



Full wwPDB EM Validation Report ⓘ

Mar 13, 2026 – 11:45 PM UTC

PDB ID : 8UHA / pdb_00008uha
EMDB ID : EMD-42267
Title : Structure of paused transcription complex Pol II-DSIF-NELF - tilted
Authors : Vos, S.M.; Su, B.G.
Deposited on : 2023-10-08
Resolution : 3.50 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:

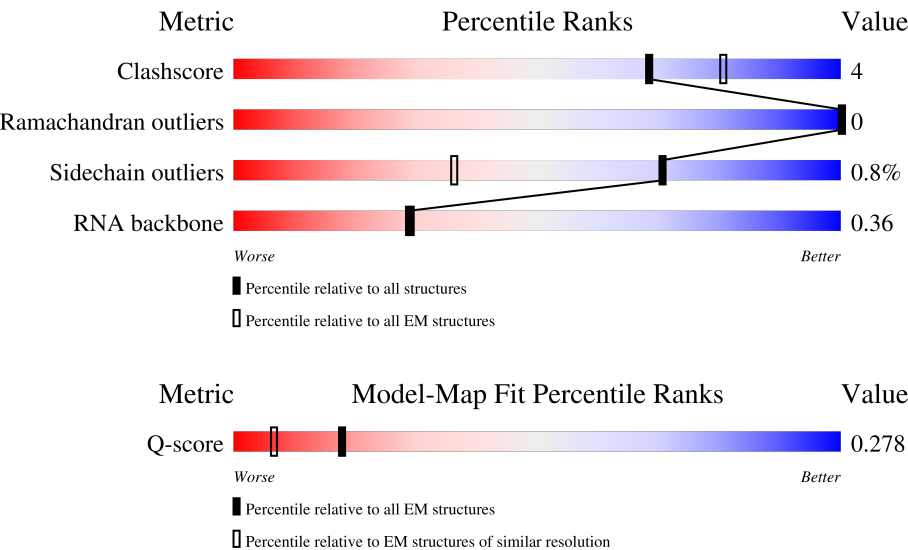
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	97%
2	Y	117	67% 91% 8%
3	Z	1087	17% 40% 57%

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Mol	Chain	Length	Quality of chain
4	W	590	
5	P	17	
6	V	580	
7	A	1970	
8	B	1174	
9	C	271	
10	D	142	
11	E	210	
12	F	127	
13	G	172	
14	H	150	
15	I	125	
16	J	67	
17	K	117	
18	L	58	
19	N	50	
20	T	50	
21	U	527	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 94681 atoms, of which 47120 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 SPT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Y	116	Total	C	H	N	O	S	0	0
			1816	570	905	159	173	9		

- Molecule 3 is a protein called Transcription elongation factor SPT5.

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

- Molecule 4 is a protein called Negative elongation factor C/D.

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

- Molecule 5 is a RNA chain called RNA.

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

- Molecule 6 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	V	550	Total	C	H	N	O	S	0	0
			8911	2825	4501	751	810	24		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	1417	Total	C	H	N	O	S	0	0
			22589	7064	11362	2008	2084	71		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	B	1136	Total	C	H	N	O	S	0	0
			18193	5739	9117	1597	1676	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	255	Total	C	H	N	O	S	0	0
			4039	1285	1995	349	404	6		

- Molecule 10 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	D	126	Total	C	H	N	O	S	0	0
			2046	642	1016	175	209	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	206	Total	C	H	N	O	S	0	0
			3414	1077	1716	294	319	8		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

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

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

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	I	114	Total	C	H	N	O	S	0	0
			1789	571	861	166	180	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	J	65	Total	C	H	N	O	S	0	0
			1050	334	535	87	88	6		

- Molecule 17 is a protein called RNA polymerase II subunit J.

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

- Molecule 18 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	44	Total	C	H	N	O	S	0	0
			752	231	379	72	64	6		

- Molecule 19 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	N	28	Total	C	H	N	O	P	0	0
			886	272	315	103	168	28		

- Molecule 20 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	38	Total	C	H	N	O	P	0	0
			1208	371	427	145	227	38		

- Molecule 21 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	196	Total	C	H	N	O	S	0	0
			3054	953	1556	253	284	8		

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

Mol	Chain	Residues	Atoms		AltConf
22	Y	1	Total	Zn	0
			1	1	
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	

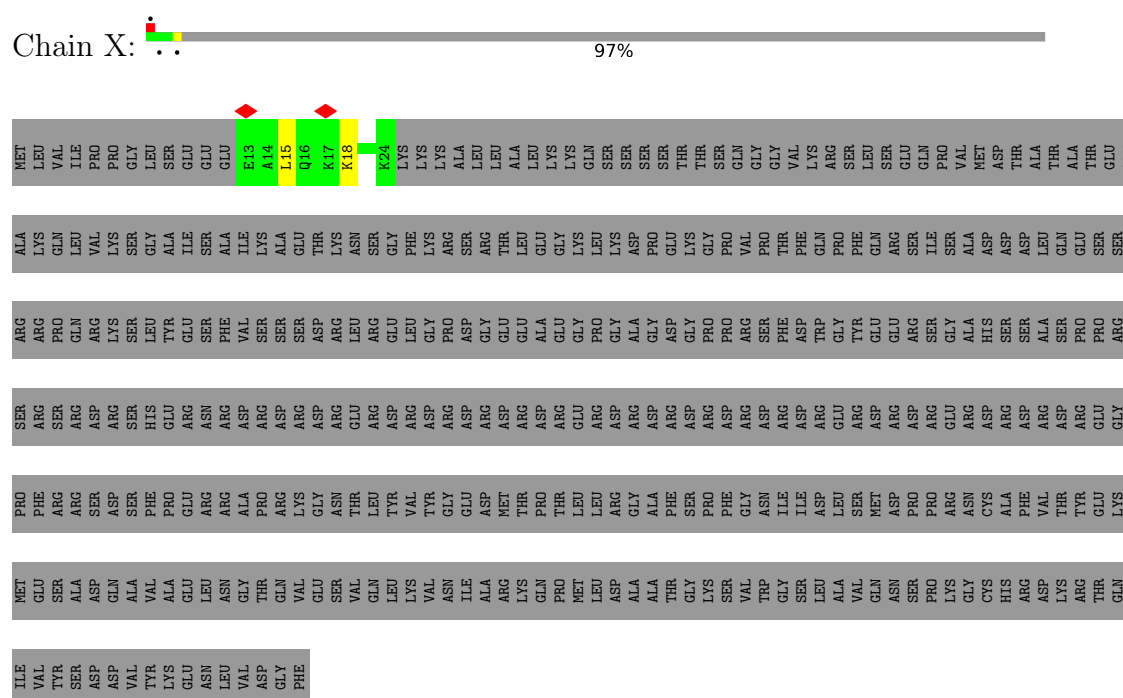
- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

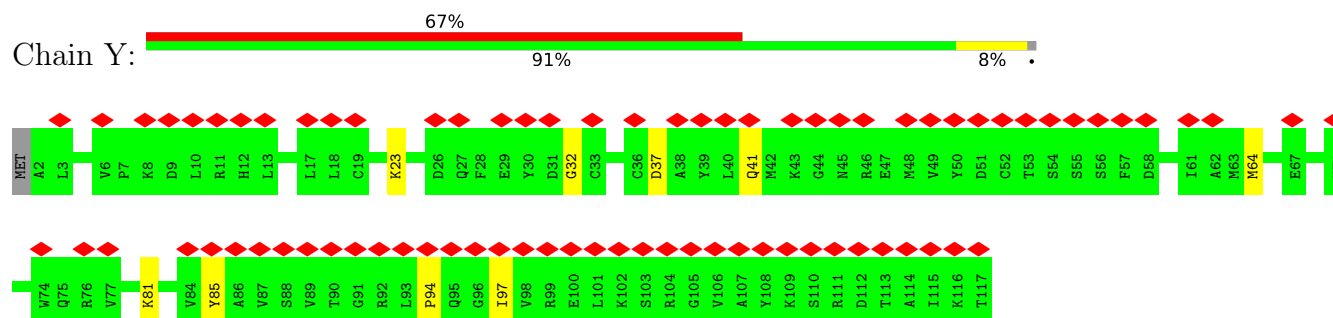
3 Residue-property plots

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

- Molecule 1: Negative elongation factor E



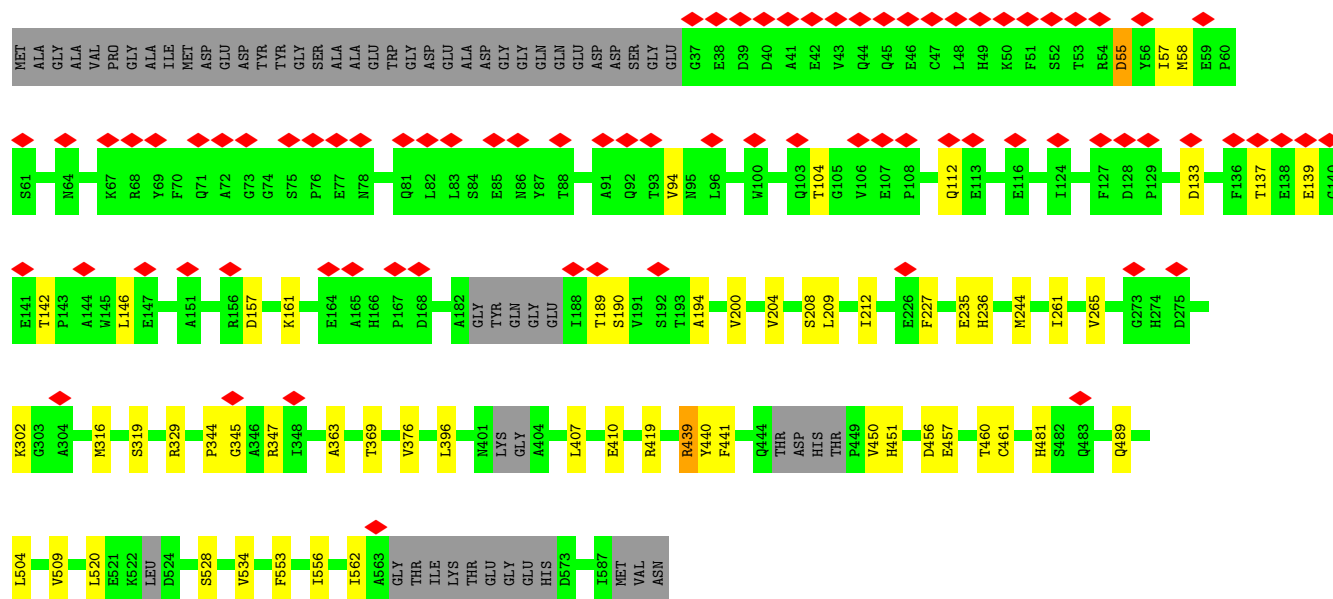
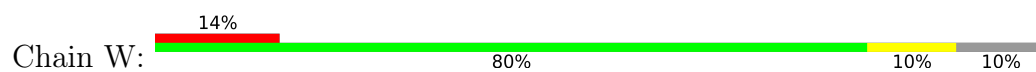
- Molecule 2: Transcription elongation factor SPT4



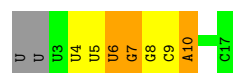
- Molecule 3: Transcription elongation factor SPT5



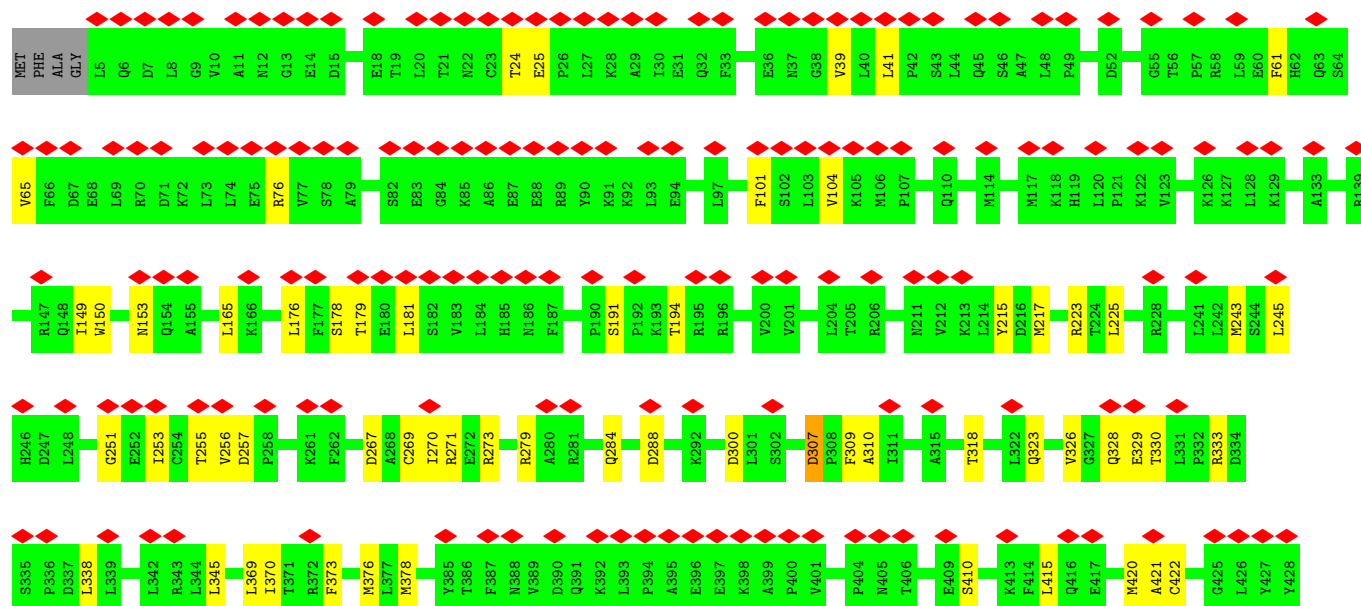
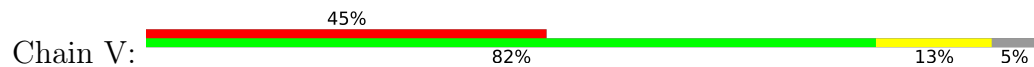
- Molecule 4: Negative elongation factor C/D

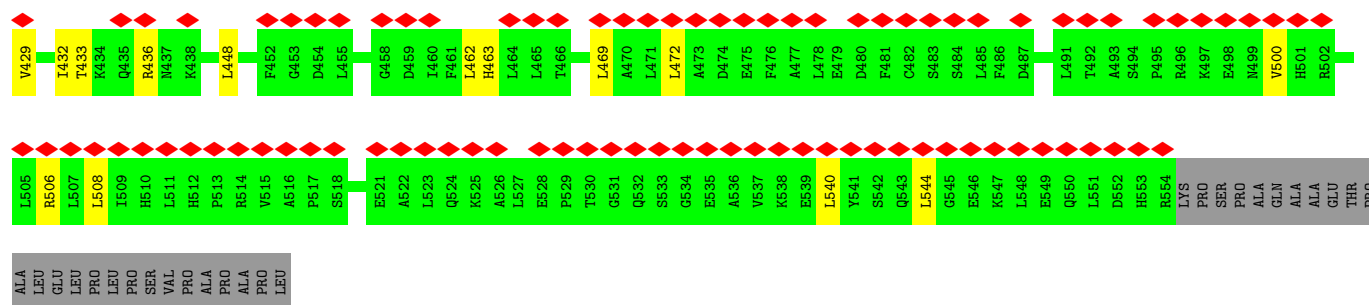


• Molecule 5: RNA



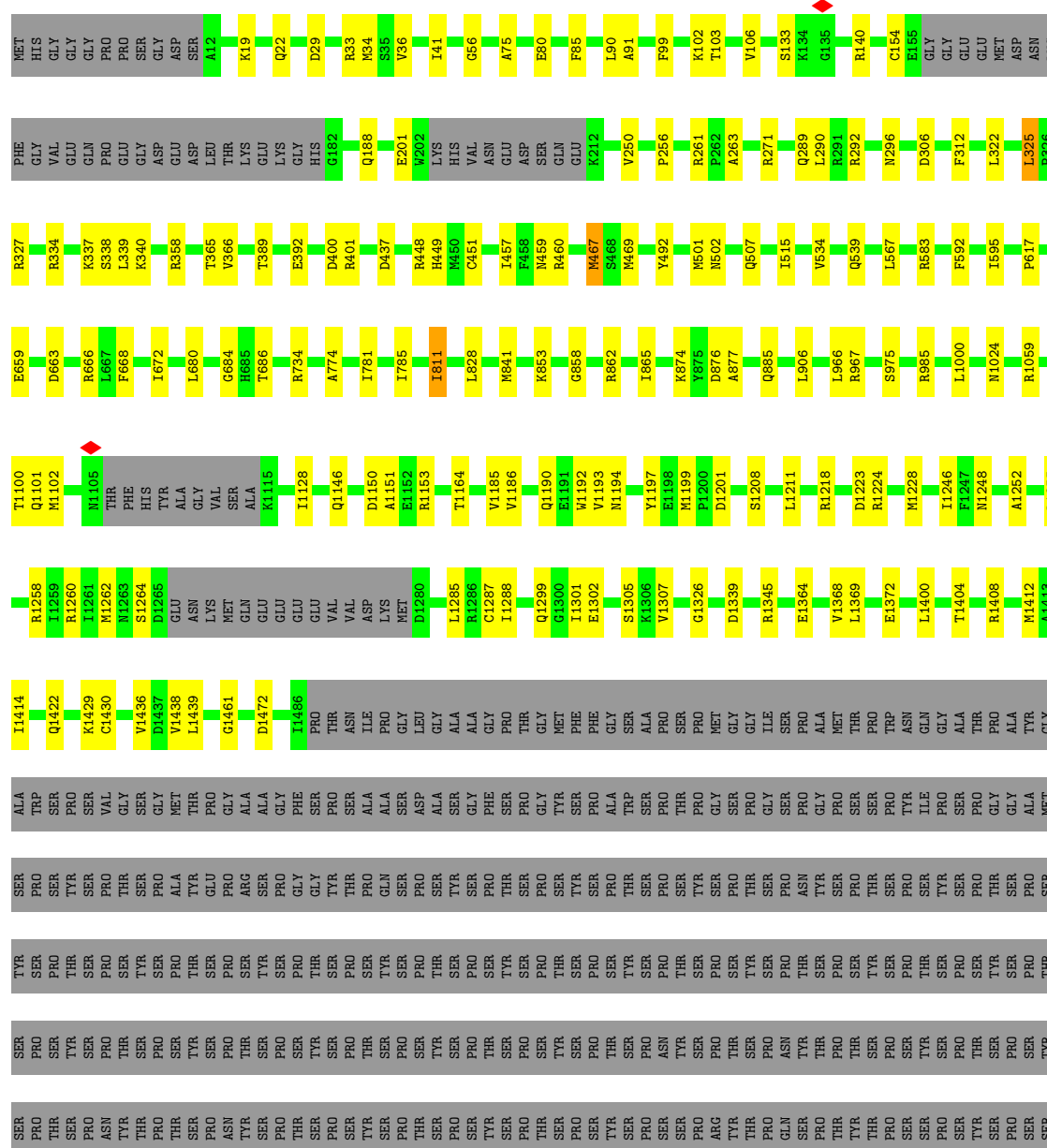
• Molecule 6: Negative elongation factor B

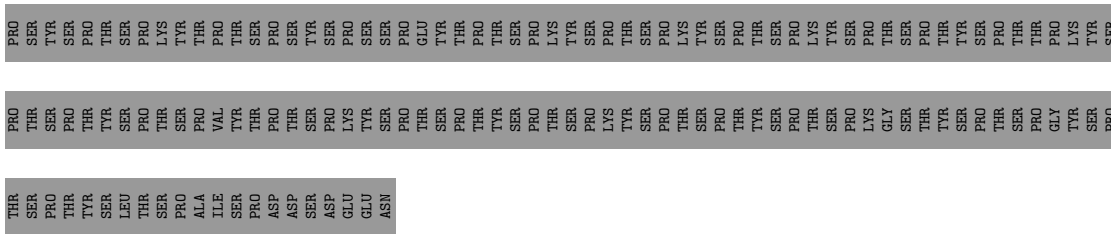




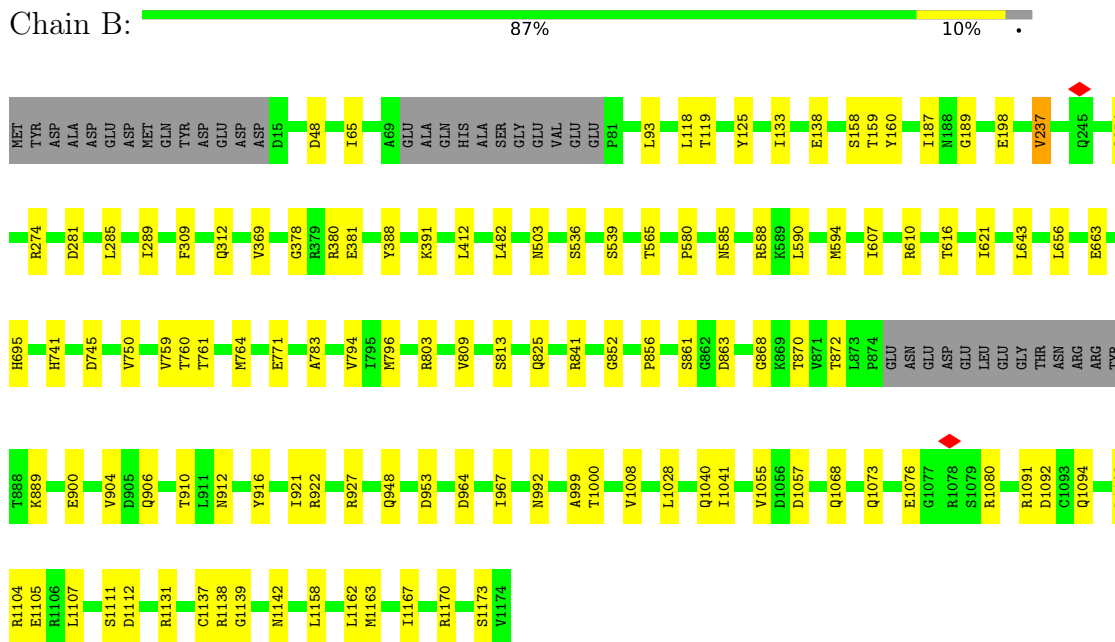
● Molecule 7: DNA-directed RNA polymerase subunit

Chain A: 64% 8% 28%

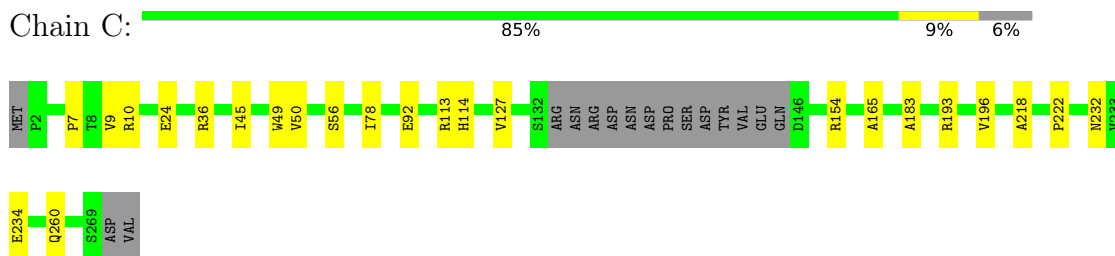




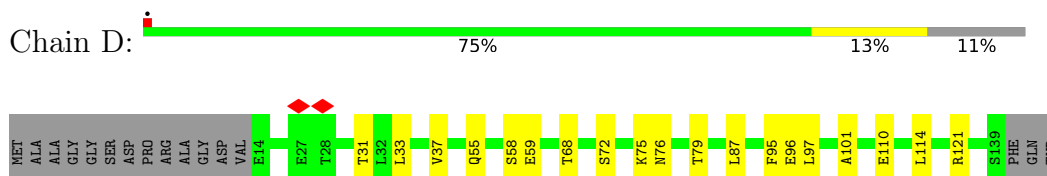
- Molecule 8: DNA-directed RNA polymerase subunit beta



- Molecule 9: DNA-directed RNA polymerase II subunit RPB3



- Molecule 10: RNA polymerase Rpb4/RPC9 core domain-containing protein



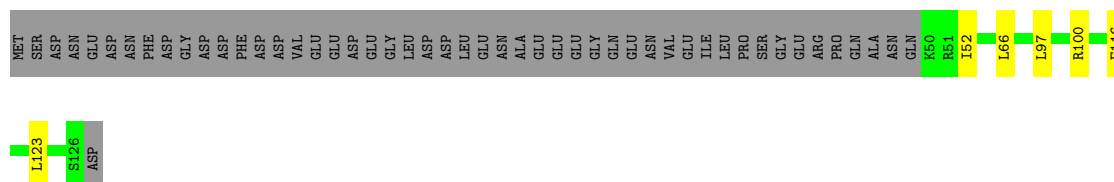
- Molecule 11: DNA-directed RNA polymerase II subunit E





- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 56% 5% 39%



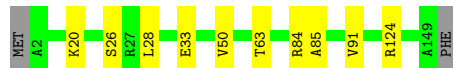
- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

Chain G: 88% 11%



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

Chain H: 92% 7%



- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

Chain I: 78% 14% 9%



- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 84% 13%

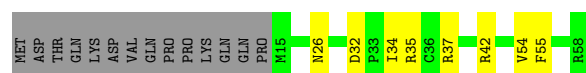


- Molecule 17: RNA polymerase II subunit J

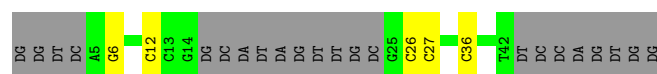
Chain K: 92% 6%



- Molecule 18: RNA polymerase II subunit K



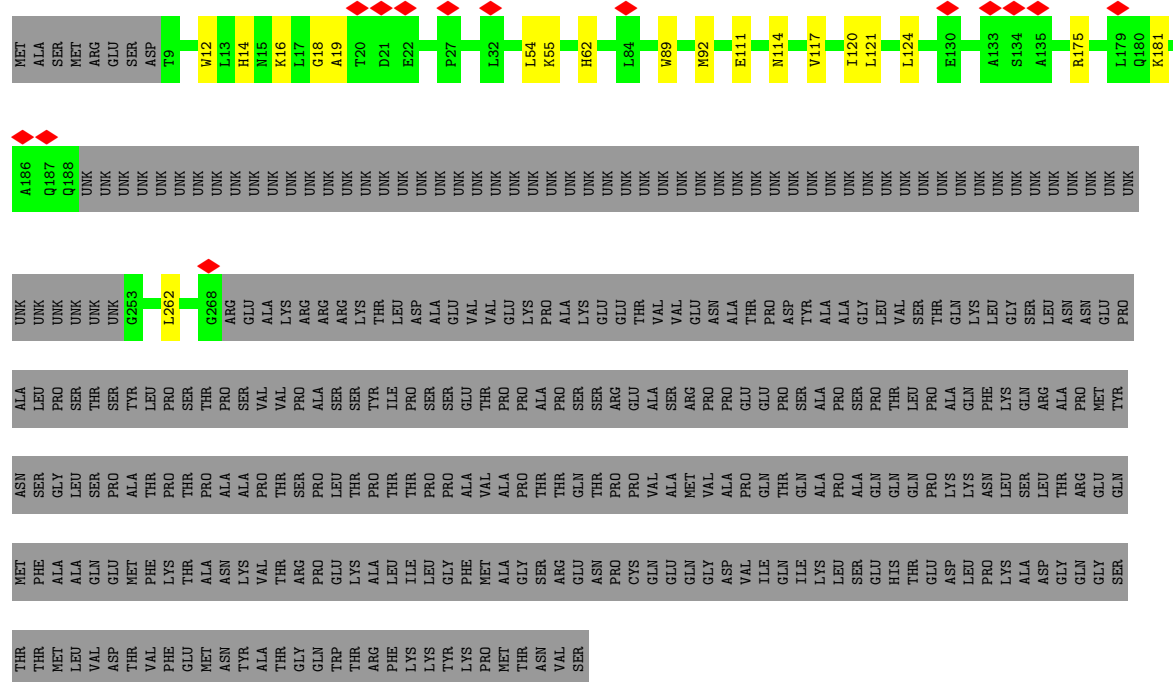
Chain N: 46% 10% 44%



Chain T: 66% 10% 24%



Chain U: 34% 1% 63%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9428	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	2.608	Depositor
Minimum map value	-1.238	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.4	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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.52	0/103	0.76	0/132
2	Y	0.16	0/927	0.32	0/1250
3	Z	0.18	0/3841	0.37	0/5167
4	W	0.21	0/4302	0.41	2/5835 (0.0%)
5	P	0.21	0/351	0.51	0/544
6	V	0.22	0/4495	0.44	0/6074
7	A	0.20	0/11431	0.42	0/15432
8	B	0.20	0/9257	0.41	0/12493
9	C	0.18	0/2087	0.39	0/2836
10	D	0.21	0/1043	0.39	0/1400
11	E	0.21	0/1727	0.41	0/2329
12	F	0.20	0/628	0.39	0/848
13	G	0.20	0/1382	0.42	0/1874
14	H	0.18	0/1207	0.41	0/1628
15	I	0.21	0/949	0.47	0/1284
16	J	0.18	0/524	0.37	0/707
17	K	0.19	0/939	0.37	0/1271
18	L	0.22	0/378	0.44	0/500
19	N	0.41	0/638	0.70	0/979
20	T	0.37	0/876	0.60	0/1350
21	U	0.22	0/1521	0.43	0/2063
All	All	0.21	0/48606	0.42	2/65996 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	345	GLY	CA-C-N	5.16	130.99	121.70
4	W	345	GLY	C-N-CA	5.16	130.99	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	103	116	120	0	0
2	Y	911	905	905	5	0
3	Z	3778	3840	3840	25	0
4	W	4217	4221	4221	38	0
5	P	316	158	158	5	0
6	V	4410	4501	4501	45	0
7	A	11227	11362	11361	104	0
8	B	9076	9117	9117	75	0
9	C	2044	1995	1995	20	0
10	D	1030	1016	1016	12	0
11	E	1698	1716	1716	12	0
12	F	618	653	653	3	0
13	G	1351	1358	1358	12	0
14	H	1186	1147	1147	6	0
15	I	928	861	860	11	0
16	J	515	535	535	8	0
17	K	920	942	942	6	0
18	L	373	379	379	5	0
19	N	571	315	317	5	0
20	T	781	427	428	5	0
21	U	1498	1556	1556	15	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	47561	47120	47125	348	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 (348) 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)
21:U:120:ILE:HG23	21:U:124:LEU:HD12	1.64	0.80
7:A:567:LEU:HD13	7:A:595:ILE:HG22	1.68	0.75
8:B:585:ASN:OD1	8:B:588:ARG:NH2	2.23	0.71
3:Z:199:LYS:NZ	3:Z:240:GLU:O	2.23	0.71
7:A:1262:MET:SD	7:A:1264:SER:OG	2.49	0.71
7:A:663:ASP:OD1	7:A:666:ARG:NH2	2.24	0.70
7:A:75:ALA:O	8:B:1131:ARG:NH1	2.24	0.70
10:D:58:SER:OG	10:D:59:GLU:OE1	2.10	0.70
7:A:460:ARG:NH1	7:A:492:TYR:O	2.25	0.69
3:Z:711:ARG:NE	9:C:92:GLU:OE2	2.24	0.69
9:C:113:ARG:NH1	9:C:114:HIS:O	2.26	0.68
8:B:794:VAL:HG12	8:B:967:ILE:HG22	1.75	0.68
7:A:1461:GLY:O	8:B:1104:ARG:NH1	2.26	0.68
4:W:419:ARG:NH1	4:W:461:CYS:SG	2.66	0.68
7:A:1100:THR:OG1	7:A:1101:GLN:OE1	2.09	0.68
8:B:309:PHE:O	8:B:312:GLN:NE2	2.27	0.68
11:E:53:PRO:O	11:E:54:ARG:NH1	2.27	0.68
7:A:1024:ASN:O	11:E:162:ARG:NH2	2.28	0.67
7:A:734:ARG:NH1	15:I:105:GLU:OE1	2.26	0.67
7:A:263:ALA:O	7:A:271:ARG:NH1	2.28	0.67
7:A:853:LYS:NZ	7:A:1102:MET:O	2.26	0.67
8:B:237:VAL:HG21	8:B:369:VAL:HG12	1.76	0.67
6:V:149:ILE:O	6:V:153:ASN:N	2.28	0.67
7:A:448:ARG:NH1	7:A:451:CYS:SG	2.68	0.67
18:L:35:ARG:O	18:L:37:ARG:NH1	2.28	0.67
14:H:63:THR:OG1	14:H:84:ARG:NH2	2.28	0.66
2:Y:81:LYS:O	2:Y:85:TYR:OH	2.12	0.66
7:A:1000:LEU:O	7:A:1059:ARG:NH2	2.29	0.66
8:B:1137:CYS:SG	8:B:1138:ARG:N	2.69	0.65
7:A:99:PHE:O	7:A:103:THR:OG1	2.11	0.64
6:V:270:ILE:HD11	6:V:309:PHE:HB2	1.79	0.64
10:D:76:ASN:O	10:D:79:THR:OG1	2.14	0.63
7:A:1364:GLU:O	7:A:1368:VAL:HG12	1.99	0.63
7:A:340:LYS:HG3	7:A:1436:VAL:HG21	1.81	0.63
9:C:7:PRO:O	17:K:104:ARG:NH1	2.31	0.63
15:I:68:ILE:O	15:I:122:ARG:NH1	2.31	0.63
8:B:927:ARG:NH2	8:B:1057:ASP:OD1	2.31	0.62
7:A:154:CYS:SG	7:A:188:GLN:NE2	2.71	0.62
7:A:1218:ARG:NH2	7:A:1252:ALA:O	2.32	0.62
4:W:94:VAL:HG11	6:V:65:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:721:ILE:O	3:Z:737:HIS:ND1	2.33	0.62
6:V:508:LEU:HB3	6:V:544:LEU:HD21	1.82	0.62
7:A:1128:ILE:HB	7:A:1414:ILE:HD13	1.81	0.62
3:Z:430:GLU:OE1	3:Z:430:GLU:N	2.33	0.61
7:A:841:MET:SD	8:B:503:ASN:ND2	2.73	0.61
6:V:269:CYS:SG	6:V:279:ARG:NE	2.73	0.61
9:C:78:ILE:HG21	9:C:127:VAL:HG13	1.82	0.61
5:P:6:U:O2'	5:P:7:G:O4'	2.14	0.61
10:D:96:GLU:OE2	10:D:121:ARG:NH1	2.34	0.61
10:D:110:GLU:OE2	13:G:144:ARG:NH1	2.33	0.61
5:P:10:A:O2'	7:A:334:ARG:NH1	2.34	0.61
8:B:759:VAL:HG12	8:B:999:ALA:HB2	1.81	0.61
10:D:72:SER:O	10:D:75:LYS:NZ	2.33	0.61
9:C:234:GLU:OE1	16:J:42:ARG:NH2	2.34	0.61
19:N:26:DC:N4	20:T:24:DG:O6	2.33	0.61
12:F:100:ARG:NH2	12:F:123:LEU:O	2.34	0.60
4:W:528:SER:OG	7:A:1151:ALA:N	2.35	0.60
16:J:19:GLU:OE1	16:J:19:GLU:N	2.35	0.60
4:W:504:LEU:HG	4:W:509:VAL:HG12	1.83	0.59
7:A:467:MET:SD	7:A:467:MET:N	2.74	0.59
6:V:24:THR:OG1	6:V:25:GLU:OE2	2.19	0.59
8:B:912:ASN:OD1	8:B:916:TYR:N	2.35	0.59
7:A:1208:SER:O	7:A:1260:ARG:NH1	2.36	0.59
4:W:133:ASP:O	4:W:137:THR:HG23	2.04	0.58
6:V:462:LEU:HD11	6:V:500:VAL:HG22	1.84	0.58
7:A:469:MET:SD	8:B:1094:GLN:NE2	2.76	0.58
7:A:358:ARG:NE	8:B:1076:GLU:OE2	2.35	0.58
8:B:380:ARG:NH1	8:B:381:GLU:O	2.37	0.58
8:B:536:SER:OG	8:B:616:THR:OG1	2.19	0.58
8:B:65:ILE:HD11	8:B:412:LEU:HG	1.85	0.58
8:B:825:GLN:NE2	8:B:872:THR:O	2.37	0.57
8:B:274:ARG:NH2	8:B:281:ASP:OD1	2.37	0.57
7:A:906:LEU:N	7:A:975:SER:OG	2.37	0.57
8:B:760:THR:OG1	8:B:764:MET:SD	2.55	0.57
8:B:741:HIS:O	8:B:922:ARG:NH2	2.38	0.57
8:B:565:THR:HG21	8:B:580:PRO:HG3	1.86	0.57
6:V:191:SER:O	6:V:194:THR:OG1	2.20	0.57
6:V:176:LEU:O	6:V:463:HIS:ND1	2.37	0.57
7:A:668:PHE:CZ	7:A:672:ILE:HD11	2.39	0.57
4:W:316:MET:O	4:W:319:SER:OG	2.22	0.56
7:A:734:ARG:NE	15:I:108:MET:SD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:376:MET:HE1	6:V:410:SER:OG	2.06	0.56
8:B:1057:ASP:O	8:B:1080:ARG:NH1	2.38	0.56
4:W:142:THR:HG21	4:W:146:LEU:HD23	1.88	0.55
6:V:61:PHE:O	6:V:65:VAL:HG22	2.05	0.55
21:U:54:LEU:HD21	21:U:89:TRP:HB3	1.88	0.55
7:A:312:PHE:CE1	7:A:325:LEU:HD22	2.42	0.55
6:V:39:VAL:HG12	6:V:41:LEU:HD12	1.89	0.55
4:W:209:LEU:HD11	21:U:124:LEU:HD13	1.89	0.55
7:A:389:THR:HG22	7:A:449:HIS:HA	1.89	0.55
7:A:1228:MET:HE2	7:A:1255:LEU:HB3	1.89	0.55
7:A:1430:CYS:SG	7:A:1439:LEU:HD21	2.46	0.55
7:A:457:ILE:HD11	7:A:515:ILE:HD12	1.89	0.54
4:W:104:THR:HG21	6:V:76:ARG:HG2	1.90	0.54
9:C:50:VAL:O	18:L:55:PHE:N	2.39	0.54
8:B:803:ARG:NH1	16:J:8:PHE:O	2.41	0.54
8:B:992:ASN:O	16:J:46:ARG:NH1	2.40	0.54
7:A:583:ARG:NH1	9:C:222:PRO:O	2.41	0.54
21:U:19:ALA:O	21:U:55:LYS:NZ	2.32	0.54
7:A:1429:LYS:HG3	7:A:1438:VAL:HG11	1.90	0.53
13:G:106:CYS:SG	13:G:107:PHE:N	2.81	0.53
9:C:78:ILE:HG21	9:C:127:VAL:CG1	2.38	0.53
7:A:289:GLN:NE2	7:A:306:ASP:OD2	2.42	0.53
15:I:23:MET:HE3	15:I:24:LEU:O	2.09	0.53
7:A:1368:VAL:HG13	7:A:1369:LEU:HD23	1.90	0.53
8:B:125:TYR:OH	21:U:262:LEU:HD22	2.08	0.53
15:I:86:CYS:SG	15:I:87:GLN:N	2.82	0.53
12:F:52:ILE:N	12:F:116:GLU:OE2	2.41	0.52
2:Y:23:LYS:NZ	2:Y:32:GLY:O	2.39	0.52
4:W:440:TYR:HH	4:W:451:HIS:HD1	1.55	0.52
7:A:967:ARG:NH2	7:A:1326:GLY:O	2.43	0.52
8:B:953:ASP:OD1	9:C:36:ARG:NH2	2.43	0.52
9:C:10:ARG:NH2	9:C:24:GLU:OE2	2.43	0.52
10:D:33:LEU:O	10:D:37:VAL:HG23	2.10	0.52
6:V:432:ILE:O	6:V:436:ARG:N	2.42	0.52
4:W:235:GLU:OE2	21:U:62:HIS:NE2	2.44	0.51
4:W:94:VAL:CG1	6:V:65:VAL:HG23	2.40	0.51
8:B:159:THR:HG23	8:B:160:TYR:CD1	2.46	0.51
8:B:872:THR:OG1	8:B:889:LYS:NZ	2.43	0.51
8:B:761:THR:HG23	8:B:1000:THR:HA	1.91	0.51
13:G:21:ASN:O	13:G:25:THR:OG1	2.23	0.51
7:A:680:LEU:O	7:A:684:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:267:ASP:OD2	6:V:271:ARG:NH2	2.44	0.51
9:C:9:VAL:HG11	17:K:105:PHE:HD1	1.76	0.51
3:Z:354:SER:HA	3:Z:359:LEU:HD23	1.93	0.51
11:E:134:GLU:OE2	11:E:181:ARG:NH2	2.42	0.51
19:N:12:DC:N4	20:T:38:DG:O6	2.44	0.51
7:A:668:PHE:CE1	7:A:672:ILE:HD11	2.46	0.50
9:C:45:ILE:HG22	9:C:165:ALA:HB1	1.93	0.50
7:A:1301:ILE:HD13	7:A:1345:ARG:HB3	1.94	0.50
8:B:745:ASP:O	8:B:813:SER:OG	2.25	0.50
4:W:457:GLU:OE1	21:U:175:ARG:NE	2.45	0.50
6:V:369:LEU:HD13	6:V:421:ALA:HB2	1.93	0.50
9:C:9:VAL:HG11	17:K:105:PHE:CD1	2.46	0.50
7:A:1190:GLN:NE2	7:A:1194:ASN:OD1	2.45	0.50
4:W:236:HIS:HB3	21:U:54:LEU:HD22	1.93	0.50
8:B:388:TYR:HE2	8:B:621:ILE:HG21	1.77	0.50
8:B:1040:GLN:NE2	9:C:196:VAL:O	2.45	0.50
8:B:254:GLN:OE1	8:B:254:GLN:N	2.41	0.50
6:V:271:ARG:NH1	11:E:67:ASP:OD1	2.45	0.50
7:A:1305:SER:OG	7:A:1339:ASP:OD2	2.17	0.50
19:N:27:DC:N4	20:T:23:DG:O6	2.45	0.50
3:Z:450:ILE:HG21	3:Z:468:LEU:HD11	1.93	0.50
7:A:592:PHE:CE2	7:A:595:ILE:HD11	2.47	0.50
7:A:659:GLU:OE2	7:A:985:ARG:NH2	2.45	0.50
7:A:1146:GLN:O	7:A:1150:ASP:N	2.44	0.50
8:B:607:ILE:HD12	15:I:75:ASP:CG	2.37	0.50
8:B:663:GLU:OE2	8:B:695:HIS:NE2	2.45	0.50
8:B:643:LEU:HD11	8:B:656:LEU:HD11	1.94	0.49
9:C:154:ARG:NH1	16:J:62:TYR:O	2.45	0.49
3:Z:719:GLY:O	9:C:49:TRP:NE1	2.45	0.49
8:B:1162:LEU:HD12	8:B:1167:ILE:HG21	1.95	0.49
13:G:17:TYR:HB3	13:G:25:THR:HG21	1.93	0.49
7:A:459:ASN:OD1	7:A:460:ARG:N	2.44	0.49
7:A:1368:VAL:HG13	7:A:1369:LEU:CD2	2.42	0.49
10:D:55:GLN:HB2	13:G:32:THR:HG22	1.95	0.49
3:Z:462:GLU:N	3:Z:462:GLU:OE1	2.45	0.49
6:V:433:THR:HG23	6:V:472:LEU:HD11	1.94	0.49
8:B:118:LEU:O	8:B:189:GLY:N	2.46	0.49
13:G:1:MET:SD	13:G:2:PHE:N	2.83	0.49
2:Y:94:PRO:HD2	2:Y:97:ILE:HD12	1.95	0.49
4:W:244:MET:SD	21:U:120:ILE:HG21	2.53	0.49
8:B:1068:GLN:N	8:B:1073:GLN:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:85:ALA:HB1	14:H:91:VAL:HG21	1.95	0.49
7:A:617:PRO:O	14:H:124:ARG:NH1	2.46	0.49
7:A:885:GLN:OE1	7:A:1408:ARG:NH2	2.46	0.49
3:Z:554:GLU:OE1	3:Z:557:THR:OG1	2.31	0.49
16:J:47:ARG:NE	16:J:48:MET:SD	2.86	0.49
3:Z:705:LEU:HG	3:Z:724:VAL:HG21	1.95	0.48
11:E:118:LEU:HD22	11:E:127:LEU:HB3	1.95	0.48
4:W:261:ILE:O	4:W:265:VAL:HG23	2.14	0.48
11:E:93:ARG:NH2	11:E:97:GLU:OE2	2.46	0.48
7:A:292:ARG:O	7:A:296:ASN:N	2.46	0.48
13:G:117:MET:SD	13:G:130:THR:OG1	2.70	0.48
4:W:396:LEU:HD22	4:W:410:GLU:HG3	1.96	0.48
4:W:407:LEU:CD1	4:W:450:VAL:HG21	2.43	0.48
10:D:87:LEU:HD11	10:D:101:ALA:HB2	1.94	0.48
21:U:117:VAL:HA	21:U:120:ILE:HD12	1.94	0.48
4:W:57:ILE:HG23	4:W:58:MET:SD	2.53	0.48
6:V:323:GLN:O	6:V:326:VAL:HG22	2.13	0.48
4:W:55:ASP:OD1	4:W:55:ASP:N	2.45	0.48
5:P:10:A:OP1	7:A:337:LYS:NZ	2.46	0.48
7:A:256:PRO:O	7:A:261:ARG:NH2	2.47	0.48
6:V:179:THR:HG23	6:V:506:ARG:HB2	1.96	0.48
8:B:48:ASP:OD1	8:B:158:SER:OG	2.32	0.48
3:Z:736:LEU:HD21	3:Z:743:ILE:HG13	1.96	0.48
8:B:1107:LEU:O	8:B:1111:SER:OG	2.32	0.48
11:E:156:VAL:O	11:E:160:LEU:HD23	2.14	0.48
7:A:91:ALA:HB3	7:A:290:LEU:HD23	1.95	0.47
13:G:28:GLN:O	13:G:32:THR:HG23	2.14	0.47
3:Z:365:ARG:HG3	3:Z:372:LEU:HD22	1.96	0.47
6:V:223:ARG:NH2	6:V:300:ASP:OD1	2.48	0.47
7:A:1218:ARG:HE	7:A:1255:LEU:HD21	1.77	0.47
7:A:858:GLY:O	7:A:862:ARG:N	2.43	0.47
8:B:1091:ARG:HG3	8:B:1103:LEU:HD11	1.95	0.47
7:A:392:GLU:OE2	7:A:448:ARG:NE	2.48	0.47
7:A:1372:GLU:HG3	11:E:193:ILE:HD13	1.95	0.47
8:B:378:GLY:HA3	15:I:102:ALA:HB3	1.97	0.47
7:A:460:ARG:HB2	7:A:501:MET:HE3	1.97	0.47
3:Z:424:ASP:HB2	3:Z:440:ILE:HD12	1.96	0.47
3:Z:631:GLU:OE1	3:Z:631:GLU:N	2.47	0.47
6:V:429:VAL:HG21	6:V:448:LEU:HD11	1.96	0.47
7:A:322:LEU:O	7:A:327:ARG:NH2	2.48	0.47
8:B:783:ALA:HB2	8:B:1041:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:112:GLN:NE2	6:V:41:LEU:HD22	2.30	0.47
6:V:245:LEU:HD13	6:V:253:ILE:HG21	1.96	0.47
4:W:481:HIS:O	4:W:489:GLN:NE2	2.48	0.47
6:V:284:GLN:NE2	6:V:288:ASP:OD2	2.48	0.47
15:I:109:ARG:NE	15:I:124:THR:OG1	2.46	0.47
2:Y:64:MET:HE2	3:Z:197:MET:HB2	1.97	0.46
7:A:34:MET:HE2	7:A:85:PHE:HB2	1.97	0.46
7:A:133:SER:O	7:A:140:ARG:NH2	2.48	0.46
15:I:69:ILE:O	15:I:72:VAL:HG22	2.15	0.46
6:V:178:SER:O	6:V:506:ARG:NH2	2.48	0.46
6:V:345:LEU:HD23	6:V:420:MET:HE1	1.97	0.46
7:A:90:LEU:HD11	7:A:250:VAL:HG12	1.98	0.46
8:B:119:THR:HG23	8:B:187:ILE:HD13	1.98	0.46
3:Z:427:GLU:OE2	3:Z:469:ARG:NH2	2.47	0.46
6:V:243:MET:SD	6:V:243:MET:N	2.89	0.46
7:A:1193:VAL:O	7:A:1197:TYR:N	2.45	0.46
7:A:1201:ASP:OD1	7:A:1201:ASP:N	2.48	0.46
4:W:200:VAL:O	4:W:204:VAL:HG23	2.16	0.46
7:A:41:ILE:HD12	7:A:56:GLY:O	2.15	0.46
6:V:215:TYR:OH	6:V:257:ASP:OD2	2.26	0.46
7:A:22:GLN:O	8:B:1170:ARG:N	2.47	0.46
14:H:33:GLU:O	21:U:12:TRP:NE1	2.46	0.46
7:A:1412:MET:SD	7:A:1422:GLN:NE2	2.85	0.46
3:Z:736:LEU:HD21	3:Z:743:ILE:CG1	2.46	0.46
11:E:83:GLY:O	11:E:86:THR:OG1	2.29	0.46
4:W:520:LEU:HD22	4:W:556:ILE:HG13	1.98	0.45
6:V:165:LEU:HD13	6:V:225:LEU:HD11	1.97	0.45
7:A:1164:THR:OG1	7:A:1299:GLN:N	2.49	0.45
6:V:369:LEU:HD12	6:V:373:PHE:HB3	1.98	0.45
4:W:329:ARG:NE	4:W:363:ALA:O	2.44	0.45
7:A:102:LYS:O	7:A:106:VAL:HG23	2.15	0.45
8:B:771:GLU:OE1	8:B:771:GLU:N	2.50	0.45
6:V:269:CYS:O	6:V:273:ARG:N	2.49	0.45
7:A:1223:ASP:OD2	7:A:1224:ARG:NH1	2.49	0.45
7:A:1285:LEU:HA	7:A:1288:ILE:HD12	1.98	0.45
7:A:1302:GLU:OE1	7:A:1302:GLU:N	2.48	0.45
4:W:369:THR:O	4:W:376:VAL:N	2.46	0.45
4:W:562:ILE:HD11	7:A:1153:ARG:HH11	1.81	0.45
8:B:198:GLU:OE2	8:B:391:LYS:NZ	2.35	0.45
7:A:539:GLN:HA	7:A:774:ALA:HB1	1.97	0.45
12:F:66:LEU:HD21	12:F:97:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:193:ARG:NH2	9:C:218:ALA:O	2.49	0.45
13:G:145:LEU:HD13	13:G:161:GLY:CA	2.47	0.45
4:W:212:ILE:HD11	4:W:227:PHE:HD2	1.82	0.45
9:C:183:ALA:HB3	9:C:232:ASN:HB3	1.99	0.45
3:Z:416:ARG:NH1	3:Z:417:GLU:O	2.51	0.44
7:A:29:ASP:OD2	7:A:33:ARG:NH2	2.49	0.44
8:B:1112:ASP:OD1	8:B:1112:ASP:N	2.51	0.44
4:W:209:LEU:HA	4:W:212:ILE:HD12	1.99	0.44
3:Z:197:MET:HE3	3:Z:201:ILE:HD11	2.00	0.44
7:A:781:ILE:HG23	7:A:785:ILE:HD12	1.99	0.44
2:Y:37:ASP:O	2:Y:41:GLN:N	2.49	0.44
8:B:852:GLY:O	8:B:868:GLY:N	2.46	0.44
8:B:1094:GLN:HB2	8:B:1103:LEU:HD12	1.99	0.44
7:A:1228:MET:HE1	7:A:1248:ASN:OD1	2.17	0.44
7:A:34:MET:HE1	8:B:1163:MET:HE1	2.00	0.44
3:Z:432:GLU:OE1	3:Z:432:GLU:N	2.44	0.44
7:A:811:ILE:HD12	15:I:79:PRO:HB3	2.00	0.44
8:B:285:LEU:O	8:B:289:ILE:N	2.50	0.44
7:A:80:GLU:OE1	8:B:1131:ARG:NH2	2.51	0.44
11:E:82:VAL:HG21	11:E:110:MET:HE3	1.99	0.44
16:J:1:MET:SD	16:J:1:MET:N	2.86	0.44
5:P:9:C:O2'	7:A:337:LYS:NZ	2.49	0.43
6:V:469:LEU:HD23	6:V:472:LEU:HD12	1.99	0.43
7:A:865:ILE:HG21	8:B:1092:ASP:CG	2.43	0.43
7:A:686:THR:HG21	8:B:1040:GLN:O	2.18	0.43
17:K:12:LEU:HD11	17:K:18:LYS:HD3	2.01	0.43
7:A:33:ARG:O	8:B:1138:ARG:NH1	2.50	0.43
8:B:906:GLN:OE1	8:B:922:ARG:NH2	2.51	0.43
19:N:36:DC:N4	20:T:14:DT:O4	2.51	0.43
4:W:534:VAL:HG23	4:W:553:PHE:CE1	2.53	0.43
13:G:108:ILE:HG22	13:G:113:ILE:HG13	2.00	0.43
7:A:36:VAL:HG22	7:A:85:PHE:O	2.18	0.43
4:W:190:SER:O	4:W:194:ALA:N	2.43	0.43
7:A:467:MET:HG2	7:A:534:VAL:HG11	2.01	0.43
7:A:1211:LEU:HD13	7:A:1258:ARG:CZ	2.48	0.43
6:V:318:THR:HG23	6:V:338:LEU:HD11	2.00	0.43
6:V:307:ASP:OD1	6:V:310:ALA:N	2.45	0.43
7:A:365:THR:OG1	7:A:366:VAL:N	2.52	0.43
8:B:861:SER:OG	8:B:863:ASP:OD1	2.36	0.43
3:Z:248:GLY:O	3:Z:252:GLN:NE2	2.51	0.43
8:B:856:PRO:HA	8:B:904:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:101:PHE:O	6:V:104:VAL:HG12	2.19	0.42
7:A:366:VAL:HG11	8:B:1055:VAL:HG12	2.01	0.42
3:Z:478:VAL:HB	3:Z:518:LEU:HD22	2.01	0.42
6:V:328:GLN:O	6:V:328:GLN:NE2	2.50	0.42
9:C:260:GLN:HB2	17:K:91:ILE:HG21	2.01	0.42
10:D:87:LEU:HD22	10:D:97:LEU:HD22	2.01	0.42
7:A:1101:GLN:OE1	7:A:1101:GLN:N	2.52	0.42
14:H:20:LYS:NZ	14:H:26:SER:OG	2.52	0.42
8:B:910:THR:OG1	18:L:42:ARG:O	2.34	0.42
11:E:180:ALA:O	11:E:184:GLY:N	2.52	0.42
13:G:30:LEU:O	13:G:34:VAL:HG22	2.19	0.42
4:W:456:ASP:O	4:W:460:THR:OG1	2.37	0.42
8:B:796:MET:SD	8:B:948:GLN:NE2	2.90	0.42
11:E:156:VAL:HG22	11:E:190:VAL:CG1	2.49	0.42
4:W:344:PRO:O	4:W:347:ARG:NH1	2.52	0.42
4:W:439:ARG:NH1	4:W:441:PHE:O	2.53	0.42
6:V:165:LEU:HD13	6:V:225:LEU:CD1	2.50	0.42
8:B:964:ASP:OD1	16:J:9:THR:OG1	2.20	0.42
18:L:32:ASP:OD1	18:L:32:ASP:N	2.53	0.42
4:W:157:ASP:OD2	4:W:161:LYS:NZ	2.52	0.42
8:B:590:LEU:O	8:B:594:MET:N	2.53	0.42
10:D:114:LEU:HD13	13:G:84:VAL:HG11	2.02	0.42
6:V:251:GLY:O	6:V:255:THR:OG1	2.16	0.41
7:A:906:LEU:HD13	7:A:966:LEU:HD13	2.02	0.41
5:P:6:U:O4'	8:B:841:ARG:NH2	2.53	0.41
10:D:68:THR:O	10:D:72:SER:N	2.53	0.41
3:Z:440:ILE:HG23	3:Z:450:ILE:HD11	2.01	0.41
7:A:33:ARG:NH1	8:B:1139:GLY:O	2.52	0.41
7:A:338:SER:OG	7:A:339:LEU:N	2.54	0.41
7:A:1192:TRP:HZ3	7:A:1246:ILE:HG22	1.85	0.41
8:B:1028:LEU:HD13	8:B:1041:ILE:HB	2.01	0.41
10:D:31:THR:HG21	10:D:95:PHE:HA	2.02	0.41
15:I:39:CYS:SG	15:I:40:ARG:N	2.93	0.41
7:A:400:ASP:OD1	7:A:401:ARG:N	2.53	0.41
7:A:1185:VAL:HG23	7:A:1186:VAL:HG23	2.02	0.41
6:V:253:ILE:HA	6:V:256:VAL:HG22	2.03	0.41
6:V:415:LEU:HD23	6:V:422:CYS:HA	2.02	0.41
7:A:1472:ASP:N	7:A:1472:ASP:OD1	2.51	0.41
14:H:28:LEU:HD11	14:H:50:VAL:HG21	2.01	0.41
17:K:105:PHE:CD2	17:K:109:ILE:HD11	2.56	0.41
4:W:534:VAL:HG23	4:W:553:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1400:LEU:O	7:A:1404:THR:HG23	2.20	0.41
4:W:209:LEU:HD21	21:U:124:LEU:HD13	2.03	0.41
21:U:111:GLU:CD	21:U:121:LEU:HD11	2.46	0.41
3:Z:227:VAL:HG21	3:Z:235:VAL:HG13	2.03	0.41
6:V:150:TRP:O	6:V:217:MET:HE1	2.21	0.41
6:V:270:ILE:HD11	6:V:309:PHE:CB	2.47	0.41
8:B:133:ILE:HG23	8:B:138:GLU:O	2.21	0.41
9:C:56:SER:O	9:C:56:SER:OG	2.39	0.41
21:U:92:MET:HE3	21:U:114:ASN:ND2	2.36	0.41
21:U:14:HIS:O	21:U:18:GLY:N	2.52	0.41
6:V:333:ARG:HE	6:V:370:ILE:HG21	1.86	0.40
8:B:565:THR:HG22	8:B:610:ARG:HB3	2.02	0.40
7:A:19:LYS:NZ	8:B:1173:SER:O	2.48	0.40
8:B:1158:LEU:O	8:B:1162:LEU:HD23	2.20	0.40
7:A:828:LEU:HD11	8:B:1008:VAL:HG11	2.02	0.40
8:B:904:VAL:HG23	8:B:921:ILE:HG23	2.03	0.40
4:W:440:TYR:OH	4:W:451:HIS:ND1	2.49	0.40
3:Z:737:HIS:NE2	18:L:54:VAL:O	2.55	0.40
7:A:507:GLN:N	8:B:1105:GLU:OE2	2.49	0.40
7:A:874:LYS:O	7:A:877:ALA:N	2.54	0.40
19:N:6:DG:O6	20:T:44:DA:N6	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	10/380 (3%)	10 (100%)	0	0	100	100
2	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
3	Z	455/1087 (42%)	434 (95%)	21 (5%)	0	100	100
4	W	518/590 (88%)	504 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	V	548/580 (94%)	536 (98%)	12 (2%)	0	100	100
7	A	1407/1970 (71%)	1355 (96%)	52 (4%)	0	100	100
8	B	1130/1174 (96%)	1071 (95%)	59 (5%)	0	100	100
9	C	251/271 (93%)	244 (97%)	7 (3%)	0	100	100
10	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
11	E	200/210 (95%)	194 (97%)	6 (3%)	0	100	100
12	F	75/127 (59%)	74 (99%)	1 (1%)	0	100	100
13	G	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
14	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
15	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
16	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
17	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
18	L	42/58 (72%)	42 (100%)	0	0	100	100
21	U	192/527 (36%)	181 (94%)	11 (6%)	0	100	100
All	All	5669/7864 (72%)	5459 (96%)	210 (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%)	9 (82%)	2 (18%)	2	10
2	Y	102/103 (99%)	102 (100%)	0	100	100
3	Z	418/940 (44%)	416 (100%)	2 (0%)	81	80
4	W	471/513 (92%)	465 (99%)	6 (1%)	61	72
6	V	493/515 (96%)	487 (99%)	6 (1%)	63	73
7	A	1248/1749 (71%)	1238 (99%)	10 (1%)	73	77
8	B	994/1027 (97%)	985 (99%)	9 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	232/248 (94%)	232 (100%)	0	100	100
10	D	116/126 (92%)	116 (100%)	0	100	100
11	E	189/192 (98%)	187 (99%)	2 (1%)	65	74
12	F	67/111 (60%)	67 (100%)	0	100	100
13	G	152/153 (99%)	152 (100%)	0	100	100
14	H	129/131 (98%)	129 (100%)	0	100	100
15	I	103/112 (92%)	103 (100%)	0	100	100
16	J	54/56 (96%)	54 (100%)	0	100	100
17	K	104/106 (98%)	103 (99%)	1 (1%)	68	75
18	L	41/55 (74%)	39 (95%)	2 (5%)	22	48
21	U	167/396 (42%)	165 (99%)	2 (1%)	63	73
All	All	5091/6864 (74%)	5049 (99%)	42 (1%)	70	77

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	15	LEU
1	X	18	LYS
3	Z	364	ASN
3	Z	738	SER
4	W	55	ASP
4	W	139	GLU
4	W	189	THR
4	W	208	SER
4	W	302	LYS
4	W	439	ARG
6	V	181	LEU
6	V	307	ASP
6	V	329	GLU
6	V	330	THR
6	V	378	MET
6	V	540	LEU
7	A	201	GLU
7	A	325	LEU
7	A	437	ASP
7	A	467	MET
7	A	502	ASN
7	A	811	ILE

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Mol	Chain	Res	Type
7	A	876	ASP
7	A	1199	MET
7	A	1287	CYS
7	A	1307	VAL
8	B	93	LEU
8	B	237	VAL
8	B	482	LEU
8	B	539	SER
8	B	750	VAL
8	B	809	VAL
8	B	870	THR
8	B	900	GLU
8	B	1142	ASN
11	E	91	CYS
11	E	108	GLN
17	K	71	ILE
18	L	26	ASN
18	L	34	ILE
21	U	16	LYS
21	U	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	364	ASN
3	Z	421	GLN
3	Z	703	ASN
4	W	250	GLN
4	W	585	ASN
6	V	6	GLN
6	V	197	GLN
6	V	294	GLN
6	V	437	ASN
6	V	543	GLN
7	A	423	ASN
7	A	493	ASN
7	A	504	HIS
7	A	742	ASN
7	A	825	ASN
7	A	888	GLN
7	A	1024	ASN
7	A	1044	HIS

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Mol	Chain	Res	Type
7	A	1146	GLN
7	A	1236	ASN
7	A	1313	GLN
7	A	1384	HIS
7	A	1417	HIS
8	B	141	GLN
8	B	486	ASN
9	C	51	GLN
14	H	76	ASN
14	H	126	GLN
15	I	46	GLN
15	I	100	HIS
17	K	29	ASN
21	U	14	HIS
21	U	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	14/17 (82%)	5 (35%)	1 (7%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	4	U
5	P	5	U
5	P	7	G
5	P	8	G
5	P	10	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	P	6	U

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 [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.

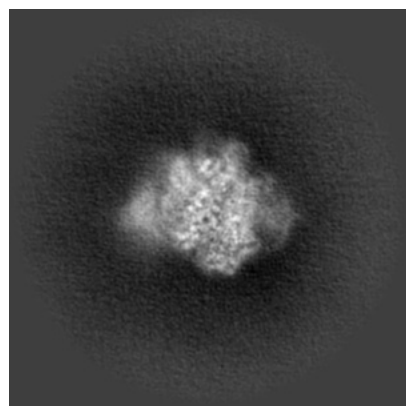
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42267. These allow visual inspection of the internal detail of the map and identification of artifacts.

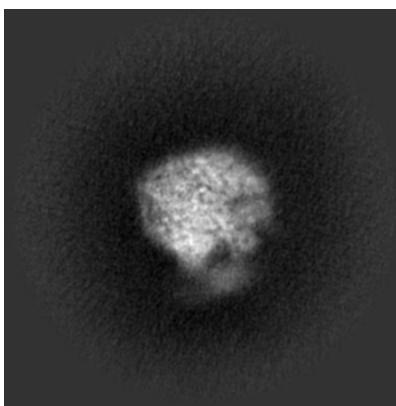
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

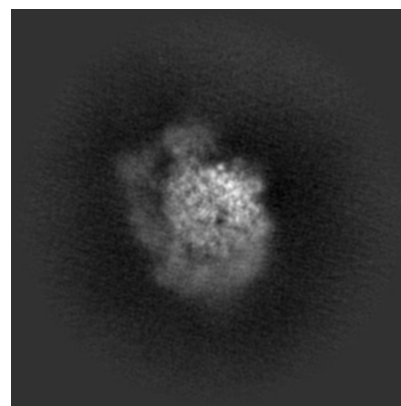
6.1.1 Primary map



X

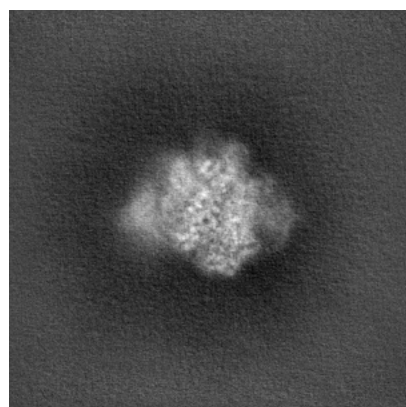


Y

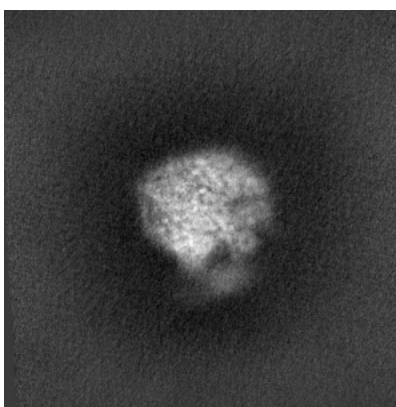


Z

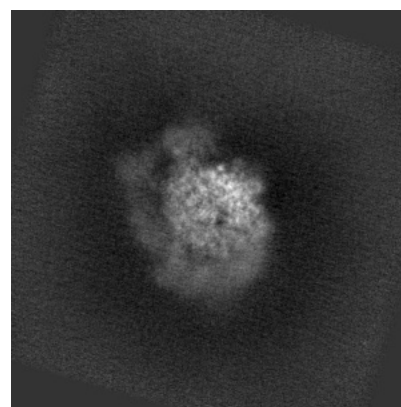
6.1.2 Raw map



X



Y

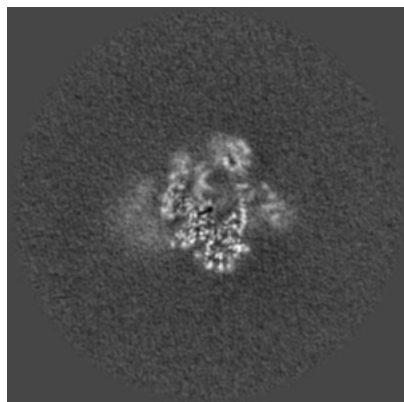


Z

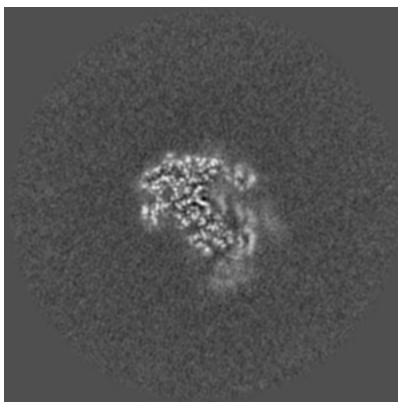
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

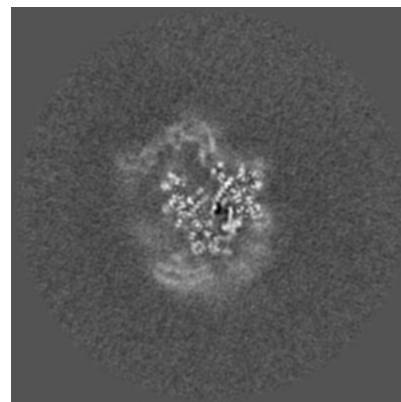
6.2.1 Primary map



X Index: 256

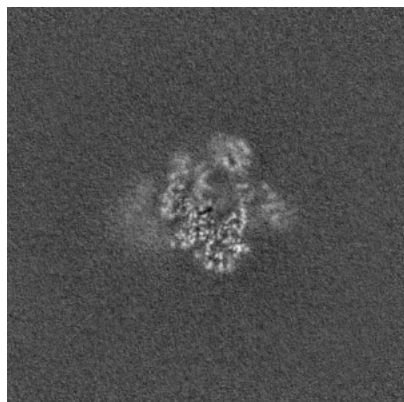


Y Index: 256

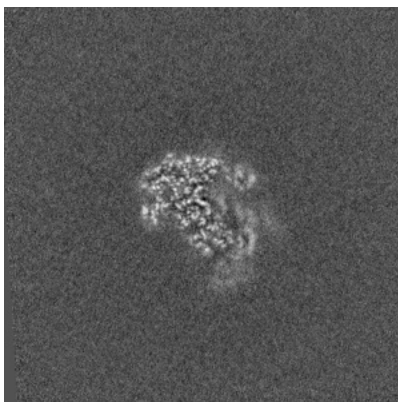


Z Index: 256

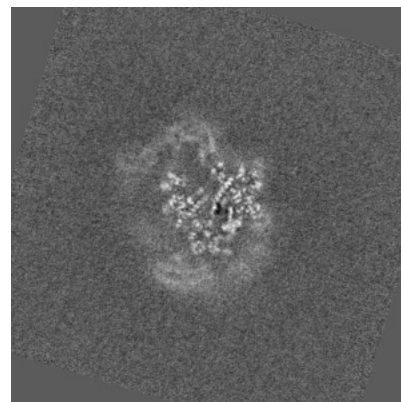
6.2.2 Raw map



X Index: 256



Y Index: 256

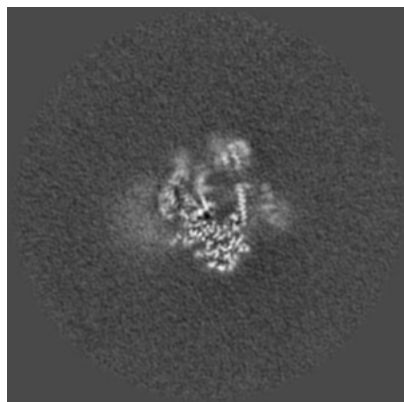


Z Index: 256

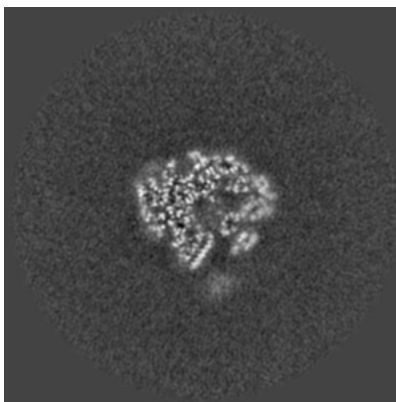
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

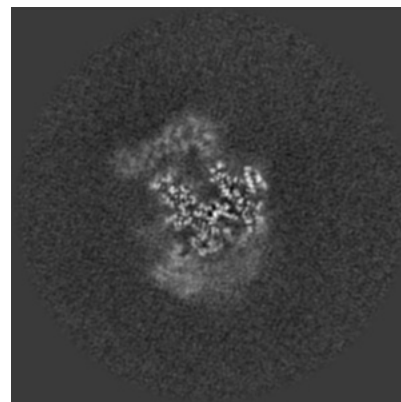
6.3.1 Primary map



X Index: 259



Y Index: 282

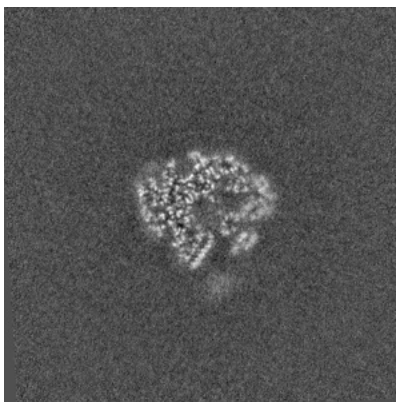


Z Index: 246

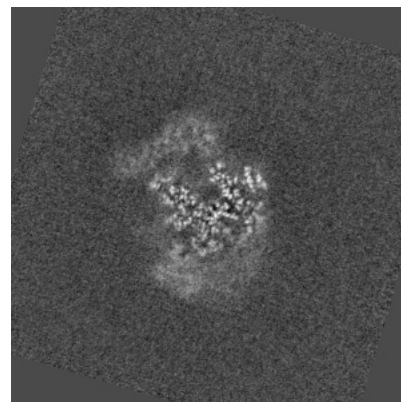
6.3.2 Raw map



X Index: 259



Y Index: 282

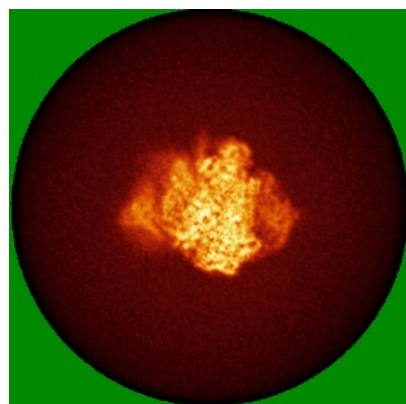


Z Index: 245

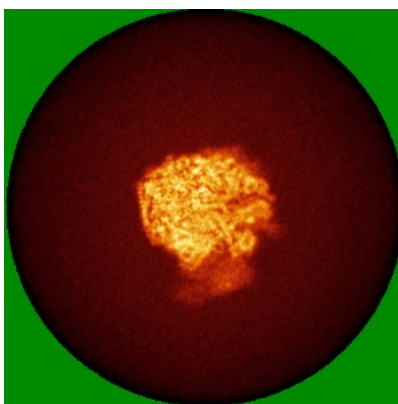
The images above show the largest variance slices of the map in three orthogonal directions.

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

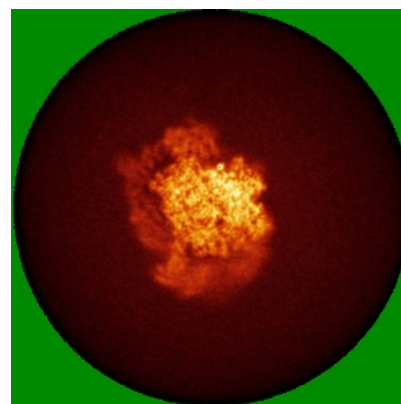
6.4.1 Primary map



X

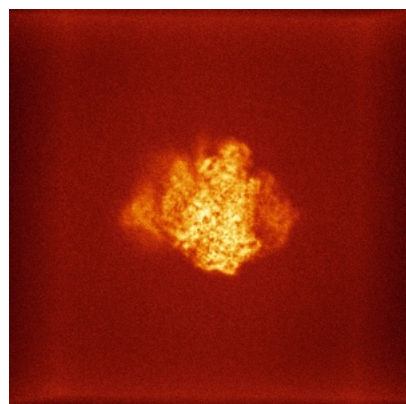


Y

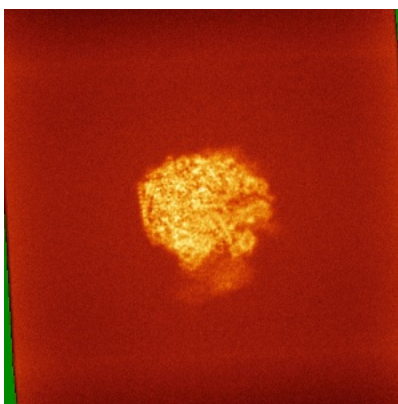


Z

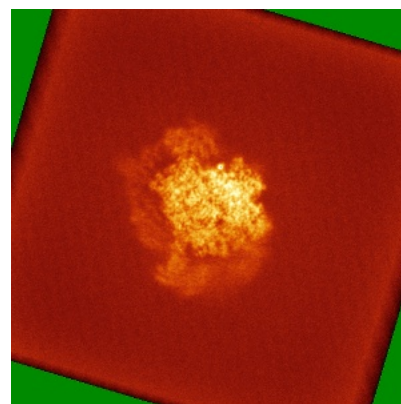
6.4.2 Raw map



X



Y

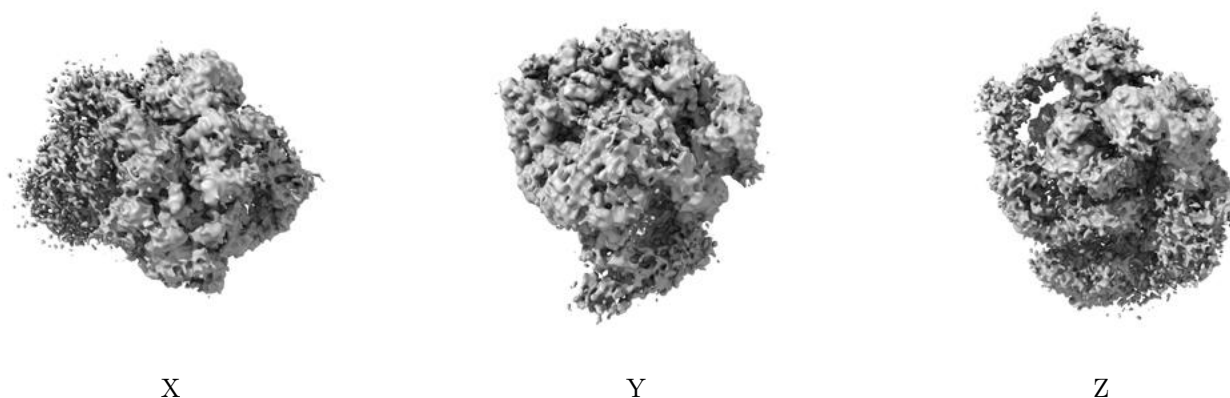


Z

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.

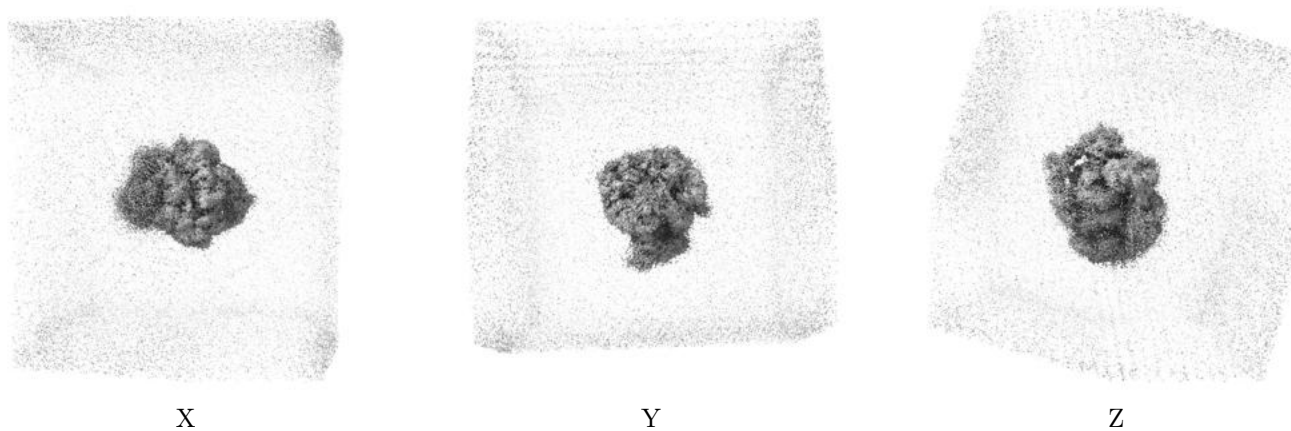
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

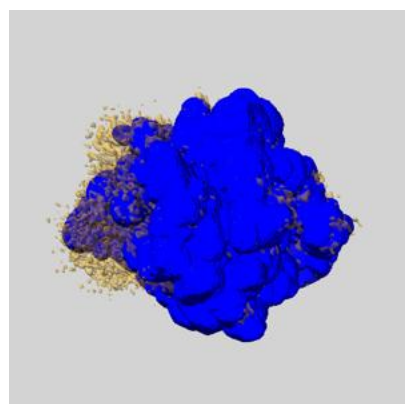
6.6 Mask visualisation [i](#)

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

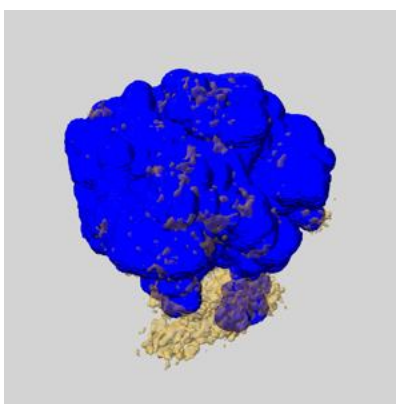
A mask typically either:

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

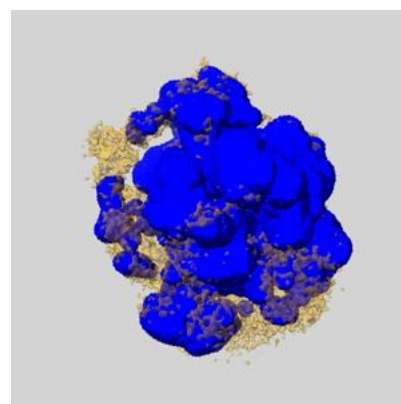
6.6.1 emd_42267_msk_1.map [i](#)



X



Y

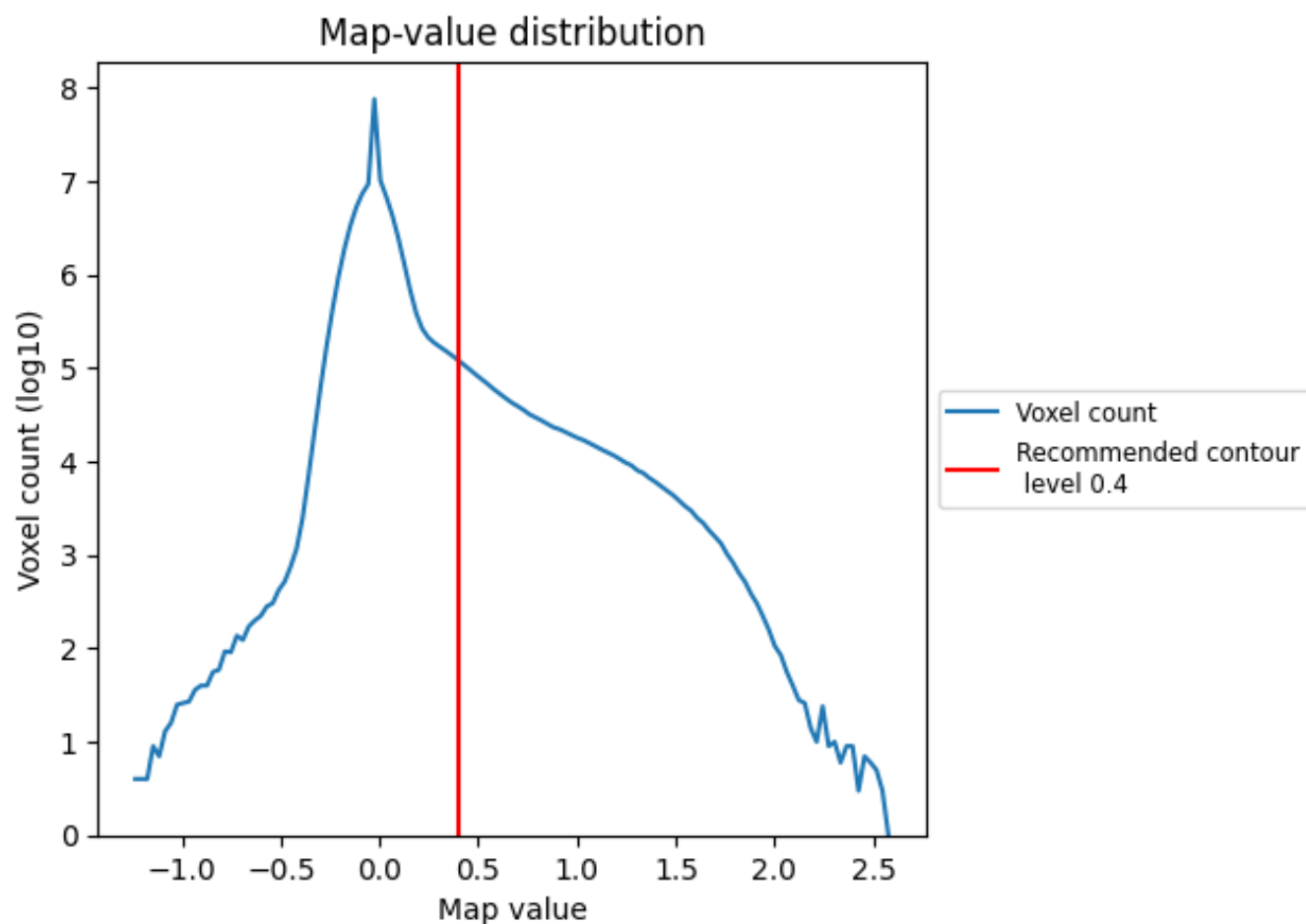


Z

7 Map analysis [i](#)

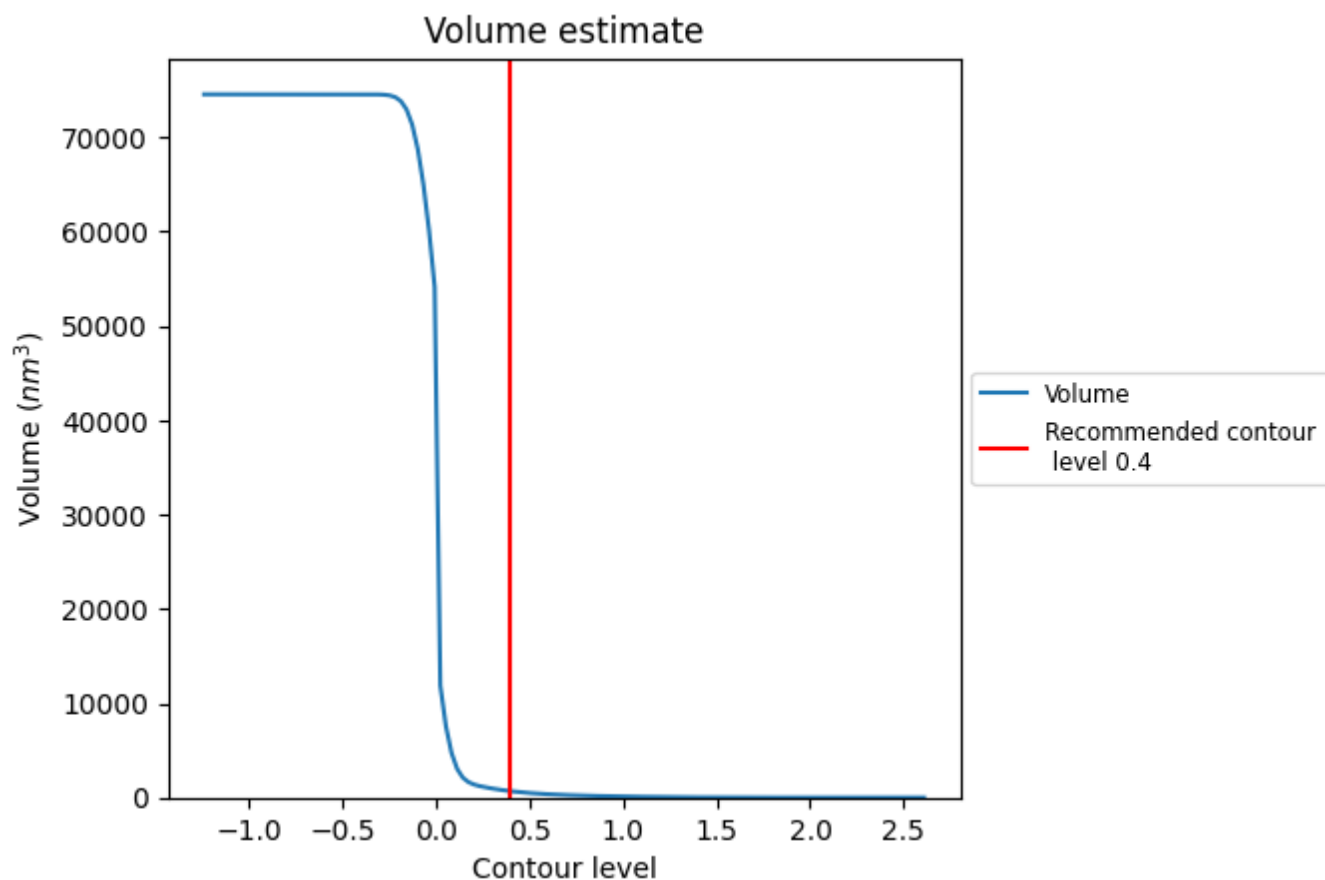
This section contains the results of statistical analysis of the map.

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.

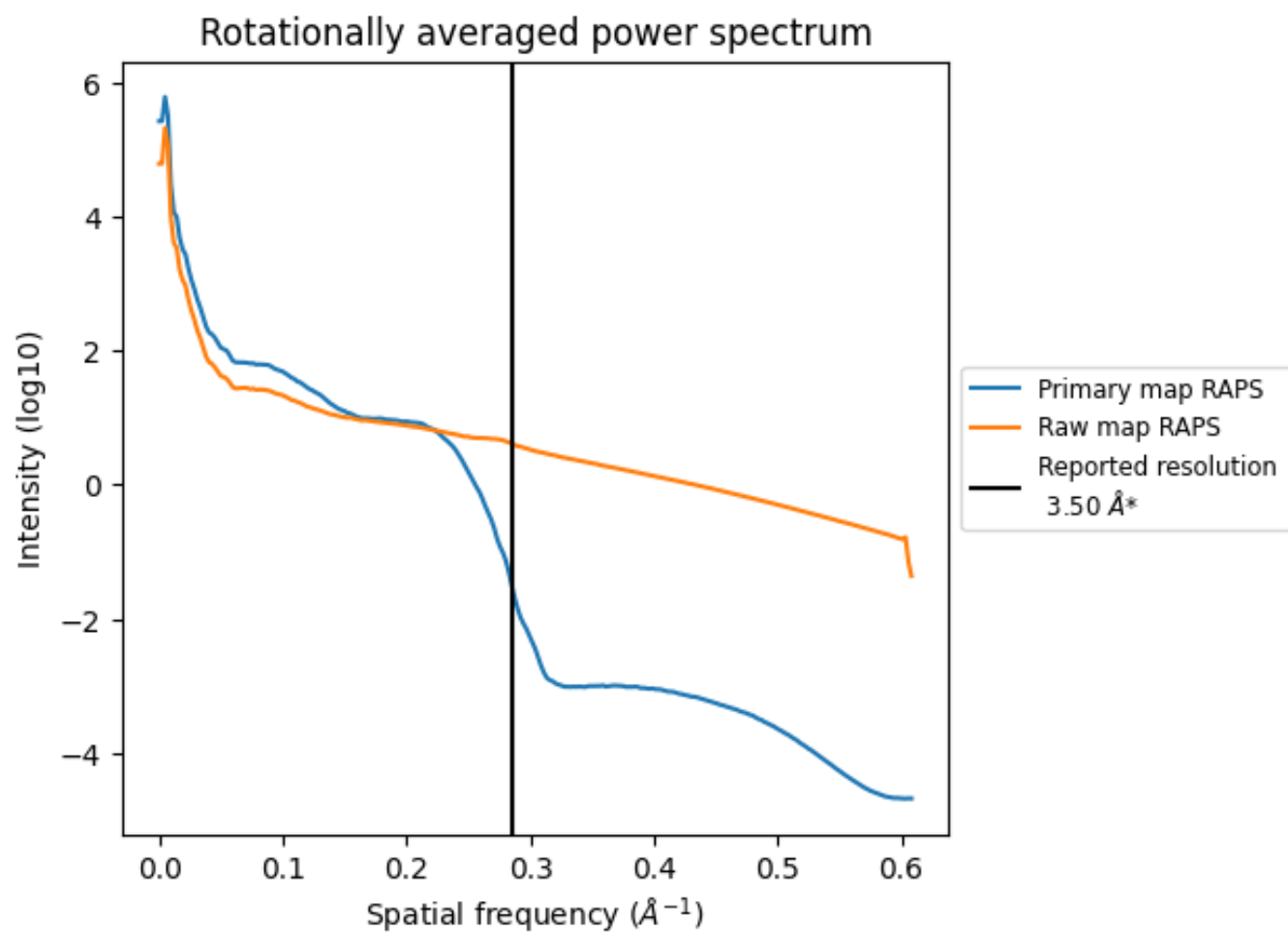
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 680 nm³; this corresponds to an approximate mass of 615 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 ⓘ

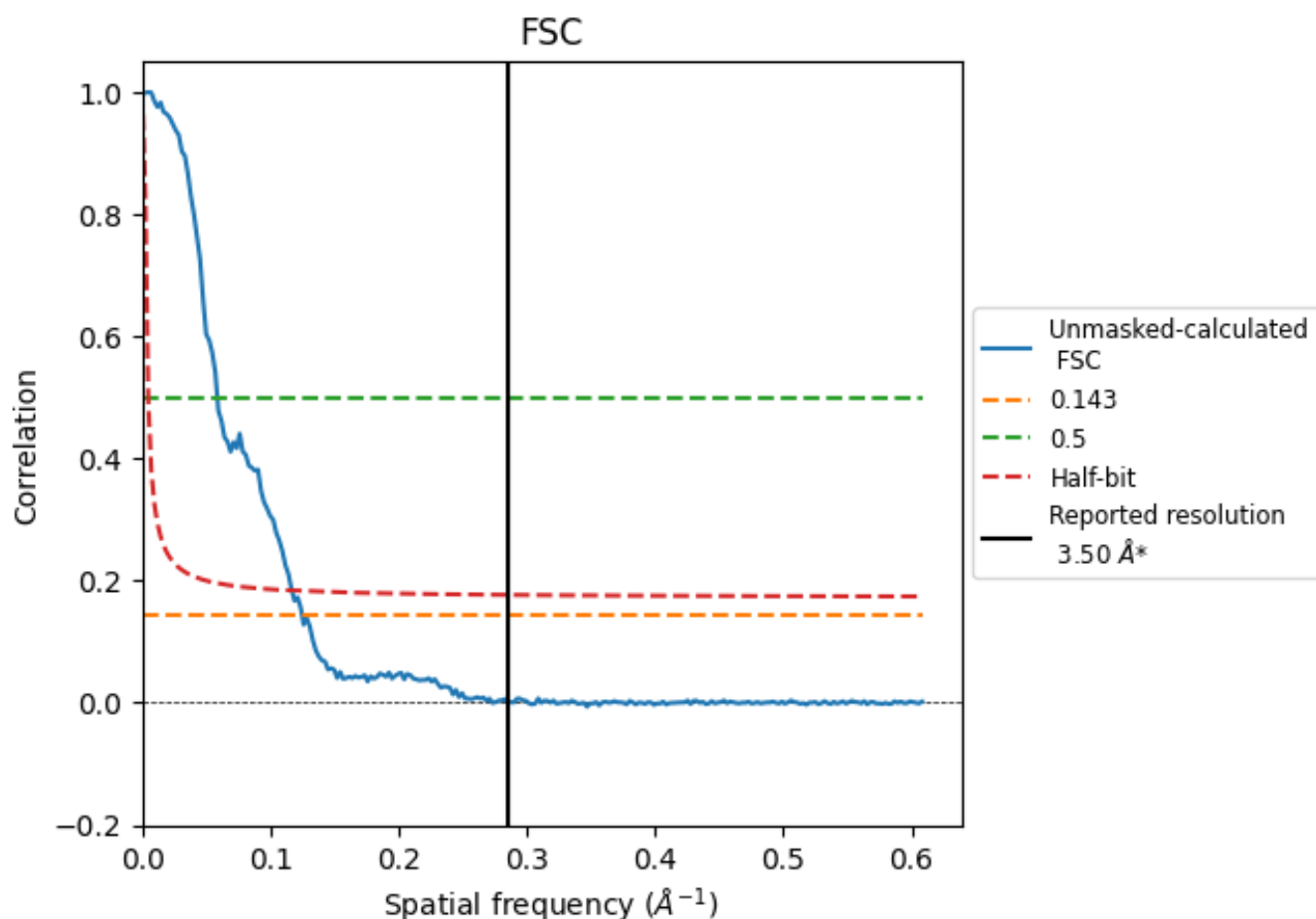


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

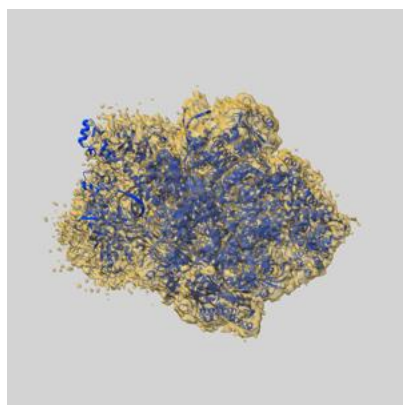
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.03	17.06	8.57

*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 8.03 differs from the reported value 3.5 by more than 10 %

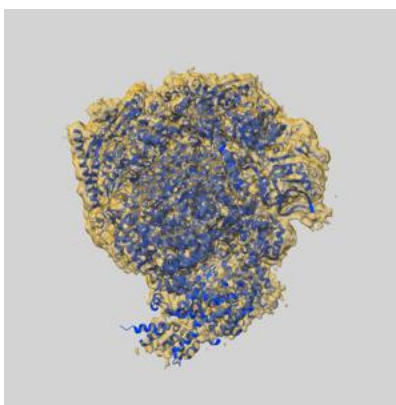
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42267 and PDB model 8UHA. Per-residue inclusion information can be found in section [3](#) on page [8](#).

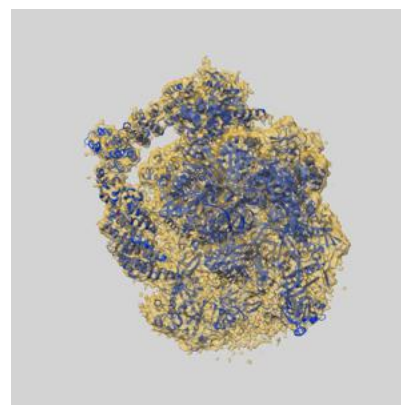
9.1 Map-model overlay [i](#)



X



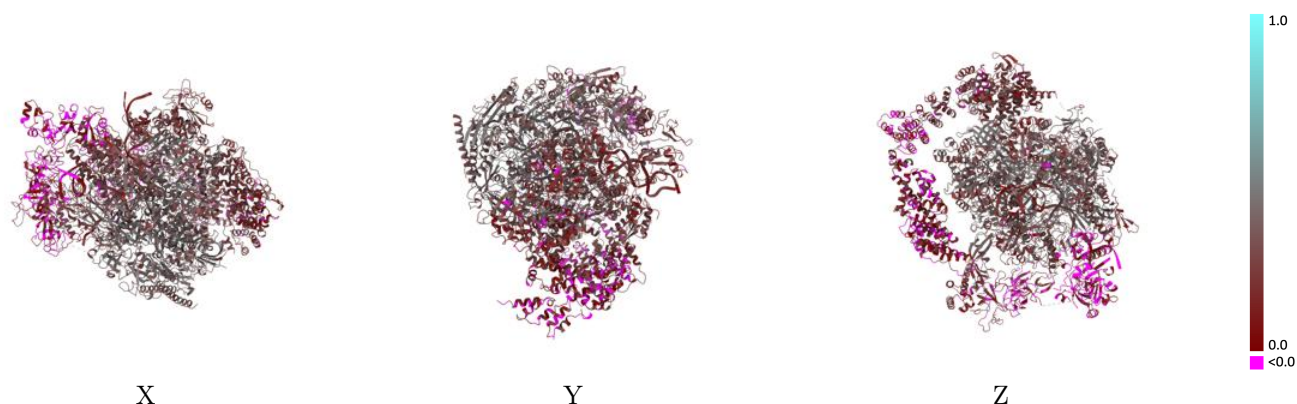
Y



Z

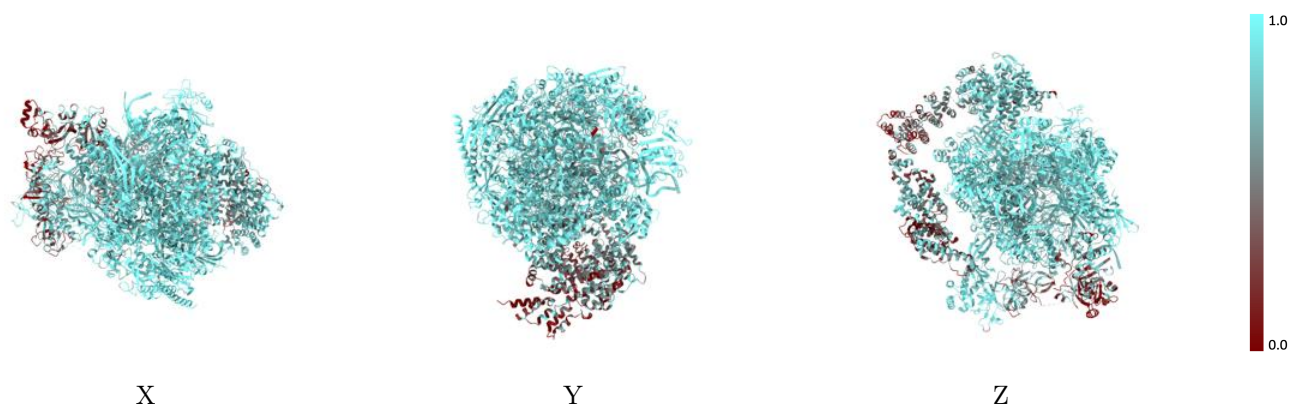
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



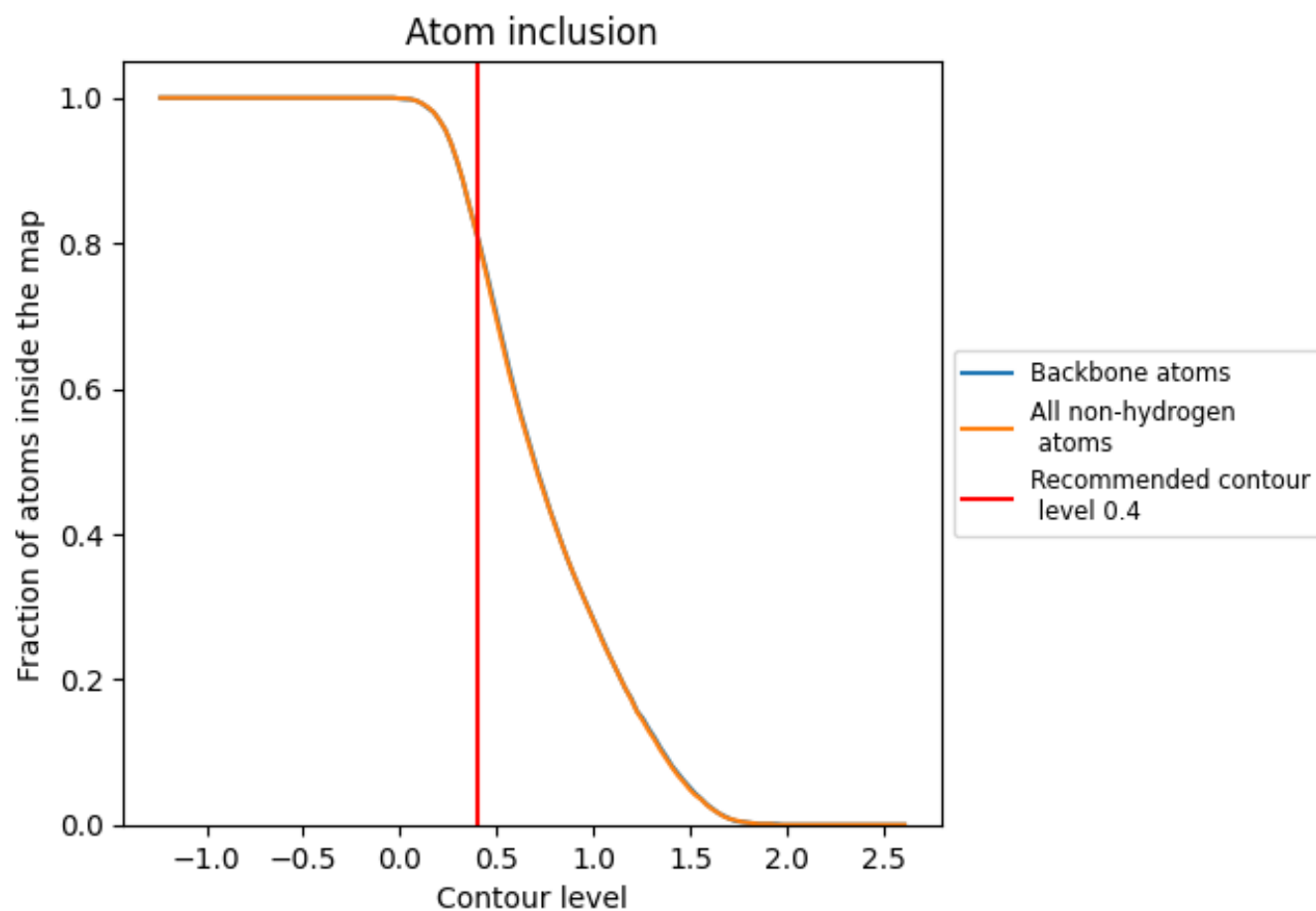
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.2780
A	 0.9100	 0.3530
B	 0.9230	 0.3730
C	 0.9610	 0.4020
D	 0.9220	 0.1800
E	 0.9370	 0.3400
F	 0.9400	 0.3890
G	 0.9450	 0.2350
H	 0.9610	 0.3820
I	 0.9600	 0.3400
J	 0.9560	 0.4040
K	 0.9530	 0.3920
L	 0.9610	 0.3730
N	 0.8350	 0.1350
P	 0.9270	 0.2830
T	 0.8590	 0.1770
U	 0.7790	 0.2070
V	 0.4500	 0.0920
W	 0.6740	 0.1990
X	 0.6120	 0.1050
Y	 0.3130	 0.0170
Z	 0.5270	 0.0910

