



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:16 AM UTC

PDB ID : 2WWB / pdb_00002wwb
EMDB ID : EMD-1652
Title : CRYO-EM STRUCTURE OF THE MAMMALIAN SEC61 COMPLEX
BOUND TO THE ACTIVELY TRANSLATING WHEAT GERM 80S RI-
BOSOME
Authors : Becker, T.; Mandon, E.; Bhushan, S.; Jarasch, A.; Armache, J.P.; Funes,
S.; Jossinet, F.; Gumbart, J.; Mielke, T.; Berninghausen, O.; Schulten, K.;
Westhof, E.; Gilmore, R.; Beckmann, R.
Deposited on : 2009-10-22
Resolution : 6.48 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:

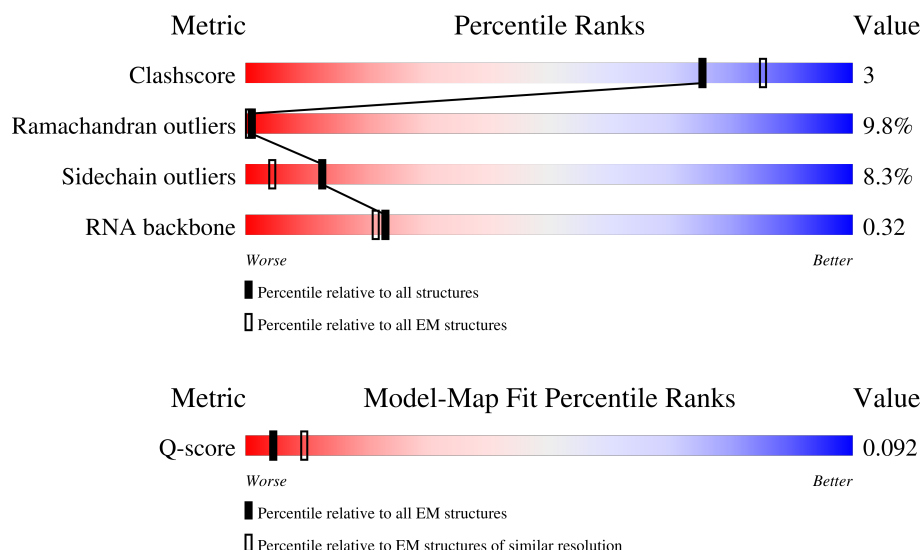
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.48 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	496 (5.98 - 6.95)

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	A	476	34% 85% 12% ..
2	B	68	26% 82% 15% .
3	C	96	19% 33% ... 63%

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Mol	Chain	Length	Quality of chain
4	D	63	
5	E	34	
6	F	25	
7	G	14	
8	H	362	
9	I	184	
10	J	189	
11	K	142	
12	L	127	
13	M	113	
14	N	120	
15	O	51	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3675	2409	591	650	25		

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	68	Total	C	N	O	S	0	0
			543	355	94	89	5		

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	36	Total	C	N	O	S	0	0
			281	188	44	47	2		

- Molecule 4 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	63	Total	C	N	O	P	0	0
			1347	603	245	436	63		

- Molecule 5 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	34	Total	C	N	O	P	0	0
			740	332	148	226	34		

- Molecule 6 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	25	Total	C	N	O	P	0	0
			536	239	99	173	25		

- Molecule 7 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	14	Total	C	N	O	P	0	0
			296	133	54	96	13		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	269	Total	C	N	O	S	0	0
			2039	1281	391	363	4		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	153	Total	C	N	O	S	0	0
			1212	756	236	219	1		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	53	Total	C	N	O	S	0	0
			410	254	83	72	1		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	83	Total	C	N	O	S	0	0
			663	424	111	126	2		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	127	Total	C	N	O	S	0	0
			1002	630	193	178	1		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	84	Total	C	N	O	S	0	0
			706	447	140	118	1		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	69	Total	C	N	O	S	0	0
			547	345	101	99	2		

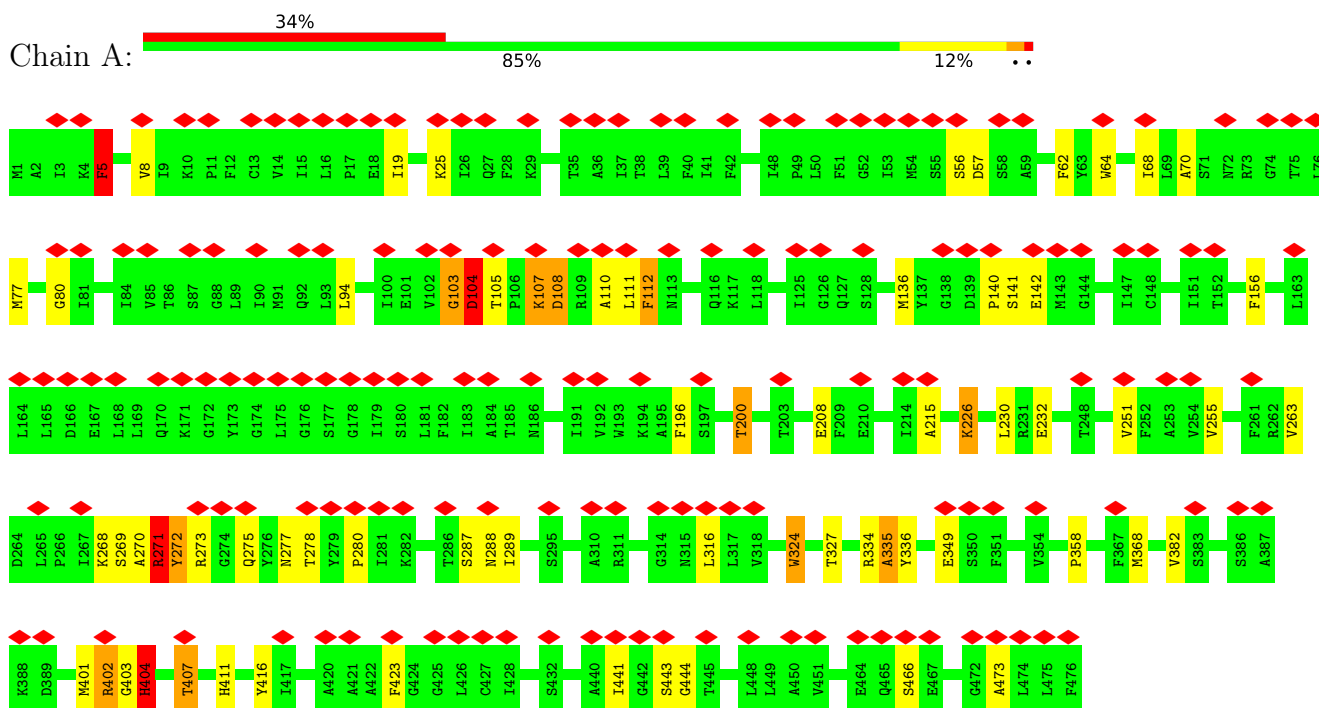
- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	37	Total	C	N	O	S	0	0
			316	200	66	48	2		

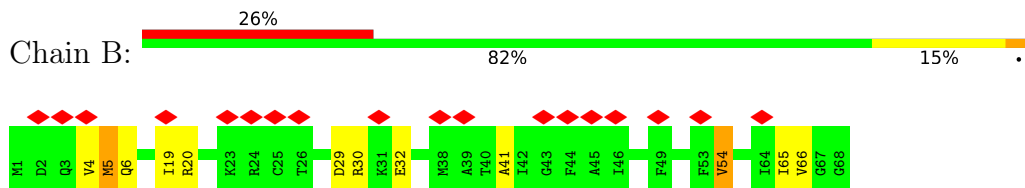
3 Residue-property plots

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.

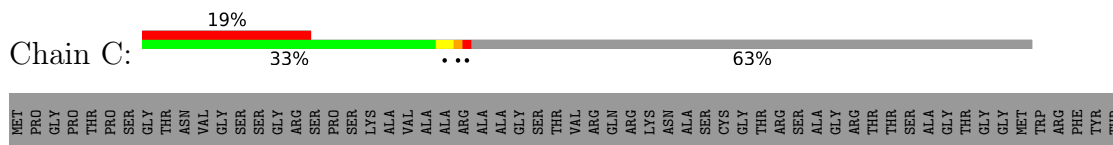
- Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1

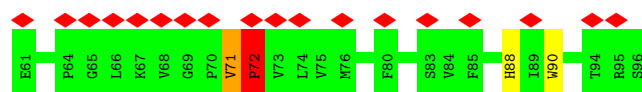


- Molecule 2: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA

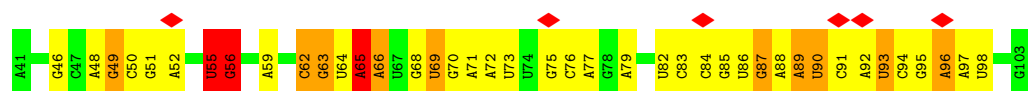


- Molecule 3: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA





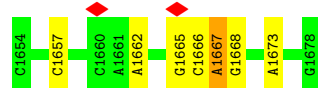
• Molecule 4: 5.8S rRNA



• Molecule 5: 25S rRNA



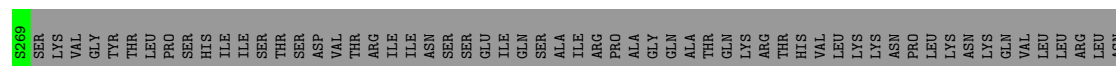
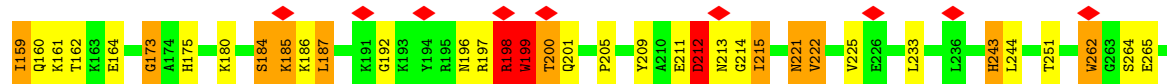
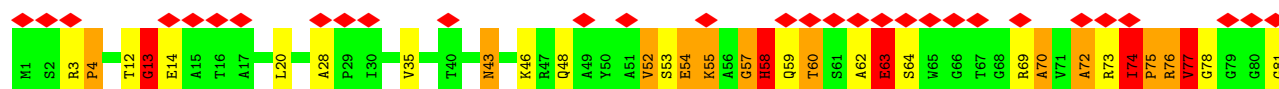
• Molecule 6: 25S rRNA



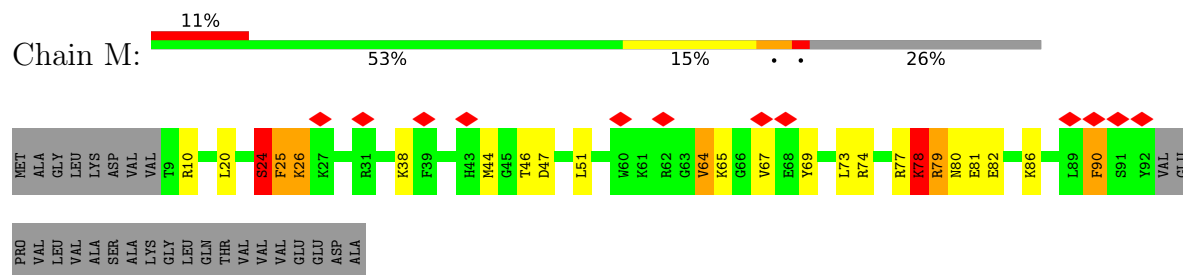
• Molecule 7: 25S rRNA



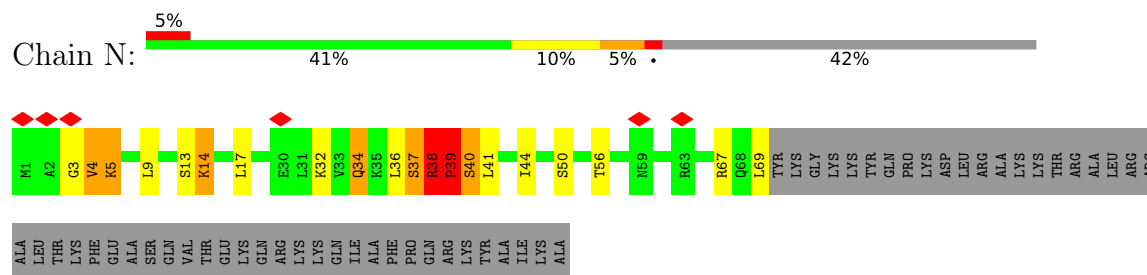
• Molecule 8: 60S RIBOSOMAL PROTEIN L4-B



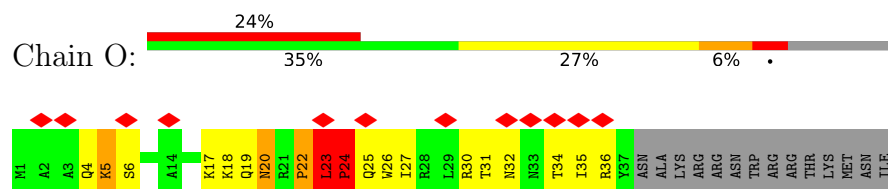
• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A



• Molecule 14: 60S RIBOSOMAL PROTEIN L35



• Molecule 15: 60S RIBOSOMAL PROTEIN L39



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	221445	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.706	Depositor
Minimum map value	-0.671	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	2.46	8/3755 (0.2%)	1.70	49/5089 (1.0%)
2	B	1.19	0/553	1.72	9/738 (1.2%)
3	C	1.10	0/289	1.62	3/391 (0.8%)
4	D	0.92	0/1508	1.30	12/2348 (0.5%)
5	E	0.91	0/833	1.16	3/1298 (0.2%)
6	F	0.91	0/599	1.07	1/932 (0.1%)
7	G	0.95	0/330	1.21	3/513 (0.6%)
8	H	1.27	0/2079	2.03	82/2817 (2.9%)
9	I	1.30	0/1235	2.00	50/1662 (3.0%)
10	J	1.28	0/412	1.46	0/551
11	K	1.15	0/670	1.66	9/903 (1.0%)
12	L	1.28	0/1013	1.81	26/1351 (1.9%)
13	M	1.37	0/719	1.79	19/959 (2.0%)
14	N	1.32	1/549 (0.2%)	2.05	24/733 (3.3%)
15	O	1.34	0/321	1.86	6/426 (1.4%)
All	All	1.60	9/14865 (0.1%)	1.69	296/20711 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
3	C	0	1
4	D	0	10
5	E	0	6
6	F	0	3
7	G	0	1
8	H	0	12
9	I	0	6
11	K	0	3
12	L	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	2
14	N	0	2
15	O	0	7
All	All	0	63

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ASP	N-CA	126.72	3.09	1.46
1	A	5	PHE	CG-CD2	20.78	1.82	1.38
1	A	5	PHE	CG-CD1	20.48	1.81	1.38
1	A	5	PHE	CD2-CE2	14.34	1.81	1.38
1	A	5	PHE	CD1-CE1	13.99	1.80	1.38
1	A	5	PHE	CE1-CZ	13.98	1.80	1.38
1	A	5	PHE	CE2-CZ	13.64	1.79	1.38
14	N	69	LEU	C-O	-11.58	1.00	1.23
1	A	104	ASP	CA-CB	7.28	1.65	1.53

All (296) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	532	A	P-O3'-C3'	13.96	141.14	120.20
1	A	103	GLY	CA-C-N	12.76	145.91	121.54
1	A	103	GLY	C-N-CA	12.76	145.91	121.54
9	I	56	ARG	CA-C-N	12.75	144.64	121.70
9	I	56	ARG	C-N-CA	12.75	144.64	121.70
8	H	184	SER	CA-C-N	11.97	143.25	121.70
8	H	184	SER	C-N-CA	11.97	143.25	121.70
4	D	90	U	P-O3'-C3'	11.63	137.65	120.20
8	H	54	GLU	CA-C-N	11.33	142.09	121.70
8	H	54	GLU	C-N-CA	11.33	142.09	121.70
4	D	93	U	P-O3'-C3'	11.32	137.18	120.20
8	H	75	PRO	CA-C-N	11.21	141.88	121.70
8	H	75	PRO	C-N-CA	11.21	141.88	121.70
4	D	69	U	P-O3'-C3'	11.19	136.98	120.20
8	H	59	GLN	CA-C-N	11.07	141.63	121.70
8	H	59	GLN	C-N-CA	11.07	141.63	121.70
9	I	36	ILE	N-CA-C	10.76	121.66	110.36
9	I	105	LYS	N-CA-C	10.64	122.64	111.14
1	A	104	ASP	N-CA-CB	10.54	128.30	110.49
4	D	65	A	P-O3'-C3'	10.30	135.65	120.20
4	D	96	A	P-O3'-C3'	10.28	135.62	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	36	ILE	CA-C-N	10.23	140.12	121.70
9	I	36	ILE	C-N-CA	10.23	140.12	121.70
4	D	55	U	P-O3'-C3'	10.08	135.32	120.20
8	H	43	ASN	CA-CB-CG	9.78	122.38	112.60
12	L	84	LYS	CA-C-N	9.37	138.56	121.70
12	L	84	LYS	C-N-CA	9.37	138.56	121.70
8	H	86	GLY	CA-C-N	9.25	138.36	121.70
8	H	86	GLY	C-N-CA	9.25	138.36	121.70
8	H	101	ALA	CA-C-N	8.97	131.05	119.84
8	H	101	ALA	C-N-CA	8.97	131.05	119.84
14	N	39	PRO	CA-C-N	8.96	137.82	121.70
14	N	39	PRO	C-N-CA	8.96	137.82	121.70
7	G	1926	G	P-O3'-C3'	8.90	133.55	120.20
9	I	36	ILE	N-CA-CB	8.88	120.37	110.51
12	L	10	SER	CA-C-N	8.89	137.69	121.70
12	L	10	SER	C-N-CA	8.89	137.69	121.70
13	M	77	ARG	CA-C-N	8.84	137.61	121.70
13	M	77	ARG	C-N-CA	8.84	137.61	121.70
12	L	11	ASP	CA-CB-CG	8.62	121.22	112.60
8	H	214	GLY	CA-C-N	8.51	137.02	121.70
8	H	214	GLY	C-N-CA	8.51	137.02	121.70
9	I	56	ARG	CB-CA-C	8.51	127.35	110.42
6	F	1667	A	P-O3'-C3'	8.38	132.77	120.20
4	D	63	G	P-O3'-C3'	8.31	132.67	120.20
8	H	159	ILE	CA-C-N	8.28	136.60	121.70
8	H	159	ILE	C-N-CA	8.28	136.60	121.70
14	N	3	GLY	CA-C-N	8.03	136.15	121.70
14	N	3	GLY	C-N-CA	8.03	136.15	121.70
4	D	89	A	P-O3'-C3'	8.01	132.21	120.20
8	H	88	GLY	CA-C-N	7.92	135.96	121.70
8	H	88	GLY	C-N-CA	7.92	135.96	121.70
5	E	560	A	P-O3'-C3'	7.92	132.08	120.20
8	H	57	GLY	CA-C-N	7.82	135.78	121.70
8	H	57	GLY	C-N-CA	7.82	135.78	121.70
15	O	31	THR	CA-C-N	7.75	135.66	121.70
15	O	31	THR	C-N-CA	7.75	135.66	121.70
1	A	104	ASP	N-CA-C	7.75	127.31	110.80
9	I	36	ILE	CA-C-O	-7.75	113.22	121.27
8	H	212	ASP	CA-C-N	7.74	132.85	121.31
8	H	212	ASP	C-N-CA	7.74	132.85	121.31
8	H	63	GLU	N-CA-C	-7.73	94.33	110.80
14	N	13	SER	CA-C-N	7.72	135.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	13	SER	C-N-CA	7.72	135.59	121.70
8	H	102	PRO	N-CA-C	7.67	128.28	112.47
1	A	104	ASP	CB-CA-C	-7.63	95.23	110.42
8	H	60	THR	N-CA-CB	7.62	124.46	111.50
9	I	3	ARG	CA-C-N	7.62	135.42	121.70
9	I	3	ARG	C-N-CA	7.62	135.42	121.70
5	E	532	A	C2'-C3'-O3'	7.60	120.89	109.50
7	G	1917	A	P-O3'-C3'	7.49	131.44	120.20
14	N	37	SER	CA-C-N	7.48	135.17	121.70
14	N	37	SER	C-N-CA	7.48	135.17	121.70
11	K	111	ASN	CA-CB-CG	7.46	120.06	112.60
8	H	105	THR	CA-C-N	7.35	134.93	121.70
8	H	105	THR	C-N-CA	7.35	134.93	121.70
9	I	105	LYS	CA-C-N	7.34	134.92	121.70
9	I	105	LYS	C-N-CA	7.34	134.92	121.70
11	K	129	ASP	CA-C-N	7.28	129.90	120.44
11	K	129	ASP	C-N-CA	7.28	129.90	120.44
9	I	9	THR	CA-C-N	7.21	134.67	121.70
9	I	9	THR	C-N-CA	7.21	134.67	121.70
12	L	83	ASP	CA-C-N	7.16	134.59	121.70
12	L	83	ASP	C-N-CA	7.16	134.59	121.70
12	L	124	GLY	CA-C-N	7.15	134.57	121.70
12	L	124	GLY	C-N-CA	7.15	134.57	121.70
8	H	175	HIS	CA-C-N	7.07	130.70	120.38
8	H	175	HIS	C-N-CA	7.07	130.70	120.38
1	A	140	PRO	N-CA-C	-7.01	106.58	114.92
9	I	66	SER	CA-C-N	7.00	134.31	121.70
9	I	66	SER	C-N-CA	7.00	134.31	121.70
2	B	4	VAL	N-CA-C	-6.98	105.98	112.96
14	N	69	LEU	CA-C-O	-6.95	108.99	120.80
8	H	89	ALA	N-CA-CB	6.90	120.76	110.40
14	N	39	PRO	CB-CA-C	6.87	122.89	111.56
8	H	262	TRP	CA-C-N	6.85	134.03	121.70
8	H	262	TRP	C-N-CA	6.85	134.03	121.70
9	I	37	ASN	N-CA-CB	6.81	122.07	110.50
12	L	85	VAL	CA-C-N	6.76	133.87	121.70
12	L	85	VAL	C-N-CA	6.76	133.87	121.70
12	L	100	HIS	CA-CB-CG	6.74	120.54	113.80
8	H	12	THR	CA-C-N	6.72	133.79	121.70
8	H	12	THR	C-N-CA	6.72	133.79	121.70
8	H	84	ARG	N-CA-CB	6.72	121.92	110.50
12	L	89	LYS	N-CA-C	-6.70	99.39	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	VAL	CA-C-N	6.66	130.44	120.31
2	B	54	VAL	C-N-CA	6.66	130.44	120.31
9	I	39	TRP	N-CA-CB	6.63	121.78	110.50
14	N	56	THR	N-CA-CB	6.51	119.80	110.16
8	H	58	HIS	N-CA-CB	6.51	121.57	110.50
2	B	65	ILE	N-CA-C	-6.50	107.53	113.71
12	L	111	LEU	N-CA-CB	6.50	119.64	109.83
14	N	34	GLN	CA-C-N	6.49	133.37	121.70
14	N	34	GLN	C-N-CA	6.49	133.37	121.70
9	I	38	GLY	CA-C-N	6.45	133.31	121.70
9	I	38	GLY	C-N-CA	6.45	133.31	121.70
13	M	26	LYS	N-CA-CB	6.39	121.28	110.49
8	H	70	ALA	N-CA-C	-6.33	97.32	110.80
1	A	288	ASN	CA-C-N	6.29	124.20	120.24
1	A	288	ASN	C-N-CA	6.29	124.20	120.24
8	H	155	ASP	CA-C-N	6.29	129.34	120.28
8	H	155	ASP	C-N-CA	6.29	129.34	120.28
8	H	13	GLY	CA-C-N	6.27	132.99	121.70
8	H	13	GLY	C-N-CA	6.27	132.99	121.70
12	L	84	LYS	N-CA-CB	6.24	121.11	110.50
13	M	25	PHE	N-CA-CB	6.22	121.08	110.50
9	I	70	THR	CA-C-N	6.21	132.88	121.70
9	I	70	THR	C-N-CA	6.21	132.88	121.70
8	H	62	ALA	CA-C-N	6.19	133.36	121.54
8	H	62	ALA	C-N-CA	6.19	133.36	121.54
9	I	71	ALA	N-CA-CB	6.18	119.67	110.40
8	H	87	GLN	N-CA-C	6.17	128.29	111.00
1	A	402	ARG	CA-C-N	6.17	126.79	119.94
1	A	402	ARG	C-N-CA	6.17	126.79	119.94
2	B	29	ASP	CA-C-N	6.16	133.31	121.54
2	B	29	ASP	C-N-CA	6.16	133.31	121.54
11	K	138	ARG	N-CA-C	-6.16	104.93	112.88
1	A	404	HIS	CB-CG-CD2	-6.15	123.20	131.20
14	N	4	VAL	N-CA-CB	6.15	121.95	111.50
14	N	14	LYS	N-CA-CB	6.13	120.92	110.50
8	H	198	ARG	CA-C-N	6.12	133.23	121.54
8	H	198	ARG	C-N-CA	6.12	133.23	121.54
8	H	158	SER	CA-C-N	6.11	128.69	120.50
8	H	158	SER	C-N-CA	6.11	128.69	120.50
12	L	110	HIS	N-CA-C	-6.09	105.02	112.88
9	I	73	GLY	CA-C-N	6.08	132.64	121.70
9	I	73	GLY	C-N-CA	6.08	132.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	MET	CA-C-N	6.06	133.11	121.54
1	A	401	MET	C-N-CA	6.06	133.11	121.54
8	H	54	GLU	N-CA-CB	6.02	120.67	110.49
15	O	5	LYS	CB-CA-C	6.01	122.39	110.42
8	H	211	GLU	CA-C-N	6.00	133.01	121.54
8	H	211	GLU	C-N-CA	6.00	133.01	121.54
13	M	24	SER	CA-C-N	6.00	132.51	121.70
13	M	24	SER	C-N-CA	6.00	132.51	121.70
15	O	5	LYS	CA-C-N	5.99	132.47	121.70
15	O	5	LYS	C-N-CA	5.99	132.47	121.70
12	L	125	LYS	N-CA-CB	5.97	120.65	110.50
8	H	185	LYS	N-CA-C	5.96	127.69	111.00
9	I	110	THR	CA-C-N	5.94	132.89	121.54
9	I	110	THR	C-N-CA	5.94	132.89	121.54
1	A	111	LEU	N-CA-C	-5.93	105.95	112.72
13	M	79	ARG	CA-C-N	5.93	129.71	120.82
13	M	79	ARG	C-N-CA	5.93	129.71	120.82
1	A	316	LEU	N-CA-C	-5.92	105.31	113.18
11	K	91	ASN	CA-C-N	5.87	128.15	120.28
11	K	91	ASN	C-N-CA	5.87	128.15	120.28
12	L	4	GLN	CA-C-N	5.86	132.25	121.70
12	L	4	GLN	C-N-CA	5.86	132.25	121.70
1	A	324	TRP	N-CA-CB	5.86	120.39	110.49
1	A	407	THR	CB-CA-C	5.86	121.98	109.10
1	A	271	ARG	N-CA-CB	5.85	119.71	110.23
9	I	7	THR	N-CA-C	5.83	123.22	110.80
8	H	55	LYS	N-CA-C	5.83	127.31	111.00
2	B	19	ILE	CA-C-N	5.81	128.53	120.29
2	B	19	ILE	C-N-CA	5.81	128.53	120.29
8	H	83	GLY	CA-C-N	5.80	132.15	121.70
8	H	83	GLY	C-N-CA	5.80	132.15	121.70
9	I	24	VAL	CA-C-N	5.78	132.58	121.54
9	I	24	VAL	C-N-CA	5.78	132.58	121.54
13	M	80	ASN	CA-C-N	5.77	132.09	121.70
13	M	80	ASN	C-N-CA	5.77	132.09	121.70
3	C	72	PRO	N-CA-C	5.76	124.33	112.47
1	A	196	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	156	PHE	CA-CB-CG	5.74	119.54	113.80
12	L	37	LYS	N-CA-C	-5.74	106.90	114.31
11	K	137	ASN	N-CA-C	-5.74	104.85	112.94
9	I	4	TYR	CA-C-N	5.72	132.00	121.70
9	I	4	TYR	C-N-CA	5.72	132.00	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	74	ILE	O-C-N	-5.68	114.62	121.10
8	H	57	GLY	N-CA-C	-5.68	99.72	113.18
12	L	31	LEU	N-CA-C	-5.66	105.69	112.59
1	A	368	MET	CA-C-N	5.65	127.86	120.28
1	A	368	MET	C-N-CA	5.65	127.86	120.28
13	M	90	PHE	CA-CB-CG	5.63	119.43	113.80
8	H	243	HIS	CA-C-N	5.62	132.28	121.54
8	H	243	HIS	C-N-CA	5.62	132.28	121.54
1	A	251	VAL	CA-C-N	5.58	127.76	120.28
1	A	251	VAL	C-N-CA	5.58	127.76	120.28
8	H	173	GLY	CA-C-N	5.57	131.73	121.70
8	H	173	GLY	C-N-CA	5.57	131.73	121.70
1	A	287	SER	CA-C-N	5.57	128.06	120.54
1	A	287	SER	C-N-CA	5.57	128.06	120.54
12	L	22	ALA	CA-C-N	5.56	126.80	119.84
12	L	22	ALA	C-N-CA	5.56	126.80	119.84
14	N	50	SER	N-CA-C	-5.56	105.62	112.90
14	N	36	LEU	CA-C-N	5.55	131.70	121.70
14	N	36	LEU	C-N-CA	5.55	131.70	121.70
12	L	27	ARG	N-CA-C	-5.55	106.47	113.18
8	H	63	GLU	N-CA-CB	5.54	119.86	110.49
13	M	24	SER	N-CA-CB	5.54	119.85	110.49
9	I	145	HIS	CA-CB-CG	5.52	119.32	113.80
8	H	143	GLU	CA-C-N	5.52	129.08	120.75
8	H	143	GLU	C-N-CA	5.52	129.08	120.75
1	A	335	ALA	CA-C-N	5.50	131.61	121.70
1	A	335	ALA	C-N-CA	5.50	131.61	121.70
13	M	65	LYS	CA-C-N	5.49	131.58	121.70
13	M	65	LYS	C-N-CA	5.49	131.58	121.70
1	A	444	GLY	CA-C-N	5.45	127.58	120.28
1	A	444	GLY	C-N-CA	5.45	127.58	120.28
13	M	64	VAL	CA-C-N	5.44	129.93	120.68
13	M	64	VAL	C-N-CA	5.44	129.93	120.68
9	I	3	ARG	CB-CA-C	5.43	121.23	110.42
13	M	81	GLU	CA-C-N	5.43	127.56	120.28
13	M	81	GLU	C-N-CA	5.43	127.56	120.28
7	G	1917	A	C2'-C3'-O3'	5.43	117.64	109.50
9	I	106	GLY	CA-C-N	5.42	131.90	121.54
9	I	106	GLY	C-N-CA	5.42	131.90	121.54
3	C	88	HIS	CA-C-N	5.41	127.87	120.35
3	C	88	HIS	C-N-CA	5.41	127.87	120.35
8	H	221	ASN	N-CA-CB	5.41	119.62	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	73	U	C5'-C4'-C3'	-5.37	107.94	116.00
14	N	40	SER	CA-C-N	5.37	131.36	121.70
14	N	40	SER	C-N-CA	5.37	131.36	121.70
4	D	49	G	P-O5'-C5'	5.36	128.94	120.90
1	A	104	ASP	CA-CB-CG	5.35	117.95	112.60
8	H	72	ALA	N-CA-CB	5.35	119.54	110.49
9	I	63	PHE	N-CA-C	-5.35	103.91	110.65
8	H	86	GLY	N-CA-C	-5.35	100.51	113.18
1	A	278	THR	N-CA-CB	5.34	119.84	111.56
14	N	67	ARG	N-CA-CB	-5.33	102.40	110.92
4	D	72	A	C5'-C4'-C3'	-5.32	108.02	116.00
2	B	6	GLN	N-CA-C	-5.32	100.83	108.60
1	A	423	PHE	CA-C-N	5.32	126.00	119.99
1	A	423	PHE	C-N-CA	5.32	126.00	119.99
8	H	92	ASN	CA-C-N	5.31	131.69	121.54
8	H	92	ASN	C-N-CA	5.31	131.69	121.54
8	H	20	LEU	CA-C-N	5.27	125.26	119.89
8	H	20	LEU	C-N-CA	5.27	125.26	119.89
9	I	57	ALA	N-CA-C	5.25	125.70	111.00
11	K	130	TYR	N-CA-CB	-5.22	102.43	110.01
15	O	20	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	416	TYR	CA-C-N	5.22	123.53	120.24
1	A	416	TYR	C-N-CA	5.22	123.53	120.24
4	D	65	A	C2'-C3'-O3'	5.22	121.53	113.70
8	H	111	VAL	N-CA-CB	5.21	119.13	111.52
9	I	56	ARG	O-C-N	-5.20	115.67	122.59
9	I	90	PHE	CA-CB-CG	5.18	118.98	113.80
9	I	9	THR	CB-CA-C	5.18	120.73	110.42
9	I	105	LYS	CA-C-O	-5.18	115.36	120.70
13	M	78	LYS	N-CA-CB	5.18	119.30	110.50
11	K	62	VAL	N-CA-CB	5.17	119.77	111.23
8	H	59	GLN	N-CA-CB	5.17	117.72	110.12
1	A	107	LYS	N-CA-CB	5.16	119.20	110.49
8	H	77	VAL	CA-CB-CG1	5.13	119.12	110.40
1	A	358	PRO	CA-C-N	5.13	127.48	120.46
1	A	358	PRO	C-N-CA	5.13	127.48	120.46
1	A	200	THR	N-CA-CB	5.11	119.13	110.49
1	A	230	LEU	N-CA-C	-5.11	106.89	112.72
1	A	441	ILE	N-CA-C	-5.11	108.00	112.90
14	N	4	VAL	CA-C-N	5.11	131.29	121.54
14	N	4	VAL	C-N-CA	5.11	131.29	121.54
8	H	213	ASN	CA-C-N	5.10	130.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	213	ASN	C-N-CA	5.10	130.88	121.70
12	L	49	PRO	CA-C-N	5.08	127.30	120.50
12	L	49	PRO	C-N-CA	5.08	127.30	120.50
1	A	208	GLU	N-CA-C	-5.07	104.39	110.88
9	I	104	ALA	CA-C-N	5.07	127.34	120.44
9	I	104	ALA	C-N-CA	5.07	127.34	120.44
1	A	289	ILE	CA-C-N	5.06	125.09	119.32
1	A	289	ILE	C-N-CA	5.06	125.09	119.32
8	H	140	HIS	CA-CB-CG	5.05	118.85	113.80
8	H	251	THR	N-CA-C	-5.04	101.71	109.52
14	N	67	ARG	N-CA-C	-5.04	106.44	112.59
1	A	215	ALA	CA-C-N	5.04	127.03	120.28
1	A	215	ALA	C-N-CA	5.04	127.03	120.28
9	I	6	ALA	CA-C-N	5.04	131.16	121.54
9	I	6	ALA	C-N-CA	5.04	131.16	121.54
9	I	3	ARG	O-C-N	-5.02	115.91	122.59
1	A	411	HIS	CA-C-N	5.02	127.00	120.28
1	A	411	HIS	C-N-CA	5.02	127.00	120.28
8	H	199	TRP	N-CA-CB	5.01	118.97	110.49
9	I	112	LEU	CA-C-N	5.01	131.11	121.54
9	I	112	LEU	C-N-CA	5.01	131.11	121.54
8	H	192	GLY	CA-C-N	5.00	126.99	120.28
8	H	192	GLY	C-N-CA	5.00	126.99	120.28

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Sidechain
1	A	270	ALA	Peptide
1	A	271	ARG	Sidechain
1	A	336	TYR	Peptide
1	A	404	HIS	Sidechain
3	C	71	VAL	Peptide
4	D	46	G	Sidechain
4	D	50	C	Sidechain
4	D	55	U	Sidechain
4	D	56	G	Sidechain
4	D	62	C	Sidechain
4	D	65	A	Sidechain
4	D	66	A	Sidechain
4	D	76	C	Sidechain

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Mol	Chain	Res	Type	Group
4	D	77	A	Sidechain
4	D	87	G	Sidechain
5	E	536	A	Sidechain
5	E	541	G	Sidechain
5	E	543	A	Sidechain
5	E	545	A	Sidechain
5	E	552	G	Sidechain
5	E	558	G	Sidechain
6	F	1662	A	Sidechain
6	F	1667	A	Sidechain
6	F	1673	A	Sidechain
7	G	1925	C	Sidechain
8	H	102	PRO	Peptide
8	H	110	ASN	Peptide
8	H	141	ARG	Sidechain
8	H	148	ILE	Peptide
8	H	187	LEU	Peptide
8	H	197	ARG	Peptide
8	H	209	TYR	Sidechain
8	H	212	ASP	Peptide
8	H	63	GLU	Peptide
8	H	73	ARG	Sidechain
8	H	76	ARG	Peptide
8	H	92	ASN	Peptide
9	I	122	ALA	Peptide
9	I	23	ARG	Sidechain
9	I	30	ARG	Sidechain
9	I	4	TYR	Sidechain
9	I	47	TYR	Sidechain
9	I	82	ARG	Sidechain
11	K	105	VAL	Peptide
11	K	57	LEU	Peptide
11	K	60	TYR	Sidechain
12	L	121	ARG	Peptide
12	L	125	LYS	Peptide
12	L	23	PRO	Peptide
12	L	40	ARG	Sidechain
12	L	52	ARG	Sidechain
13	M	10	ARG	Sidechain
13	M	74	ARG	Sidechain
14	N	32	LYS	Peptide
14	N	38	ARG	Sidechain

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Mol	Chain	Res	Type	Group
15	O	19	GLN	Peptide
15	O	23	LEU	Peptide
15	O	24	PRO	Peptide
15	O	30	ARG	Sidechain
15	O	32	ASN	Peptide
15	O	36	ARG	Peptide
15	O	4	GLN	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	A	3675	0	3798	45	0
2	B	543	0	577	1	0
3	C	281	0	294	0	0
4	D	1347	0	678	2	0
5	E	740	0	369	1	0
6	F	536	0	272	1	0
7	G	296	0	154	0	0
8	H	2039	0	2106	16	0
9	I	1212	0	1231	9	0
10	J	410	0	452	0	0
11	K	663	0	699	5	0
12	L	1002	0	1093	2	0
13	M	706	0	741	3	0
14	N	547	0	613	8	0
15	O	316	0	349	2	0
All	All	14313	0	13426	86	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 3.

All (86) 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)
1:A:5:PHE:CD2	1:A:5:PHE:CE2	1.81	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CD1	1:A:5:PHE:CE1	1.80	1.66
1:A:5:PHE:CE2	1:A:5:PHE:CZ	1.79	1.64
1:A:5:PHE:CD1	1:A:5:PHE:CG	1.81	1.61
1:A:5:PHE:CE1	1:A:5:PHE:CZ	1.80	1.61
1:A:5:PHE:CD2	1:A:5:PHE:CG	1.82	1.59
1:A:5:PHE:CZ	1:A:104:ASP:HA	1.56	1.37
1:A:5:PHE:CE1	1:A:104:ASP:HA	1.82	1.14
1:A:5:PHE:CG	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CD2	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CE1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CD1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CE2	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CZ	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CD1	1:A:104:ASP:N	2.32	0.96
1:A:5:PHE:CD2	1:A:104:ASP:N	2.33	0.96
1:A:5:PHE:CG	1:A:104:ASP:N	2.33	0.95
1:A:5:PHE:CE2	1:A:104:ASP:N	2.35	0.94
1:A:5:PHE:CE1	1:A:104:ASP:N	2.37	0.93
1:A:5:PHE:CZ	1:A:104:ASP:N	2.39	0.90
1:A:5:PHE:CE2	1:A:104:ASP:HA	2.14	0.82
1:A:5:PHE:CD1	1:A:104:ASP:C	2.62	0.78
11:K:100:LYS:HA	11:K:105:VAL:HG22	1.67	0.76
1:A:5:PHE:CD2	1:A:104:ASP:CB	2.72	0.72
1:A:268:LYS:HB2	14:N:38:ARG:HH21	1.65	0.61
1:A:5:PHE:CE2	1:A:104:ASP:HB2	2.36	0.60
5:E:539:U:H3	5:E:546:G:H1	1.50	0.59
1:A:5:PHE:CE2	1:A:104:ASP:CB	2.86	0.58
1:A:5:PHE:CD2	1:A:103:GLY:C	2.81	0.57
9:I:57:ALA:HB3	9:I:82:ARG:O	2.06	0.56
1:A:277:ASN:H	14:N:38:ARG:HH22	1.56	0.55
12:L:56:VAL:HG22	12:L:106:ILE:HG22	1.88	0.54
14:N:39:PRO:HB2	14:N:40:SER:C	2.32	0.54
1:A:94:LEU:HB3	1:A:112:PHE:CG	2.42	0.54
1:A:277:ASN:H	14:N:38:ARG:NH2	2.07	0.53
8:H:184:SER:HA	8:H:186:LYS:H	1.73	0.53
1:A:275:GLN:HB3	14:N:38:ARG:CZ	2.40	0.52
11:K:105:VAL:HG23	11:K:106:ASP:HA	1.91	0.52
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.92	0.52
13:M:44:MET:HE1	13:M:78:LYS:HB2	1.93	0.51
8:H:58:HIS:CG	8:H:58:HIS:O	2.64	0.51
14:N:41:LEU:H	14:N:44:ILE:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:52:VAL:HG22	8:H:53:SER:H	1.76	0.50
8:H:198:ARG:CG	8:H:199:TRP:H	2.24	0.50
1:A:5:PHE:CD1	1:A:5:PHE:CB	2.84	0.50
2:B:20:ARG:HA	11:K:137:ASN:HD21	1.76	0.50
9:I:3:ARG:HB2	9:I:4:TYR:HA	1.95	0.49
8:H:63:GLU:CD	8:H:64:SER:H	2.20	0.49
1:A:404:HIS:CE1	6:F:1657:C:H1'	2.48	0.49
8:H:184:SER:HA	8:H:186:LYS:N	2.28	0.49
8:H:57:GLY:HA3	8:H:58:HIS:HB2	1.95	0.48
1:A:268:LYS:CB	14:N:38:ARG:HH21	2.27	0.48
1:A:94:LEU:HB3	1:A:112:PHE:CD1	2.49	0.47
8:H:83:GLY:HA3	8:H:84:ARG:HB2	1.96	0.47
14:N:39:PRO:HA	14:N:41:LEU:HD22	1.96	0.47
9:I:9:THR:HG23	9:I:10:ASN:HA	1.98	0.46
13:M:82:GLU:H	13:M:82:GLU:CD	2.22	0.46
1:A:273:ARG:HA	1:A:273:ARG:HE	1.81	0.46
1:A:5:PHE:CG	1:A:104:ASP:C	2.93	0.45
9:I:108:ASP:HB2	9:I:109:ALA:HA	1.97	0.45
1:A:5:PHE:CD2	1:A:104:ASP:HB2	2.52	0.45
1:A:5:PHE:CD2	1:A:103:GLY:O	2.70	0.45
1:A:269:SER:HB2	1:A:403:GLY:H	1.82	0.45
13:M:44:MET:HE3	13:M:46:THR:HB	1.99	0.45
8:H:152:VAL:HG12	8:H:153:SER:H	1.83	0.44
9:I:51:VAL:HG13	9:I:57:ALA:H	1.83	0.44
1:A:64:TRP:H	1:A:334:ARG:HE	1.65	0.44
1:A:271:ARG:HD3	1:A:272:TYR:CE2	2.53	0.44
8:H:77:VAL:HG13	8:H:78:GLY:N	2.32	0.44
8:H:222:VAL:HB	8:H:225:VAL:HG12	1.99	0.43
8:H:74:ILE:H	8:H:75:PRO:HA	1.83	0.43
11:K:105:VAL:HG23	11:K:106:ASP:CA	2.49	0.43
11:K:73:MET:HA	11:K:73:MET:HE2	2.02	0.42
1:A:108:ASP:HB2	1:A:112:PHE:CE1	2.55	0.42
9:I:107:LEU:HD12	9:I:107:LEU:H	1.85	0.42
9:I:24:VAL:HG11	9:I:87:SER:HA	2.02	0.42
12:L:10:SER:N	12:L:11:ASP:HB2	2.35	0.42
8:H:74:ILE:N	8:H:75:PRO:HA	2.35	0.41
8:H:13:GLY:H	8:H:14:GLU:HB2	1.86	0.41
4:D:55:U:C2	4:D:56:G:C8	3.08	0.41
9:I:40:GLU:H	9:I:40:GLU:CD	2.29	0.41
1:A:272:TYR:CE2	15:O:24:PRO:HG3	2.55	0.41
9:I:138:LYS:H	9:I:138:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:CE2	1:A:136:MET:HE3	2.56	0.41
8:H:199:TRP:HA	8:H:200:THR:HB	2.02	0.41
4:D:75:G:C2	15:O:27:ILE:HD13	2.56	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	A	474/476 (100%)	402 (85%)	46 (10%)	26 (6%)	1	14
2	B	66/68 (97%)	60 (91%)	2 (3%)	4 (6%)	1	12
3	C	34/96 (35%)	27 (79%)	4 (12%)	3 (9%)	0	8
8	H	267/362 (74%)	181 (68%)	38 (14%)	48 (18%)	0	2
9	I	151/184 (82%)	119 (79%)	15 (10%)	17 (11%)	0	5
10	J	51/189 (27%)	46 (90%)	4 (8%)	1 (2%)	6	31
11	K	81/142 (57%)	73 (90%)	5 (6%)	3 (4%)	2	19
12	L	125/127 (98%)	101 (81%)	9 (7%)	15 (12%)	0	4
13	M	82/113 (73%)	65 (79%)	8 (10%)	9 (11%)	0	5
14	N	67/120 (56%)	59 (88%)	3 (4%)	5 (8%)	1	10
15	O	35/51 (69%)	26 (74%)	0	9 (26%)	0	1
All	All	1433/1928 (74%)	1159 (81%)	134 (9%)	140 (10%)	1	7

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	104	ASP
1	A	108	ASP

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Mol	Chain	Res	Type
1	A	110	ALA
1	A	142	GLU
1	A	280	PRO
1	A	402	ARG
1	A	466	SER
1	A	473	ALA
2	B	30	ARG
2	B	41	ALA
3	C	71	VAL
3	C	72	PRO
8	H	3	ARG
8	H	28	ALA
8	H	54	GLU
8	H	55	LYS
8	H	58	HIS
8	H	60	THR
8	H	63	GLU
8	H	69	ARG
8	H	70	ALA
8	H	72	ALA
8	H	74	ILE
8	H	76	ARG
8	H	87	GLN
8	H	89	ALA
8	H	98	ARG
8	H	102	PRO
8	H	103	THR
8	H	146	PRO
8	H	185	LYS
8	H	187	LEU
8	H	198	ARG
8	H	199	TRP
8	H	200	THR
8	H	212	ASP
8	H	222	VAL
8	H	244	LEU
8	H	262	TRP
9	I	37	ASN
9	I	57	ALA
9	I	67	ILE
9	I	107	LEU
9	I	111	LYS

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Mol	Chain	Res	Type
9	I	113	TYR
9	I	123	PRO
9	I	143	PRO
12	L	23	PRO
12	L	85	VAL
12	L	125	LYS
13	M	78	LYS
13	M	79	ARG
13	M	90	PHE
14	N	4	VAL
14	N	14	LYS
14	N	39	PRO
15	O	20	ASN
15	O	22	PRO
15	O	23	LEU
1	A	107	LYS
1	A	141	SER
1	A	200	THR
1	A	226	LYS
1	A	324	TRP
2	B	66	VAL
8	H	13	GLY
8	H	81	GLY
8	H	93	MET
8	H	160	GLN
8	H	173	GLY
8	H	264	SER
9	I	7	THR
9	I	71	ALA
11	K	62	VAL
12	L	6	LEU
12	L	11	ASP
12	L	45	ILE
12	L	46	LYS
12	L	87	LYS
12	L	96	PRO
12	L	113	LYS
12	L	122	LYS
13	M	25	PHE
13	M	26	LYS
13	M	69	TYR
14	N	37	SER

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Mol	Chain	Res	Type
15	O	5	LYS
15	O	6	SER
15	O	24	PRO
1	A	57	ASP
1	A	70	ALA
1	A	335	ALA
1	A	349	GLU
2	B	5	MET
8	H	107	ARG
8	H	132	ALA
8	H	221	ASN
8	H	265	GLU
9	I	2	ALA
9	I	3	ARG
9	I	25	SER
9	I	54	HIS
11	K	109	LYS
12	L	36	SER
12	L	84	LYS
14	N	5	LYS
15	O	25	GLN
1	A	105	THR
1	A	272	TYR
3	C	90	TRP
8	H	101	ALA
8	H	131	VAL
8	H	215	ILE
9	I	39	TRP
11	K	131	ASP
12	L	97	ILE
13	M	24	SER
1	A	19	ILE
1	A	77	MET
1	A	443	SER
8	H	52	VAL
8	H	84	ARG
8	H	106	TRP
8	H	196	ASN
9	I	131	ARG
10	J	19	LYS
12	L	86	THR
15	O	34	THR

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Mol	Chain	Res	Type
1	A	382	VAL
8	H	4	PRO
8	H	205	PRO
13	M	51	LEU
13	M	64	VAL
1	A	80	GLY
9	I	84	PRO
15	O	35	ILE
8	H	86	GLY
1	A	8	VAL
8	H	77	VAL

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	A	398/398 (100%)	389 (98%)	9 (2%)	44	64
2	B	59/59 (100%)	56 (95%)	3 (5%)	21	42
3	C	32/74 (43%)	31 (97%)	1 (3%)	35	56
8	H	209/288 (73%)	186 (89%)	23 (11%)	6	20
9	I	124/146 (85%)	105 (85%)	19 (15%)	3	12
10	J	44/154 (29%)	41 (93%)	3 (7%)	14	36
11	K	74/118 (63%)	63 (85%)	11 (15%)	3	12
12	L	110/110 (100%)	96 (87%)	14 (13%)	4	16
13	M	74/97 (76%)	67 (90%)	7 (10%)	8	25
14	N	62/105 (59%)	56 (90%)	6 (10%)	8	24
15	O	33/46 (72%)	28 (85%)	5 (15%)	3	12
All	All	1219/1595 (76%)	1118 (92%)	101 (8%)	12	30

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	25	LYS
1	A	68	ILE
1	A	226	LYS
1	A	232	GLU
1	A	255	VAL
1	A	263	VAL
1	A	327	THR
1	A	407	THR
2	B	5	MET
2	B	32	GLU
2	B	54	VAL
3	C	72	PRO
8	H	4	PRO
8	H	35	VAL
8	H	43	ASN
8	H	46	LYS
8	H	48	GLN
8	H	77	VAL
8	H	98	ARG
8	H	103	THR
8	H	119	ARG
8	H	131	VAL
8	H	136	LEU
8	H	140	HIS
8	H	145	ILE
8	H	155	ASP
8	H	159	ILE
8	H	161	LYS
8	H	162	THR
8	H	164	GLU
8	H	180	LYS
8	H	201	GLN
8	H	215	ILE
8	H	233	LEU
8	H	243	HIS
9	I	36	ILE
9	I	40	GLU
9	I	43	LYS
9	I	46	LYS
9	I	51	VAL
9	I	54	HIS
9	I	59	PRO

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Mol	Chain	Res	Type
9	I	66	SER
9	I	67	ILE
9	I	72	GLN
9	I	76	PHE
9	I	79	THR
9	I	80	LYS
9	I	94	LEU
9	I	107	LEU
9	I	112	LEU
9	I	120	ASN
9	I	144	SER
9	I	149	VAL
10	J	39	ASN
10	J	47	ASN
10	J	53	LYS
11	K	65	GLN
11	K	67	ILE
11	K	70	GLU
11	K	74	LYS
11	K	100	LYS
11	K	111	ASN
11	K	114	VAL
11	K	117	ASN
11	K	120	LYS
11	K	123	TYR
11	K	135	ILE
12	L	28	ARG
12	L	37	LYS
12	L	52	ARG
12	L	57	LEU
12	L	64	LYS
12	L	77	LYS
12	L	87	LYS
12	L	95	VAL
12	L	98	ASN
12	L	108	LYS
12	L	111	LEU
12	L	113	LYS
12	L	122	LYS
12	L	125	LYS
13	M	20	LEU
13	M	24	SER

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Mol	Chain	Res	Type
13	M	38	LYS
13	M	47	ASP
13	M	67	VAL
13	M	73	LEU
13	M	86	LYS
14	N	5	LYS
14	N	9	LEU
14	N	17	LEU
14	N	34	GLN
14	N	38	ARG
14	N	39	PRO
15	O	17	LYS
15	O	18	LYS
15	O	22	PRO
15	O	23	LEU
15	O	26	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	47	GLN
1	A	72	ASN
1	A	92	GLN
1	A	113	ASN
1	A	170	GLN
1	A	202	ASN
1	A	218	HIS
1	A	259	GLN
1	A	275	GLN
1	A	277	ASN
1	A	343	HIS
1	A	360	HIS
1	A	397	GLN
1	A	398	GLN
2	B	13	GLN
2	B	58	HIS
8	H	5	GLN
8	H	18	ASN
8	H	36	HIS
8	H	43	ASN
8	H	175	HIS

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Mol	Chain	Res	Type
8	H	213	ASN
9	I	116	HIS
9	I	120	ASN
9	I	133	HIS
12	L	4	GLN
12	L	91	ASN
12	L	98	ASN
13	M	15	ASN
14	N	20	GLN
14	N	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63 (98%)	28 (45%)	10 (16%)
5	E	33/34 (97%)	9 (27%)	3 (9%)
6	F	24/25 (96%)	3 (12%)	0
7	G	14/14 (100%)	6 (42%)	2 (14%)
All	All	133/136 (97%)	46 (34%)	15 (11%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	49	G
4	D	51	G
4	D	52	A
4	D	56	G
4	D	59	A
4	D	62	C
4	D	63	G
4	D	64	U
4	D	66	A
4	D	68	G
4	D	70	G
4	D	71	A
4	D	79	A
4	D	82	U
4	D	83	C
4	D	84	C
4	D	85	G

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Mol	Chain	Res	Type
4	D	86	U
4	D	87	G
4	D	88	A
4	D	90	U
4	D	91	C
4	D	92	A
4	D	94	C
4	D	95	G
4	D	97	A
4	D	98	U
5	E	532	A
5	E	533	A
5	E	534	G
5	E	553	A
5	E	556	A
5	E	557	A
5	E	558	G
5	E	560	A
5	E	561	C
6	F	1665	G
6	F	1666	C
6	F	1668	G
7	G	1918	C
7	G	1921	G
7	G	1922	U
7	G	1927	C
7	G	1929	G
7	G	1930	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	51	G
4	D	55	U
4	D	63	G
4	D	65	A
4	D	69	U
4	D	89	A
4	D	90	U
4	D	93	U
4	D	96	A

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Mol	Chain	Res	Type
5	E	532	A
5	E	558	G
5	E	560	A
7	G	1917	A
7	G	1926	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

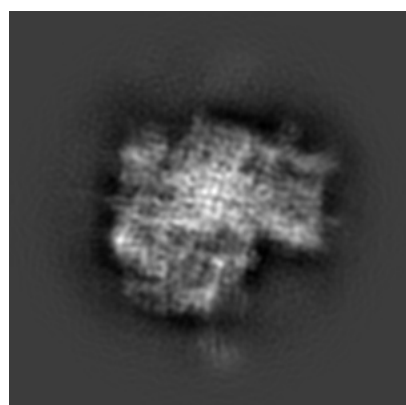
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1652. These allow visual inspection of the internal detail of the map and identification of artifacts.

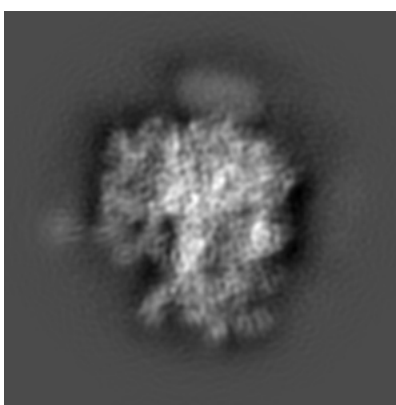
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

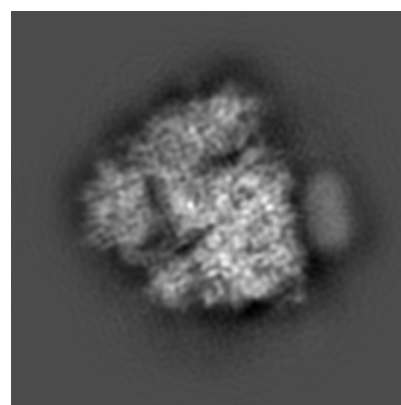
6.1.1 Primary map



X



Y

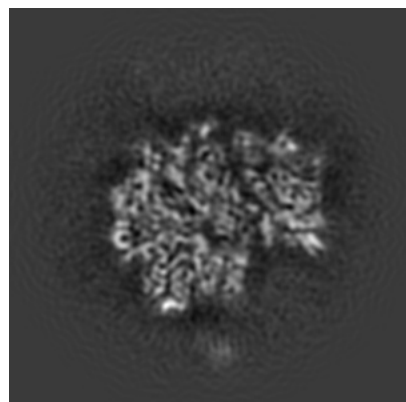


Z

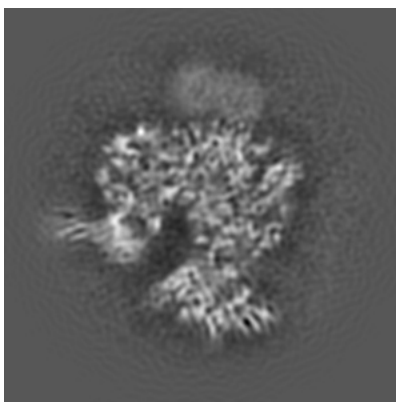
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

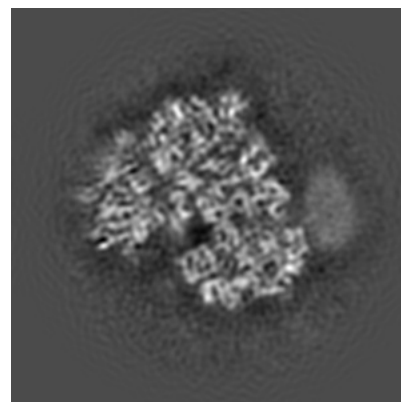
6.2.1 Primary map



X Index: 184



Y Index: 184

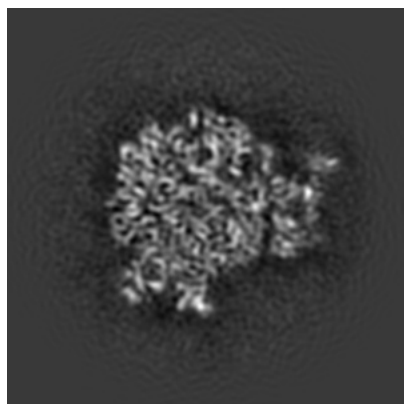


Z Index: 184

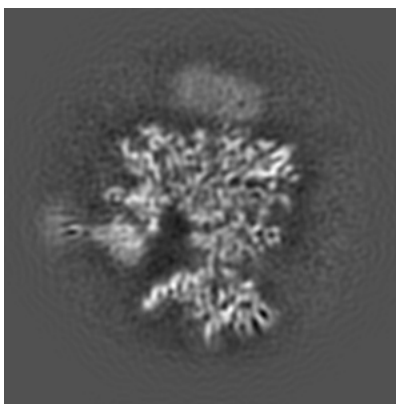
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

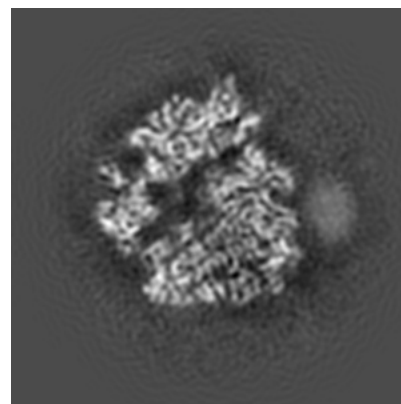
6.3.1 Primary map



X Index: 214



Y Index: 191

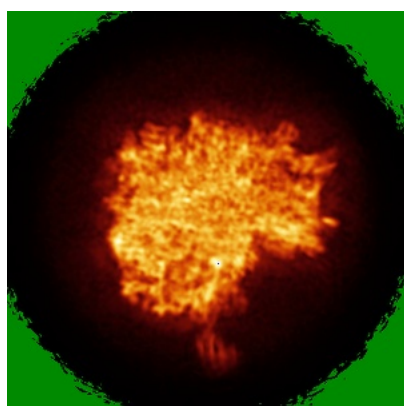


Z Index: 168

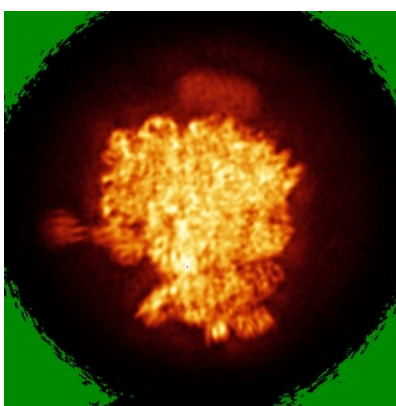
The images above show the largest variance slices of the map in three orthogonal directions.

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

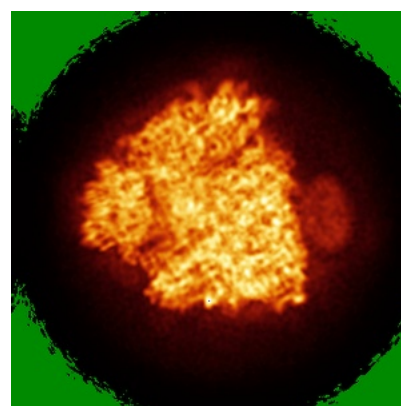
6.4.1 Primary map



X



Y



Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

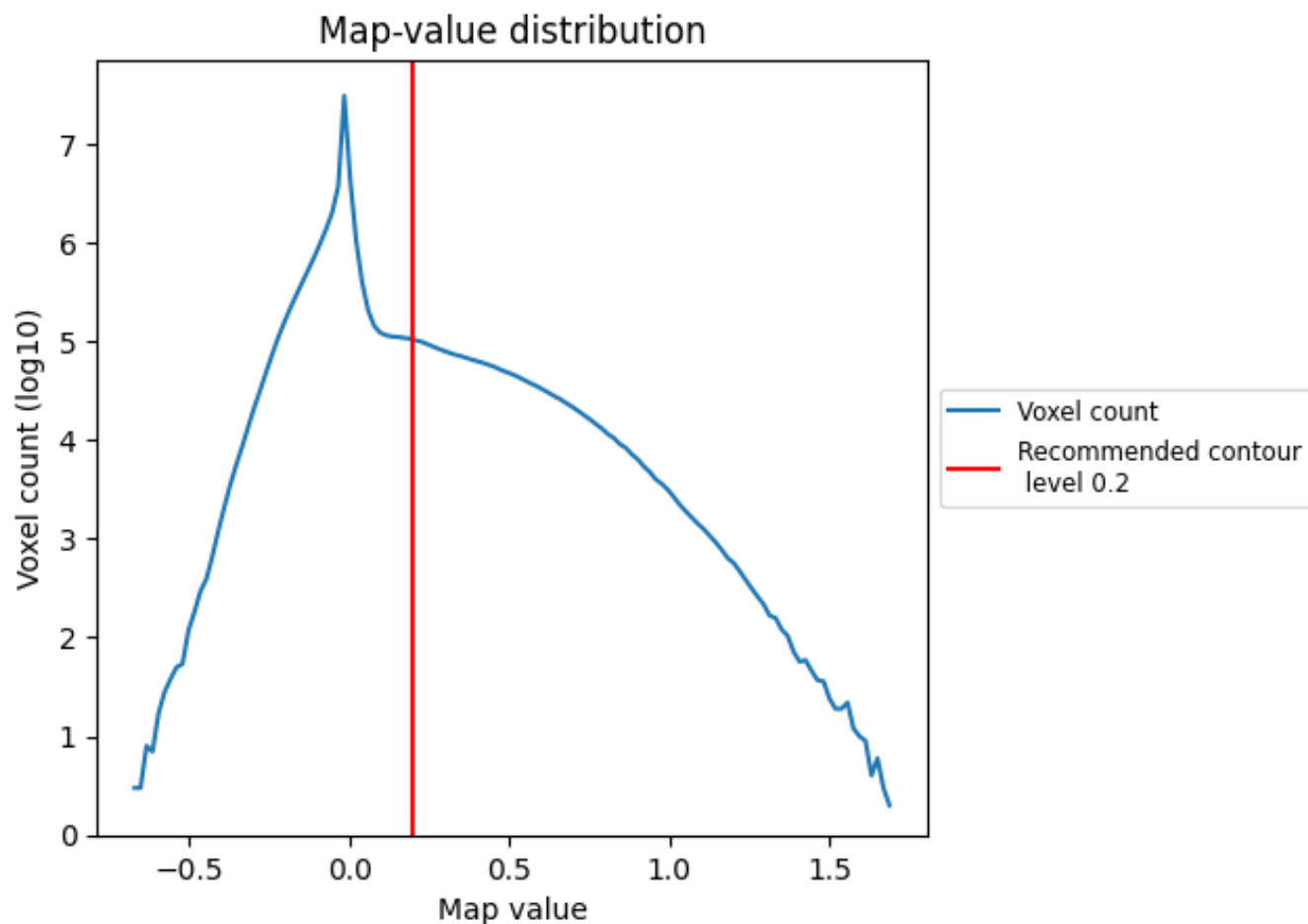
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

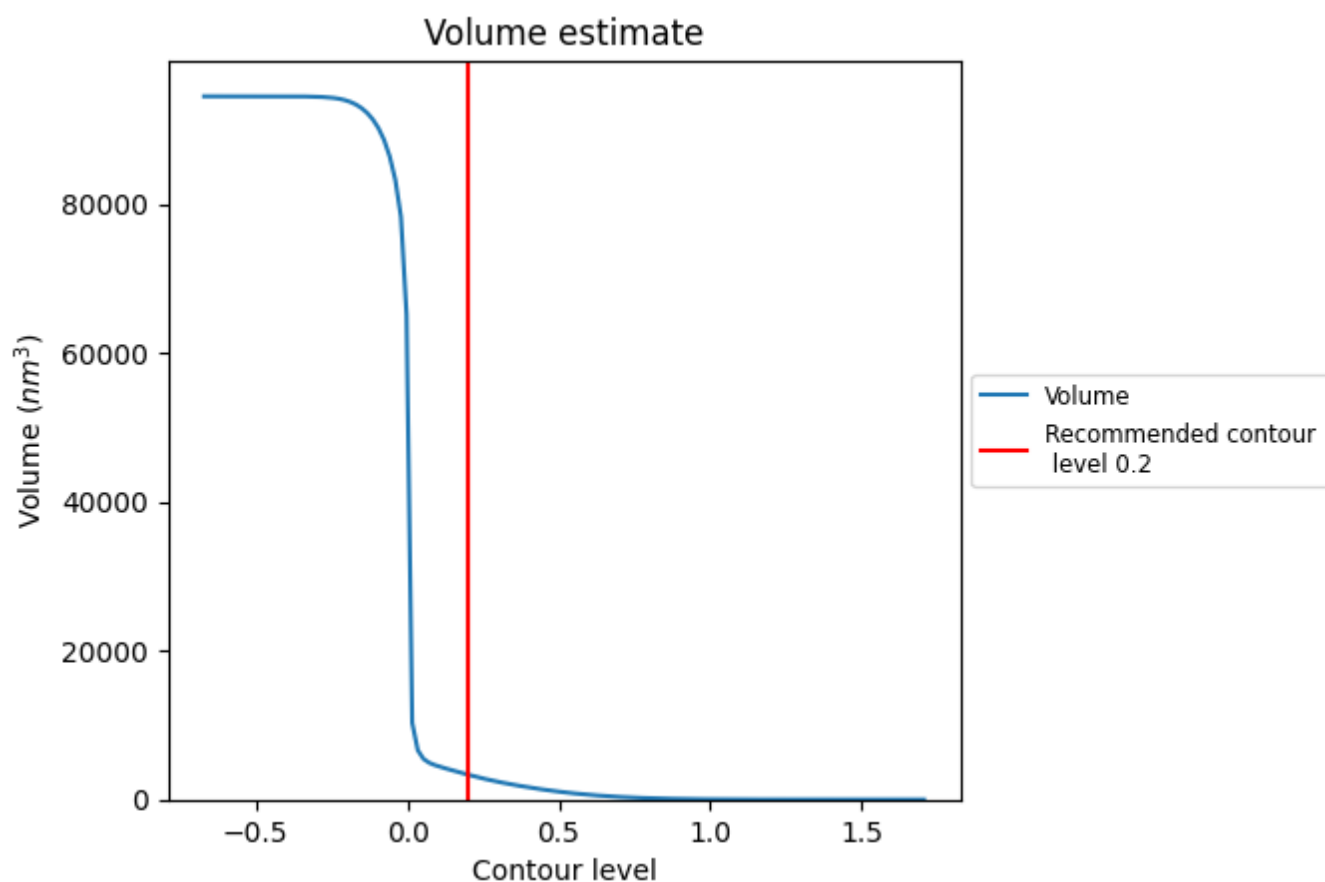
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

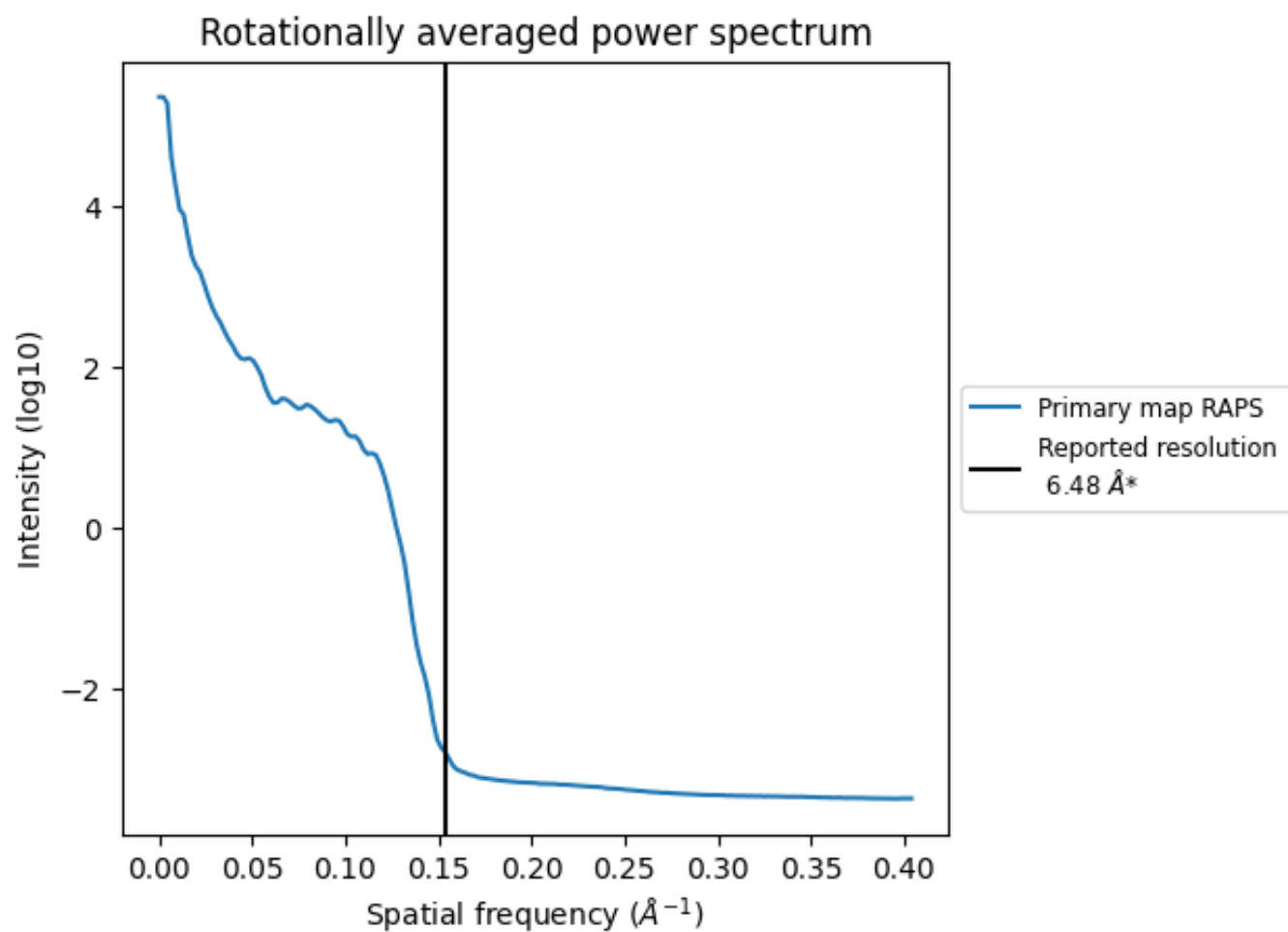
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3348 nm^3 ; this corresponds to an approximate mass of 3024 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 0.154 Å⁻¹

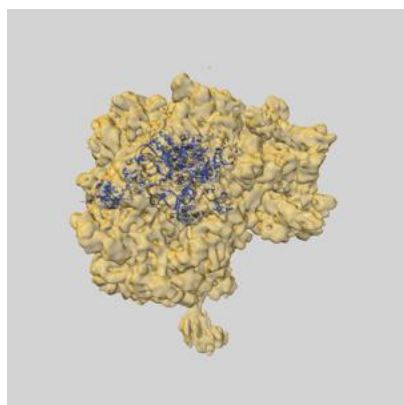
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

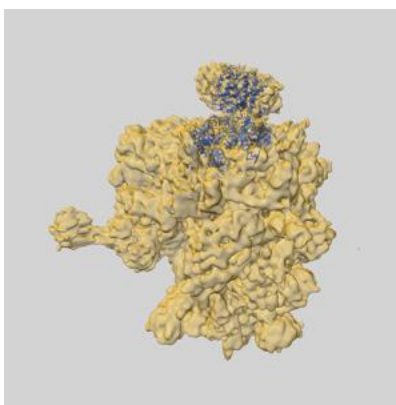
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1652 and PDB model 2WWB. Per-residue inclusion information can be found in section [3](#) on page [7](#).

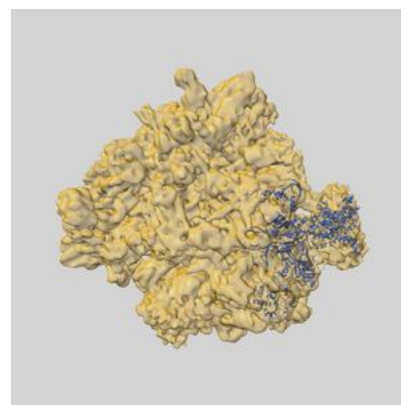
9.1 Map-model overlay [i](#)



X



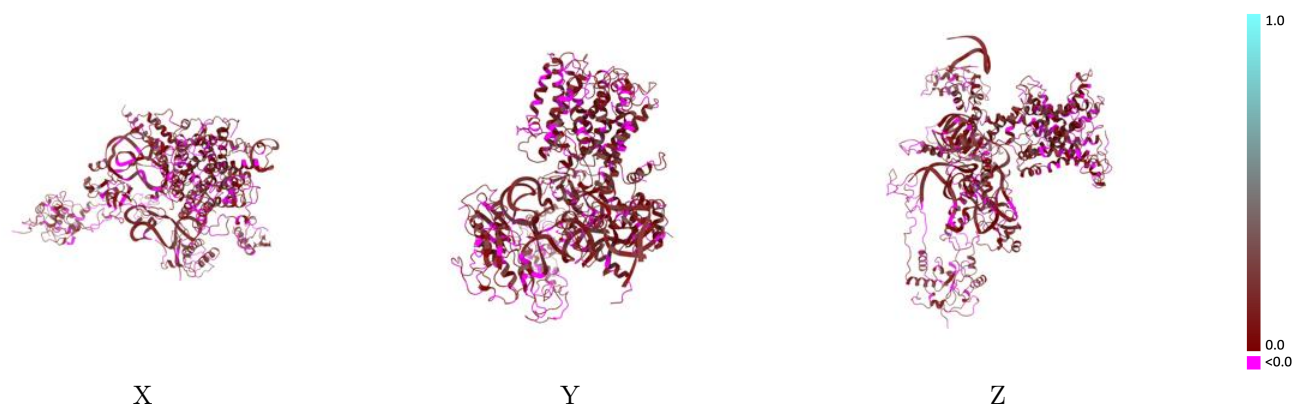
Y



Z

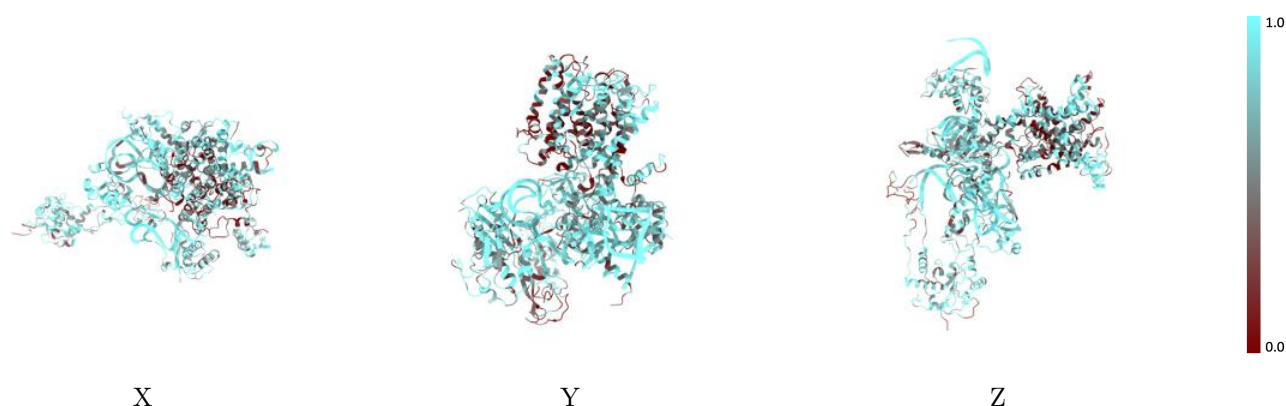
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



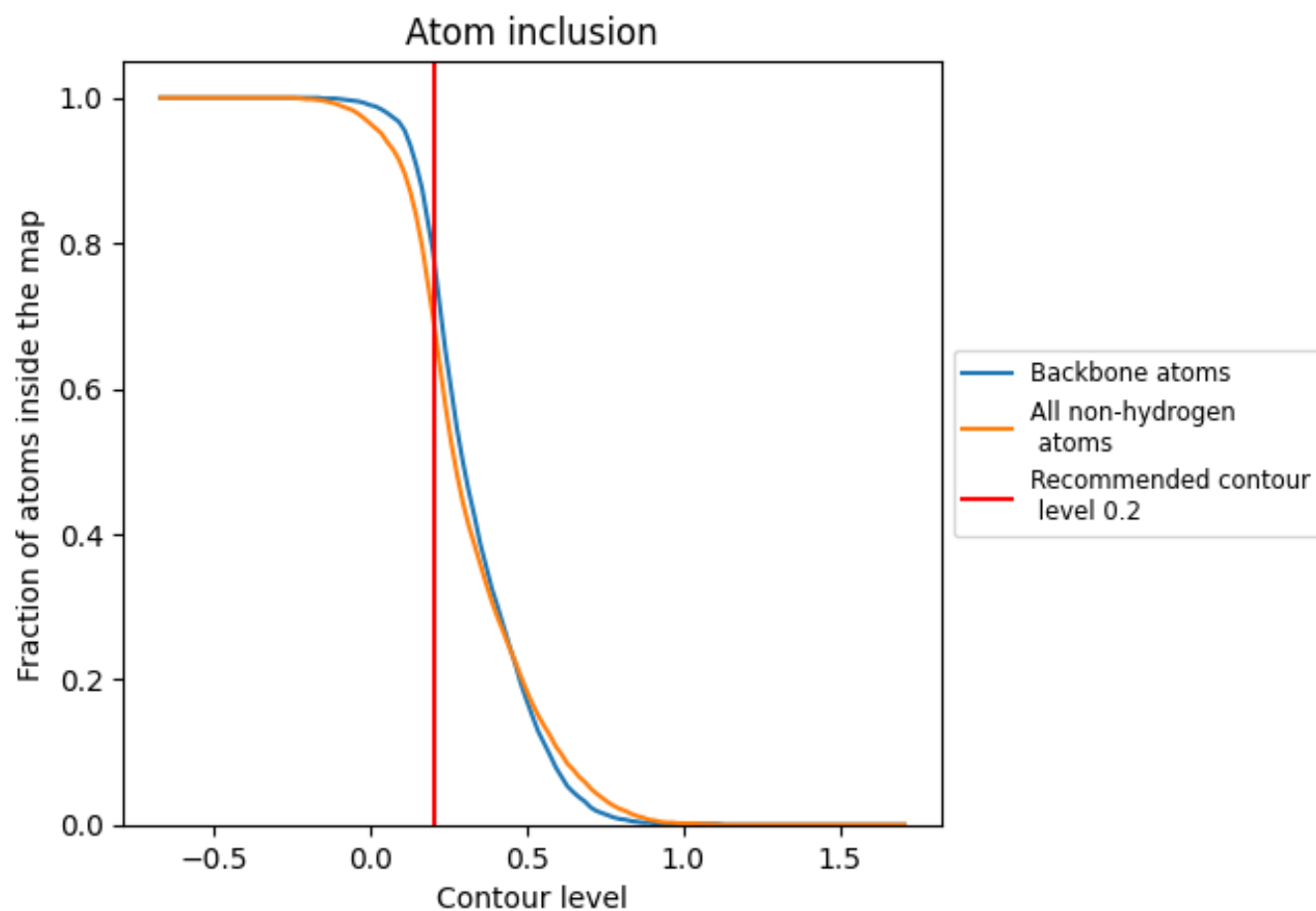
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.0920
A	 0.5780	 0.0860
B	 0.6690	 0.1140
C	 0.3970	 0.0410
D	 0.8190	 0.0880
E	 0.9350	 0.1460
F	 0.8770	 0.1340
G	 0.9430	 0.1730
H	 0.6630	 0.0690
I	 0.6890	 0.0790
J	 0.6670	 0.1180
K	 0.6500	 0.0970
L	 0.8560	 0.0970
M	 0.7070	 0.0760
N	 0.7430	 0.0920
O	 0.5690	 0.0980

