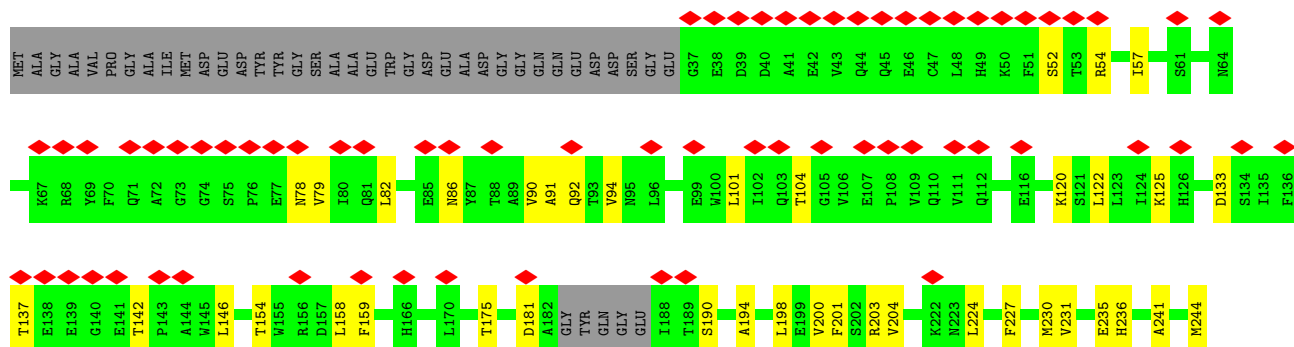
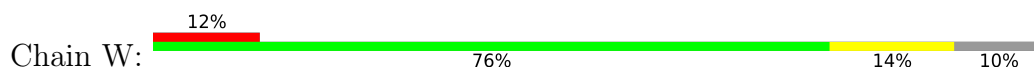
Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Zn	0
			2	2	
22	B	1	Total	Zn	0
			1	1	
22	C	1	Total	Zn	0
			1	1	
22	I	2	Total	Zn	0
			2	2	
22	J	1	Total	Zn	0
			1	1	
22	L	1	Total	Zn	0
			1	1	
22	Y	1	Total	Zn	0
			1	1	

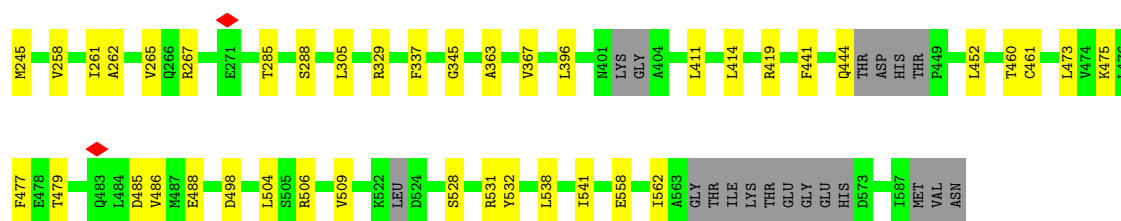
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

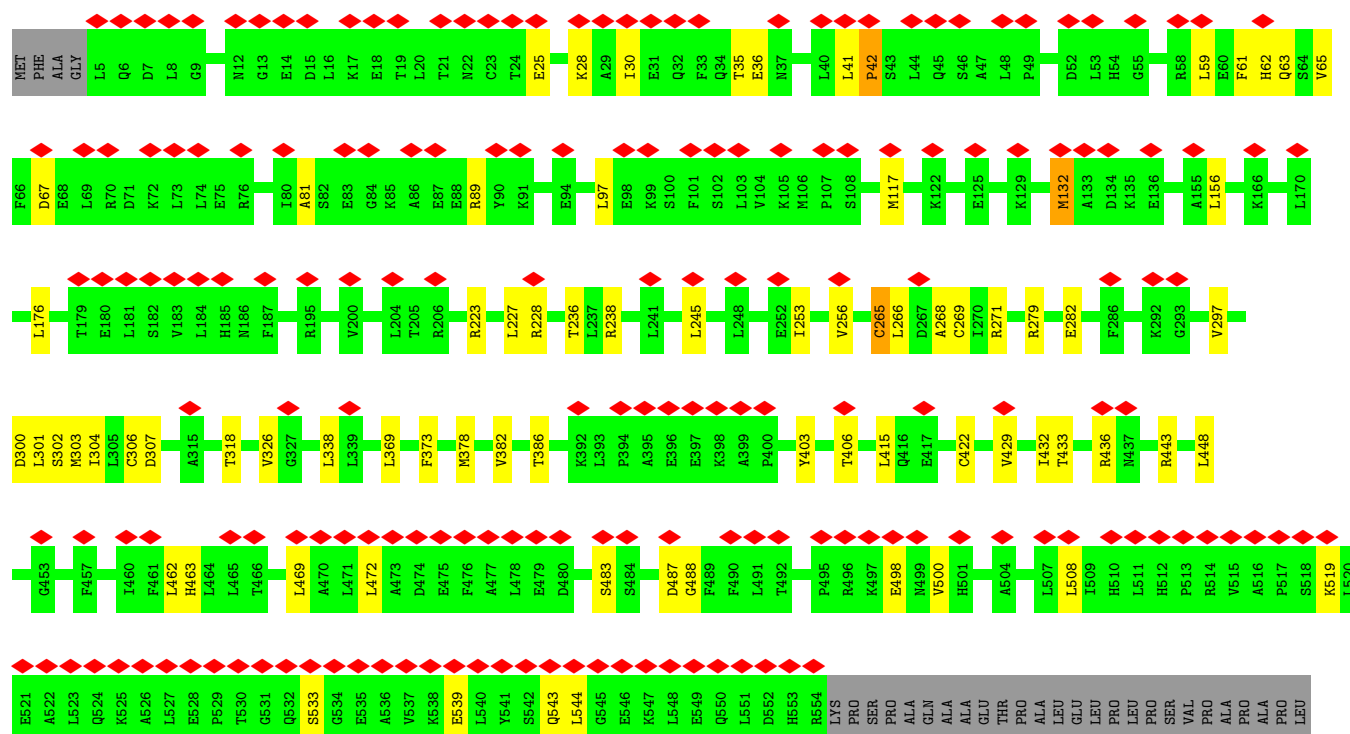
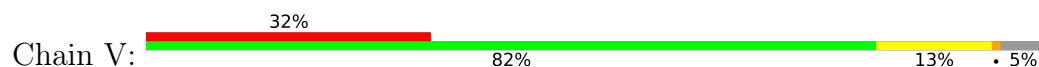


• Molecule 3: Negative elongation factor C/D

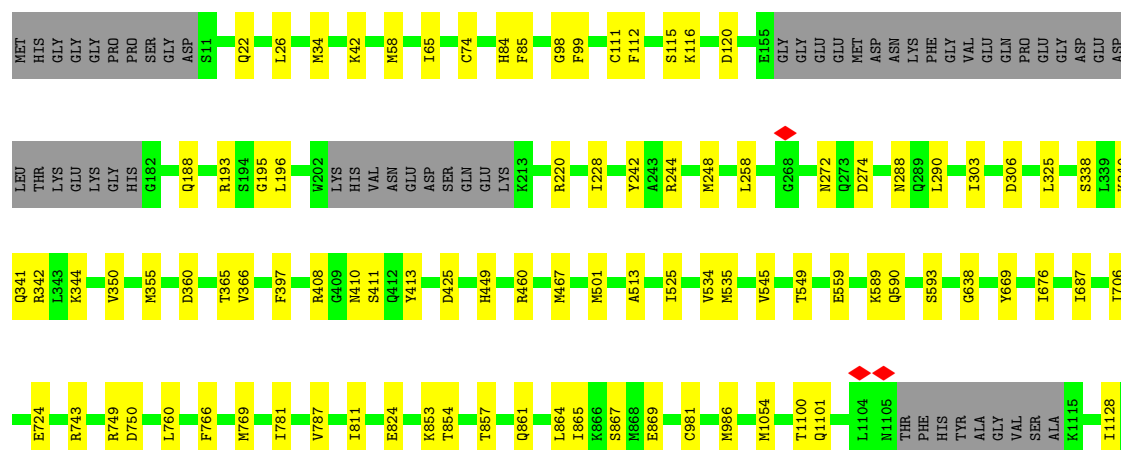


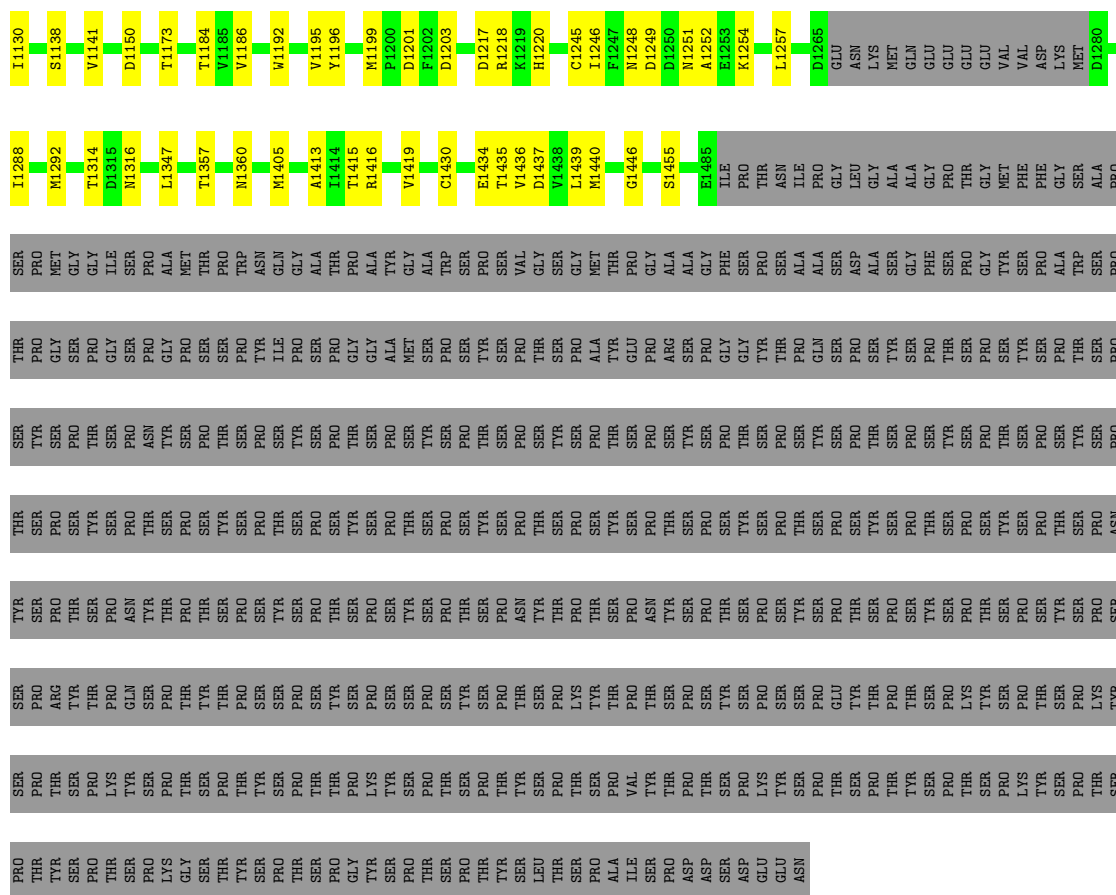


• Molecule 4: Negative elongation factor B



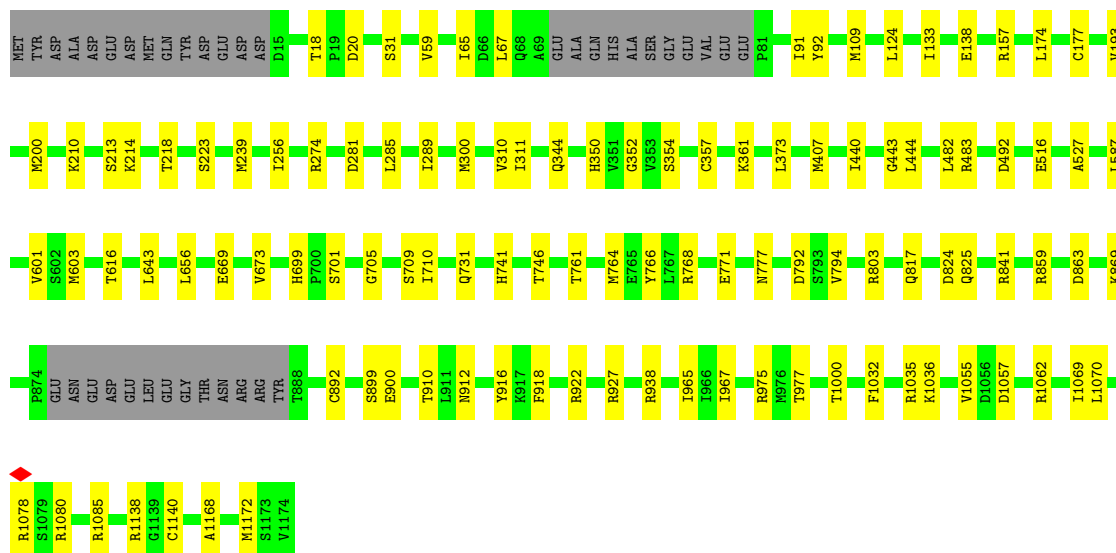
• Molecule 5: DNA-directed RNA polymerase subunit





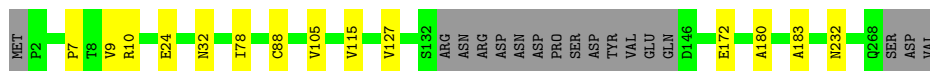
• Molecule 6: DNA-directed RNA polymerase subunit beta

Chain B: 87% 9% .

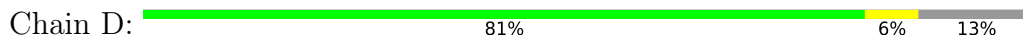


• Molecule 7: DNA-directed RNA polymerase II subunit RPB3

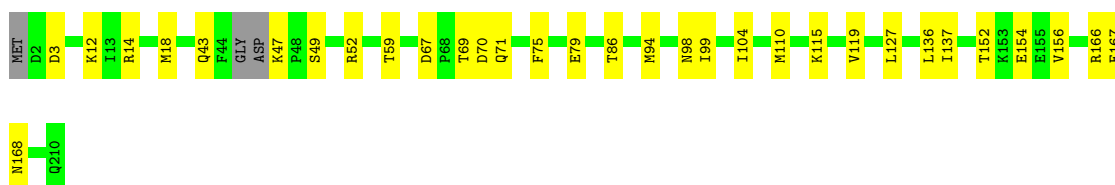
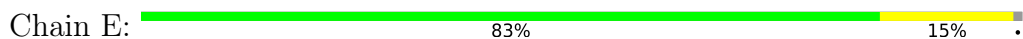
Chain C: 89% 5% 6%



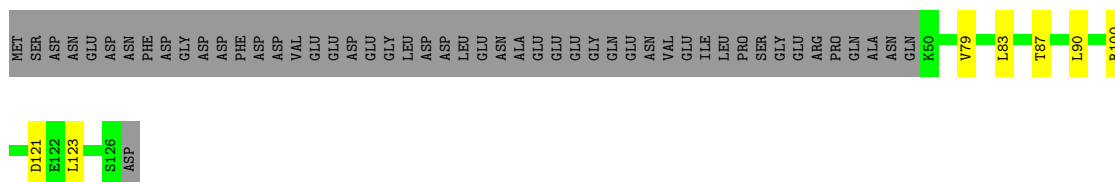
- Molecule 8: RNA polymerase Rpb4/RPC9 core domain-containing protein



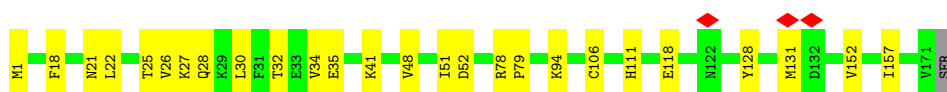
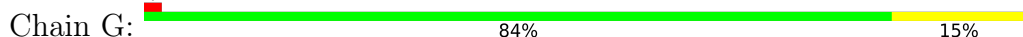
- Molecule 9: DNA-directed RNA polymerase II subunit E



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 11: DNA-directed RNA polymerase II subunit RPB7



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC3

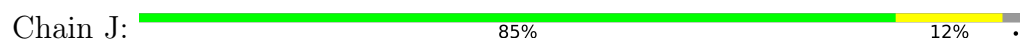


- Molecule 13: DNA-directed RNA polymerase II subunit RPB9

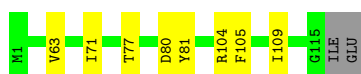




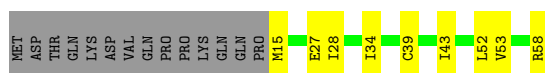
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC5



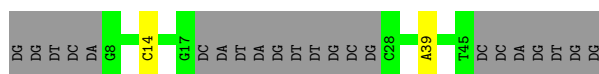
- Molecule 15: RNA polymerase II subunit J



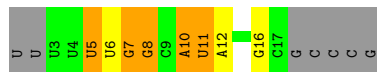
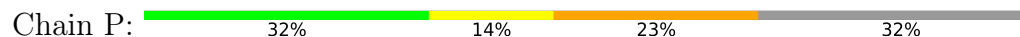
- Molecule 16: RNA polymerase II subunit K



- Molecule 17: Non-template DNA



- Molecule 18: RNA



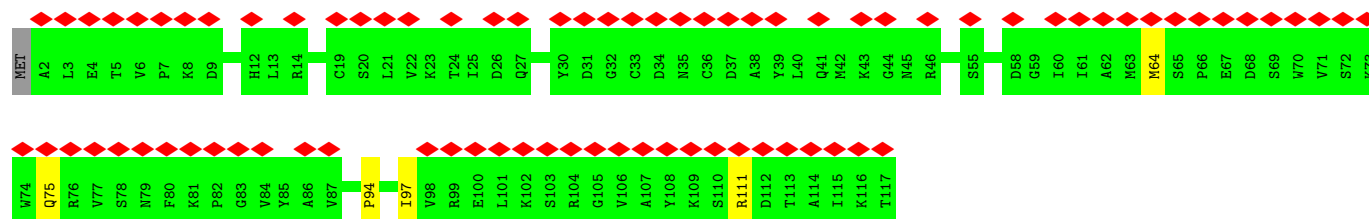
- Molecule 19: Template DNA



- Molecule 20: Negative elongation factor A



- Molecule 21: Transcription elongation factor SPT4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.780	Depositor
Minimum map value	-0.819	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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, 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	X	0.63	0/103	0.94	0/132
2	Z	0.22	0/3841	0.46	0/5167
3	W	0.28	0/4302	0.51	3/5835 (0.1%)
4	V	0.54	3/4495 (0.1%)	0.73	4/6074 (0.1%)
5	A	0.25	0/11420	0.51	2/15418 (0.0%)
6	B	0.25	0/9257	0.49	0/12493
7	C	0.22	0/2081	0.46	0/2828
8	D	0.27	0/1025	0.50	0/1376
9	E	0.26	0/1739	0.51	0/2347
10	F	0.22	0/628	0.49	0/848
11	G	0.27	0/1382	0.52	0/1874
12	H	0.21	0/1207	0.46	0/1628
13	I	0.26	0/949	0.59	0/1284
14	J	0.24	0/524	0.50	0/707
15	K	0.25	0/939	0.48	0/1271
16	L	0.26	0/378	0.49	0/500
17	N	0.44	0/636	0.71	0/976
18	P	0.37	0/351	0.74	0/544
19	T	0.45	0/878	0.73	1/1353 (0.1%)
20	U	0.28	0/1544	0.56	0/2094
21	Y	0.22	0/927	0.42	0/1250
All	All	0.30	3/48606 (0.0%)	0.54	10/65999 (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
6	B	0	1
13	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	U	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	42	PRO	CB-CG	27.41	2.86	1.49
4	V	42	PRO	CG-CD	-12.06	1.09	1.50
4	V	42	PRO	N-CD	6.90	1.57	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	42	PRO	CB-CG-CD	-33.15	0.03	106.10
4	V	42	PRO	CA-N-CD	-12.74	94.16	112.00
4	V	42	PRO	CA-CB-CG	-10.79	84.00	104.50
4	V	42	PRO	N-CA-CB	-10.72	93.22	103.51
19	T	36	DC	P-O3'-C3'	5.80	128.90	120.20
5	A	861	GLN	CB-CG-CD	5.37	121.74	112.60
5	A	1128	ILE	CA-CB-CG1	5.16	119.16	110.40
3	W	345	GLY	CA-C-N	5.12	130.91	121.70
3	W	345	GLY	C-N-CA	5.12	130.91	121.70
3	W	488	GLU	CB-CG-CD	5.08	121.23	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	1138	ARG	Sidechain
13	I	122	ARG	Sidechain
20	U	182	SER	Mainchain

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	103	116	120	3	0
2	Z	3778	3840	3840	31	0
3	W	4217	4221	4221	51	0
4	V	4410	4499	4499	48	0
5	A	11216	11342	11342	94	0
6	B	9076	9113	9116	71	0
7	C	2038	1989	1989	10	0
8	D	1012	1004	1004	7	0
9	E	1709	1729	1729	19	0
10	F	618	653	653	5	0
11	G	1351	1358	1358	16	0
12	H	1186	1147	1147	2	0
13	I	928	859	859	12	0
14	J	515	534	534	7	0
15	K	920	942	942	6	0
16	L	373	378	378	6	0
17	N	570	316	318	2	0
18	P	316	158	158	6	0
19	T	782	426	427	6	0
20	U	1521	1571	1571	18	0
21	Y	911	907	907	3	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	C	1	0	0	0	0
22	I	2	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	Y	1	0	0	0	0
23	A	1	0	0	0	0
All	All	47560	47102	47112	368	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 (368) 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:A:350:VAL:HG11	5:A:1435:THR:HG21	1.56	0.86
3:W:94:VAL:HG21	4:V:65:VAL:HG23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:841:ARG:NH1	18:P:5:U:O2	2.14	0.79
5:A:26:LEU:HD13	6:B:1168:ALA:HB2	1.68	0.76
6:B:357:CYS:SG	6:B:361:LYS:NZ	2.62	0.72
8:D:44:ARG:NH2	11:G:35:GLU:OE2	2.23	0.71
10:F:100:ARG:NH2	10:F:123:LEU:O	2.24	0.70
2:Z:199:LYS:NZ	2:Z:240:GLU:O	2.26	0.69
6:B:483:ARG:NH2	6:B:527:ALA:O	2.25	0.69
4:V:236:THR:OG1	4:V:307:ASP:OD1	2.07	0.68
6:B:274:ARG:NH2	6:B:281:ASP:OD1	2.26	0.68
3:W:198:LEU:O	3:W:201:PHE:N	2.27	0.67
5:A:22:GLN:NE2	5:A:1446:GLY:O	2.27	0.67
11:G:1:MET:N	11:G:78:ARG:O	2.27	0.67
3:W:498:ASP:OD1	3:W:532:TYR:OH	2.10	0.66
6:B:223:SER:OG	6:B:350:HIS:ND1	2.23	0.66
9:E:167:GLU:N	9:E:167:GLU:OE1	2.29	0.66
2:Z:736:LEU:O	6:B:859:ARG:NH2	2.29	0.66
5:A:111:CYS:SG	5:A:188:GLN:NE2	2.68	0.66
4:V:61:PHE:O	4:V:65:VAL:HG22	1.95	0.66
9:E:110:MET:HE1	9:E:115:LYS:HB2	1.78	0.65
3:W:245:MET:HG3	3:W:258:VAL:HG12	1.78	0.65
6:B:869:LYS:NZ	6:B:892:CYS:SG	2.68	0.65
5:A:513:ALA:HB2	10:F:90:LEU:HD21	1.77	0.65
5:A:1130:ILE:HD13	5:A:1413:ALA:HA	1.78	0.65
11:G:21:ASN:O	11:G:25:THR:OG1	2.13	0.64
5:A:112:PHE:O	5:A:220:ARG:NH2	2.30	0.64
2:Z:733:ARG:NH1	5:A:411:SER:O	2.30	0.64
8:D:34:ASN:O	8:D:68:THR:OG1	2.17	0.64
7:C:78:ILE:HG21	7:C:127:VAL:HG22	1.80	0.63
18:P:10:A:O2'	18:P:11:U:OP1	2.13	0.63
3:W:82:LEU:O	3:W:86:ASN:ND2	2.32	0.63
4:V:508:LEU:HB3	4:V:544:LEU:HD21	1.80	0.63
2:Z:427:GLU:OE2	2:Z:469:ARG:NH2	2.32	0.63
3:W:528:SER:OG	5:A:1150:ASP:OD1	2.11	0.63
5:A:74:CYS:SG	5:A:84:HIS:CE1	2.92	0.63
4:V:25:GLU:OE2	4:V:28:LYS:N	2.31	0.62
6:B:1032:PHE:O	7:C:32:ASN:ND2	2.33	0.62
9:E:3:ASP:OD1	9:E:49:SER:N	2.33	0.61
6:B:731:GLN:NE2	18:P:16:G:OP1	2.32	0.61
9:E:94:MET:O	9:E:98:ASN:N	2.33	0.61
2:Z:735:GLU:OE1	6:B:859:ARG:NH2	2.33	0.61
3:W:133:ASP:O	3:W:137:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:792:ASP:OD2	6:B:975:ARG:NH2	2.34	0.61
14:J:19:GLU:OE2	14:J:19:GLU:N	2.32	0.61
5:A:193:ARG:NH2	5:A:195:GLY:O	2.34	0.61
6:B:705:GLY:O	6:B:709:SER:OG	2.17	0.60
11:G:78:ARG:NH1	11:G:79:PRO:O	2.34	0.60
20:U:54:LEU:HD21	20:U:89:TRP:HB3	1.83	0.60
5:A:1288:ILE:HG22	5:A:1292:MET:HE2	1.82	0.60
13:I:86:CYS:SG	13:I:87:GLN:N	2.75	0.60
6:B:768:ARG:NH1	6:B:771:GLU:OE2	2.35	0.60
9:E:12:LYS:NZ	9:E:136:LEU:O	2.30	0.59
16:L:15:MET:N	16:L:27:GLU:OE2	2.36	0.59
5:A:1314:THR:OG1	5:A:1316:ASN:OD1	2.18	0.59
5:A:467:MET:HG2	5:A:534:VAL:HG21	1.84	0.59
6:B:31:SER:HG	6:B:766:TYR:HH	1.49	0.59
3:W:504:LEU:HG	3:W:509:VAL:HG12	1.84	0.59
5:A:58:MET:HG2	5:A:258:LEU:HD11	1.85	0.59
10:F:100:ARG:NH2	10:F:121:ASP:O	2.36	0.59
14:J:31:GLU:OE2	14:J:31:GLU:N	2.35	0.59
6:B:344:GLN:NE2	6:B:354:SER:O	2.35	0.59
5:A:535:MET:O	5:A:669:TYR:OH	2.20	0.58
5:A:854:THR:O	5:A:857:THR:OG1	2.21	0.58
6:B:927:ARG:NH2	6:B:1057:ASP:OD1	2.37	0.58
13:I:85:PRO:O	13:I:87:GLN:NE2	2.36	0.58
5:A:1173:THR:OG1	13:I:56:ASN:OD1	2.22	0.57
6:B:1035:ARG:NH1	6:B:1036:LYS:O	2.37	0.57
8:D:25:GLU:OE1	11:G:41:LYS:NZ	2.37	0.57
5:A:549:THR:O	5:A:589:LYS:NZ	2.34	0.57
7:C:180:ALA:O	14:J:42:ARG:NH2	2.37	0.57
3:W:244:MET:SD	3:W:244:MET:N	2.78	0.57
5:A:338:SER:OG	5:A:341:GLN:NE2	2.37	0.57
3:W:236:HIS:HB3	20:U:54:LEU:HD22	1.86	0.57
15:K:77:THR:OG1	15:K:81:TYR:O	2.10	0.57
13:I:60:HIS:O	13:I:60:HIS:ND1	2.36	0.57
3:W:285:THR:O	3:W:288:SER:OG	2.23	0.56
2:Z:741:GLN:NE2	2:Z:742:THR:O	2.39	0.56
4:V:433:THR:HG23	4:V:472:LEU:HD11	1.88	0.56
4:V:176:LEU:O	4:V:463:HIS:ND1	2.38	0.55
9:E:67:ASP:OD2	9:E:70:ASP:N	2.38	0.55
5:A:58:MET:HE3	5:A:65:ILE:HD13	1.88	0.55
7:C:10:ARG:NH2	7:C:24:GLU:OE2	2.40	0.55
9:E:47:LYS:O	9:E:52:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:14:HIS:O	20:U:18:GLY:N	2.39	0.55
20:U:92:MET:SD	20:U:92:MET:N	2.80	0.55
2:Z:725:LYS:NZ	6:B:863:ASP:OD2	2.39	0.54
3:W:267:ARG:NH2	20:U:139:LEU:HD11	2.23	0.54
6:B:699:HIS:ND1	6:B:701:SER:OG	2.37	0.54
8:D:44:ARG:NH1	11:G:48:VAL:O	2.40	0.54
6:B:899:SER:OG	6:B:900:GLU:OE1	2.22	0.54
2:Z:718:LYS:NZ	7:C:88:CYS:O	2.40	0.54
3:W:200:VAL:O	3:W:204:VAL:HG23	2.08	0.54
7:C:183:ALA:HB3	7:C:232:ASN:HB3	1.90	0.54
9:E:154:GLU:OE2	9:E:154:GLU:N	2.36	0.54
5:A:1245:CYS:HB2	5:A:1257:LEU:HD11	1.90	0.54
5:A:1430:CYS:O	5:A:1435:THR:HG22	2.08	0.54
6:B:133:ILE:HG23	6:B:138:GLU:O	2.08	0.54
13:I:15:ARG:HB3	13:I:24:LEU:HD12	1.90	0.54
13:I:18:GLN:OE1	13:I:44:TYR:OH	2.13	0.53
6:B:746:THR:HG21	19:T:33:DA:OP2	2.08	0.53
2:Z:554:GLU:OE1	2:Z:557:THR:OG1	2.26	0.53
4:V:432:ILE:O	4:V:436:ARG:N	2.39	0.53
5:A:559:GLU:N	5:A:559:GLU:OE1	2.42	0.53
11:G:30:LEU:O	11:G:34:VAL:HG22	2.09	0.53
4:V:429:VAL:HG21	4:V:448:LEU:HD11	1.91	0.53
5:A:706:ILE:HD11	5:A:787:VAL:HG21	1.89	0.53
5:A:1100:THR:OG1	5:A:1101:GLN:OE1	2.26	0.53
4:V:35:THR:OG1	4:V:36:GLU:OE1	2.20	0.53
4:V:97:LEU:HD11	4:V:117:MET:HE2	1.89	0.53
5:A:344:LYS:NZ	19:T:24:DG:OP2	2.28	0.53
3:W:54:ARG:O	4:V:59:LEU:HD22	2.09	0.53
6:B:900:GLU:OE1	6:B:900:GLU:N	2.41	0.53
21:Y:94:PRO:HD2	21:Y:97:ILE:HD12	1.91	0.53
4:V:268:ALA:O	4:V:271:ARG:NH1	2.42	0.53
4:V:539:GLU:OE2	4:V:543:GLN:NE2	2.42	0.53
20:U:45:PHE:O	20:U:53:LYS:NZ	2.39	0.53
3:W:441:PHE:O	5:A:743:ARG:NH1	2.42	0.52
5:A:34:MET:HE1	5:A:85:PHE:HB2	1.91	0.52
5:A:1248:ASN:ND2	5:A:1254:LYS:O	2.43	0.52
17:N:39:DA:N6	19:T:13:DC:N3	2.57	0.52
4:V:318:THR:HG23	4:V:338:LEU:HD11	1.91	0.52
2:Z:705:LEU:HG	2:Z:724:VAL:HG21	1.91	0.52
3:W:235:GLU:HB3	20:U:58:LEU:HD22	1.90	0.52
4:V:245:LEU:HD13	4:V:253:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:369:LEU:HD12	4:V:373:PHE:HB3	1.90	0.52
15:K:80:ASP:OD1	15:K:80:ASP:N	2.42	0.52
4:V:406:THR:O	4:V:443:ARG:NE	2.32	0.52
2:Z:745:VAL:HG23	2:Z:750:LEU:HD21	1.92	0.52
3:W:120:LYS:NZ	3:W:154:THR:O	2.43	0.52
12:H:115:TYR:OH	12:H:124:ARG:NH2	2.43	0.52
6:B:824:ASP:OD1	6:B:825:GLN:N	2.43	0.52
6:B:91:ILE:HG23	6:B:124:LEU:HD11	1.92	0.52
6:B:407:MET:HE3	6:B:440:ILE:HA	1.92	0.52
1:X:19:PHE:HE1	4:V:382:VAL:HG21	1.75	0.51
6:B:310:VAL:HG23	6:B:311:ILE:HD12	1.92	0.51
3:W:444:GLN:NE2	5:A:724:GLU:O	2.43	0.51
5:A:1130:ILE:HD11	5:A:1405:MET:HE1	1.93	0.51
11:G:152:VAL:HG22	11:G:157:ILE:HG12	1.92	0.51
6:B:65:ILE:HG22	6:B:67:LEU:HD23	1.91	0.51
4:V:487:ASP:OD2	4:V:519:LYS:NZ	2.44	0.51
6:B:109:MET:HE3	6:B:109:MET:HA	1.92	0.51
21:Y:64:MET:SD	21:Y:64:MET:N	2.84	0.51
5:A:525:ILE:O	5:A:534:VAL:HG22	2.10	0.51
9:E:115:LYS:O	9:E:119:VAL:HG23	2.11	0.51
20:U:41:ILE:HD13	20:U:56:LEU:HD21	1.91	0.51
2:Z:450:ILE:HG21	2:Z:468:LEU:HD11	1.92	0.51
6:B:516:GLU:OE1	6:B:516:GLU:N	2.40	0.51
1:X:19:PHE:CE1	4:V:382:VAL:HG21	2.46	0.51
6:B:407:MET:HE1	6:B:444:LEU:N	2.25	0.51
6:B:741:HIS:O	6:B:922:ARG:NH2	2.43	0.51
2:Z:424:ASP:HB2	2:Z:440:ILE:HD12	1.93	0.50
5:A:760:LEU:HD11	5:A:781:ILE:HG21	1.92	0.50
11:G:118:GLU:HB2	11:G:131:MET:HE1	1.94	0.50
4:V:462:LEU:HD11	4:V:500:VAL:HG22	1.93	0.50
5:A:274:ASP:OD2	5:A:342:ARG:NH2	2.45	0.49
6:B:1069:ILE:HD12	6:B:1070:LEU:N	2.27	0.49
3:W:485:ASP:OD1	3:W:486:VAL:N	2.45	0.49
4:V:227:LEU:HD23	4:V:228:ARG:NH1	2.27	0.49
4:V:238:ARG:NE	4:V:303:MET:HE1	2.28	0.49
20:U:19:ALA:O	20:U:55:LYS:NZ	2.39	0.49
4:V:266:LEU:HD22	4:V:304:ILE:HG22	1.94	0.49
5:A:116:LYS:NZ	5:A:120:ASP:OD1	2.46	0.49
5:A:1130:ILE:HD11	5:A:1405:MET:CE	2.41	0.49
9:E:14:ARG:NH1	9:E:43:GLN:OE1	2.45	0.49
11:G:27:LYS:HG2	11:G:51:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:513:VAL:HG21	2:Z:518:LEU:HD21	1.95	0.49
3:W:245:MET:SD	3:W:262:ALA:N	2.85	0.49
6:B:352:GLY:O	6:B:361:LYS:NZ	2.43	0.49
9:E:18:MET:HA	9:E:18:MET:HE2	1.95	0.49
2:Z:554:GLU:OE2	2:Z:559:GLN:NE2	2.46	0.49
5:A:467:MET:SD	5:A:467:MET:N	2.86	0.49
7:C:7:PRO:O	15:K:104:ARG:NH1	2.46	0.48
2:Z:390:LEU:HD23	2:Z:393:LEU:HD12	1.95	0.48
4:V:132:MET:HE2	4:V:132:MET:HA	1.95	0.48
16:L:28:ILE:HG21	16:L:34:ILE:HG22	1.94	0.48
20:U:141:CYS:HB3	20:U:149:LEU:HD11	1.95	0.48
3:W:159:PHE:CD2	3:W:175:THR:HG21	2.48	0.48
4:V:415:LEU:HD23	4:V:422:CYS:HA	1.95	0.48
6:B:18:THR:OG1	6:B:20:ASP:OD1	2.25	0.48
5:A:1249:ASP:OD2	5:A:1251:ASN:ND2	2.47	0.48
6:B:239:MET:HE1	6:B:300:MET:HE2	1.95	0.48
3:W:531:ARG:NH2	3:W:562:ILE:HD13	2.28	0.48
20:U:76:MET:O	20:U:80:GLN:NE2	2.46	0.48
20:U:54:LEU:O	20:U:58:LEU:HD12	2.13	0.48
3:W:120:LYS:HG3	3:W:158:LEU:HD13	1.95	0.48
6:B:777:ASN:O	14:J:47:ARG:NH1	2.47	0.48
6:B:899:SER:OG	6:B:1080:ARG:NH1	2.46	0.48
5:A:589:LYS:NZ	5:A:638:GLY:O	2.46	0.47
6:B:803:ARG:NH1	14:J:9:THR:O	2.48	0.47
11:G:28:GLN:O	11:G:32:THR:HG23	2.13	0.47
3:W:142:THR:HG21	3:W:146:LEU:HD23	1.96	0.47
3:W:329:ARG:NE	3:W:363:ALA:O	2.43	0.47
4:V:81:ALA:O	4:V:89:ARG:NH1	2.47	0.47
4:V:469:LEU:HD23	4:V:472:LEU:HD12	1.95	0.47
5:A:350:VAL:HG11	5:A:1435:THR:CG2	2.36	0.47
4:V:132:MET:HE3	4:V:156:LEU:HD22	1.97	0.47
19:T:19:DT:H2'	19:T:20:DT:H71	1.97	0.47
5:A:272:ASN:OD1	18:P:8:G:N2	2.48	0.47
6:B:285:LEU:O	6:B:289:ILE:N	2.47	0.47
21:Y:75:GLN:O	21:Y:111:ARG:NH1	2.48	0.47
4:V:63:GLN:NE2	4:V:67:ASP:OD2	2.47	0.47
3:W:92:GLN:OE1	3:W:92:GLN:N	2.46	0.47
4:V:223:ARG:NH2	4:V:300:ASP:OD1	2.48	0.47
6:B:794:VAL:HG13	6:B:965:ILE:HG23	1.96	0.47
6:B:587:LEU:HB3	6:B:603:MET:HE3	1.97	0.46
5:A:1192:TRP:HZ3	5:A:1246:ILE:HG22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:669:GLU:O	6:B:673:VAL:HG23	2.15	0.46
4:V:483:SER:O	4:V:488:GLY:N	2.47	0.46
5:A:98:GLY:HA3	5:A:1440:MET:HE2	1.97	0.46
5:A:590:GLN:O	5:A:593:SER:OG	2.29	0.46
2:Z:473:LYS:O	2:Z:492:ILE:HD11	2.15	0.46
2:Z:737:HIS:NE2	16:L:53:VAL:HG23	2.31	0.46
5:A:65:ILE:HD11	5:A:258:LEU:HG	1.96	0.46
5:A:1201:ASP:OD1	5:A:1201:ASP:N	2.48	0.46
2:Z:260:MET:O	2:Z:263:VAL:HG22	2.16	0.46
3:W:122:LEU:HD23	3:W:125:LYS:HZ2	1.80	0.46
4:V:41:LEU:HA	4:V:42:PRO:HG3	1.97	0.46
13:I:17:CYS:HA	13:I:24:LEU:HD21	1.98	0.46
5:A:1347:LEU:HB3	9:E:137:ILE:HD13	1.98	0.45
6:B:1085:ARG:N	19:T:29:DA:OP1	2.46	0.45
3:W:460:THR:O	3:W:506:ARG:NH2	2.50	0.45
3:W:101:LEU:O	3:W:104:THR:OG1	2.33	0.45
12:H:40:ILE:HD12	12:H:124:ARG:HD2	1.98	0.45
5:A:853:LYS:O	5:A:857:THR:N	2.48	0.45
5:A:1138:SER:N	5:A:1360:ASN:OD1	2.49	0.45
3:W:94:VAL:CG2	4:V:65:VAL:HG23	2.43	0.45
5:A:865:ILE:O	5:A:869:GLU:N	2.50	0.45
6:B:601:VAL:HG22	6:B:616:THR:HG23	1.98	0.45
6:B:1172:MET:HA	6:B:1172:MET:HE3	1.98	0.45
3:W:245:MET:SD	3:W:262:ALA:HB2	2.57	0.45
5:A:34:MET:C	5:A:34:MET:HE2	2.41	0.45
7:C:105:VAL:HG11	7:C:115:VAL:HG22	1.98	0.45
4:V:265:CYS:O	4:V:268:ALA:N	2.50	0.45
5:A:749:ARG:NH2	5:A:750:ASP:OD1	2.50	0.45
6:B:59:VAL:HG21	6:B:91:ILE:HD11	1.99	0.45
2:Z:278:TRP:HZ2	2:Z:396:PHE:HB2	1.80	0.45
5:A:195:GLY:C	5:A:196:LEU:HD12	2.42	0.45
6:B:841:ARG:NH1	18:P:5:U:O2'	2.49	0.45
3:W:181:ASP:OD1	3:W:203:ARG:NH2	2.49	0.45
5:A:1199:MET:HE3	5:A:1199:MET:N	2.32	0.45
2:Z:753:VAL:HG11	16:L:52:LEU:HD21	1.98	0.44
3:W:538:LEU:HD23	3:W:541:ILE:HD11	1.98	0.44
5:A:290:LEU:HD11	5:A:303:ILE:HG23	1.99	0.44
6:B:761:THR:HG23	6:B:1000:THR:HA	1.99	0.44
14:J:44:CYS:SG	14:J:45:CYS:N	2.91	0.44
5:A:355:MET:HE2	5:A:355:MET:HA	1.99	0.44
5:A:1130:ILE:N	5:A:1130:ILE:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:864:LEU:O	5:A:867:SER:OG	2.32	0.44
7:C:9:VAL:HG11	15:K:105:PHE:CD1	2.53	0.44
5:A:460:ARG:HB2	5:A:501:MET:HE3	1.99	0.44
5:A:545:VAL:HB	5:A:676:ILE:HD13	1.99	0.44
20:U:85:ASP:O	20:U:91:LEU:HD21	2.18	0.44
1:X:22:LEU:HD13	4:V:386:THR:HA	1.99	0.44
6:B:771:GLU:O	14:J:55:LEU:HD21	2.18	0.44
10:F:79:VAL:HG11	10:F:83:LEU:HD23	2.00	0.44
15:K:105:PHE:CE2	15:K:109:ILE:HD11	2.52	0.44
7:C:172:GLU:OE2	16:L:58:ARG:NH2	2.49	0.44
5:A:350:VAL:CG1	5:A:1435:THR:HG21	2.39	0.43
6:B:157:ARG:NH2	6:B:177:CYS:O	2.51	0.43
6:B:794:VAL:HG22	6:B:967:ILE:HG22	2.00	0.43
6:B:912:ASN:OD1	6:B:916:TYR:N	2.49	0.43
8:D:31:THR:O	8:D:84:ARG:NH2	2.50	0.43
2:Z:540:VAL:O	2:Z:548:GLY:N	2.45	0.43
3:W:558:GLU:N	3:W:558:GLU:OE1	2.51	0.43
5:A:1196:TYR:CD2	5:A:1246:ILE:HG23	2.53	0.43
6:B:109:MET:HE2	6:B:174:LEU:HD13	2.00	0.43
6:B:210:LYS:HD2	6:B:218:THR:HG21	1.99	0.43
9:E:152:THR:O	9:E:156:VAL:HG23	2.18	0.43
20:U:17:LEU:O	20:U:55:LYS:NZ	2.48	0.43
6:B:256:ILE:HD11	6:B:373:LEU:HD21	1.99	0.43
17:N:14:DC:N4	19:T:38:DG:O6	2.52	0.43
20:U:179:LEU:O	20:U:183:THR:HG23	2.18	0.43
3:W:57:ILE:HD11	4:V:30:ILE:HD11	1.99	0.43
3:W:396:LEU:HD12	3:W:414:LEU:HD21	2.01	0.43
5:A:115:SER:OG	5:A:115:SER:O	2.36	0.43
6:B:213:SER:OG	6:B:214:LYS:N	2.51	0.43
3:W:419:ARG:NH1	3:W:461:CYS:SG	2.91	0.43
5:A:99:PHE:HB3	5:A:248:MET:HE3	2.01	0.43
5:A:340:LYS:HG3	5:A:1436:VAL:HG11	2.00	0.43
13:I:120:GLY:O	13:I:122:ARG:NH1	2.51	0.43
5:A:410:ASN:OD1	5:A:449:HIS:NE2	2.47	0.43
5:A:397:PHE:HB3	10:F:87:THR:HG23	2.00	0.43
5:A:1184:THR:OG1	5:A:1186:VAL:O	2.34	0.43
5:A:1416:ARG:NH1	5:A:1434:GLU:OE2	2.47	0.43
5:A:1415:THR:O	5:A:1419:VAL:HG12	2.18	0.43
4:V:282:GLU:CD	9:E:69:THR:HG21	2.43	0.43
5:A:1435:THR:O	5:A:1439:LEU:HD23	2.18	0.43
9:E:71:GLN:HB2	9:E:99:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:94:LYS:O	11:G:128:TYR:OH	2.37	0.43
6:B:643:LEU:HD11	6:B:656:LEU:HD11	2.00	0.42
13:I:109:ARG:NH2	13:I:124:THR:OG1	2.51	0.42
15:K:63:VAL:HG12	15:K:71:ILE:HG22	2.01	0.42
2:Z:495:VAL:HG22	2:Z:500:VAL:HG13	2.00	0.42
13:I:91:HIS:CG	13:I:116:ALA:HB2	2.54	0.42
3:W:190:SER:O	3:W:194:ALA:N	2.46	0.42
3:W:367:VAL:HG22	20:U:148:ALA:HB2	2.02	0.42
5:A:196:LEU:HD13	5:A:325:LEU:HD11	2.02	0.42
5:A:869:GLU:OE2	5:A:1455:SER:N	2.45	0.42
5:A:1218:ARG:NH2	5:A:1252:ALA:O	2.53	0.42
13:I:13:GLY:O	13:I:14:ILE:HD13	2.20	0.42
2:Z:726:ASP:O	2:Z:733:ARG:N	2.52	0.42
3:W:231:VAL:HG13	3:W:241:ALA:HB3	2.02	0.42
5:A:981:CYS:HB3	5:A:986:MET:HE1	2.02	0.42
3:W:245:MET:HG2	3:W:262:ALA:HB2	2.02	0.42
3:W:475:LYS:O	3:W:479:THR:HG23	2.19	0.42
4:V:403:TYR:OH	4:V:443:ARG:NH1	2.52	0.42
5:A:687:ILE:HD12	5:A:769:MET:HE1	2.01	0.42
5:A:811:ILE:HD12	13:I:79:PRO:HB3	2.01	0.42
6:B:407:MET:HE1	6:B:443:GLY:HA3	2.02	0.42
6:B:710:ILE:HA	6:B:764:MET:HE2	2.02	0.42
11:G:22:LEU:O	11:G:26:VAL:HG23	2.20	0.42
3:W:91:ALA:HB2	4:V:62:HIS:CE1	2.55	0.42
4:V:227:LEU:HD23	4:V:228:ARG:HH11	1.84	0.42
5:A:687:ILE:HD11	5:A:766:PHE:CE2	2.55	0.42
5:A:1217:ASP:OD2	5:A:1220:HIS:ND1	2.53	0.42
6:B:200:MET:HE3	6:B:492:ASP:OD2	2.20	0.42
6:B:764:MET:HE1	6:B:938:ARG:NH1	2.34	0.42
6:B:910:THR:HG22	16:L:43:ILE:HA	2.02	0.42
20:U:96:ILE:HG12	20:U:110:LEU:HD11	2.01	0.42
2:Z:440:ILE:HG23	2:Z:450:ILE:HD11	2.01	0.42
3:W:120:LYS:CG	3:W:158:LEU:HD13	2.50	0.42
4:V:326:VAL:HG12	4:V:378:MET:CG	2.49	0.42
5:A:42:LYS:O	5:A:288:ASN:ND2	2.48	0.42
5:A:366:VAL:HG22	6:B:1055:VAL:HG23	2.01	0.42
8:D:76:ASN:O	8:D:79:THR:OG1	2.25	0.42
5:A:360:ASP:OD1	6:B:1062:ARG:NE	2.47	0.41
5:A:787:VAL:HG22	5:A:824:GLU:O	2.20	0.41
5:A:1437:ASP:N	5:A:1437:ASP:OD1	2.52	0.41
8:D:125:GLU:OE1	8:D:125:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:604:ASP:OD1	2:Z:605:GLY:N	2.53	0.41
6:B:817:GLN:HA	6:B:918:PHE:HB2	2.03	0.41
2:Z:493:VAL:HG11	11:G:111:HIS:HB3	2.02	0.41
5:A:1195:VAL:O	5:A:1199:MET:HE1	2.20	0.41
9:E:79:GLU:OE1	9:E:79:GLU:N	2.54	0.41
4:V:498:GLU:OE1	4:V:533:SER:OG	2.39	0.41
6:B:92:TYR:O	6:B:124:LEU:HD12	2.21	0.41
9:E:104:ILE:HD11	9:E:127:LEU:HD23	2.03	0.41
11:G:18:PHE:HA	11:G:22:LEU:HD12	2.02	0.41
2:Z:493:VAL:HG11	11:G:111:HIS:CB	2.51	0.41
3:W:78:ASN:OD1	3:W:79:VAL:N	2.54	0.41
4:V:253:ILE:HA	4:V:256:VAL:HG22	2.02	0.41
5:A:1141:VAL:HA	5:A:1357:THR:HG23	2.02	0.41
3:W:52:SER:O	3:W:86:ASN:ND2	2.53	0.41
5:A:290:LEU:HD13	5:A:306:ASP:HB3	2.02	0.41
6:B:1078:ARG:NH2	18:P:7:G:O5'	2.53	0.41
3:W:473:LEU:O	3:W:477:PHE:N	2.52	0.41
4:V:302:SER:O	4:V:306:CYS:N	2.54	0.41
5:A:408:ARG:NH2	5:A:413:TYR:O	2.54	0.41
5:A:1054:MET:HE3	5:A:1054:MET:HA	2.02	0.41
2:Z:710:VAL:HB	2:Z:750:LEU:HD12	2.02	0.41
3:W:90:VAL:O	3:W:94:VAL:HG23	2.21	0.41
3:W:224:LEU:O	3:W:227:PHE:N	2.51	0.41
4:V:269:CYS:SG	4:V:279:ARG:NE	2.90	0.41
5:A:228:ILE:O	5:A:244:ARG:NH2	2.48	0.41
6:B:975:ARG:HB3	6:B:977:THR:HG23	2.02	0.41
9:E:59:THR:HG22	9:E:75:PHE:HA	2.03	0.41
20:U:145:ASN:OD1	20:U:145:ASN:N	2.53	0.41
5:A:1201:ASP:N	5:A:1203:ASP:OD1	2.54	0.40
3:W:261:ILE:O	3:W:265:VAL:HG23	2.20	0.40
4:V:297:VAL:O	4:V:301:LEU:N	2.42	0.40
5:A:365:THR:OG1	5:A:366:VAL:N	2.53	0.40
2:Z:189:GLU:N	2:Z:189:GLU:OE1	2.54	0.40
2:Z:561:LEU:HD21	2:Z:636:PHE:HA	2.02	0.40
3:W:305:LEU:HD11	3:W:337:PHE:HD1	1.86	0.40
5:A:425:ASP:N	5:A:425:ASP:OD1	2.55	0.40
6:B:193:VAL:CG2	6:B:482:LEU:HD23	2.51	0.40
9:E:166:ARG:NH1	9:E:168:ASN:OD1	2.54	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	X	10/380 (3%)	10 (100%)	0	0	100	100
2	Z	455/1087 (42%)	435 (96%)	20 (4%)	0	100	100
3	W	518/590 (88%)	504 (97%)	14 (3%)	0	100	100
4	V	548/580 (94%)	539 (98%)	9 (2%)	0	100	100
5	A	1406/1970 (71%)	1355 (96%)	51 (4%)	0	100	100
6	B	1130/1174 (96%)	1076 (95%)	54 (5%)	0	100	100
7	C	250/271 (92%)	245 (98%)	5 (2%)	0	100	100
8	D	122/142 (86%)	118 (97%)	4 (3%)	0	100	100
9	E	203/210 (97%)	198 (98%)	5 (2%)	0	100	100
10	F	75/127 (59%)	72 (96%)	3 (4%)	0	100	100
11	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
12	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
13	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
14	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
15	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
16	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
20	U	195/527 (37%)	186 (95%)	9 (5%)	0	100	100
21	Y	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
All	All	5671/7864 (72%)	5468 (96%)	203 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	X	11/331 (3%)	11 (100%)	0	100	100
2	Z	418/940 (44%)	416 (100%)	2 (0%)	81	93
3	W	471/513 (92%)	468 (99%)	3 (1%)	78	92
4	V	493/515 (96%)	491 (100%)	2 (0%)	84	94
5	A	1247/1749 (71%)	1246 (100%)	1 (0%)	88	97
6	B	994/1027 (97%)	993 (100%)	1 (0%)	88	97
7	C	231/248 (93%)	231 (100%)	0	100	100
8	D	114/126 (90%)	114 (100%)	0	100	100
9	E	190/192 (99%)	189 (100%)	1 (0%)	81	93
10	F	67/111 (60%)	67 (100%)	0	100	100
11	G	152/153 (99%)	150 (99%)	2 (1%)	61	86
12	H	129/131 (98%)	129 (100%)	0	100	100
13	I	103/112 (92%)	103 (100%)	0	100	100
14	J	54/56 (96%)	54 (100%)	0	100	100
15	K	104/106 (98%)	104 (100%)	0	100	100
16	L	41/55 (74%)	40 (98%)	1 (2%)	43	77
20	U	170/396 (43%)	170 (100%)	0	100	100
21	Y	102/103 (99%)	102 (100%)	0	100	100
All	All	5091/6864 (74%)	5078 (100%)	13 (0%)	84	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	278	TRP
2	Z	359	LEU
3	W	230	MET
3	W	411	LEU
3	W	452	LEU
4	V	132	MET
4	V	265	CYS
5	A	242	TYR
6	B	1140	CYS
9	E	86	THR
11	G	52	ASP

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Mol	Chain	Res	Type
11	G	106	CYS
16	L	39	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	559	GLN
3	W	103	GLN
3	W	278	GLN
3	W	339	GLN
3	W	350	GLN
3	W	395	ASN
3	W	444	GLN
3	W	551	GLN
4	V	388	ASN
4	V	405	ASN
4	V	418	GLN
4	V	437	ASN
5	A	152	ASN
5	A	562	ASN
5	A	740	GLN
5	A	792	ASN
5	A	1244	ASN
5	A	1384	HIS
6	B	52	GLN
6	B	370	HIS
6	B	838	GLN
6	B	1009	GLN
6	B	1101	GLN
7	C	265	HIS
8	D	19	GLN
9	E	71	GLN
9	E	116	GLN
13	I	32	ASN
13	I	118	HIS
15	K	29	ASN
15	K	69	HIS
20	U	15	ASN
20	U	107	ASN
20	U	114	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	P	14/22 (63%)	7 (50%)	1 (7%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	P	5	U
18	P	6	U
18	P	7	G
18	P	8	G
18	P	10	A
18	P	11	U
18	P	12	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	P	10	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

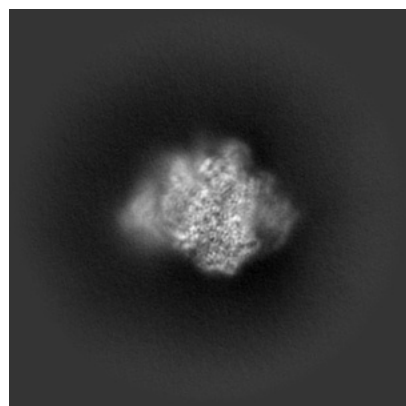
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42270. These allow visual inspection of the internal detail of the map and identification of artifacts.

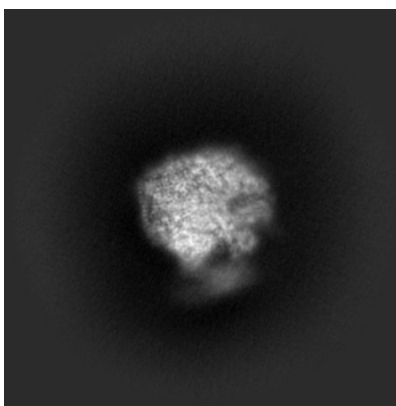
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

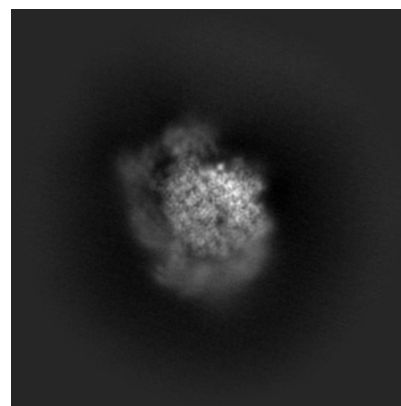
6.1.1 Primary map



X

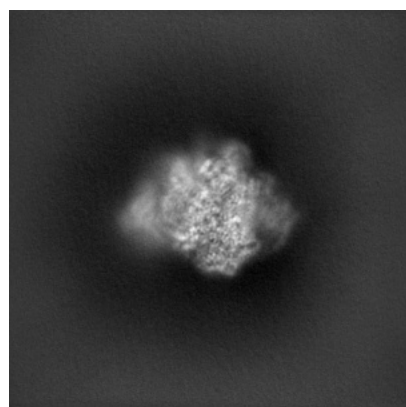


Y

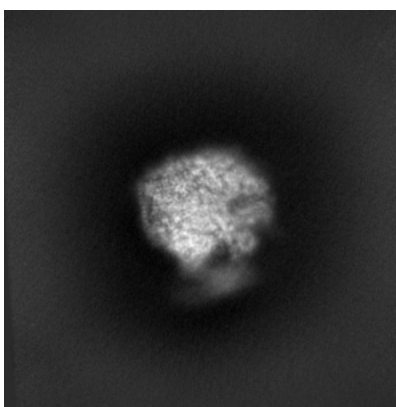


Z

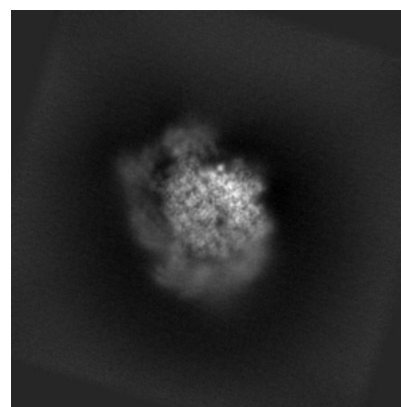
6.1.2 Raw map



X



Y

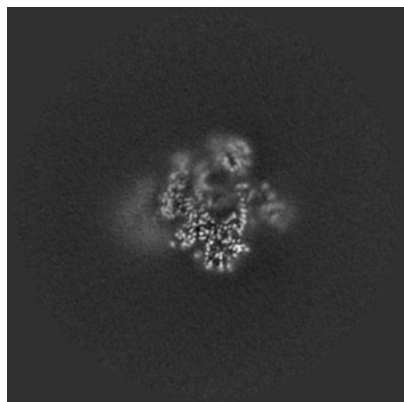


Z

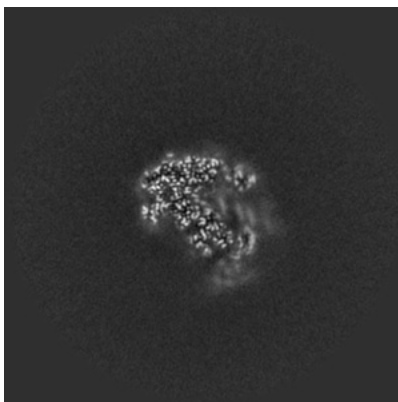
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

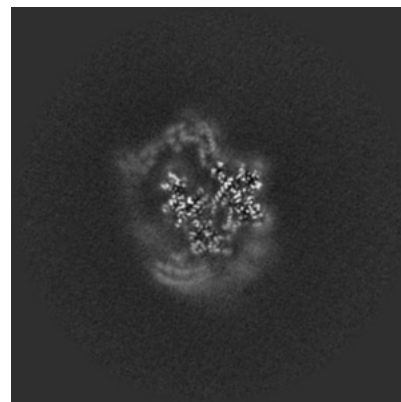
6.2.1 Primary map



X Index: 256

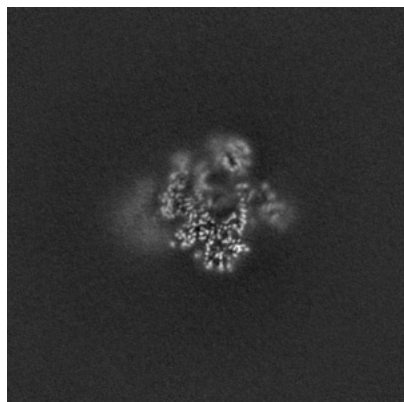


Y Index: 256

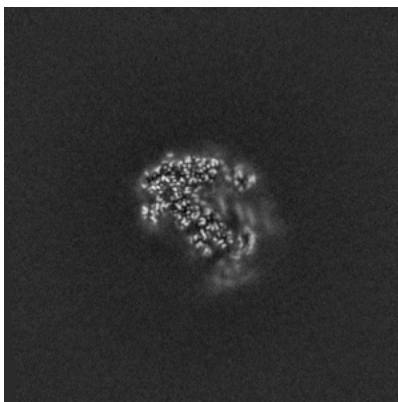


Z Index: 256

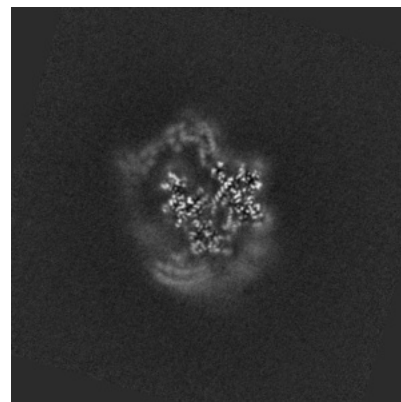
6.2.2 Raw map



X Index: 256



Y Index: 256

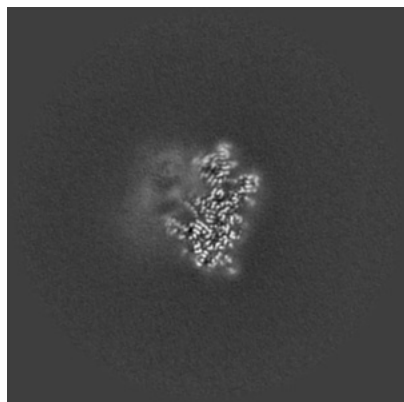


Z Index: 256

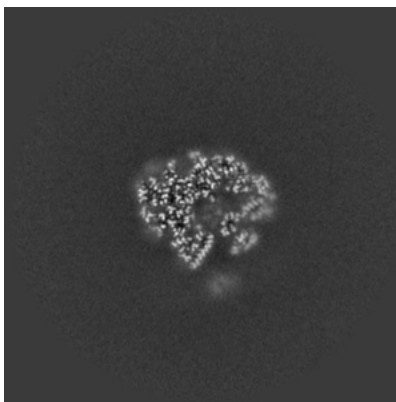
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

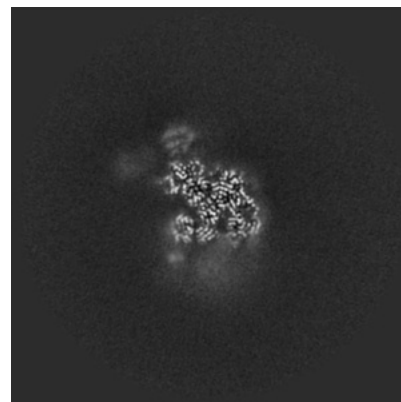
6.3.1 Primary map



X Index: 289

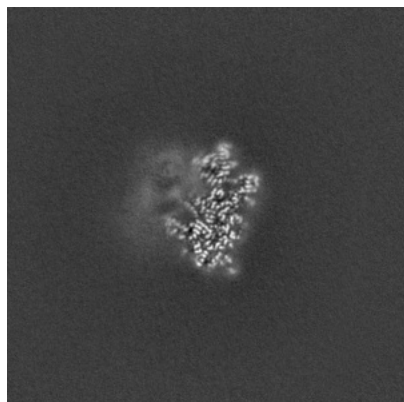


Y Index: 281

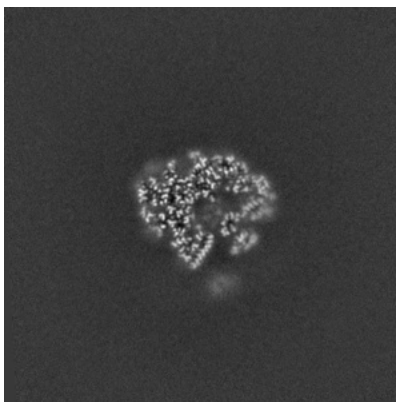


Z Index: 221

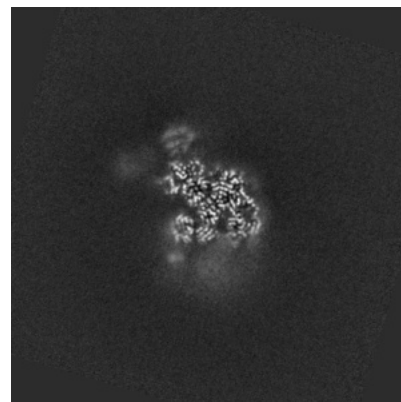
6.3.2 Raw map



X Index: 289



Y Index: 281

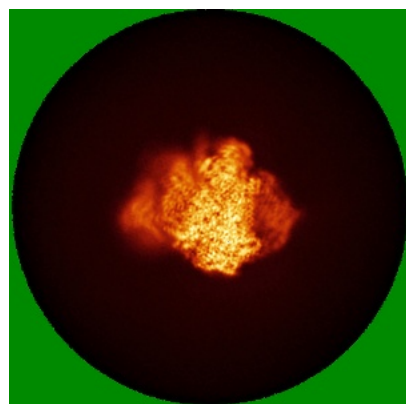


Z Index: 221

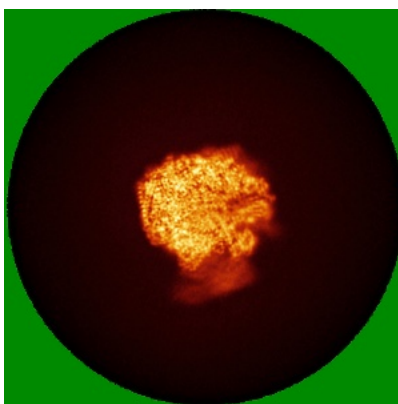
The images above show the largest variance slices of the map in three orthogonal directions.

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

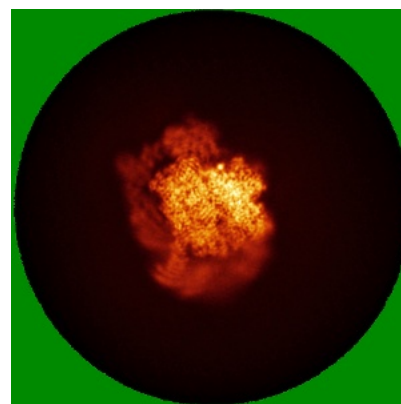
6.4.1 Primary map



X

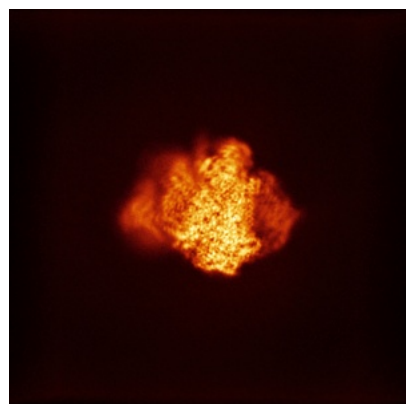


Y

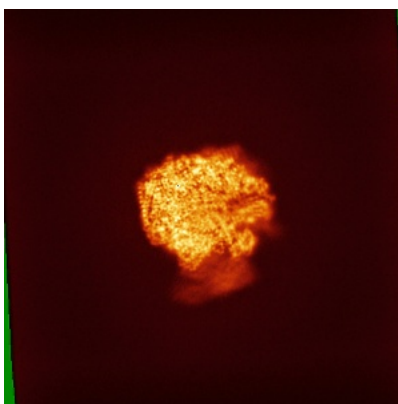


Z

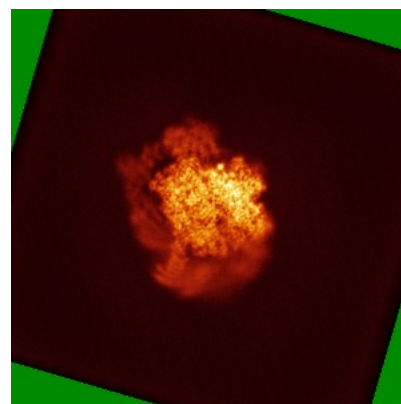
6.4.2 Raw map



X



Y

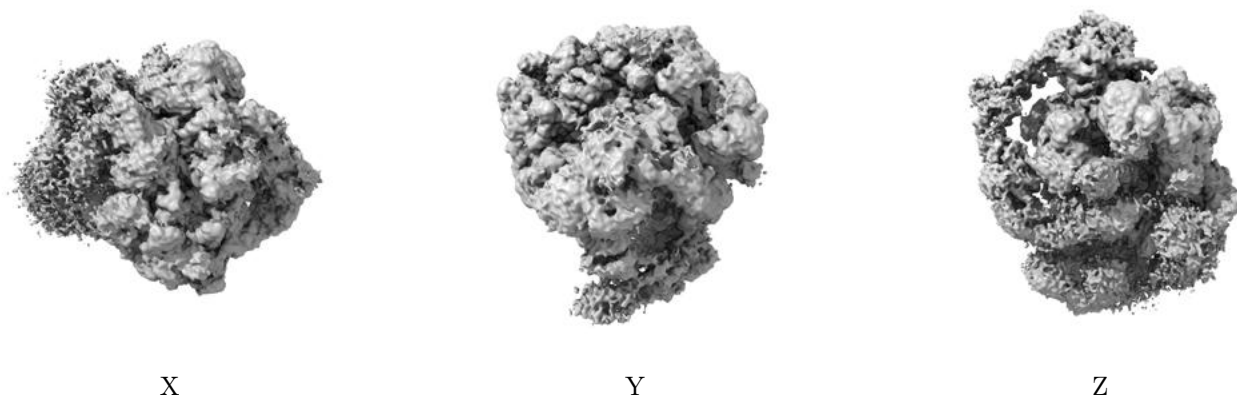


Z

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.

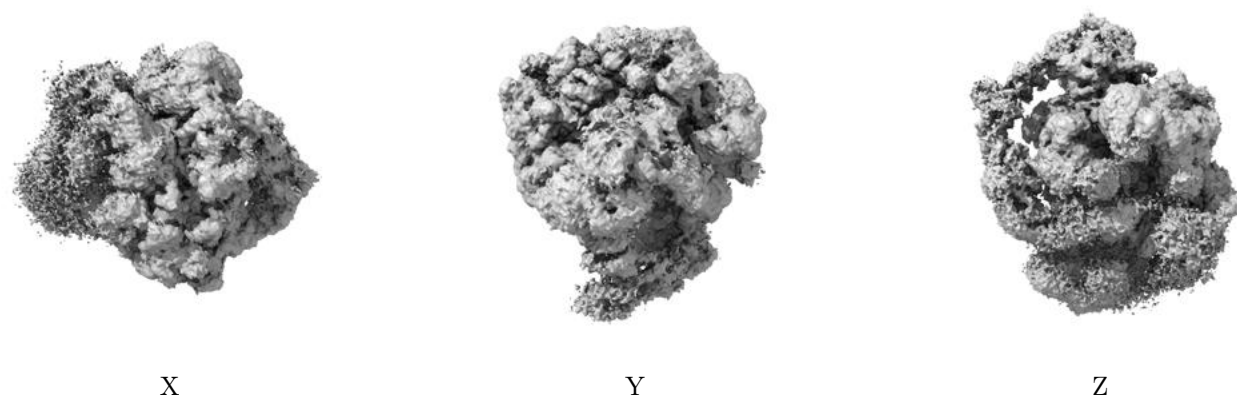
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

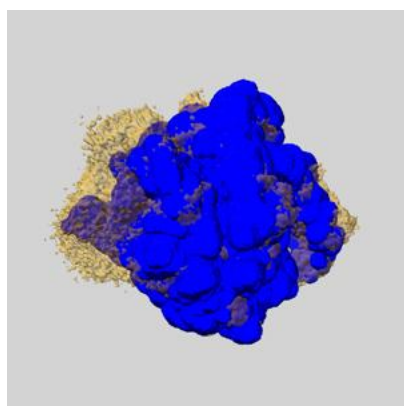
6.6 Mask visualisation [i](#)

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

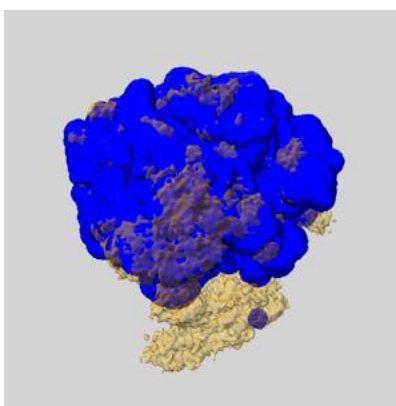
A mask typically either:

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

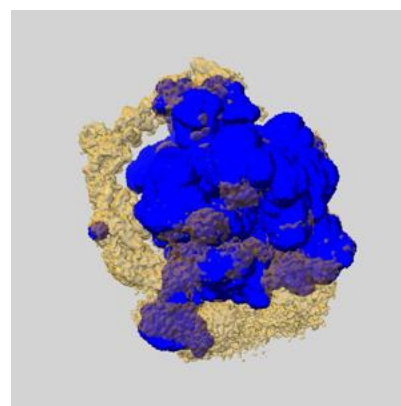
6.6.1 emd_42270_msk_1.map [i](#)



X



Y

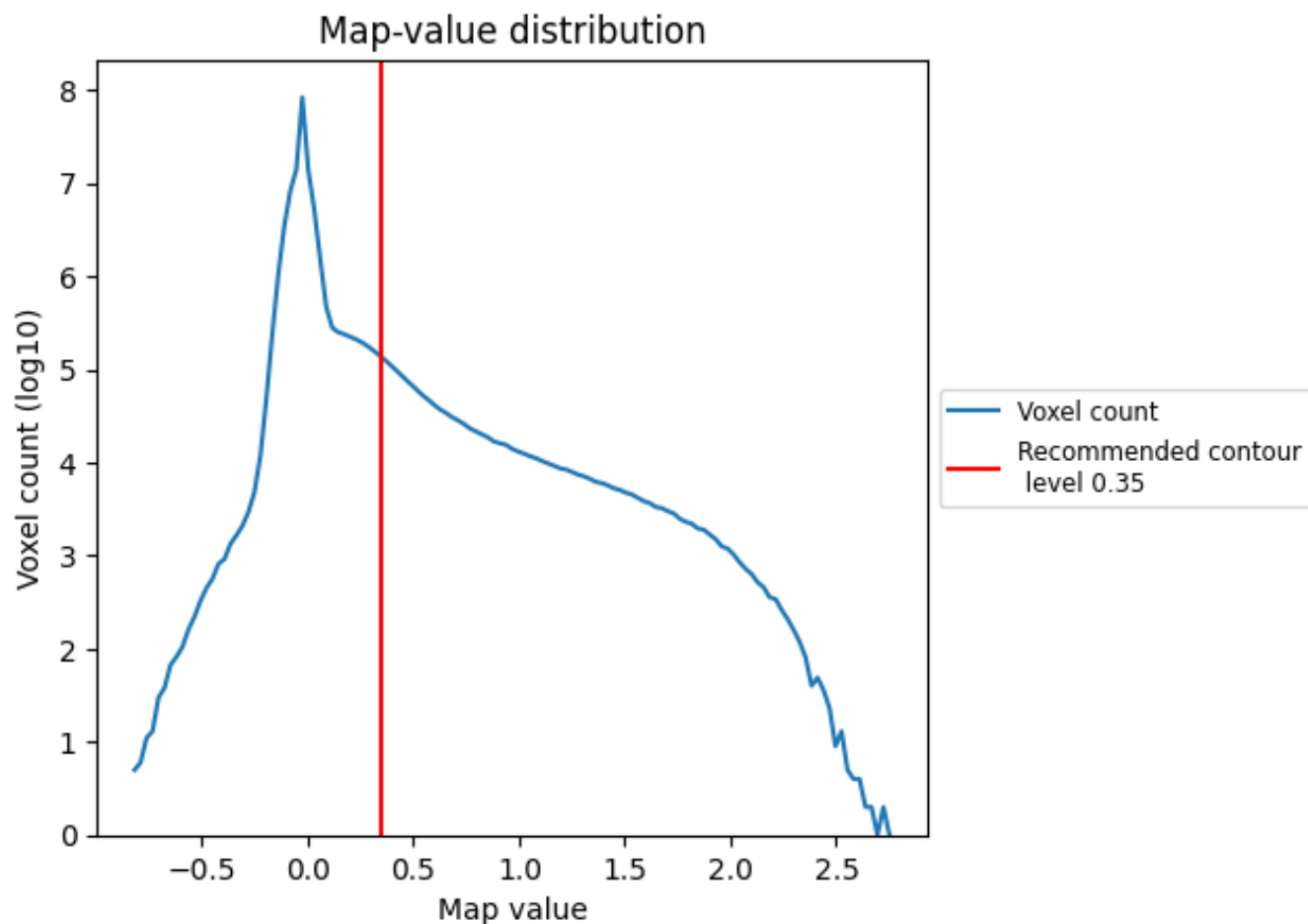


Z

7 Map analysis [i](#)

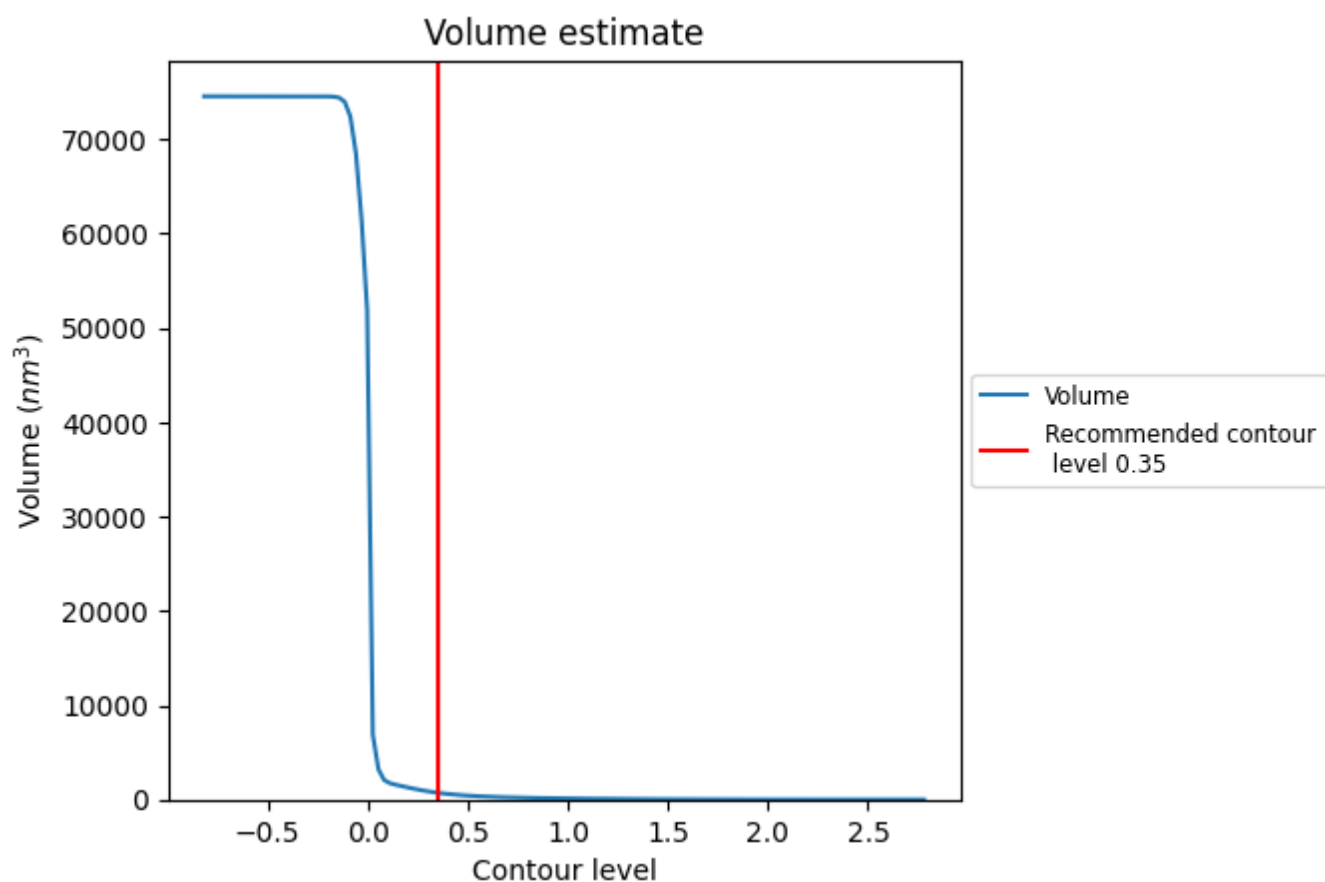
This section contains the results of statistical analysis of the map.

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.

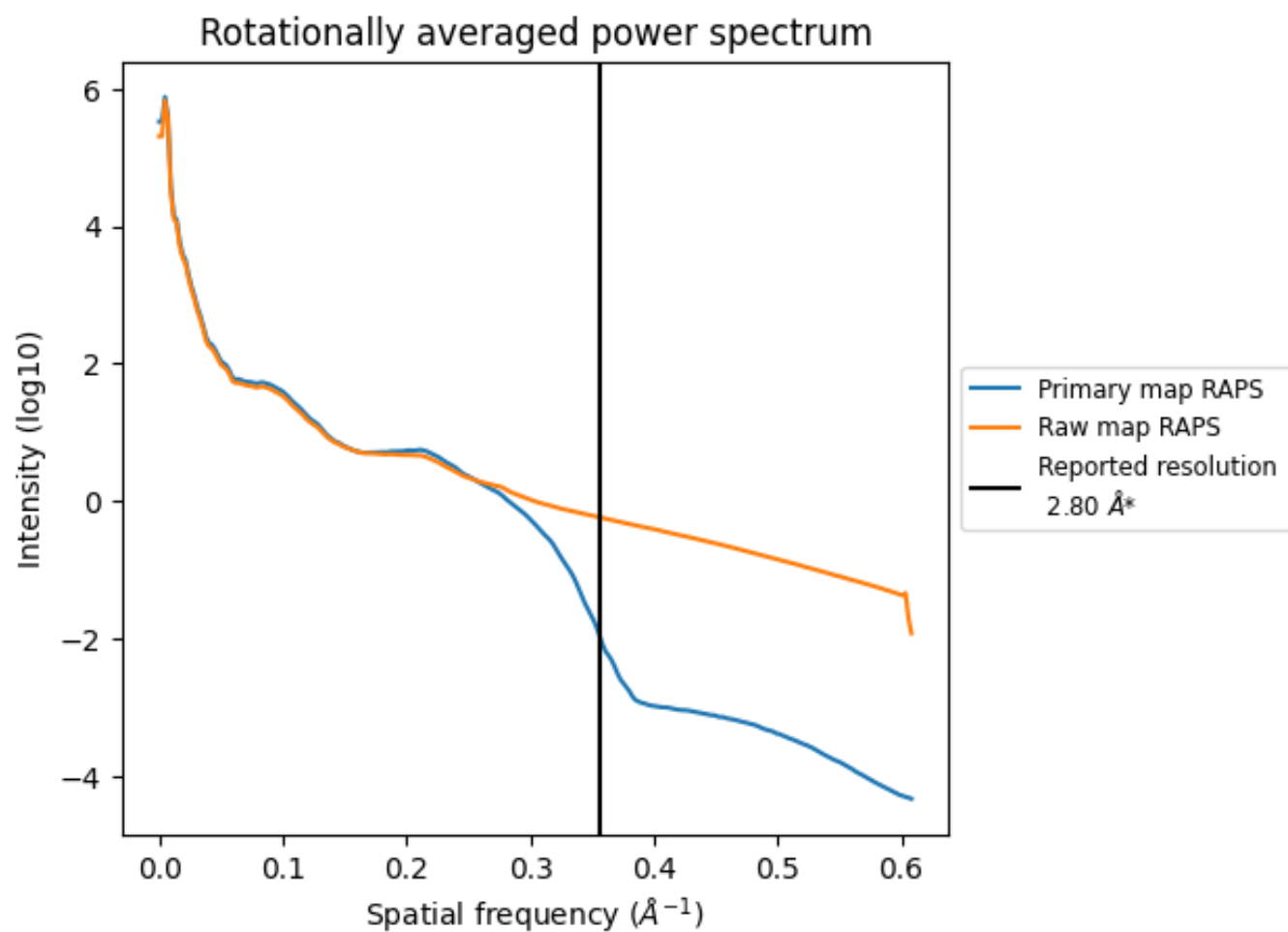
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 717 nm³; this corresponds to an approximate mass of 647 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 ⓘ

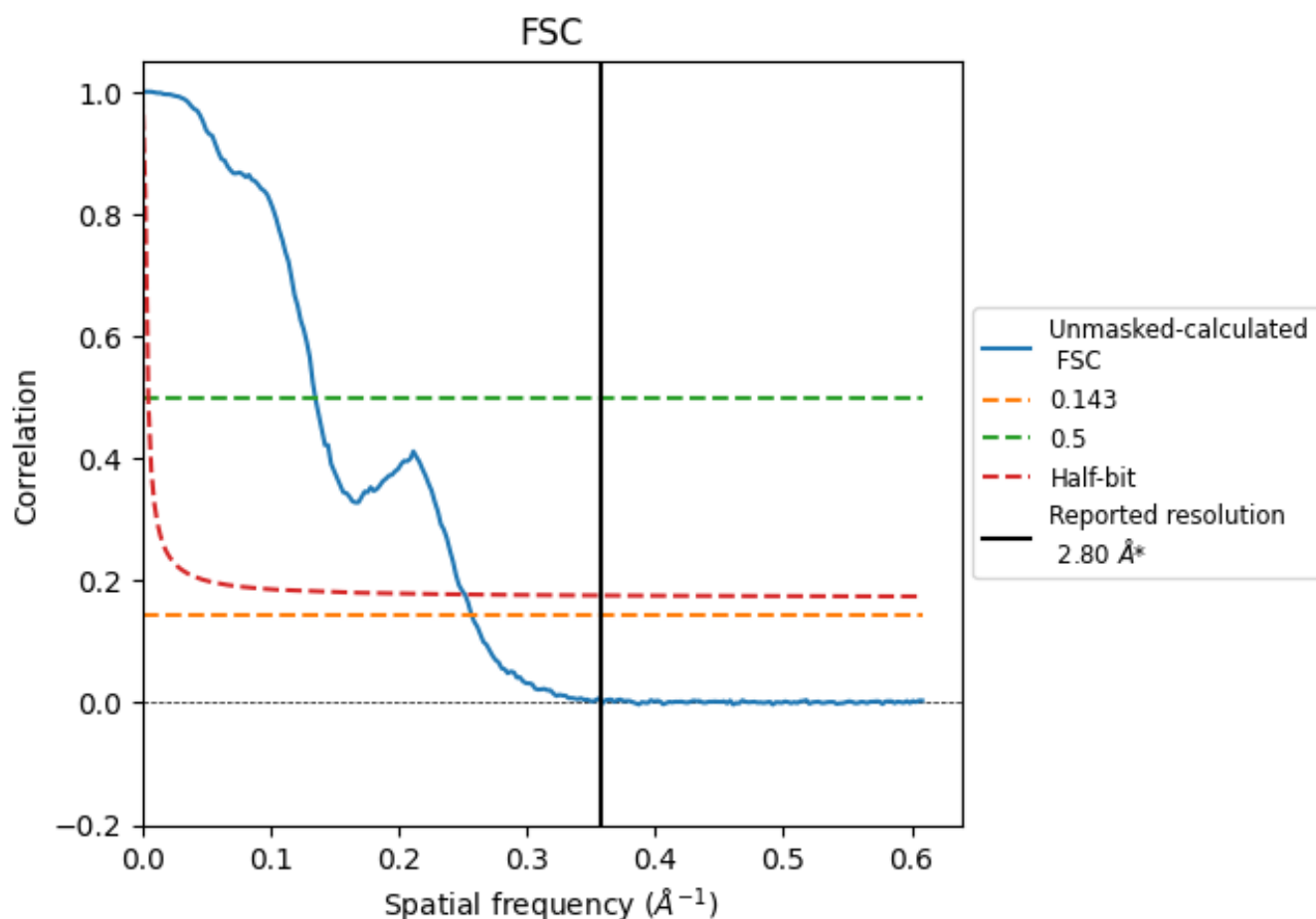


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

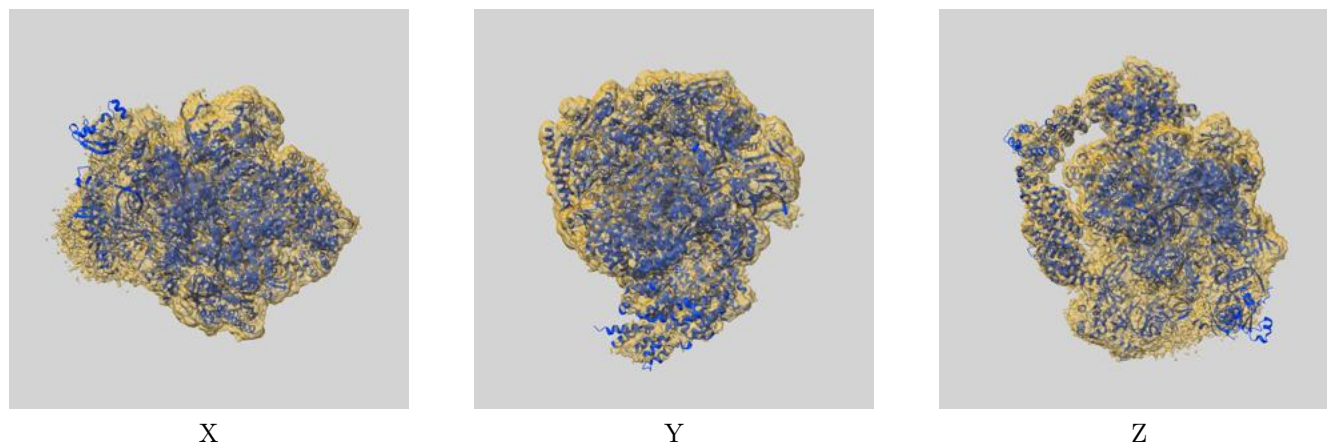
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	7.41	3.98

*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 3.89 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

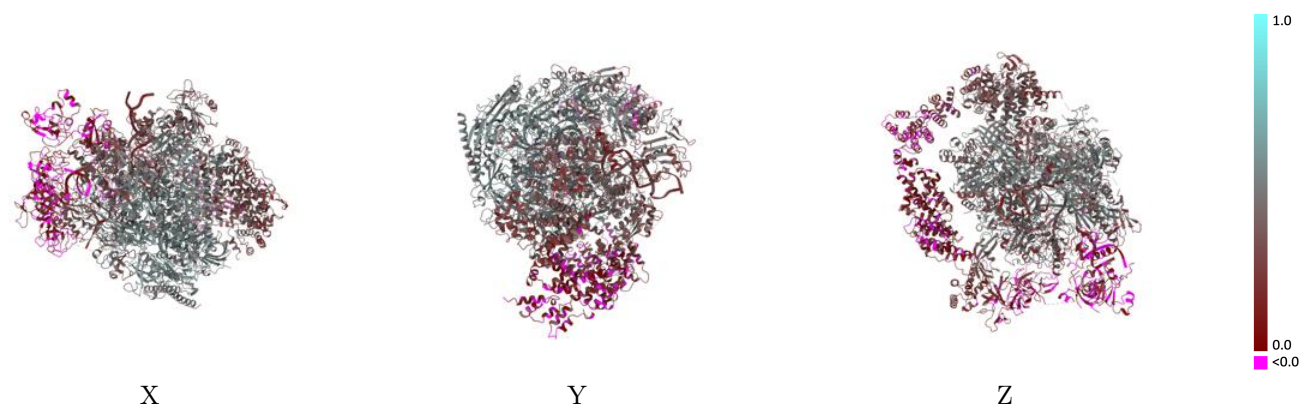
This section contains information regarding the fit between EMDB map EMD-42270 and PDB model 8UHD. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



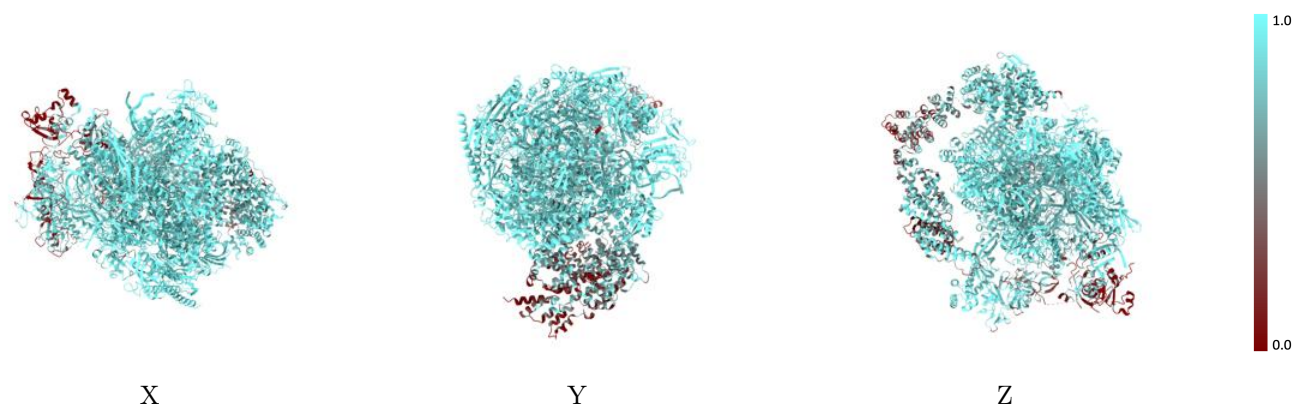
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



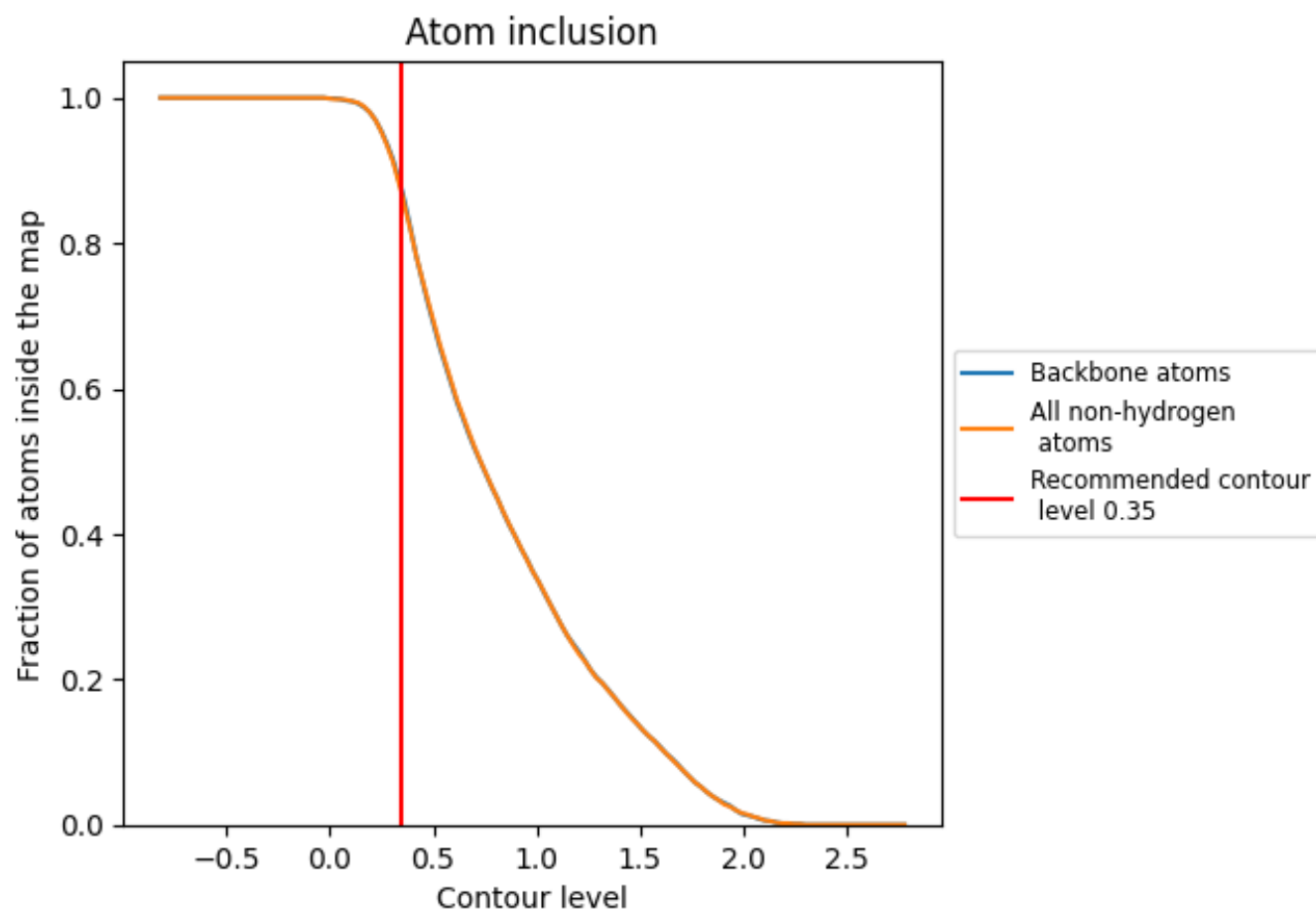
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.3540
A	 0.9570	 0.4520
B	 0.9710	 0.4800
C	 0.9880	 0.5100
D	 0.9720	 0.2000
E	 0.9630	 0.4270
F	 0.9900	 0.4970
G	 0.9710	 0.2560
H	 0.9770	 0.4880
I	 0.9860	 0.4240
J	 0.9920	 0.5230
K	 0.9840	 0.5080
L	 0.9970	 0.4690
N	 0.9190	 0.1840
P	 0.9750	 0.3560
T	 0.9480	 0.2730
U	 0.8740	 0.2760
V	 0.5540	 0.1150
W	 0.7560	 0.2720
X	 0.8740	 0.1330
Y	 0.2720	 0.0730
Z	 0.6150	 0.0830

