



Full wwPDB EM Validation Report ⓘ

Mar 14, 2024 – 05:10 PM EDT

PDB ID : 8UHA
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:

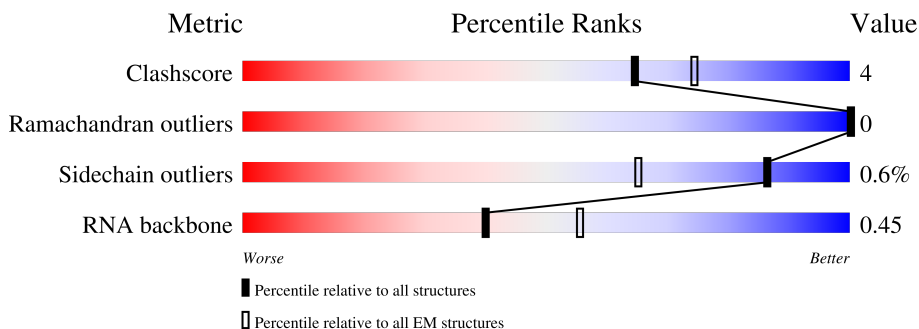
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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% (poor fit), 96%
3	Z	1087	17% (poor fit), 39%, 57%
4	W	590	14% (poor fit), 77%, 12%, 10%
5	P	17	41%, 24%, 18%, 6%, 12%
6	V	580	44% (poor fit), 82%, 13%, 5%
7	A	1970	63%, 9%, 28%

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Mol	Chain	Length	Quality of chain
8	B	1174	 86% 11%
9	C	271	 85% 9% 6%
10	D	142	 73% 16% 11%
11	E	210	 87% 11%
12	F	127	 54% 7% 39%
13	G	172	 85% 15%
14	H	150	 91% 8%
15	I	125	 78% 14% 9%
16	J	67	 84% 13%
17	K	117	 92% 6%
18	L	58	 67% 9% 24%
19	N	50	 46% 10% 44%
20	T	50	 66% 10% 24%
21	U	528	 34% 63%

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 94684 atoms, of which 47123 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
			Total	C	H	N	O		
1	X	12	218	68	115	19	16	0	0

- Molecule 2 is a protein called Transcription elongation factor SPT4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	Z	471	7617	2404	3839	664	693	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	W	530	8432	2699	4215	704	790	24	0	0

- Molecule 5 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
5	P	15	475	141	159	50	110	15	0	0

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	A	1417	22591	7064	11364	2008	2084	71	0	0

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	C	255	4041	1285	1997	349	404	6	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	I	114	1793	571	865	166	180	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	J	65	1051	334	536	87	88	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	L	44	753	231	380	72	64	6	0	0

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

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

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

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

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

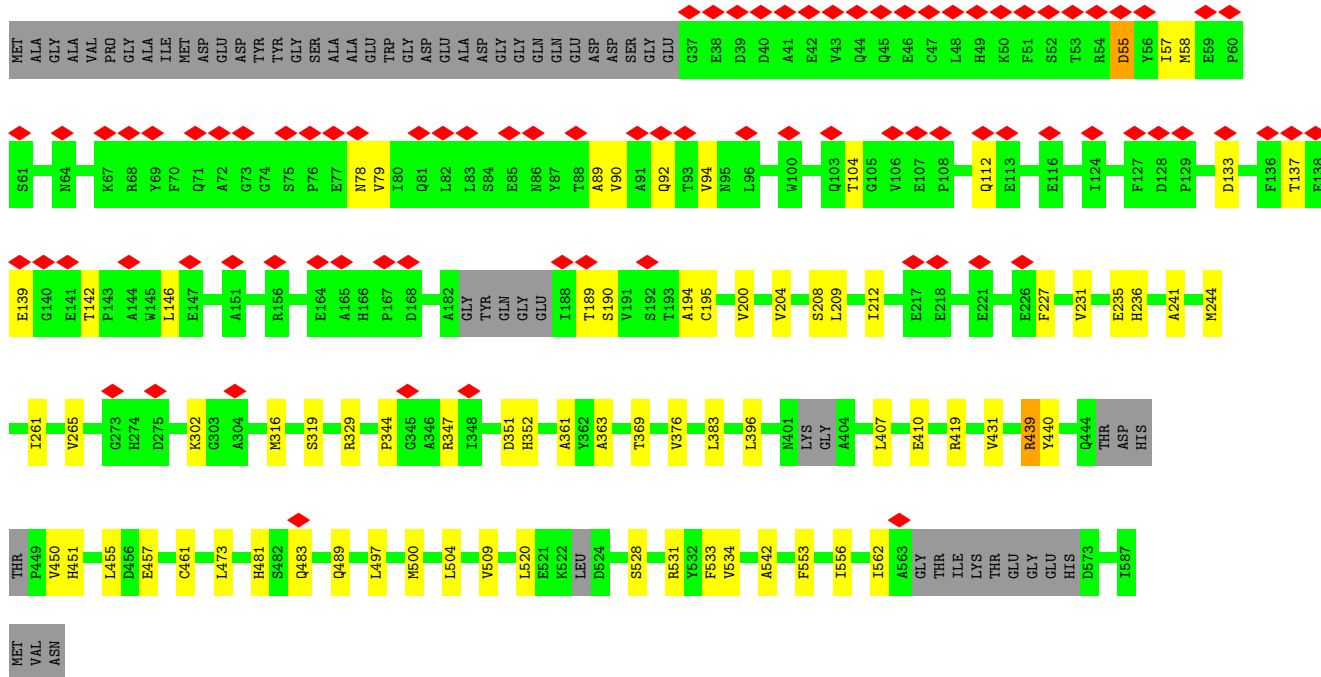
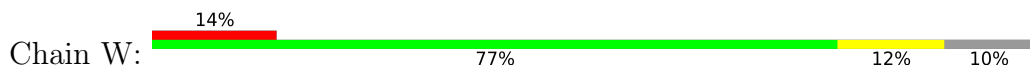
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	196	3054	953	1556	253	284	8	0	0

- Molecule 22 is ZINC ION (three-letter code: 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 (three-letter code: MG) (formula: Mg).

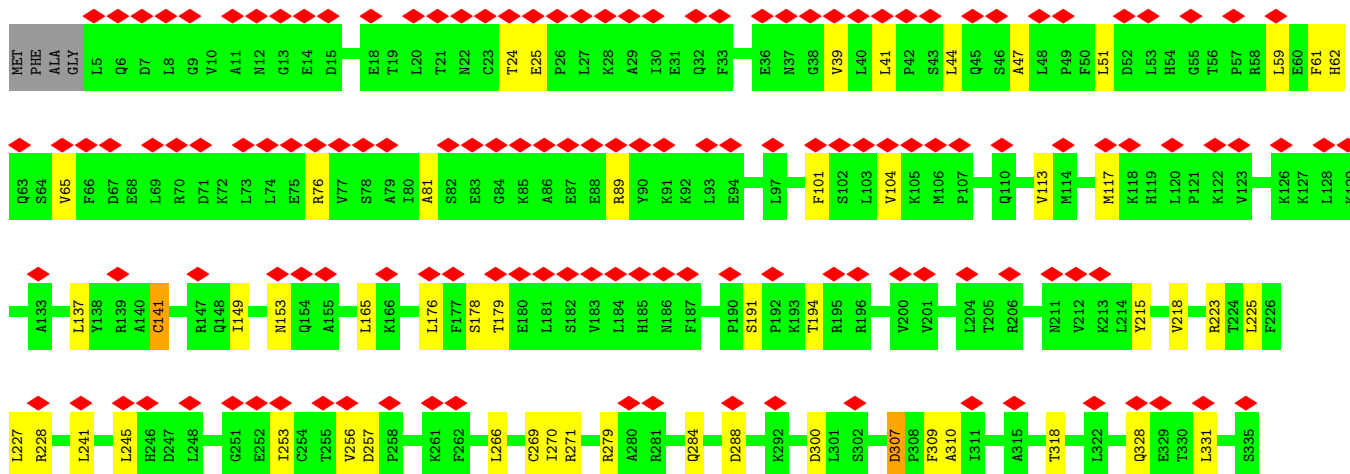
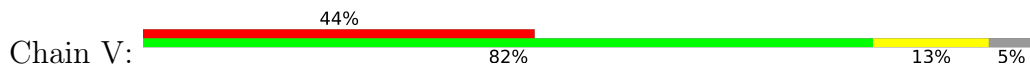
Mol	Chain	Residues	Atoms		AltConf
23	P	1	Total	Mg	0
			1	1	

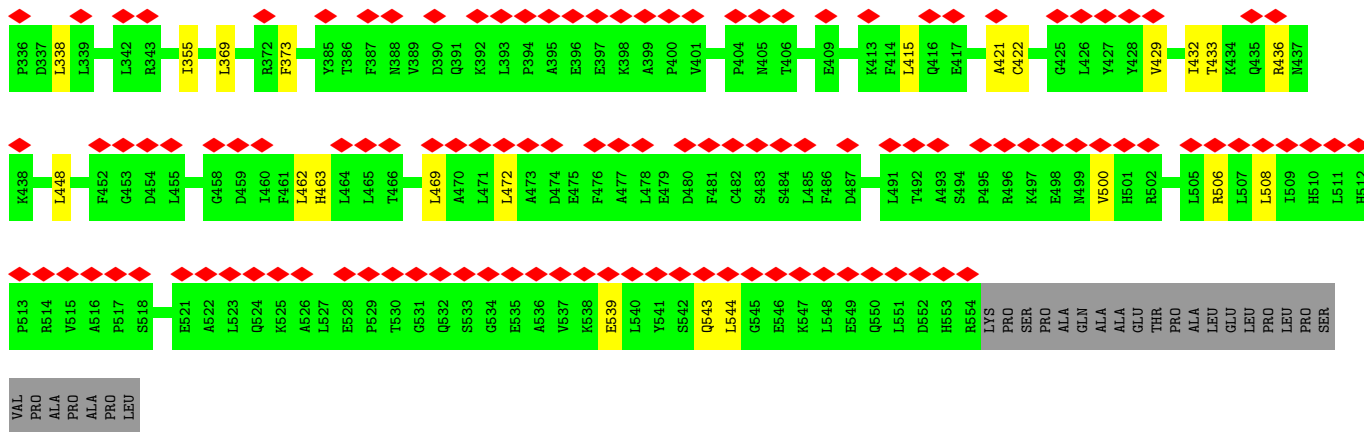


• Molecule 5: RNA

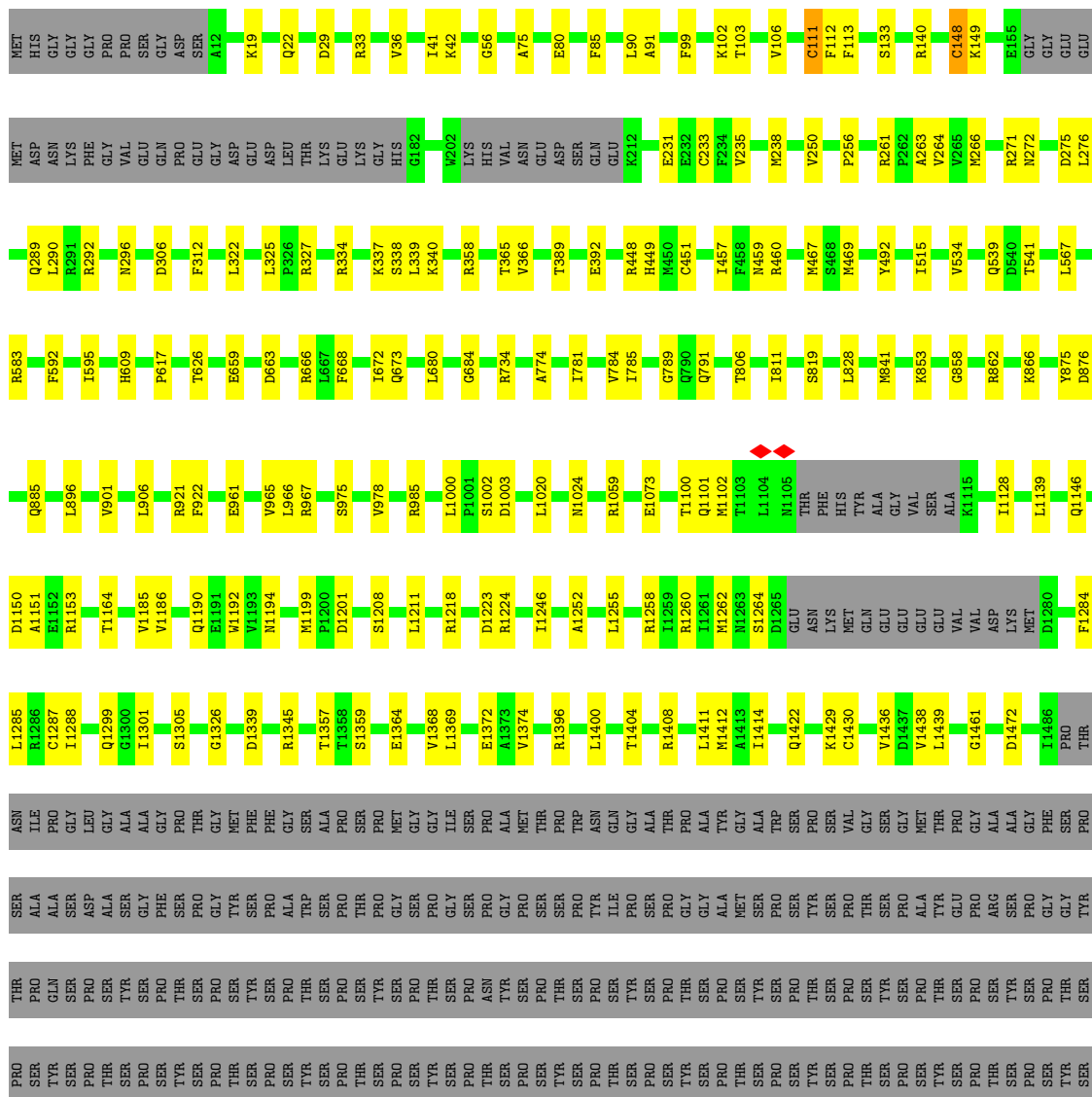


• Molecule 6: Negative elongation factor B





• Molecule 7: DNA-directed RNA polymerase subunit

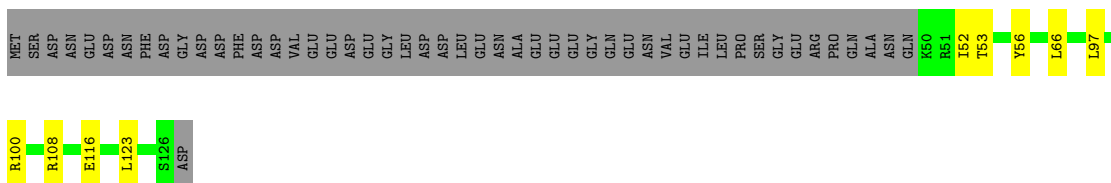


GLN
TYR


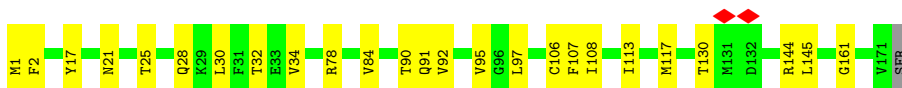
- Molecule 11: DNA-directed RNA polymerase II subunit E

Chain E:  87% 11%

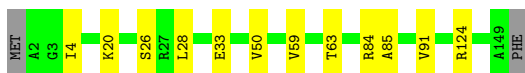
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  54% 7% 39%

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

Chain G:  85% 15%

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

Chain H:  91% 8%

- 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

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 i

5.1 Standard geometry i

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	0.59	0/103	1.14	0/132
2	Y	0.31	0/927	0.61	0/1250
3	Z	0.29	0/3841	0.61	0/5167
4	W	0.31	0/4302	0.56	0/5835
5	P	0.36	0/351	1.16	2/544 (0.4%)
6	V	0.32	0/4495	0.62	0/6074
7	A	0.29	0/11431	0.63	0/15432
8	B	0.30	0/9257	0.63	0/12493
9	C	0.29	0/2087	0.60	0/2836
10	D	0.32	0/1043	0.61	0/1400
11	E	0.30	0/1727	0.62	0/2329
12	F	0.29	0/628	0.64	0/848
13	G	0.32	0/1382	0.60	0/1874
14	H	0.29	0/1207	0.63	0/1628
15	I	0.30	0/949	0.62	0/1284
16	J	0.32	0/524	0.60	0/707
17	K	0.31	0/939	0.53	0/1271
18	L	0.31	0/378	0.78	0/500
19	N	0.96	0/638	1.15	1/979 (0.1%)
20	T	0.90	1/876 (0.1%)	1.10	0/1350
21	U	0.32	0/1521	0.58	0/2063
All	All	0.34	1/48606 (0.0%)	0.65	3/65996 (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
1	X	0	1
7	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	37	DC	C1'-N1	5.65	1.56	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	6	U	P-O3'-C3'	6.02	126.92	119.70
19	N	38	DG	O4'-C1'-N9	5.35	111.75	108.00
5	P	17	C	C2-N1-C1'	5.24	124.56	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	875	TYR	Peptide
1	X	21	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	103	115	120	2	0
2	Y	911	905	905	2	0
3	Z	3778	3839	3840	26	0
4	W	4217	4215	4221	48	0
5	P	316	159	158	9	0
6	V	4410	4501	4501	50	0
7	A	11227	11364	11362	116	0
8	B	9076	9117	9117	81	0
9	C	2044	1997	1995	21	0
10	D	1030	1016	1016	14	0
11	E	1698	1716	1716	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	618	653	653	5	0
13	G	1351	1358	1358	18	0
14	H	1186	1147	1147	7	0
15	I	928	865	861	12	0
16	J	515	536	535	8	0
17	K	920	942	942	5	0
18	L	373	380	379	3	0
19	N	571	315	317	4	0
20	T	781	427	428	4	0
21	U	1498	1556	1556	19	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	P	1	0	0	0	0
All	All	47561	47123	47127	394	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 (394) 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	1.59	0.83
19:N:36:DC:O2	20:T:15:DG:N2	2.18	0.76
3:Z:199:LYS:NZ	3:Z:240:GLU:O	2.22	0.73
7:A:567:LEU:HD13	7:A:595:ILE:HG22	1.69	0.73
7:A:75:ALA:O	8:B:1131:ARG:NH1	2.23	0.72
8:B:1137:CYS:SG	8:B:1138:ARG:N	2.62	0.72
7:A:1262:MET:SD	7:A:1264:SER:OG	2.49	0.71
7:A:853:LYS:NZ	7:A:1102:MET:O	2.23	0.71
7:A:663:ASP:OD1	7:A:666:ARG:NH2	2.24	0.70
8:B:309:PHE:O	8:B:312:GLN:NE2	2.25	0.70
7:A:1100:THR:OG1	7:A:1101:GLN:OE1	2.09	0.69
7:A:460:ARG:NH1	7:A:492:TYR:O	2.25	0.69
9:C:113:ARG:NH1	9:C:114:HIS:O	2.26	0.69
8:B:794:VAL:HG12	8:B:967:ILE:HG22	1.75	0.69
4:W:419:ARG:NH1	4:W:461:CYS:SG	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:35:ARG:O	18:L:37:ARG:NH1	2.26	0.69
6:V:149:ILE:O	6:V:153:ASN:N	2.27	0.68
7:A:263:ALA:O	7:A:271:ARG:NH1	2.27	0.68
5:P:6:U:O2'	5:P:7:G:O4'	2.11	0.68
7:A:1461:GLY:O	8:B:1104:ARG:NH1	2.27	0.67
8:B:927:ARG:NH2	8:B:1057:ASP:OD1	2.27	0.67
8:B:223:SER:OG	8:B:350:HIS:ND1	2.24	0.67
7:A:1000:LEU:O	7:A:1059:ARG:NH2	2.28	0.66
7:A:734:ARG:NH1	15:I:105:GLU:OE1	2.28	0.66
11:E:53:PRO:O	11:E:54:ARG:NH1	2.28	0.66
4:W:94:VAL:HG11	6:V:65:VAL:HG23	1.77	0.66
3:Z:711:ARG:NE	9:C:92:GLU:OE1	2.30	0.65
8:B:237:VAL:HG21	8:B:369:VAL:HG12	1.77	0.65
10:D:58:SER:OG	10:D:59:GLU:OE1	2.15	0.65
14:H:63:THR:OG1	14:H:84:ARG:NH2	2.30	0.65
7:A:111:CYS:SG	7:A:113:PHE:N	2.71	0.64
7:A:1364:GLU:O	7:A:1368:VAL:HG12	1.98	0.64
7:A:358:ARG:NE	8:B:1076:GLU:OE2	2.31	0.64
7:A:1128:ILE:HB	7:A:1414:ILE:HD13	1.80	0.63
8:B:759:VAL:HG12	8:B:999:ALA:HB2	1.81	0.63
9:C:78:ILE:HG21	9:C:127:VAL:HG13	1.80	0.63
3:Z:736:LEU:HD21	3:Z:743:ILE:HG13	1.81	0.63
3:Z:721:ILE:O	3:Z:737:HIS:ND1	2.31	0.63
7:A:340:LYS:HG3	7:A:1436:VAL:HG21	1.80	0.63
10:D:76:ASN:O	10:D:79:THR:OG1	2.16	0.63
7:A:841:MET:SD	8:B:503:ASN:ND2	2.72	0.62
10:D:110:GLU:OE2	13:G:144:ARG:NH1	2.31	0.62
9:C:7:PRO:O	17:K:104:ARG:NH1	2.32	0.62
4:W:104:THR:HG21	6:V:76:ARG:HG2	1.82	0.62
7:A:1024:ASN:O	11:E:162:ARG:NH2	2.33	0.62
6:V:508:LEU:HB3	6:V:544:LEU:HD21	1.82	0.62
4:W:504:LEU:HG	4:W:509:VAL:HG12	1.81	0.62
8:B:274:ARG:NH2	8:B:281:ASP:OD1	2.33	0.62
10:D:96:GLU:OE2	10:D:121:ARG:NH1	2.33	0.61
19:N:26:DC:N4	20:T:24:DG:O6	2.32	0.61
3:Z:430:GLU:OE1	3:Z:430:GLU:N	2.33	0.61
7:A:609:HIS:ND1	7:A:626:THR:OG1	2.34	0.61
5:P:10:A:O2'	7:A:334:ARG:NH1	2.34	0.61
7:A:1218:ARG:NH2	7:A:1252:ALA:O	2.34	0.61
8:B:585:ASN:OD1	8:B:588:ARG:NH2	2.34	0.61
8:B:380:ARG:NH1	8:B:381:GLU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:536:SER:OG	8:B:616:THR:OG1	2.17	0.60
2:Y:81:LYS:O	2:Y:85:TYR:OH	2.11	0.60
8:B:1057:ASP:O	8:B:1080:ARG:NH1	2.34	0.60
7:A:467:MET:SD	7:A:467:MET:N	2.75	0.60
4:W:209:LEU:HD11	21:U:124:LEU:HD13	1.84	0.60
4:W:528:SER:OG	7:A:1151:ALA:N	2.35	0.60
6:V:328:GLN:O	6:V:328:GLN:NE2	2.35	0.60
12:F:100:ARG:NH2	12:F:123:LEU:O	2.34	0.60
15:I:68:ILE:O	15:I:122:ARG:NH1	2.35	0.60
4:W:133:ASP:O	4:W:137:THR:HG23	2.02	0.59
8:B:65:ILE:HD11	8:B:412:LEU:HG	1.84	0.59
6:V:270:ILE:HD11	6:V:309:PHE:HB2	1.84	0.59
6:V:462:LEU:HD11	6:V:500:VAL:HG22	1.84	0.59
8:B:861:SER:OG	8:B:863:ASP:OD1	2.20	0.59
10:D:72:SER:O	10:D:75:LYS:NZ	2.36	0.58
15:I:86:CYS:SG	15:I:87:GLN:N	2.76	0.58
16:J:19:GLU:OE1	16:J:19:GLU:N	2.34	0.58
8:B:565:THR:HG21	8:B:580:PRO:HG3	1.86	0.58
8:B:825:GLN:NE2	8:B:872:THR:O	2.36	0.58
3:Z:354:SER:HA	3:Z:359:LEU:HD23	1.86	0.58
7:A:1430:CYS:SG	7:A:1439:LEU:HD21	2.43	0.58
6:V:176:LEU:O	6:V:463:HIS:ND1	2.36	0.57
4:W:316:MET:O	4:W:319:SER:OG	2.21	0.57
7:A:1208:SER:O	7:A:1260:ARG:NH1	2.37	0.57
4:W:142:THR:HG21	4:W:146:LEU:HD23	1.86	0.57
8:B:125:TYR:OH	21:U:262:LEU:HD22	2.04	0.57
6:V:61:PHE:O	6:V:65:VAL:HG22	2.04	0.57
9:C:78:ILE:HG21	9:C:127:VAL:CG1	2.35	0.57
7:A:906:LEU:N	7:A:975:SER:OG	2.37	0.57
7:A:1218:ARG:HE	7:A:1255:LEU:HD21	1.70	0.57
21:U:54:LEU:HD21	21:U:89:TRP:HB3	1.87	0.57
4:W:261:ILE:O	4:W:265:VAL:HG23	2.05	0.56
9:C:45:ILE:HG22	9:C:165:ALA:HB1	1.87	0.56
7:A:469:MET:SD	8:B:1094:GLN:NE2	2.78	0.56
7:A:811:ILE:HD12	15:I:79:PRO:HB3	1.88	0.56
2:Y:94:PRO:HD2	2:Y:97:ILE:HD12	1.87	0.56
9:C:10:ARG:NH2	9:C:24:GLU:OE2	2.39	0.56
3:Z:736:LEU:HD21	3:Z:743:ILE:CG1	2.36	0.56
4:W:244:MET:SD	21:U:120:ILE:HG21	2.46	0.56
5:P:9:C:O2'	7:A:337:LYS:NZ	2.39	0.56
8:B:912:ASN:OD1	8:B:916:TYR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:307:ASP:OD2	6:V:310:ALA:N	2.38	0.56
4:W:112:GLN:NE2	6:V:41:LEU:HD22	2.21	0.55
8:B:643:LEU:HD11	8:B:656:LEU:HD11	1.89	0.55
7:A:289:GLN:NE2	7:A:306:ASP:OD2	2.40	0.55
7:A:312:PHE:CE1	7:A:325:LEU:HD22	2.42	0.55
7:A:668:PHE:CZ	7:A:672:ILE:HD11	2.40	0.55
6:V:39:VAL:HG12	6:V:41:LEU:HD12	1.88	0.55
7:A:389:THR:HG22	7:A:449:HIS:HA	1.89	0.55
12:F:52:ILE:N	12:F:116:GLU:OE2	2.39	0.55
5:P:10:A:OP1	7:A:337:LYS:NZ	2.37	0.55
8:B:953:ASP:OD1	9:C:36:ARG:NH2	2.40	0.55
11:E:118:LEU:HD22	11:E:127:LEU:HB3	1.89	0.55
7:A:1368:VAL:HG13	7:A:1369:LEU:HD23	1.89	0.54
7:A:1400:LEU:O	7:A:1404:THR:HG23	2.07	0.54
9:C:9:VAL:HG11	17:K:105:PHE:HD1	1.72	0.54
8:B:964:ASP:OD1	16:J:9:THR:OG1	2.18	0.54
6:V:269:CYS:SG	6:V:279:ARG:NE	2.78	0.54
6:V:369:LEU:HD12	6:V:373:PHE:HB3	1.90	0.54
4:W:94:VAL:CG1	6:V:65:VAL:HG23	2.37	0.53
9:C:50:VAL:O	18:L:55:PHE:N	2.40	0.53
13:G:117:MET:SD	13:G:130:THR:OG1	2.65	0.53
6:V:433:THR:HG23	6:V:472:LEU:HD11	1.91	0.53
8:B:741:HIS:O	8:B:922:ARG:NH2	2.40	0.53
13:G:1:MET:N	13:G:78:ARG:O	2.42	0.53
19:N:27:DC:N4	20:T:23:DG:O6	2.41	0.53
7:A:256:PRO:O	7:A:261:ARG:NH2	2.42	0.53
7:A:1429:LYS:HG3	7:A:1438:VAL:HG11	1.90	0.53
8:B:872:THR:OG1	8:B:889:LYS:NZ	2.41	0.53
8:B:118:LEU:O	8:B:189:GLY:N	2.42	0.53
7:A:906:LEU:HD13	7:A:966:LEU:HD13	1.91	0.53
12:F:53:THR:OG1	12:F:116:GLU:OE1	2.12	0.53
4:W:440:TYR:HH	4:W:451:HIS:HD1	1.55	0.52
13:G:1:MET:SD	13:G:2:PHE:N	2.80	0.52
7:A:734:ARG:NE	15:I:108:MET:SD	2.81	0.52
13:G:106:CYS:SG	13:G:107:PHE:N	2.82	0.52
7:A:1223:ASP:OD2	7:A:1224:ARG:NH1	2.42	0.52
3:Z:450:ILE:HG21	3:Z:468:LEU:HD11	1.91	0.52
7:A:1146:GLN:O	7:A:1150:ASP:N	2.41	0.52
8:B:159:THR:HG23	8:B:160:TYR:CD1	2.45	0.52
8:B:992:ASN:O	16:J:46:ARG:NH1	2.42	0.52
9:C:9:VAL:HG11	17:K:105:PHE:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:183:ALA:HB3	9:C:232:ASN:HB3	1.92	0.52
7:A:1305:SER:OG	7:A:1339:ASP:OD2	2.16	0.52
8:B:761:THR:HG23	8:B:1000:THR:HA	1.91	0.52
6:V:369:LEU:HD13	6:V:421:ALA:HB2	1.90	0.52
3:Z:554:GLU:OE1	3:Z:557:THR:OG1	2.28	0.51
4:W:236:HIS:HB3	21:U:54:LEU:HD22	1.92	0.51
7:A:1412:MET:SD	7:A:1422:GLN:NE2	2.83	0.51
3:Z:705:LEU:HG	3:Z:724:VAL:HG21	1.92	0.51
7:A:1301:ILE:HD13	7:A:1345:ARG:HB3	1.92	0.51
4:W:396:LEU:HD22	4:W:410:GLU:HG3	1.92	0.51
7:A:231:GLU:O	7:A:235:VAL:HG23	2.10	0.51
7:A:1190:GLN:NE2	7:A:1194:ASN:OD1	2.44	0.51
21:U:17:LEU:O	21:U:55:LYS:NZ	2.40	0.51
6:V:432:ILE:O	6:V:436:ARG:N	2.42	0.51
7:A:668:PHE:CE1	7:A:672:ILE:HD11	2.45	0.51
14:H:85:ALA:HB1	14:H:91:VAL:HG21	1.92	0.51
6:V:179:THR:HG23	6:V:506:ARG:HB2	1.93	0.51
7:A:467:MET:HG2	7:A:534:VAL:HG11	1.91	0.51
10:D:55:GLN:HB2	13:G:32:THR:HG22	1.93	0.51
6:V:24:THR:OG1	6:V:25:GLU:OE2	2.28	0.51
8:B:1068:GLN:N	8:B:1073:GLN:O	2.40	0.51
7:A:292:ARG:O	7:A:296:ASN:N	2.43	0.51
8:B:388:TYR:HE2	8:B:621:ILE:HG21	1.76	0.51
7:A:1372:GLU:HG3	11:E:193:ILE:HD13	1.91	0.51
12:F:66:LEU:HD21	12:F:97:LEU:HD22	1.93	0.51
7:A:33:ARG:O	8:B:1138:ARG:NH1	2.43	0.51
8:B:48:ASP:OD1	8:B:158:SER:OG	2.29	0.50
8:B:127:ASP:OD2	8:B:145:GLN:NE2	2.45	0.50
8:B:1040:GLN:NE2	9:C:196:VAL:O	2.45	0.50
19:N:12:DC:N4	20:T:38:DG:O6	2.45	0.50
4:W:200:VAL:O	4:W:204:VAL:HG23	2.11	0.50
7:A:457:ILE:HD11	7:A:515:ILE:HD12	1.92	0.50
8:B:803:ARG:NH1	16:J:8:PHE:O	2.45	0.50
11:E:93:ARG:NH2	11:E:97:GLU:OE2	2.44	0.50
5:P:8:G:H1'	7:A:264:VAL:HG21	1.92	0.50
7:A:617:PRO:O	14:H:124:ARG:NH1	2.45	0.50
8:B:1162:LEU:HD12	8:B:1167:ILE:HG21	1.94	0.50
10:D:34:ASN:OD1	10:D:102:ASN:ND2	2.45	0.50
11:E:134:GLU:OE2	11:E:181:ARG:NH2	2.43	0.50
7:A:885:GLN:OE1	7:A:1408:ARG:NH2	2.45	0.50
13:G:28:GLN:O	13:G:32:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:223:ARG:NH2	6:V:300:ASP:OD1	2.45	0.50
7:A:111:CYS:SG	7:A:112:PHE:N	2.84	0.50
7:A:592:PHE:CE2	7:A:595:ILE:HD11	2.47	0.50
10:D:33:LEU:O	10:D:37:VAL:HG23	2.12	0.50
3:Z:432:GLU:OE1	3:Z:432:GLU:N	2.44	0.49
3:Z:719:GLY:O	9:C:49:TRP:NE1	2.45	0.49
14:H:20:LYS:NZ	14:H:26:SER:OG	2.45	0.49
4:W:457:GLU:OE1	21:U:175:ARG:NE	2.46	0.49
7:A:366:VAL:HG11	8:B:1055:VAL:HG12	1.94	0.49
4:W:329:ARG:NE	4:W:363:ALA:O	2.41	0.49
15:I:109:ARG:NE	15:I:124:THR:OG1	2.43	0.49
8:B:119:THR:HG23	8:B:187:ILE:HD13	1.94	0.49
8:B:1091:ARG:HG3	8:B:1103:LEU:HD11	1.94	0.49
4:W:407:LEU:CD1	4:W:450:VAL:HG21	2.42	0.49
4:W:520:LEU:HD22	4:W:556:ILE:HG13	1.94	0.49
7:A:539:GLN:HA	7:A:774:ALA:HB1	1.93	0.49
13:G:145:LEU:HD13	13:G:161:GLY:HA2	1.94	0.49
7:A:459:ASN:OD1	7:A:460:ARG:N	2.44	0.49
8:B:254:GLN:OE1	8:B:254:GLN:N	2.43	0.49
4:W:481:HIS:O	4:W:489:GLN:NE2	2.46	0.49
7:A:659:GLU:OE2	7:A:985:ARG:NH2	2.45	0.49
6:V:271:ARG:NH1	11:E:67:ASP:OD1	2.46	0.49
3:Z:462:GLU:N	3:Z:462:GLU:OE1	2.45	0.48
7:A:322:LEU:O	7:A:327:ARG:NH2	2.47	0.48
7:A:967:ARG:NH2	7:A:1326:GLY:O	2.47	0.48
3:Z:416:ARG:NH1	3:Z:417:GLU:O	2.47	0.48
7:A:583:ARG:NH1	9:C:222:PRO:O	2.43	0.48
3:Z:424:ASP:HB2	3:Z:440:ILE:HD12	1.95	0.48
9:C:193:ARG:NH2	9:C:218:ALA:O	2.46	0.48
4:W:562:ILE:HD11	7:A:1153:ARG:HH11	1.78	0.48
6:V:191:SER:O	6:V:194:THR:OG1	2.21	0.48
4:W:344:PRO:O	4:W:347:ARG:NH1	2.45	0.48
11:E:83:GLY:O	11:E:86:THR:OG1	2.29	0.48
9:C:234:GLU:OE1	16:J:42:ARG:NH2	2.47	0.47
3:Z:427:GLU:OE2	3:Z:469:ARG:NH2	2.46	0.47
6:V:245:LEU:HD13	6:V:253:ILE:HG21	1.95	0.47
8:B:771:GLU:OE1	8:B:771:GLU:N	2.48	0.47
4:W:369:THR:O	4:W:376:VAL:N	2.45	0.47
7:A:90:LEU:HD11	7:A:250:VAL:HG12	1.96	0.47
7:A:1101:GLN:OE1	7:A:1101:GLN:N	2.47	0.47
17:K:12:LEU:HD11	17:K:18:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:783:ALA:HB2	8:B:1041:ILE:HG23	1.96	0.47
13:G:145:LEU:HD13	13:G:161:GLY:CA	2.44	0.47
3:Z:248:GLY:O	3:Z:252:GLN:NE2	2.47	0.47
3:Z:365:ARG:HG3	3:Z:372:LEU:HD22	1.96	0.47
6:V:191:SER:N	6:V:194:THR:OG1	2.48	0.47
6:V:215:TYR:OH	6:V:257:ASP:OD2	2.24	0.47
7:A:99:PHE:O	7:A:103:THR:OG1	2.22	0.47
7:A:1368:VAL:HG13	7:A:1369:LEU:CD2	2.44	0.47
8:B:663:GLU:OE2	8:B:695:HIS:NE2	2.45	0.47
1:X:24:LYS:O	1:X:24:LYS:NZ	2.38	0.47
10:D:87:LEU:HD11	10:D:101:ALA:HB2	1.97	0.47
21:U:117:VAL:HA	21:U:120:ILE:HD12	1.96	0.47
7:A:29:ASP:OD2	7:A:33:ARG:NH2	2.47	0.46
8:B:55:VAL:O	8:B:59:VAL:HG23	2.16	0.46
8:B:852:GLY:O	8:B:868:GLY:N	2.45	0.46
14:H:33:GLU:O	21:U:12:TRP:NE1	2.45	0.46
6:V:178:SER:O	6:V:506:ARG:NH2	2.47	0.46
8:B:906:GLN:OE1	8:B:922:ARG:NH2	2.48	0.46
9:C:154:ARG:NH1	16:J:62:TYR:O	2.48	0.46
8:B:56:GLN:NE2	8:B:60:GLU:OE2	2.48	0.46
8:B:607:ILE:HD12	15:I:75:ASP:CG	2.36	0.46
13:G:17:TYR:HB3	13:G:25:THR:HG21	1.97	0.46
7:A:102:LYS:O	7:A:106:VAL:HG23	2.14	0.46
6:V:429:VAL:HG21	6:V:448:LEU:HD11	1.96	0.46
7:A:1192:TRP:HZ3	7:A:1246:ILE:HG22	1.80	0.46
15:I:69:ILE:O	15:I:72:VAL:HG22	2.16	0.46
3:Z:631:GLU:OE1	3:Z:631:GLU:N	2.48	0.46
4:W:235:GLU:OE2	21:U:62:HIS:NE2	2.49	0.46
7:A:1211:LEU:HD13	7:A:1258:ARG:CZ	2.45	0.46
3:Z:508:MET:SD	13:G:95:VAL:HG11	2.55	0.46
4:W:57:ILE:HG23	4:W:58:MET:SD	2.55	0.46
8:B:378:GLY:HA3	15:I:102:ALA:HB3	1.98	0.46
8:B:856:PRO:HA	8:B:904:VAL:HG13	1.97	0.46
7:A:680:LEU:O	7:A:684:GLY:N	2.43	0.46
6:V:415:LEU:HD23	6:V:422:CYS:HA	1.98	0.46
7:A:392:GLU:OE2	7:A:448:ARG:NE	2.49	0.46
7:A:609:HIS:ND1	7:A:626:THR:O	2.49	0.46
8:B:565:THR:HG22	8:B:610:ARG:HB3	1.98	0.46
8:B:1094:GLN:HB2	8:B:1103:LEU:HD12	1.98	0.46
7:A:806:THR:OG1	7:A:819:SER:O	2.28	0.45
7:A:828:LEU:HD11	8:B:1008:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1285:LEU:HA	7:A:1288:ILE:HD12	1.98	0.45
15:I:26:PRO:HB2	15:I:35:LEU:HD11	1.98	0.45
7:A:1139:LEU:HD23	7:A:1359:SER:HB2	1.98	0.45
13:G:21:ASN:O	13:G:25:THR:OG1	2.29	0.45
4:W:534:VAL:HG23	4:W:553:PHE:HE1	1.82	0.45
7:A:858:GLY:O	7:A:862:ARG:N	2.44	0.45
7:A:1164:THR:OG1	7:A:1299:GLN:N	2.48	0.45
7:A:1201:ASP:OD1	7:A:1201:ASP:N	2.49	0.45
6:V:284:GLN:NE2	6:V:288:ASP:OD2	2.50	0.45
7:A:36:VAL:HG22	7:A:85:PHE:O	2.16	0.45
7:A:41:ILE:HD12	7:A:56:GLY:O	2.16	0.45
7:A:91:ALA:HB3	7:A:290:LEU:HD23	1.98	0.45
1:X:24:LYS:HG2	6:V:331:LEU:HD13	1.98	0.45
7:A:233:CYS:O	7:A:238:MET:N	2.50	0.45
6:V:218:VAL:HG11	6:V:241:LEU:HD13	1.98	0.45
16:J:47:ARG:NE	16:J:48:MET:SD	2.89	0.45
7:A:448:ARG:NH1	7:A:451:CYS:SG	2.89	0.45
8:B:796:MET:SD	8:B:948:GLN:NE2	2.88	0.45
8:B:1107:LEU:O	8:B:1111:SER:OG	2.35	0.45
10:D:114:LEU:HD13	13:G:84:VAL:HG11	1.99	0.45
21:U:14:HIS:O	21:U:18:GLY:N	2.48	0.45
7:A:133:SER:O	7:A:140:ARG:NH2	2.49	0.45
6:V:469:LEU:HD23	6:V:472:LEU:HD12	1.98	0.45
11:E:118:LEU:HD22	11:E:127:LEU:CB	2.47	0.45
21:U:41:ILE:HG21	21:U:56:LEU:HD21	1.98	0.45
7:A:22:GLN:O	8:B:1170:ARG:N	2.49	0.44
4:W:190:SER:O	4:W:194:ALA:N	2.42	0.44
4:W:439:ARG:NE	4:W:483:GLN:OE1	2.50	0.44
7:A:1374:VAL:HG11	7:A:1411:LEU:HD21	2.00	0.44
4:W:195:CYS:O	21:U:89:TRP:NE1	2.50	0.44
7:A:896:LEU:O	7:A:1396:ARG:NH1	2.51	0.44
8:B:760:THR:OG1	8:B:764:MET:SD	2.58	0.44
8:B:1028:LEU:HD13	8:B:1041:ILE:HB	1.98	0.44
10:D:105:PRO:O	10:D:131:LEU:HD13	2.18	0.44
6:V:318:THR:HG23	6:V:338:LEU:HD11	1.99	0.44
8:B:590:LEU:O	8:B:594:MET:N	2.51	0.44
10:D:103:LEU:HD13	13:G:84:VAL:HG13	2.00	0.44
13:G:30:LEU:O	13:G:34:VAL:HG22	2.17	0.44
7:A:1284:PHE:CE2	7:A:1288:ILE:HD11	2.53	0.44
7:A:1472:ASP:N	7:A:1472:ASP:OD1	2.49	0.44
8:B:94:SER:HB3	21:U:262:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:19:ALA:O	21:U:55:LYS:NZ	2.33	0.44
4:W:89:ALA:HB1	4:W:92:GLN:HB3	2.00	0.44
7:A:781:ILE:HG23	7:A:785:ILE:HD12	2.00	0.44
7:A:961:GLU:O	7:A:965:VAL:HG23	2.18	0.44
6:V:113:VAL:HG12	6:V:117:MET:SD	2.57	0.44
7:A:921:ARG:NH1	7:A:922:PHE:O	2.51	0.44
5:P:9:C:O2'	5:P:10:A:OP1	2.32	0.43
12:F:56:TYR:O	12:F:108:ARG:NH2	2.50	0.43
6:V:253:ILE:HA	6:V:256:VAL:HG22	2.00	0.43
6:V:266:LEU:O	6:V:270:ILE:HG22	2.18	0.43
7:A:19:LYS:NZ	8:B:1173:SER:O	2.48	0.43
13:G:108:ILE:HG22	13:G:113:ILE:HG13	1.99	0.43
3:Z:478:VAL:HB	3:Z:518:LEU:HD22	1.99	0.43
4:W:351:ASP:OD1	4:W:352:HIS:N	2.51	0.43
14:H:28:LEU:HD11	14:H:50:VAL:HG21	1.99	0.43
4:W:439:ARG:CD	4:W:483:GLN:OE1	2.67	0.43
4:W:236:HIS:CB	21:U:54:LEU:HD22	2.48	0.43
6:V:101:PHE:O	6:V:104:VAL:HG12	2.18	0.43
8:B:311:ILE:O	8:B:312:GLN:NE2	2.51	0.43
8:B:607:ILE:HD12	15:I:75:ASP:OD1	2.19	0.43
21:U:85:ASP:O	21:U:91:LEU:HD21	2.18	0.43
4:W:361:ALA:HB3	4:W:383:LEU:HD12	2.01	0.43
4:W:55:ASP:HB2	6:V:59:LEU:HD13	2.01	0.43
8:B:133:ILE:HG23	8:B:138:GLU:O	2.19	0.43
10:D:31:THR:HG21	10:D:95:PHE:HA	2.00	0.43
13:G:92:VAL:HG22	13:G:97:LEU:HD22	1.99	0.43
11:E:156:VAL:O	11:E:160:LEU:HD23	2.19	0.43
8:B:859:ARG:HG2	8:B:903:ILE:HG13	2.01	0.42
6:V:41:LEU:HD13	6:V:44:LEU:HD11	2.01	0.42
6:V:165:LEU:HD13	6:V:225:LEU:HD11	2.00	0.42
6:V:227:LEU:HD23	6:V:228:ARG:NH1	2.35	0.42
11:E:180:ALA:O	11:E:184:GLY:N	2.52	0.42
4:W:473:LEU:HD13	4:W:500:MET:SD	2.59	0.42
6:V:47:ALA:O	6:V:51:LEU:N	2.46	0.42
7:A:862:ARG:O	7:A:866:LYS:NZ	2.41	0.42
9:C:260:GLN:HB2	17:K:91:ILE:HG21	2.01	0.42
11:E:156:VAL:HG22	11:E:190:VAL:CG1	2.49	0.42
4:W:431:VAL:HG11	4:W:455:LEU:HD21	2.02	0.42
5:P:8:G:C1'	7:A:264:VAL:HG21	2.49	0.42
7:A:789:GLY:O	7:A:791:GLN:NE2	2.52	0.42
11:E:3:ASP:OD1	11:E:49:SER:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:196:LEU:HD23	3:Z:215:VAL:HG21	2.02	0.42
3:Z:561:LEU:HD21	3:Z:636:PHE:HA	2.02	0.42
4:W:534:VAL:HG23	4:W:553:PHE:CE1	2.54	0.42
6:V:137:LEU:O	6:V:141:CYS:N	2.53	0.42
7:A:365:THR:OG1	7:A:366:VAL:N	2.53	0.42
6:V:227:LEU:HD22	6:V:355:ILE:HG22	2.01	0.42
7:A:80:GLU:OE1	8:B:1131:ARG:NH2	2.53	0.42
7:A:1357:THR:O	11:E:142:HIS:NE2	2.46	0.42
8:B:1112:ASP:OD1	8:B:1112:ASP:N	2.53	0.42
10:D:68:THR:O	10:D:72:SER:N	2.53	0.42
18:L:32:ASP:OD1	18:L:32:ASP:N	2.53	0.42
7:A:901:VAL:HB	7:A:978:VAL:HG12	2.01	0.41
5:P:6:U:O4'	8:B:841:ARG:NH2	2.53	0.41
8:B:289:ILE:HG22	8:B:291:ASP:O	2.20	0.41
6:V:270:ILE:HD11	6:V:309:PHE:CB	2.49	0.41
3:Z:340:PHE:HE2	3:Z:359:LEU:HD12	1.86	0.41
4:W:440:TYR:OH	4:W:451:HIS:ND1	2.47	0.41
4:W:542:ALA:HB3	21:U:164:GLN:O	2.21	0.41
5:P:9:C:HO2'	5:P:10:A:P	2.42	0.41
6:V:81:ALA:O	6:V:89:ARG:NH1	2.53	0.41
8:B:157:ARG:NE	8:B:180:ASP:O	2.53	0.41
11:E:94:MET:O	11:E:98:ASN:N	2.53	0.41
4:W:212:ILE:HD11	4:W:227:PHE:HD2	1.84	0.41
3:Z:440:ILE:HG23	3:Z:450:ILE:HD11	2.02	0.41
7:A:1185:VAL:HG23	7:A:1186:VAL:HG23	2.02	0.41
6:V:165:LEU:HD13	6:V:225:LEU:CD1	2.51	0.41
7:A:275:ASP:OD1	7:A:276:LEU:N	2.54	0.41
8:B:1158:LEU:O	8:B:1162:LEU:HD23	2.20	0.41
6:V:539:GLU:OE2	6:V:543:GLN:NE2	2.54	0.41
7:A:541:THR:HG21	7:A:673:GLN:HG2	2.03	0.41
8:B:904:VAL:HG23	8:B:921:ILE:HG23	2.03	0.41
9:C:154:ARG:NE	16:J:60:LEU:O	2.54	0.41
4:W:531:ARG:CZ	4:W:562:ILE:HD12	2.51	0.41
4:W:231:VAL:HG13	4:W:241:ALA:HB3	2.03	0.40
13:G:90:THR:OG1	13:G:91:GLN:N	2.54	0.40
14:H:4:ILE:HG23	14:H:59:VAL:HG13	2.03	0.40
3:Z:740:CYS:HA	8:B:901:THR:HG21	2.03	0.40
4:W:78:ASN:OD1	4:W:79:VAL:N	2.54	0.40
7:A:784:VAL:HG23	8:B:978:ILE:HG13	2.03	0.40
7:A:1002:SER:OG	7:A:1003:ASP:N	2.54	0.40
7:A:1020:LEU:HD21	7:A:1073:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:266:MET:SD	7:A:272:ASN:ND2	2.94	0.40
9:C:16:ASP:OD1	9:C:240:ARG:NH2	2.54	0.40
4:W:90:VAL:HG12	6:V:62:HIS:HB3	2.03	0.40
4:W:497:LEU:HD13	4:W:533:PHE:HB2	2.02	0.40
7:A:148:CYS:SG	7:A:149:LYS:N	2.94	0.40
8:B:285:LEU:O	8:B:289:ILE:N	2.54	0.40
8:B:718:GLN:O	8:B:721:ARG:N	2.49	0.40
8:B:1109:GLU:OE1	8:B:1109:GLU:N	2.55	0.40
15:I:54:TYR:OH	15:I:56:ASN:ND2	2.54	0.40
7:A:338:SER:OG	7:A:339:LEU:N	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%)	6 (60%)	4 (40%)	0	100	100
2	Y	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
3	Z	455/1087 (42%)	435 (96%)	20 (4%)	0	100	100
4	W	518/590 (88%)	506 (98%)	12 (2%)	0	100	100
6	V	548/580 (94%)	535 (98%)	13 (2%)	0	100	100
7	A	1407/1970 (71%)	1357 (96%)	50 (4%)	0	100	100
8	B	1130/1174 (96%)	1075 (95%)	55 (5%)	0	100	100
9	C	251/271 (93%)	242 (96%)	9 (4%)	0	100	100
10	D	124/142 (87%)	117 (94%)	7 (6%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	110 (97%)	3 (3%)	0	100	100
18	L	42/58 (72%)	42 (100%)	0	0	100	100
21	U	192/528 (36%)	182 (95%)	10 (5%)	0	100	100
All	All	5669/7865 (72%)	5459 (96%)	210 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	11/331 (3%)	6 (54%)	5 (46%)	0	0
2	Y	102/103 (99%)	102 (100%)	0	100	100
3	Z	418/940 (44%)	415 (99%)	3 (1%)	84	93
4	W	471/513 (92%)	465 (99%)	6 (1%)	69	86
6	V	493/515 (96%)	491 (100%)	2 (0%)	91	96
7	A	1248/1749 (71%)	1242 (100%)	6 (0%)	88	94
8	B	994/1027 (97%)	989 (100%)	5 (0%)	88	94
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%)	188 (100%)	1 (0%)	88	94
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	K	104/106 (98%)	102 (98%)	2 (2%)	57	80
18	L	41/55 (74%)	40 (98%)	1 (2%)	49	76
21	U	167/451 (37%)	167 (100%)	0	100	100
All	All	5091/6919 (74%)	5060 (99%)	31 (1%)	86	94

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	13	GLU
1	X	15	LEU
1	X	21	LYS
1	X	23	LYS
1	X	24	LYS
3	Z	300	GLN
3	Z	703	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	141	CYS
6	V	307	ASP
7	A	42	LYS
7	A	111	CYS
7	A	148	CYS
7	A	876	ASP
7	A	1199	MET
7	A	1287	CYS
8	B	870	THR
8	B	918	PHE
8	B	975	ARG
8	B	1052	LYS
8	B	1142	ASN
11	E	108	GLN
17	K	71	ILE
17	K	84	GLN
18	L	26	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
17	K	84	GLN

5.3.3 RNA [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

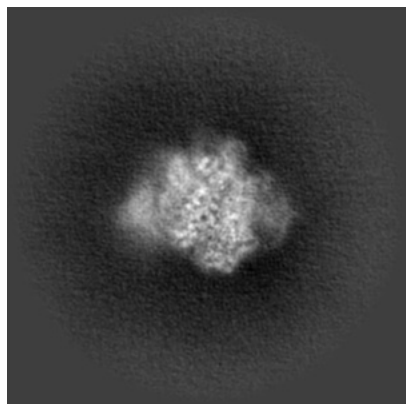
6 Map visualisation [i](#)

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.

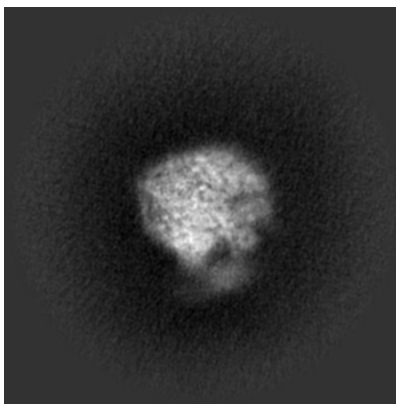
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

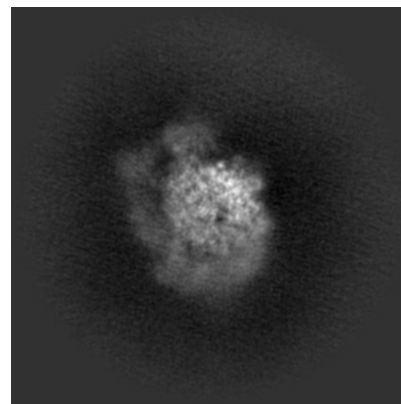
6.1.1 Primary map



X

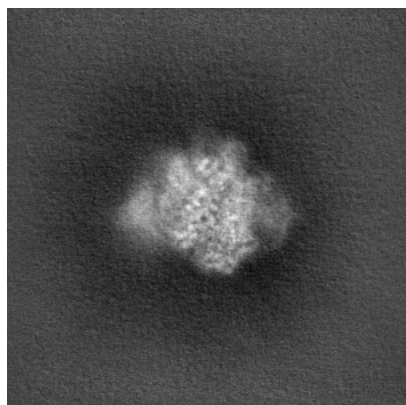


Y

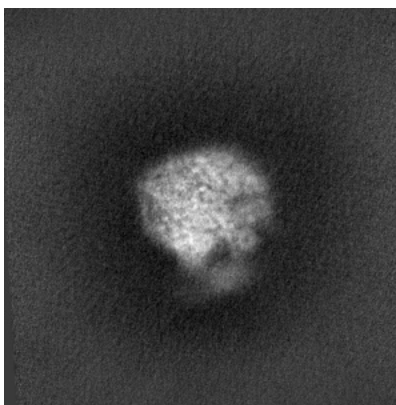


Z

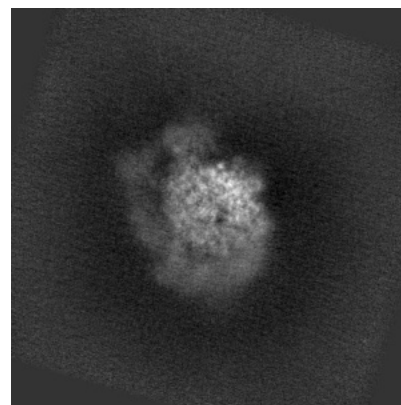
6.1.2 Raw map



X



Y

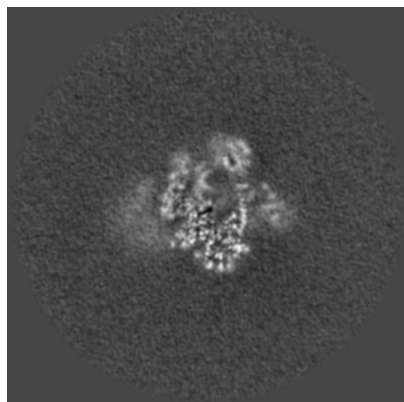


Z

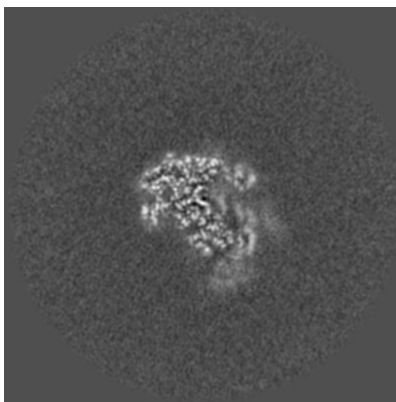
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

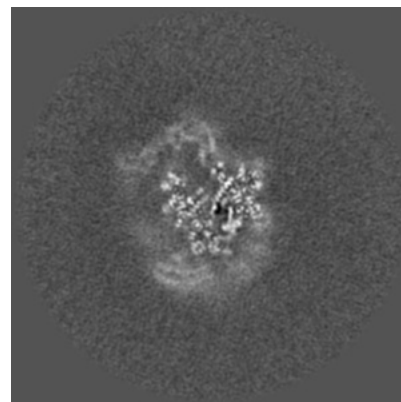
6.2.1 Primary map



X Index: 256



Y Index: 256

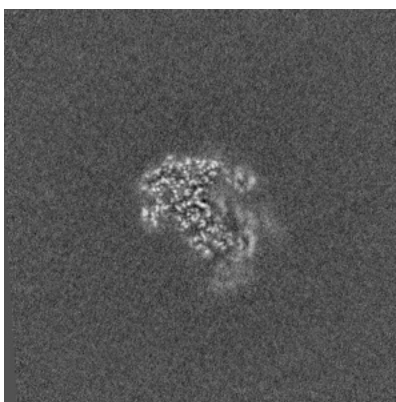


Z Index: 256

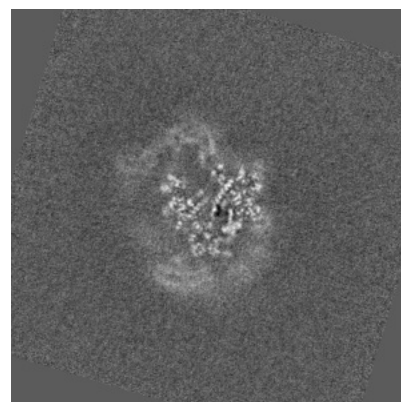
6.2.2 Raw map



X Index: 256



Y Index: 256

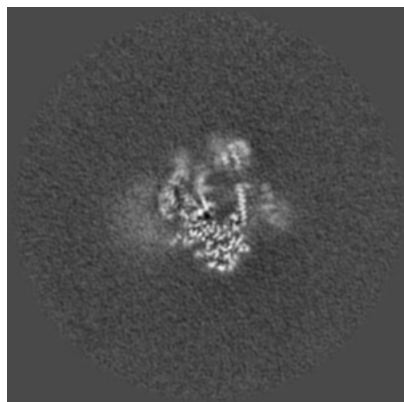


Z Index: 256

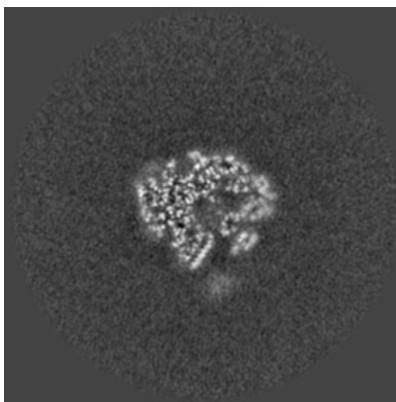
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

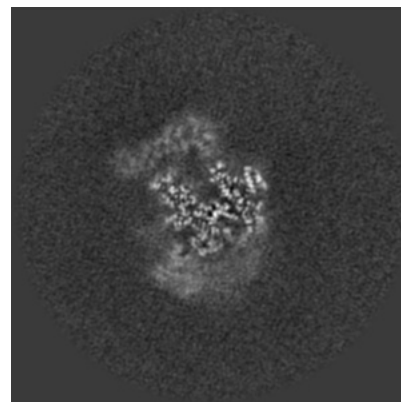
6.3.1 Primary map



X Index: 259

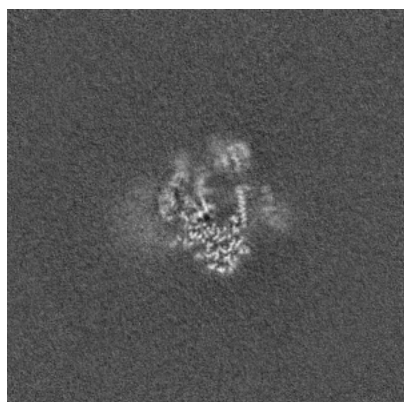


Y Index: 282

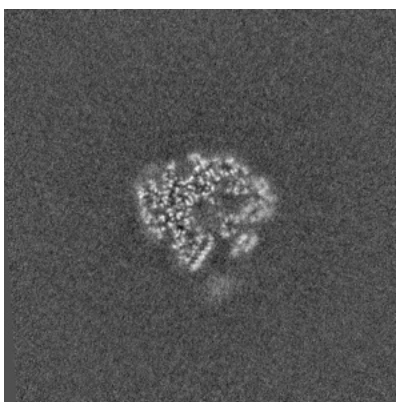


Z Index: 246

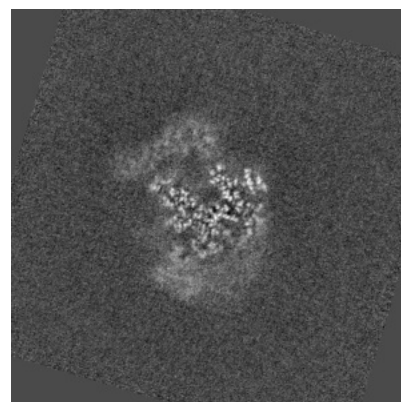
6.3.2 Raw map



X Index: 259



Y Index: 282

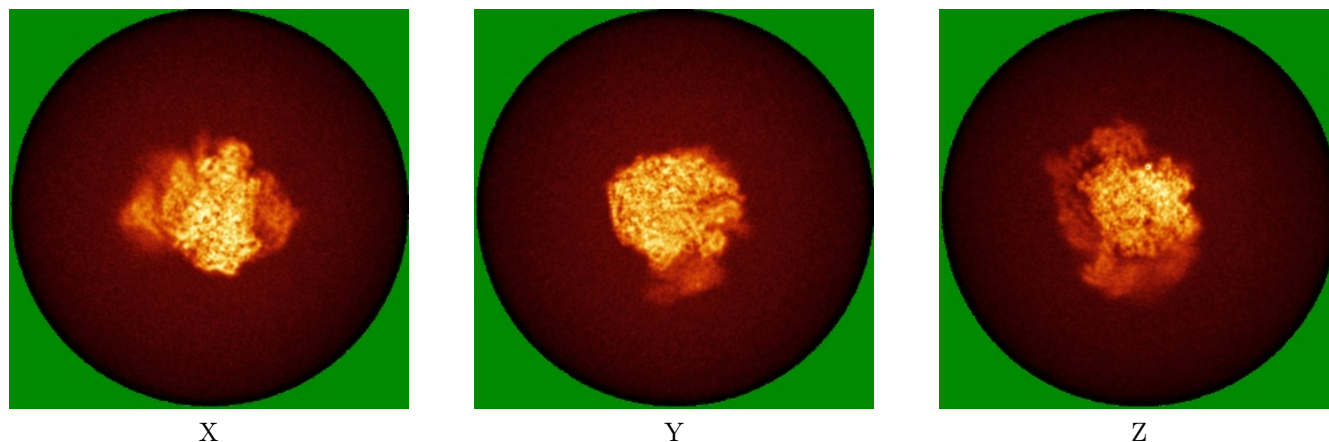


Z Index: 245

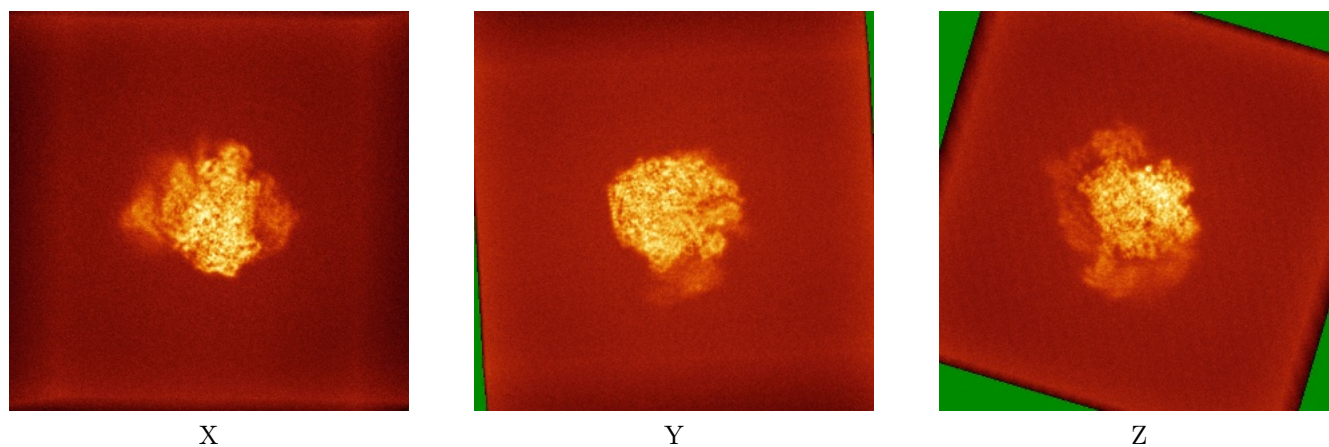
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



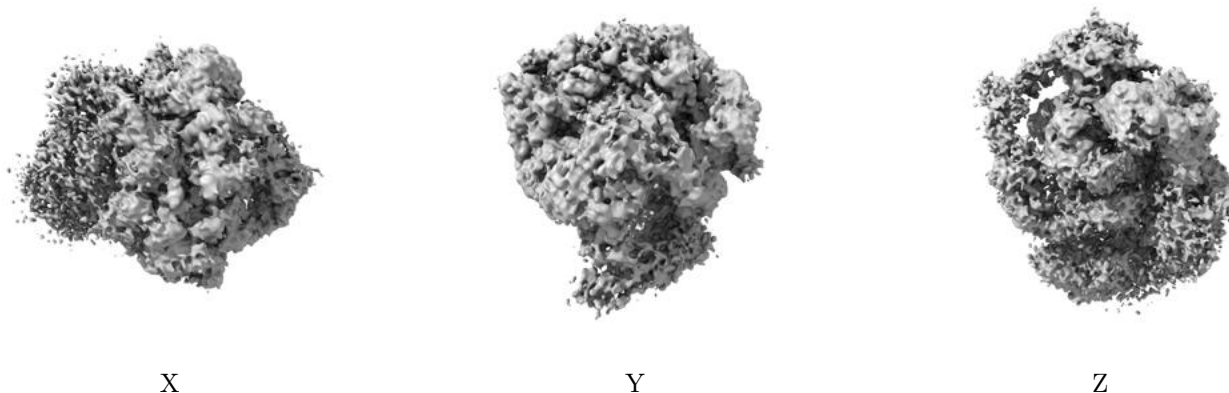
6.4.2 Raw map



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.

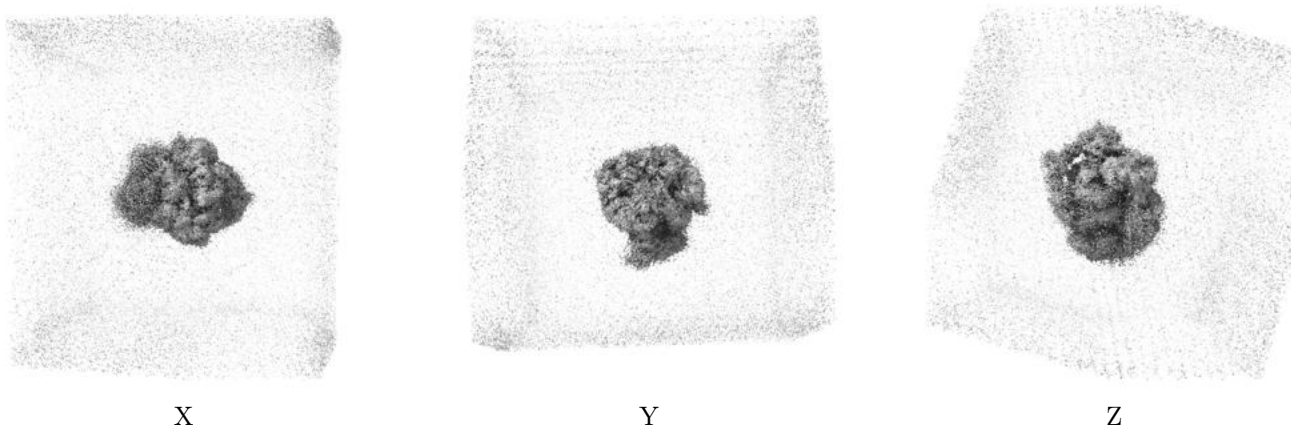
6.5 Orthogonal surface views [i](#)

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.

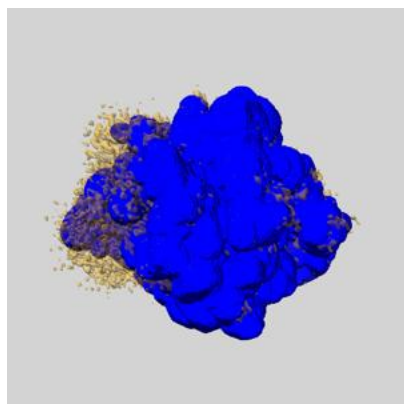
6.6 Mask visualisation [i](#)

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

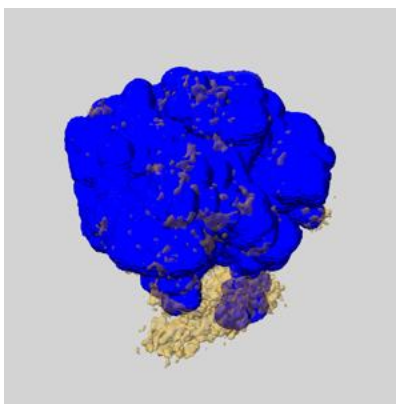
A mask typically either:

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

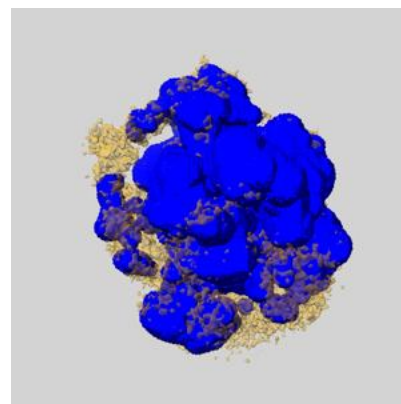
6.6.1 emd_42267_msk_1.map [i](#)



X



Y

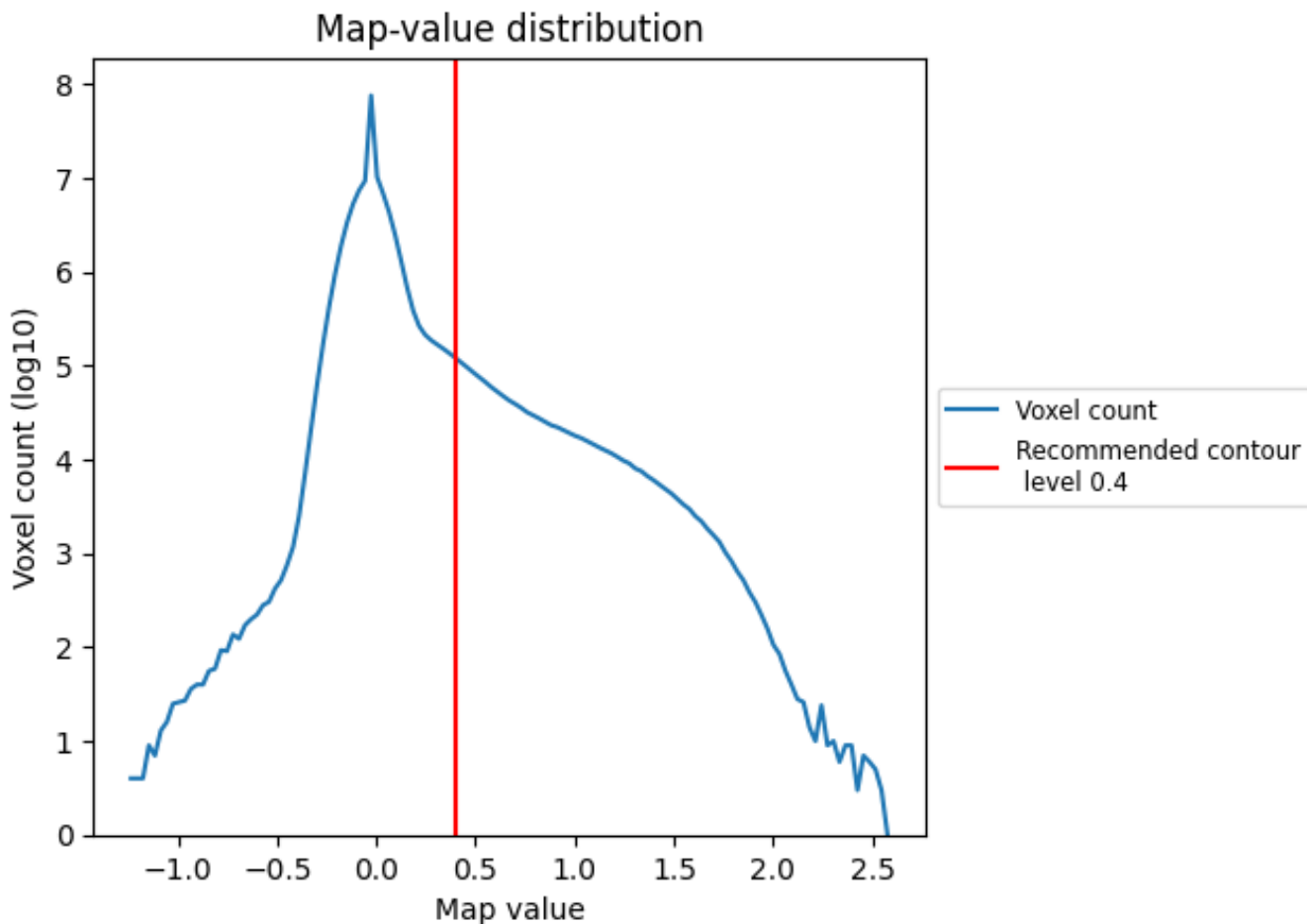


Z

7 Map analysis [i](#)

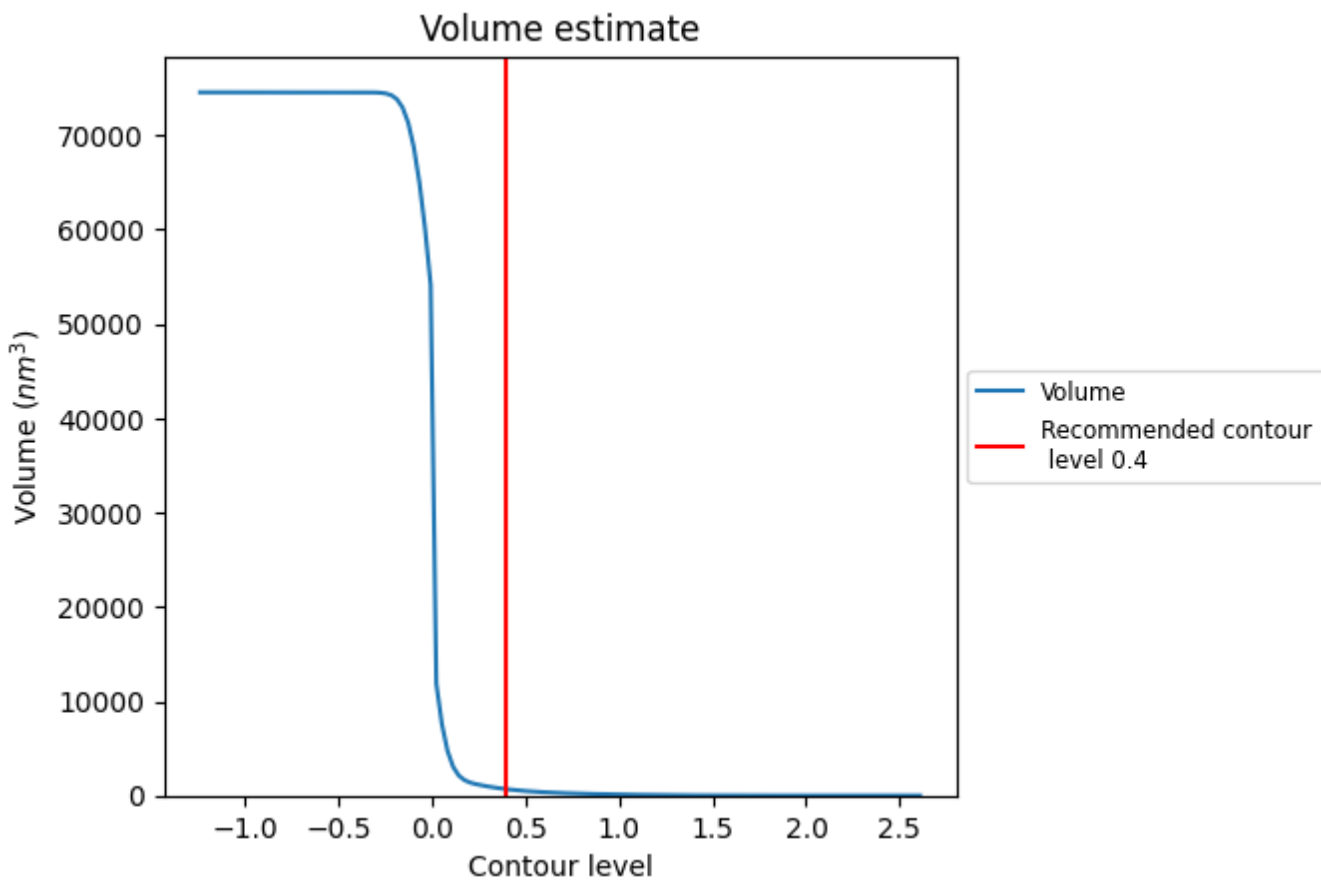
This section contains the results of statistical analysis of the map.

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.

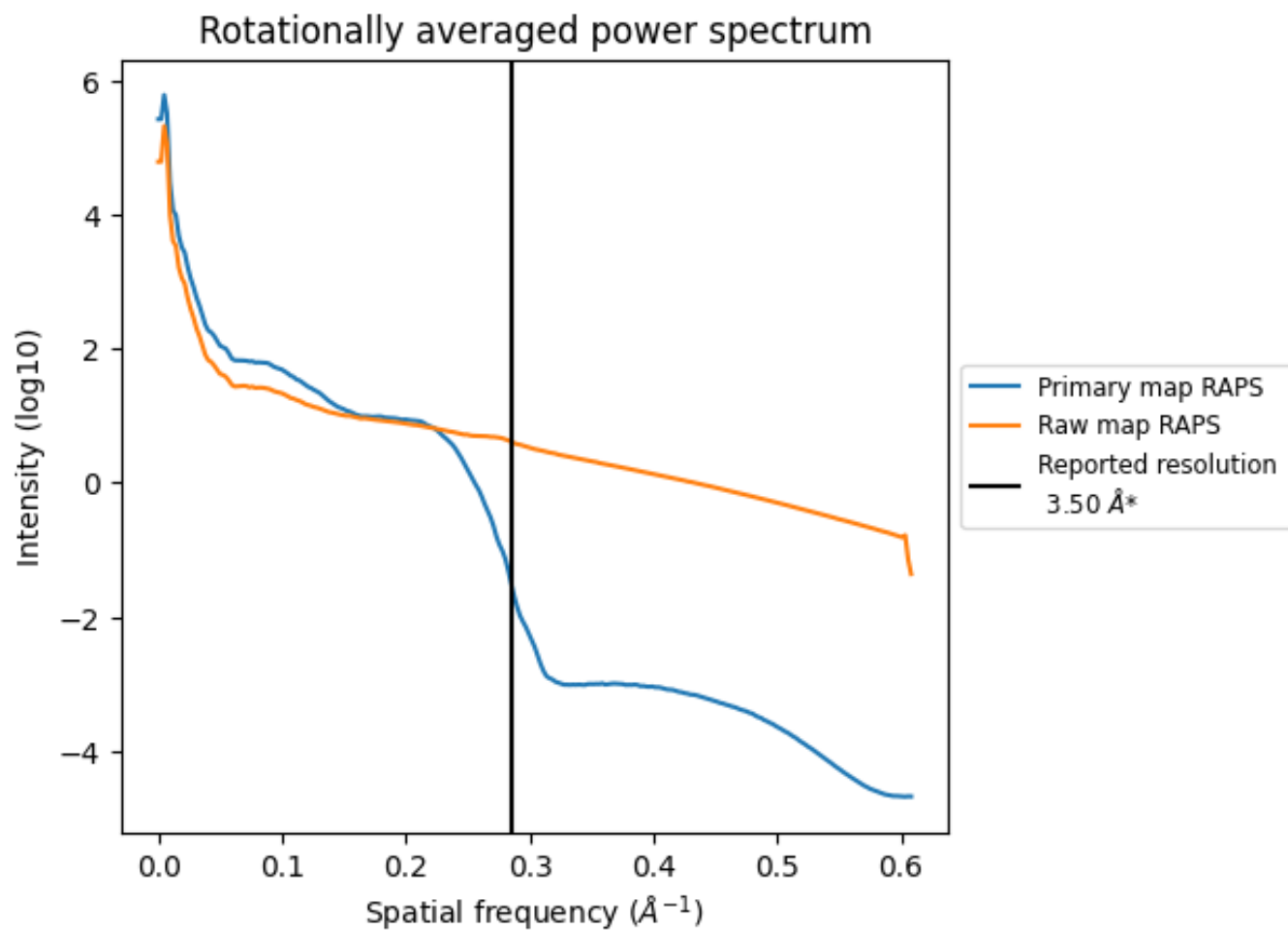
7.2 Volume estimate [i](#)



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 (i)

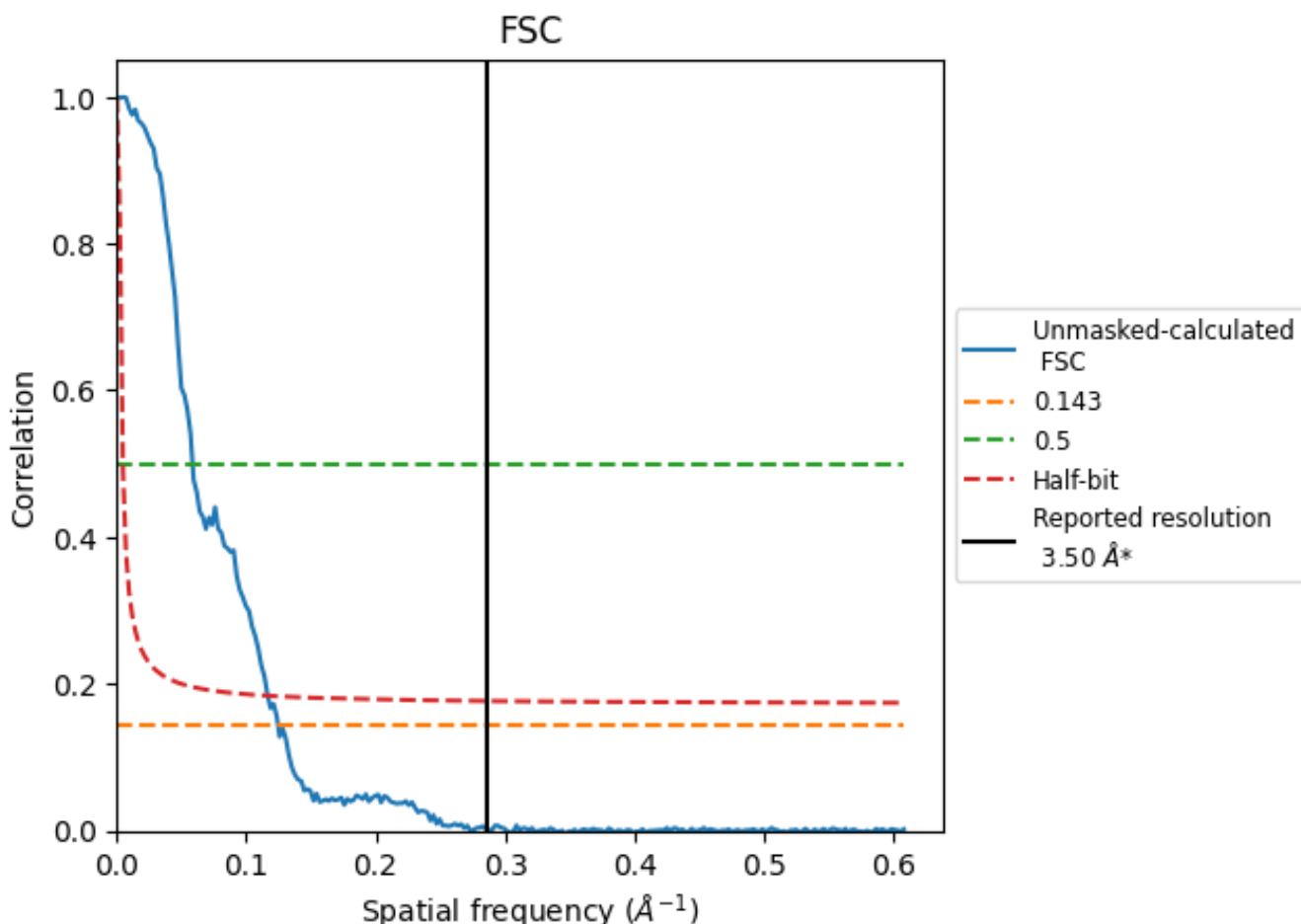


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

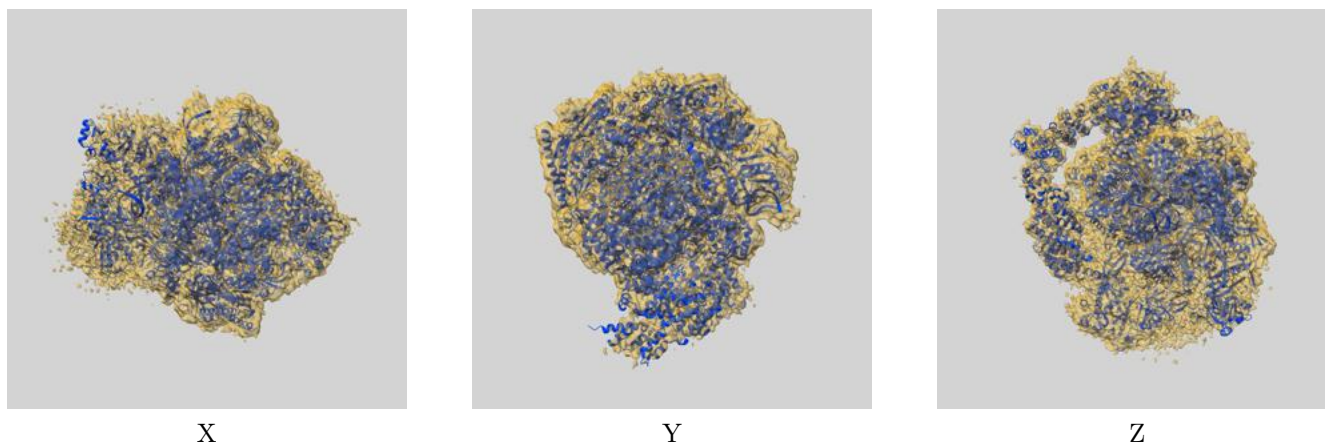
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.03	17.06	8.57

*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](#)

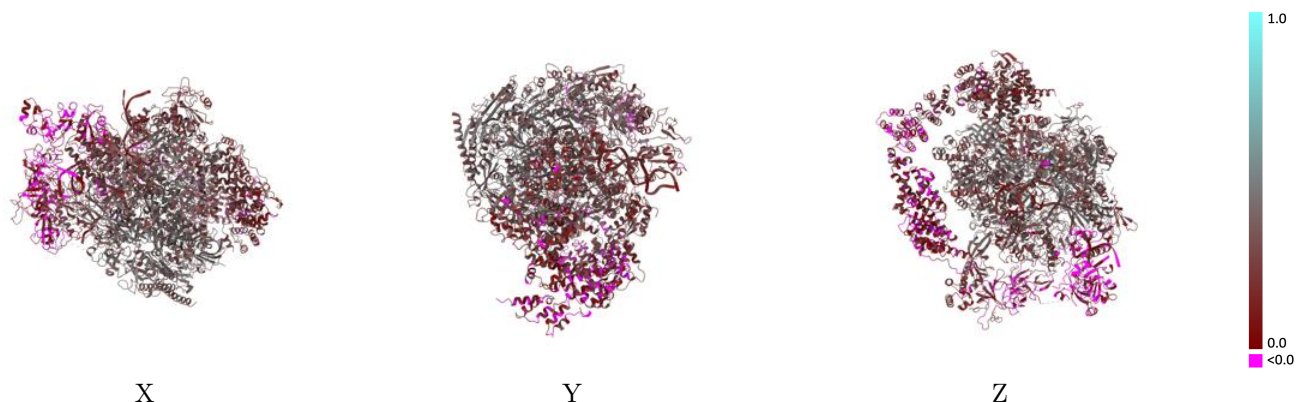
This section contains information regarding the fit between EMDB map EMD-42267 and PDB model 8UHA. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



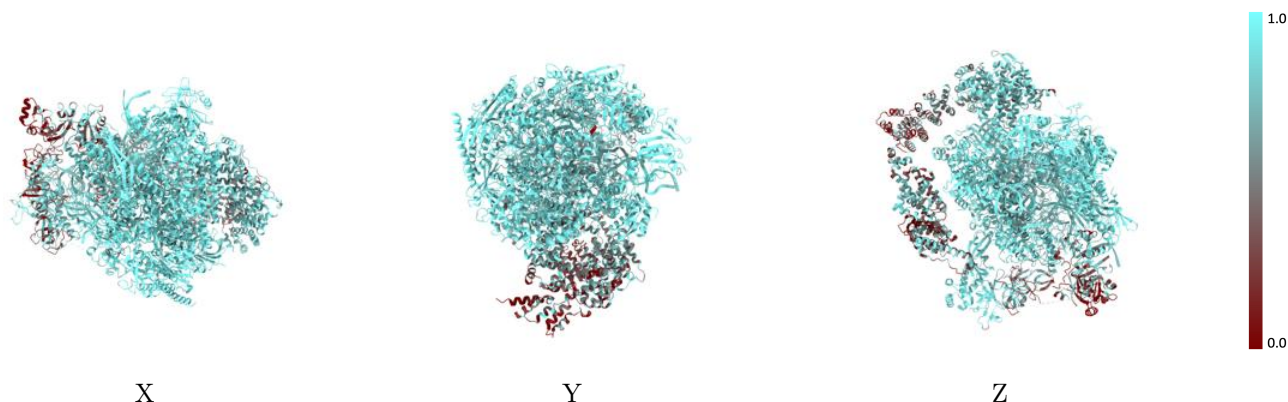
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



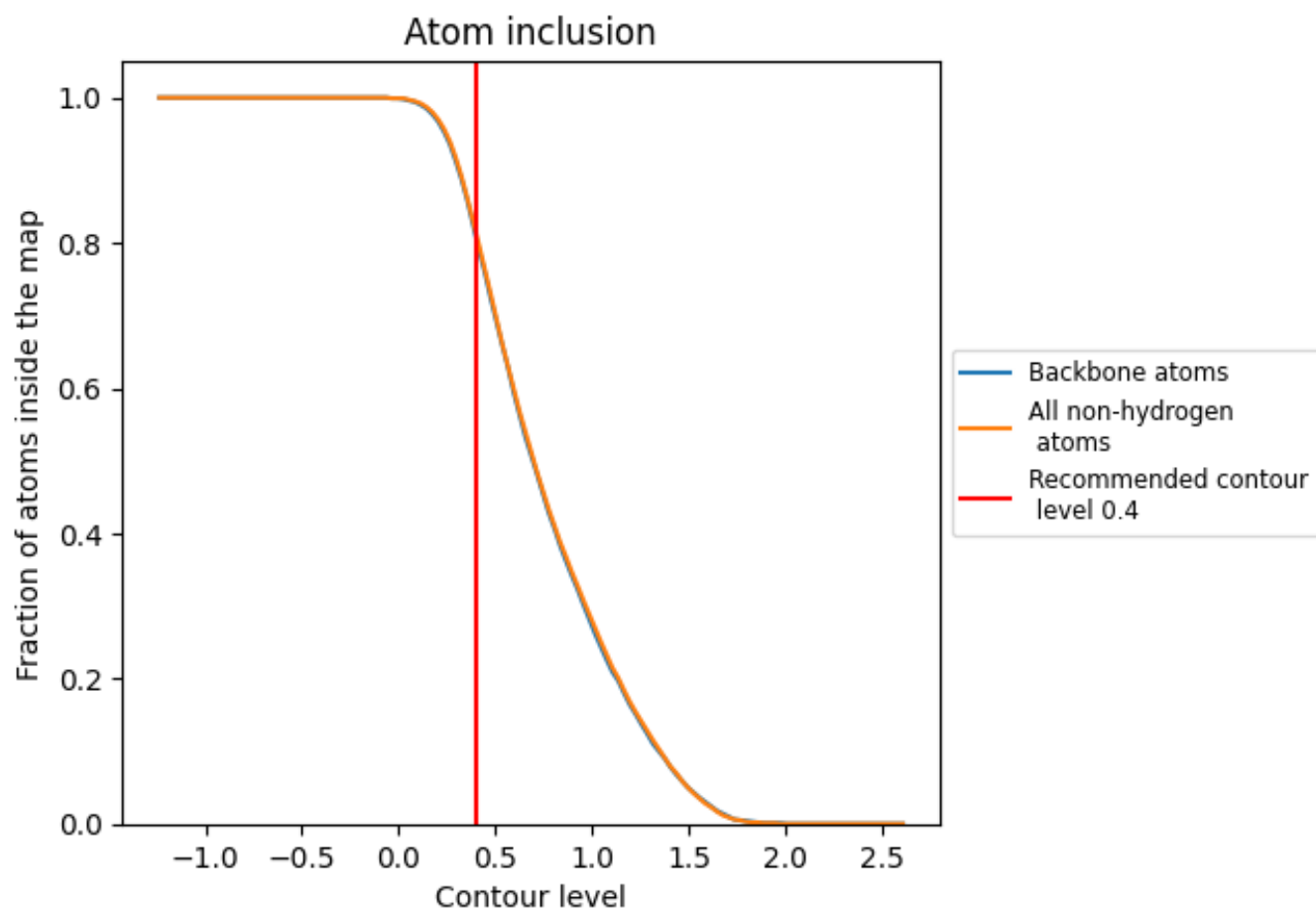
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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













































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	 0.8140	 0.2800
A	 0.9120	 0.3550
B	 0.9260	 0.3750
C	 0.9620	 0.4030
D	 0.9230	 0.1830
E	 0.9390	 0.3420
F	 0.9450	 0.3900
G	 0.9480	 0.2390
H	 0.9620	 0.3840
I	 0.9640	 0.3420
J	 0.9600	 0.4050
K	 0.9530	 0.3940
L	 0.9640	 0.3740
N	 0.8350	 0.1370
P	 0.9270	 0.2850
T	 0.8570	 0.1780
U	 0.7820	 0.2080
V	 0.4520	 0.0950
W	 0.6770	 0.2000
X	 0.7860	 0.2600
Y	 0.3130	 0.0170
Z	 0.5290	 0.0920

