Full wwPDB EM Validation Report

Nov 20, 2022 – 05:18 AM EST

PDB ID	:	7SBA
EMDB ID	:	EMD-24974
Title	:	Structure of type I-D Cascade bound to a dsDNA target
Authors	:	Schwartz, E.A.; Taylor, D.W.
Deposited on	:	2021-09-24
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

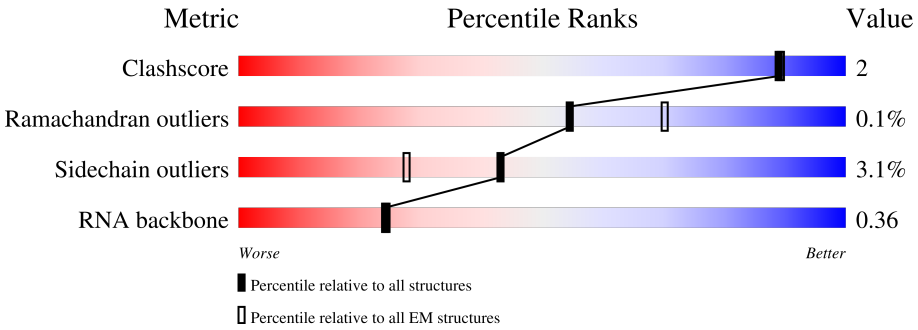
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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 <=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	329	88% 9%
1	B	329	91% 6%
1	C	329	88% 9%
1	D	329	90% 7%
1	E	329	6% 88% 9%
1	F	329	7% 88% 8%
1	G	329	20% 88% 8%

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Mol	Chain	Length	Quality of chain
2	H	254	85% 8% 6%
3	I	975	5% 84% 8% 8%
4	J	146	34% 89% 10%
4	K	146	77% 88% 10%
5	X	16	12% 12% 44% 38% 6%
6	Y	13	46% 23% 62% 15%
7	Z	43	21% 42% 30% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 30651 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 Cas7d.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	B	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	C	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	D	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	E	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	F	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		
1	G	320	Total	C	N	O	S	0	0
			2503	1572	429	490	12		

- Molecule 2 is a protein called Cas5d.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	238	Total	C	N	O	S	0	0
			1929	1249	328	347	5		

- Molecule 3 is a protein called Cas10d.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	899	Total	C	N	O	S	0	0
			7323	4709	1240	1356	18		

- Molecule 4 is a protein called Cas11d.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	146	Total	C	N	O	S	0	0
			1194	751	209	229	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	146	Total	C	N	O	S	0	0
			1194	751	209	229	5		

- Molecule 5 is a DNA chain called DNA target strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	16	Total	C	N	O	P	0	0
			325	156	66	88	15		

- Molecule 6 is a DNA chain called DNA non-target strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	13	Total	C	N	O	P	0	0
			261	128	40	81	12		

- Molecule 7 is a RNA chain called crRNA.

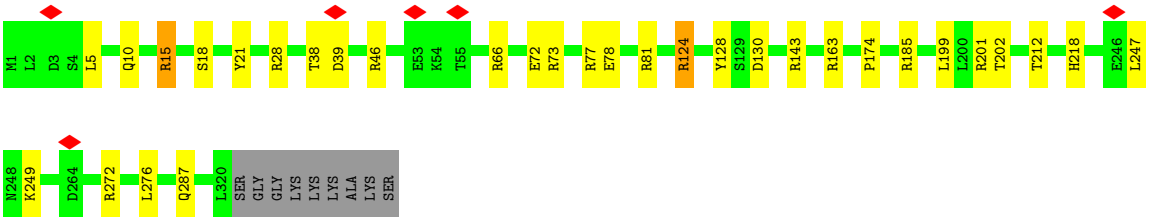
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	43	Total	C	N	O	P	0	0
			904	405	152	305	42		

3 Residue-property plots (i)

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

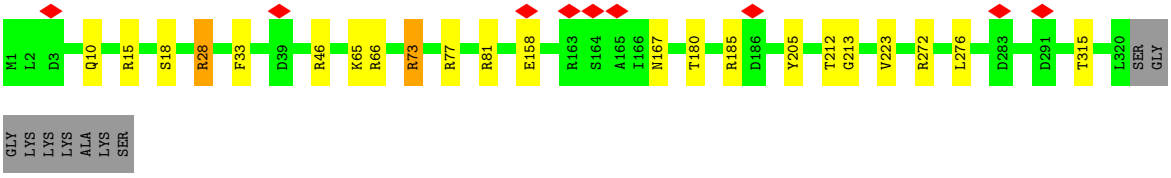
- Molecule 1: Cas7d

Chain A:



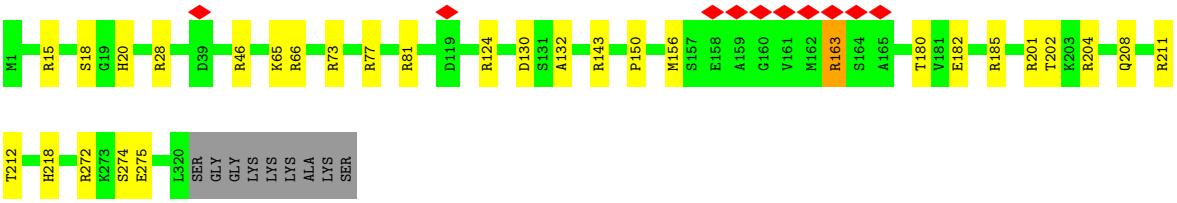
- Molecule 1: Cas7d

Chain B:



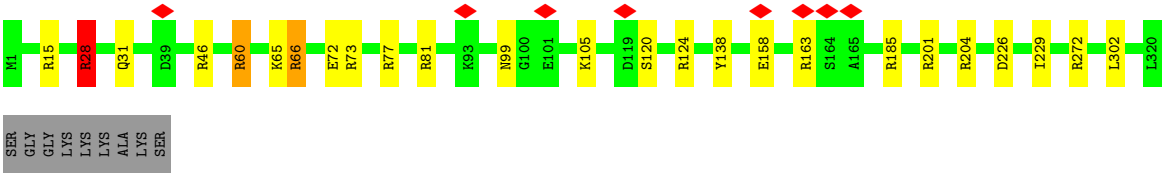
- Molecule 1: Cas7d

Chain C:

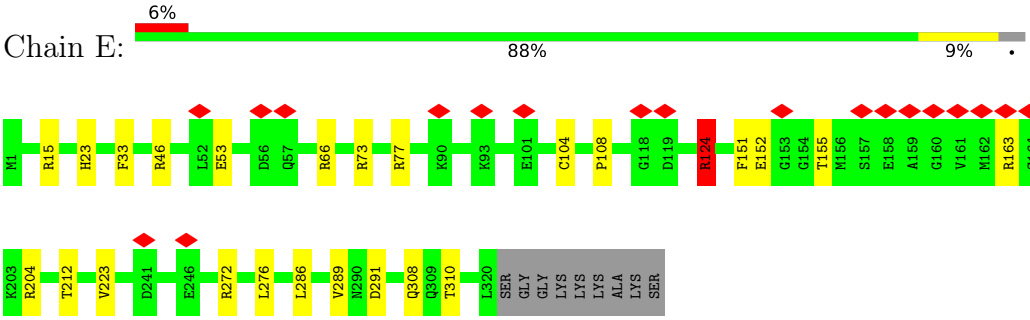


- Molecule 1: Cas7d

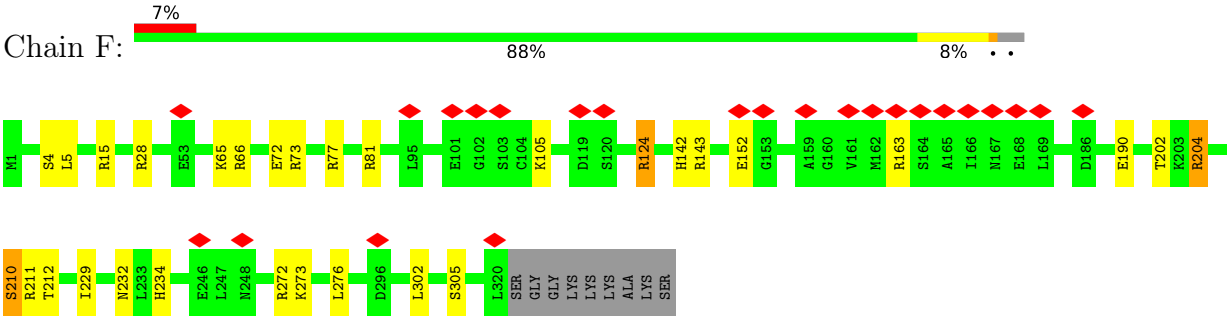
Chain D:



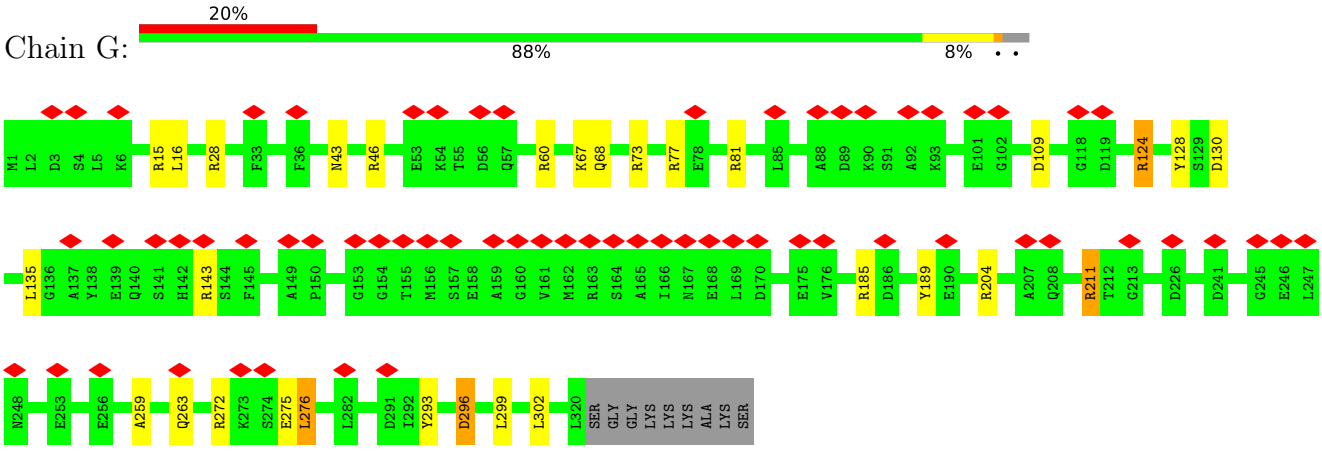
• Molecule 1: Cas7d



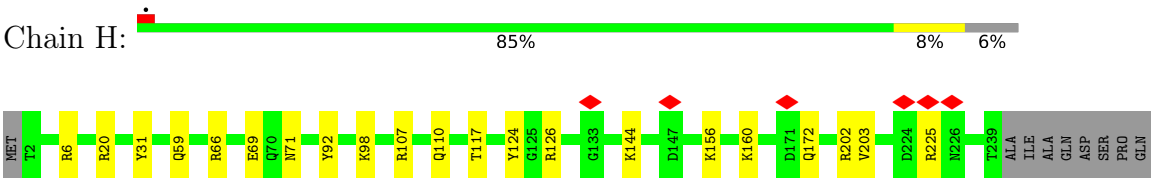
• Molecule 1: Cas7d



• Molecule 1: Cas7d

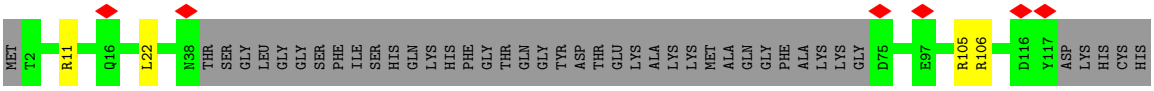


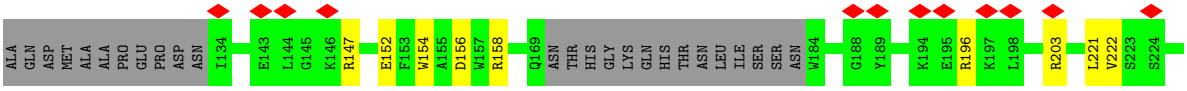
• Molecule 2: Cas5d

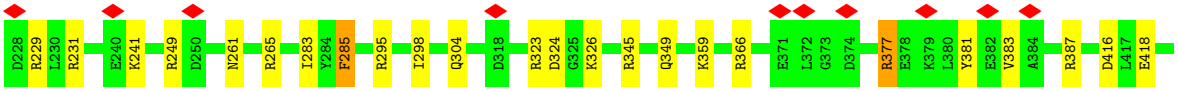


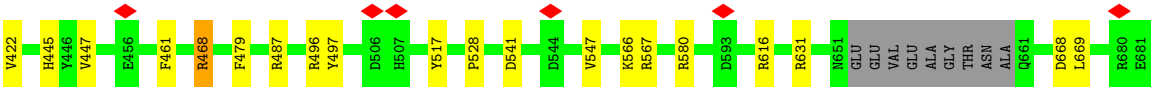
• Molecule 3: Cas10d

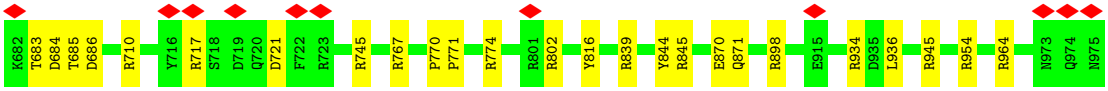
Chain I:





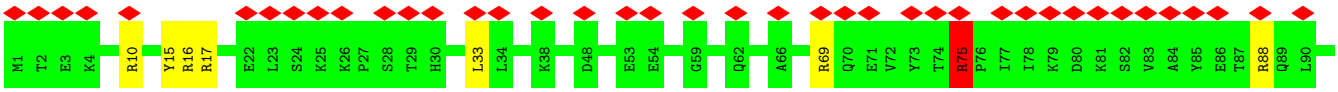


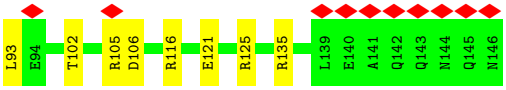




• Molecule 4: Cas11d

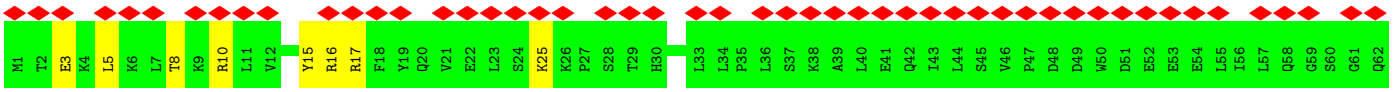
Chain J:

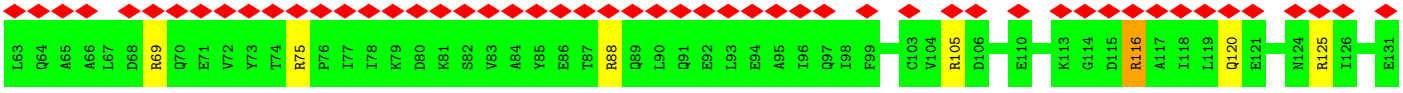


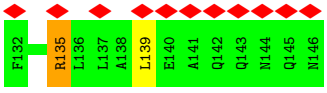


• Molecule 4: Cas11d

Chain K:

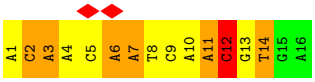






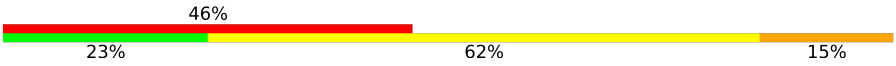
• Molecule 5: DNA target strand

Chain X:



• Molecule 6: DNA non-target strand

Chain Y:



• Molecule 7: crRNA

Chain Z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	336400	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 ($e^-/Å^2$)	41.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.550	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	459.8, 459.8, 459.8	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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	0.66	0/2549	1.13	20/3442 (0.6%)
1	B	0.67	0/2549	1.11	14/3442 (0.4%)
1	C	0.67	0/2549	1.10	16/3442 (0.5%)
1	D	0.68	0/2549	1.12	16/3442 (0.5%)
1	E	0.66	0/2549	1.12	14/3442 (0.4%)
1	F	0.69	0/2549	1.11	14/3442 (0.4%)
1	G	0.69	0/2549	1.12	17/3442 (0.5%)
2	H	0.71	0/1988	1.10	6/2706 (0.2%)
3	I	0.65	0/7487	1.10	40/10153 (0.4%)
4	J	0.67	0/1209	1.14	10/1624 (0.6%)
4	K	0.68	0/1209	1.12	10/1624 (0.6%)
5	X	1.59	0/366	2.49	34/562 (6.0%)
6	Y	1.50	0/290	2.12	18/446 (4.0%)
7	Z	1.50	2/1007 (0.2%)	2.40	66/1566 (4.2%)
All	All	0.74	2/31399 (0.0%)	1.23	295/42775 (0.7%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	2
2	H	0	1
3	I	0	5
4	J	0	1
5	X	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	Y	0	2
7	Z	0	10
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	8	C	C4-N4	-5.17	1.29	1.33
7	Z	25	G	C2-N2	-5.06	1.29	1.34

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	73	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	D	73	ARG	NE-CZ-NH1	-12.56	114.02	120.30
1	B	73	ARG	NE-CZ-NH1	-12.51	114.05	120.30
1	G	73	ARG	NE-CZ-NH1	-12.33	114.14	120.30
7	Z	7	A	N1-C6-N6	-11.39	111.77	118.60
1	A	124	ARG	NE-CZ-NH1	10.96	125.78	120.30
7	Z	32	C	N3-C2-O2	-10.71	114.41	121.90
5	X	6	DA	N1-C6-N6	-10.68	112.19	118.60
1	C	73	ARG	NE-CZ-NH2	10.66	125.63	120.30
5	X	11	DA	N1-C6-N6	-10.52	112.29	118.60
1	D	73	ARG	NE-CZ-NH2	10.40	125.50	120.30
6	Y	8	DA	N1-C6-N6	-10.27	112.44	118.60
7	Z	3	U	O4'-C1'-N1	10.22	116.38	108.20
5	X	11	DA	O4'-C1'-N9	10.22	115.15	108.00
5	X	10	DA	N1-C6-N6	-10.18	112.49	118.60
1	A	73	ARG	NE-CZ-NH2	10.06	125.33	120.30
5	X	4	DA	N1-C6-N6	-9.63	112.82	118.60
1	A	66	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	B	73	ARG	NE-CZ-NH2	9.53	125.06	120.30
7	Z	32	C	N1-C2-O2	9.52	124.61	118.90
1	D	15	ARG	NE-CZ-NH1	9.44	125.02	120.30
7	Z	8	C	N3-C2-O2	-9.43	115.30	121.90
4	J	75	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	G	272	ARG	NE-CZ-NH2	9.34	124.97	120.30
7	Z	5	A	N1-C6-N6	-9.32	113.00	118.60
7	Z	38	A	N1-C6-N6	-9.19	113.08	118.60
7	Z	37	A	N1-C6-N6	-9.18	113.09	118.60
3	I	954	ARG	NE-CZ-NH1	9.17	124.89	120.30
7	Z	1	A	N1-C6-N6	-9.09	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	272	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	E	201	ARG	NE-CZ-NH1	8.94	124.77	120.30
4	K	116	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	124	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	F	28	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	272	ARG	NE-CZ-NH2	8.67	124.64	120.30
6	Y	8	DA	O4'-C1'-N9	8.62	114.04	108.00
1	F	15	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	D	272	ARG	NE-CZ-NH2	8.57	124.58	120.30
7	Z	14	U	N3-C2-O2	-8.55	116.21	122.20
1	F	272	ARG	NE-CZ-NH2	8.55	124.57	120.30
2	H	6	ARG	NE-CZ-NH1	8.48	124.54	120.30
7	Z	10	A	N1-C6-N6	-8.43	113.54	118.60
5	X	1	DA	N1-C6-N6	-8.35	113.59	118.60
1	E	15	ARG	NE-CZ-NH1	8.34	124.47	120.30
3	I	487	ARG	NE-CZ-NH1	8.26	124.43	120.30
7	Z	6	A	N1-C6-N6	-8.24	113.66	118.60
7	Z	3	U	N3-C2-O2	-8.23	116.44	122.20
7	Z	37	A	C5'-C4'-C3'	-8.22	102.86	116.00
1	A	272	ARG	NE-CZ-NH2	8.21	124.41	120.30
5	X	7	DA	N1-C6-N6	-8.12	113.73	118.60
1	D	204	ARG	NE-CZ-NH1	8.07	124.34	120.30
5	X	2	DC	N3-C2-O2	-7.96	116.33	121.90
3	I	387	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	H	20	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	B	46	ARG	NE-CZ-NH1	7.89	124.25	120.30
4	J	135	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	F	77	ARG	NE-CZ-NH1	7.86	124.23	120.30
7	Z	1	A	C5-C6-N1	7.86	121.63	117.70
1	E	73	ARG	NE-CZ-NH2	7.85	124.22	120.30
5	X	4	DA	C5-C6-N1	7.80	121.60	117.70
1	B	66	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	H	126	ARG	NE-CZ-NH1	7.79	124.20	120.30
3	I	203	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	272	ARG	NE-CZ-NH2	7.70	124.15	120.30
7	Z	13	G	O4'-C1'-N9	7.67	114.34	108.20
7	Z	7	A	C5-C6-N1	7.67	121.54	117.70
5	X	10	DA	C4-C5-C6	-7.67	113.17	117.00
3	I	631	ARG	NE-CZ-NH2	7.65	124.13	120.30
6	Y	8	DA	C5-C6-N1	7.61	121.50	117.70
5	X	10	DA	C5-C6-N1	7.61	121.50	117.70
7	Z	42	C	N3-C2-O2	-7.61	116.58	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	323	ARG	NE-CZ-NH1	7.60	124.10	120.30
5	X	6	DA	C4-C5-C6	-7.54	113.23	117.00
3	I	377	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	G	272	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	B	28	ARG	NE-CZ-NH1	7.48	124.04	120.30
7	Z	8	C	N1-C2-O2	7.47	123.38	118.90
3	I	285	PHE	N-CA-C	-7.46	90.87	111.00
3	I	964	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	C	211	ARG	NE-CZ-NH1	7.44	124.02	120.30
7	Z	10	A	C5-C6-N1	7.43	121.42	117.70
1	E	77	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	81	ARG	NE-CZ-NH1	7.38	123.99	120.30
3	I	710	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	81	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	66	ARG	NE-CZ-NH2	-7.35	116.62	120.30
7	Z	38	A	C5-C6-N1	7.35	121.37	117.70
7	Z	37	A	C5-C6-N1	7.34	121.37	117.70
1	D	185	ARG	NE-CZ-NH2	7.30	123.95	120.30
3	I	345	ARG	NE-CZ-NH1	7.27	123.94	120.30
4	J	17	ARG	NE-CZ-NH1	7.25	123.92	120.30
5	X	4	DA	C4-C5-C6	-7.23	113.39	117.00
7	Z	31	G	O4'-C1'-N9	7.23	113.98	108.20
1	D	124	ARG	NE-CZ-NH1	7.21	123.91	120.30
5	X	3	DA	N1-C6-N6	-7.21	114.27	118.60
4	K	16	ARG	NE-CZ-NH2	7.21	123.90	120.30
3	I	496	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	C	143	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	46	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	H	225	ARG	NE-CZ-NH1	7.18	123.89	120.30
3	I	366	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	F	66	ARG	NE-CZ-NH2	7.16	123.88	120.30
5	X	11	DA	O4'-C1'-C2'	-7.13	100.20	105.90
1	E	163	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	15	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	46	ARG	NE-CZ-NH1	7.09	123.84	120.30
3	I	767	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	H	202	ARG	NE-CZ-NH1	7.05	123.82	120.30
4	K	75	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	163	ARG	NE-CZ-NH1	7.01	123.81	120.30
3	I	265	ARG	NE-CZ-NH1	6.99	123.80	120.30
7	Z	8	C	C6-N1-C2	-6.95	117.52	120.30
1	A	77	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	36	C	N3-C2-O2	-6.93	117.05	121.90
5	X	3	DA	C4-C5-C6	-6.93	113.54	117.00
1	B	185	ARG	NE-CZ-NH2	6.90	123.75	120.30
5	X	5	DC	N3-C2-O2	-6.90	117.07	121.90
5	X	3	DA	C5-C6-N1	6.89	121.14	117.70
7	Z	38	A	C4-C5-C6	-6.89	113.56	117.00
1	G	28	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	I	323	ARG	NE-CZ-NH2	-6.85	116.88	120.30
3	I	231	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	I	11	ARG	NE-CZ-NH1	6.83	123.72	120.30
6	Y	10	DT	N3-C2-O2	-6.83	118.20	122.30
7	Z	37	A	O4'-C1'-N9	6.81	113.65	108.20
4	K	69	ARG	NE-CZ-NH1	6.80	123.70	120.30
5	X	2	DC	O4'-C1'-N1	6.79	112.75	108.00
3	I	468	ARG	NE-CZ-NH1	6.79	123.69	120.30
5	X	1	DA	C5-C6-N1	6.78	121.09	117.70
1	G	73	ARG	NE-CZ-NH2	6.72	123.66	120.30
7	Z	5	A	C5-C6-N1	6.72	121.06	117.70
4	K	135	ARG	NE-CZ-NH1	6.72	123.66	120.30
5	X	11	DA	C5-C6-N1	6.70	121.05	117.70
1	G	124	ARG	NE-CZ-NH1	6.69	123.64	120.30
7	Z	34	U	N3-C2-O2	-6.64	117.55	122.20
1	F	73	ARG	NE-CZ-NH2	6.64	123.62	120.30
7	Z	7	A	C4-C5-C6	-6.63	113.69	117.00
1	A	73	ARG	CD-NE-CZ	6.63	132.88	123.60
7	Z	22	C	N3-C2-O2	-6.62	117.26	121.90
4	J	10	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	73	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	F	163	ARG	NE-CZ-NH1	6.58	123.59	120.30
5	X	1	DA	C4-C5-C6	-6.57	113.72	117.00
3	I	845	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	201	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	G	204	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	I	196	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	60	ARG	NE-CZ-NH1	6.52	123.56	120.30
7	Z	5	A	C4-C5-C6	-6.52	113.74	117.00
3	I	567	ARG	NE-CZ-NH1	6.50	123.55	120.30
6	Y	9	DT	C6-C5-C7	-6.49	119.01	122.90
1	C	28	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	E	73	ARG	NE-CZ-NH1	-6.49	117.06	120.30
3	I	934	ARG	NE-CZ-NH1	6.47	123.53	120.30
3	I	106	ARG	NE-CZ-NH1	6.46	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	272	ARG	NE-CZ-NH1	-6.42	117.09	120.30
7	Z	30	C	N3-C2-O2	-6.40	117.42	121.90
7	Z	21	C	N3-C2-O2	-6.40	117.42	121.90
1	A	143	ARG	NE-CZ-NH1	6.39	123.50	120.30
6	Y	5	DT	C6-C5-C7	-6.36	119.08	122.90
6	Y	9	DT	N3-C2-O2	-6.36	118.49	122.30
1	G	81	ARG	NE-CZ-NH1	6.33	123.46	120.30
7	Z	6	A	C5-C6-N1	6.33	120.86	117.70
7	Z	41	C	N3-C2-O2	-6.33	117.47	121.90
4	K	88	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	D	163	ARG	NE-CZ-NH1	6.32	123.46	120.30
6	Y	10	DT	C6-C5-C7	-6.30	119.12	122.90
1	E	66	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	F	124	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	46	ARG	NE-CZ-NH1	6.27	123.44	120.30
7	Z	20	C	N3-C2-O2	-6.27	117.51	121.90
5	X	14	DT	C6-C5-C7	-6.24	119.16	122.90
3	I	802	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	81	ARG	NE-CZ-NH1	6.21	123.41	120.30
5	X	6	DA	C5-C6-N1	6.19	120.80	117.70
5	X	7	DA	C5-C6-N1	6.19	120.79	117.70
1	F	143	ARG	NE-CZ-NH1	6.18	123.39	120.30
5	X	14	DT	N3-C2-O2	-6.18	118.59	122.30
4	J	69	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	I	158	ARG	NE-CZ-NH1	6.14	123.37	120.30
3	I	295	ARG	NE-CZ-NH1	6.13	123.36	120.30
7	Z	19	C	O4'-C1'-N1	6.12	113.10	108.20
7	Z	34	U	O4'-C1'-N1	6.10	113.08	108.20
1	A	66	ARG	NE-CZ-NH1	-6.10	117.25	120.30
5	X	12	DC	N3-C2-O2	-6.09	117.63	121.90
6	Y	6	DT	C6-C5-C7	-6.08	119.25	122.90
7	Z	19	C	N3-C2-O2	-6.08	117.65	121.90
6	Y	6	DT	N3-C2-O2	-6.07	118.66	122.30
4	K	125	ARG	NE-CZ-NH1	6.06	123.33	120.30
7	Z	39	U	N3-C2-O2	-6.06	117.95	122.20
6	Y	11	DT	C6-C5-C7	-6.04	119.27	122.90
5	X	7	DA	C4-C5-C6	-6.01	114.00	117.00
6	Y	4	DG	O4'-C1'-N9	6.01	112.21	108.00
1	F	5	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	124	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
5	X	8	DT	C6-C5-C7	-5.97	119.32	122.90
1	D	66	ARG	NE-CZ-NH2	5.95	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	32	C	N3-C4-N4	-5.88	113.89	118.00
1	G	185	ARG	NE-CZ-NH2	5.86	123.23	120.30
3	I	229	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	77	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	D	81	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	28	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
4	K	10	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	H	107	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	185	ARG	NE-CZ-NH2	5.78	123.19	120.30
5	X	6	DA	C6-C5-N7	5.77	136.34	132.30
5	X	7	DA	P-O3'-C3'	5.77	126.62	119.70
6	Y	8	DA	C4-C5-C6	-5.76	114.12	117.00
1	C	163	ARG	NE-CZ-NH1	5.75	123.18	120.30
5	X	11	DA	C4-C5-C6	-5.74	114.13	117.00
7	Z	8	C	N1-C1'-C2'	5.74	121.46	114.00
3	I	839	ARG	NE-CZ-NH1	5.73	123.17	120.30
3	I	616	ARG	NE-CZ-NH2	5.73	123.16	120.30
6	Y	7	DG	O4'-C1'-N9	5.72	112.00	108.00
6	Y	7	DG	C5-C6-N1	5.71	114.36	111.50
7	Z	26	C	N3-C2-O2	-5.71	117.90	121.90
1	D	73	ARG	CD-NE-CZ	5.71	131.59	123.60
3	I	945	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	77	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	15	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	J	105	ARG	NE-CZ-NH1	5.67	123.14	120.30
3	I	717	ARG	NE-CZ-NH2	5.66	123.13	120.30
4	J	16	ARG	NE-CZ-NH1	5.65	123.12	120.30
7	Z	39	U	C3'-C2'-C1'	-5.65	96.98	101.50
1	E	204	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	28	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
7	Z	39	U	N1-C1'-C2'	5.64	121.33	114.00
7	Z	15	U	C3'-C2'-C1'	-5.62	97.00	101.50
4	J	125	ARG	NE-CZ-NH1	5.62	123.11	120.30
7	Z	37	A	C4-C5-C6	-5.61	114.19	117.00
7	Z	42	C	N1-C2-O2	5.59	122.25	118.90
7	Z	10	A	C4-C5-C6	-5.59	114.21	117.00
1	G	276	LEU	CA-CB-CG	5.58	128.14	115.30
1	E	185	ARG	NE-CZ-NH2	5.58	123.09	120.30
3	I	147	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	204	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	G	211	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	E	15	ARG	NE-CZ-NH2	-5.55	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	2	DC	N1-C2-O2	5.55	122.23	118.90
1	F	73	ARG	CD-NE-CZ	5.55	131.37	123.60
7	Z	32	C	N1-C1'-C2'	5.51	121.17	114.00
4	J	88	ARG	NE-CZ-NH1	5.49	123.05	120.30
3	I	745	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	204	ARG	NE-CZ-NH1	5.48	123.04	120.30
7	Z	6	A	C4-C5-C6	-5.46	114.27	117.00
1	D	77	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	276	LEU	CA-CB-CG	5.43	127.78	115.30
6	Y	7	DG	N1-C6-O6	-5.43	116.64	119.90
4	K	17	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	124	ARG	NE-CZ-NH1	5.41	123.00	120.30
7	Z	8	C	O3'-P-O5'	-5.41	93.73	104.00
7	Z	11	U	N3-C2-O2	-5.40	118.42	122.20
6	Y	11	DT	N3-C2-O2	-5.40	119.06	122.30
1	G	77	ARG	NE-CZ-NH1	5.37	122.99	120.30
3	I	105	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	5	LEU	CA-CB-CG	5.37	127.64	115.30
3	I	964	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	201	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	I	898	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	G	60	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	F	81	ARG	NE-CZ-NH1	5.31	122.96	120.30
4	K	105	ARG	NE-CZ-NH1	5.30	122.95	120.30
4	J	116	ARG	NE-CZ-NH1	5.29	122.95	120.30
7	Z	14	U	N1-C1'-C2'	5.29	120.88	114.00
7	Z	34	U	C5'-C4'-O4'	5.29	115.45	109.10
7	Z	9	G	N1-C6-O6	-5.28	116.73	119.90
3	I	580	ARG	NE-CZ-NH1	5.28	122.94	120.30
7	Z	28	G	C5'-C4'-O4'	5.25	115.40	109.10
3	I	249	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	73	ARG	CD-NE-CZ	5.24	130.94	123.60
1	D	28	ARG	NE-CZ-NH2	5.22	122.91	120.30
7	Z	30	C	N1-C2-O2	5.21	122.03	118.90
7	Z	25	G	N1-C6-O6	-5.18	116.79	119.90
6	Y	11	DT	O4'-C1'-N1	5.18	111.63	108.00
1	C	66	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	G	143	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	I	774	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	G	124	ARG	CD-NE-CZ	5.14	130.80	123.60
1	G	60	ARG	CD-NE-CZ	5.14	130.79	123.60
1	B	15	ARG	NE-CZ-NH1	5.13	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	201	ARG	NE-CZ-NH1	5.11	122.86	120.30
5	X	8	DT	N3-C2-O2	-5.11	119.23	122.30
1	C	185	ARG	NE-CZ-NH2	5.10	122.85	120.30
7	Z	21	C	O4'-C1'-N1	5.09	112.27	108.20
1	A	28	ARG	NE-CZ-NH1	5.07	122.83	120.30
7	Z	1	A	C4-C5-C6	-5.06	114.47	117.00
7	Z	14	U	N1-C2-O2	5.04	126.33	122.80
7	Z	32	C	C6-N1-C2	-5.04	118.28	120.30
1	E	46	ARG	NE-CZ-NH1	5.04	122.82	120.30
7	Z	18	G	N1-C6-O6	-5.03	116.88	119.90
7	Z	36	C	N1-C2-O2	5.03	121.92	118.90
1	B	205	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	G	46	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	128	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	TYR	Sidechain
1	B	73	ARG	Sidechain
1	C	163	ARG	Sidechain
1	D	28	ARG	Sidechain
1	E	124	ARG	Sidechain
1	F	204	ARG	Sidechain
1	G	189	TYR	Sidechain
1	G	293	TYR	Sidechain
2	H	92	TYR	Sidechain
3	I	468	ARG	Sidechain
3	I	497	TYR	Sidechain
3	I	517	TYR	Sidechain
3	I	816	TYR	Sidechain
3	I	844	TYR	Sidechain
4	J	15	TYR	Sidechain
5	X	12	DC	Sidechain
5	X	13	DG	Sidechain
5	X	2	DC	Sidechain
5	X	3	DA	Sidechain
5	X	6	DA	Sidechain
5	X	7	DA	Sidechain
6	Y	11	DT	Sidechain
6	Y	5	DT	Sidechain

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Mol	Chain	Res	Type	Group
7	Z	13	G	Sidechain
7	Z	14	U	Sidechain
7	Z	19	C	Sidechain
7	Z	2	C	Sidechain
7	Z	20	C	Sidechain
7	Z	25	G	Sidechain
7	Z	32	C	Sidechain
7	Z	37	A	Sidechain
7	Z	41	C	Sidechain
7	Z	43	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2503	0	2454	8	0
1	B	2503	0	2454	13	0
1	C	2503	0	2454	5	0
1	D	2503	0	2454	2	0
1	E	2503	0	2454	17	0
1	F	2503	0	2454	9	0
1	G	2503	0	2454	10	0
2	H	1929	0	1877	7	0
3	I	7323	0	7311	39	0
4	J	1194	0	1219	3	0
4	K	1194	0	1219	6	0
5	X	325	0	180	11	0
6	Y	261	0	152	12	0
7	Z	904	0	454	9	0
All	All	30651	0	29590	107	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 2.

All (107) 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)
3:I:221:LEU:HD23	3:I:283:ILE:CD1	1.71	1.18
3:I:771:PRO:HA	6:Y:13:DT:C7	1.82	1.10
3:I:261:ASN:HD22	3:I:668:ASP:HB3	1.06	1.09
3:I:221:LEU:HD23	3:I:283:ILE:HD13	1.29	1.07
3:I:770:PRO:O	6:Y:13:DT:C7	2.04	1.04
5:X:14:DT:O4	6:Y:2:DA:N6	1.96	0.98
3:I:770:PRO:O	6:Y:13:DT:H72	1.65	0.96
5:X:9:DC:H5	7:Z:9:G:H1	0.97	0.95
1:G:15:ARG:O	1:G:16:LEU:HD12	1.67	0.94
1:A:212:THR:CG2	1:B:65:LYS:HD3	1.97	0.94
1:E:212:THR:HG23	1:F:65:LYS:HD2	1.50	0.93
1:E:155:THR:HG22	7:Z:41:C:H1'	1.50	0.91
4:K:135:ARG:O	4:K:139:LEU:HG	1.73	0.88
1:B:212:THR:HG22	1:B:213:GLY:N	1.90	0.86
3:I:261:ASN:ND2	3:I:668:ASP:HB3	1.90	0.84
1:E:155:THR:HG22	7:Z:41:C:C1'	2.07	0.84
3:I:771:PRO:HA	6:Y:13:DT:H71	1.61	0.82
1:E:212:THR:CG2	1:F:65:LYS:HD2	2.11	0.81
1:A:212:THR:HG23	1:B:65:LYS:HD3	1.63	0.79
3:I:770:PRO:O	6:Y:13:DT:H71	1.82	0.79
3:I:221:LEU:CD2	3:I:283:ILE:HG12	2.13	0.79
3:I:221:LEU:HD21	3:I:283:ILE:HG12	1.67	0.77
1:B:33:PHE:O	1:B:212:THR:CG2	2.36	0.74
5:X:9:DC:H5	7:Z:9:G:N1	1.82	0.73
1:E:155:THR:CG2	7:Z:41:C:H1'	2.18	0.73
1:B:33:PHE:O	1:B:212:THR:HG21	1.88	0.72
1:C:208:GLN:O	1:C:212:THR:HG22	1.89	0.72
1:G:15:ARG:HG2	1:G:16:LEU:HD13	1.72	0.72
1:E:151:PHE:CZ	1:G:16:LEU:HD11	2.25	0.72
3:I:383:VAL:O	3:I:383:VAL:HG12	1.89	0.72
1:D:28:ARG:NH2	1:D:72:GLU:OE2	2.22	0.72
1:G:15:ARG:C	1:G:16:LEU:HD12	2.09	0.71
1:B:212:THR:CG2	1:B:213:GLY:N	2.53	0.71
3:I:221:LEU:HD23	3:I:283:ILE:CG1	2.20	0.71
1:B:212:THR:OG1	1:C:65:LYS:HD2	1.92	0.70
1:G:15:ARG:HG2	1:G:16:LEU:CD1	2.23	0.69
1:A:212:THR:HG21	1:B:65:LYS:HD3	1.75	0.69
1:B:10:GLN:NE2	1:B:18:SER:OG	2.25	0.69
3:I:383:VAL:CG1	3:I:447:VAL:HG12	2.23	0.69
3:I:221:LEU:CD2	3:I:283:ILE:CD1	2.63	0.68
1:A:15:ARG:NH2	2:H:69:GLU:OE1	2.28	0.67
4:K:5:LEU:HA	4:K:8:THR:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:221:LEU:CD2	3:I:283:ILE:CG1	2.74	0.66
3:I:771:PRO:HA	6:Y:13:DT:H73	1.76	0.64
3:I:261:ASN:HD22	3:I:668:ASP:CB	1.97	0.64
4:J:93:LEU:HD22	4:K:139:LEU:HD21	1.78	0.63
3:I:528:PRO:CD	3:I:541:ASP:OD1	2.48	0.62
1:B:28:ARG:HH11	1:B:180:THR:HG21	1.66	0.61
1:E:212:THR:CG2	1:F:65:LYS:CD	2.78	0.61
2:H:66:ARG:HA	2:H:71:ASN:HD21	1.67	0.59
5:X:14:DT:O4	6:Y:2:DA:C6	2.56	0.59
3:I:221:LEU:HD23	3:I:283:ILE:HD11	1.81	0.58
2:H:110:GLN:HG2	5:X:9:DC:H5"	1.87	0.57
2:H:124:TYR:CE1	5:X:9:DC:C6	2.94	0.56
3:I:261:ASN:HD21	3:I:669:LEU:N	2.04	0.55
3:I:221:LEU:CD2	3:I:283:ILE:HD13	2.20	0.54
1:E:155:THR:HG22	7:Z:41:C:O4'	2.08	0.54
3:I:383:VAL:O	3:I:383:VAL:CG1	2.55	0.54
1:D:138:TYR:CE2	4:K:120:GLN:HG3	2.43	0.53
3:I:771:PRO:CA	6:Y:13:DT:C7	2.73	0.53
3:I:528:PRO:CG	3:I:541:ASP:OD1	2.57	0.53
2:H:110:GLN:CG	5:X:9:DC:H5"	2.39	0.53
1:E:151:PHE:CE1	1:G:16:LEU:HD11	2.44	0.52
3:I:383:VAL:HG11	3:I:447:VAL:HG12	1.90	0.52
3:I:771:PRO:CA	6:Y:13:DT:H71	2.37	0.52
1:E:23:HIS:HD1	1:E:183:SER:CB	2.19	0.52
4:K:5:LEU:O	4:K:8:THR:HG22	2.10	0.52
3:I:683:THR:CG2	3:I:685:THR:HG22	2.40	0.51
1:A:72:GLU:OE2	1:A:199:LEU:HD23	2.10	0.51
1:G:259:ALA:O	1:G:263:GLN:HG3	2.10	0.51
3:I:383:VAL:HG12	3:I:447:VAL:HG12	1.91	0.51
5:X:14:DT:C4	6:Y:2:DA:N1	2.78	0.51
3:I:261:ASN:ND2	3:I:669:LEU:N	2.59	0.50
1:E:212:THR:HG21	1:F:65:LYS:CD	2.42	0.50
3:I:528:PRO:HG3	3:I:541:ASP:OD1	2.12	0.50
1:E:152:GLU:HG3	1:G:16:LEU:CD2	2.41	0.50
3:I:683:THR:HG22	3:I:685:THR:HG22	1.95	0.49
1:B:10:GLN:NE2	1:B:18:SER:HG	2.12	0.48
1:A:124:ARG:HH21	7:Z:2:C:P	2.37	0.47
1:E:223:VAL:HG13	1:E:276:LEU:CD2	2.45	0.47
3:I:221:LEU:HD12	3:I:222:VAL:HG23	1.98	0.46
4:J:93:LEU:HD22	4:K:139:LEU:CD2	2.45	0.46
1:F:211:ARG:HH21	7:Z:43:U:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:HB2	1:C:180:THR:HG22	1.99	0.44
2:H:31:TYR:CE1	2:H:203:VAL:HG11	2.52	0.44
3:I:566:LYS:HE2	5:X:12:DC:O5'	2.17	0.44
1:E:108:PRO:HA	1:E:310:THR:HG21	1.99	0.44
1:G:296:ASP:HA	1:G:299:LEU:HB3	2.00	0.44
3:I:683:THR:HG22	3:I:684:ASP:N	2.32	0.44
1:E:212:THR:HG21	1:F:65:LYS:HD3	1.99	0.43
3:I:422:VAL:HG21	3:I:445:HIS:CD2	2.53	0.43
1:F:210:SER:HA	1:G:128:TYR:CD2	2.53	0.43
2:H:124:TYR:HE1	5:X:9:DC:C6	2.37	0.42
3:I:566:LYS:HZ3	5:X:11:DA:H2"	1.85	0.42
3:I:261:ASN:ND2	3:I:669:LEU:H	2.17	0.41
4:J:75:ARG:HG2	4:J:75:ARG:HH11	1.85	0.41
1:B:212:THR:CG2	1:B:213:GLY:H	2.30	0.41
1:C:18:SER:OG	1:C:20:HIS:HD2	2.04	0.41
1:A:38:THR:HG22	7:Z:9:G:H5'	2.03	0.41
1:B:223:VAL:HG13	1:B:276:LEU:HD23	2.03	0.41
1:A:10:GLN:NE2	1:A:18:SER:OG	2.54	0.41
1:F:273:LYS:HB3	1:F:276:LEU:HD11	2.03	0.41
1:E:286:LEU:HA	1:E:289:VAL:HG12	2.03	0.40
1:E:23:HIS:CE1	1:E:183:SER:HG	2.19	0.40
1:C:150:PRO:HA	1:C:156:MET:SD	2.61	0.40
3:I:771:PRO:HA	6:Y:13:DT:H72	1.89	0.40
1:F:190:GLU:OE1	1:F:305:SER:HB3	2.21	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	318/329 (97%)	309 (97%)	8 (2%)	1 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	318/329 (97%)	304 (96%)	14 (4%)	0	100	100
1	C	318/329 (97%)	308 (97%)	10 (3%)	0	100	100
1	D	318/329 (97%)	303 (95%)	14 (4%)	1 (0%)	41	71
1	E	318/329 (97%)	308 (97%)	9 (3%)	1 (0%)	41	71
1	F	318/329 (97%)	303 (95%)	14 (4%)	1 (0%)	41	71
1	G	318/329 (97%)	288 (91%)	30 (9%)	0	100	100
2	H	236/254 (93%)	227 (96%)	9 (4%)	0	100	100
3	I	889/975 (91%)	860 (97%)	29 (3%)	0	100	100
4	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
4	K	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
All	All	3639/3824 (95%)	3482 (96%)	153 (4%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	PRO
1	E	33	PHE
1	D	229	ILE
1	F	229	ILE

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	A	273/279 (98%)	265 (97%)	8 (3%)	42	76
1	B	273/279 (98%)	270 (99%)	3 (1%)	73	92
1	C	273/279 (98%)	267 (98%)	6 (2%)	52	81
1	D	273/279 (98%)	263 (96%)	10 (4%)	34	68
1	E	273/279 (98%)	267 (98%)	6 (2%)	52	81
1	F	273/279 (98%)	261 (96%)	12 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	273/279 (98%)	261 (96%)	12 (4%)	28 61
2	H	205/219 (94%)	198 (97%)	7 (3%)	37 71
3	I	792/855 (93%)	768 (97%)	24 (3%)	41 75
4	J	130/130 (100%)	125 (96%)	5 (4%)	33 67
4	K	130/130 (100%)	126 (97%)	4 (3%)	40 74
All	All	3168/3287 (96%)	3071 (97%)	97 (3%)	43 74

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	78	GLU
1	A	130	ASP
1	A	202	THR
1	A	218	HIS
1	A	247	LEU
1	A	249	LYS
1	A	287	GLN
1	B	158	GLU
1	B	167	ASN
1	B	315	THR
1	C	130	ASP
1	C	182	GLU
1	C	202	THR
1	C	218	HIS
1	C	274	SER
1	C	275	GLU
1	D	31	GLN
1	D	60	ARG
1	D	65	LYS
1	D	66	ARG
1	D	99	ASN
1	D	105	LYS
1	D	120	SER
1	D	158	GLU
1	D	226	ASP
1	D	302	LEU
1	E	53	GLU
1	E	104	CYS
1	E	124	ARG

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Mol	Chain	Res	Type
1	E	202	THR
1	E	291	ASP
1	E	308	GLN
1	F	4	SER
1	F	72	GLU
1	F	105	LYS
1	F	124	ARG
1	F	142	HIS
1	F	152	GLU
1	F	202	THR
1	F	210	SER
1	F	212	THR
1	F	232	ASN
1	F	234	HIS
1	F	302	LEU
1	G	43	ASN
1	G	67	LYS
1	G	68	GLN
1	G	109	ASP
1	G	124	ARG
1	G	130	ASP
1	G	135	LEU
1	G	211	ARG
1	G	275	GLU
1	G	276	LEU
1	G	296	ASP
1	G	302	LEU
2	H	59	GLN
2	H	98	LYS
2	H	117	THR
2	H	144	LYS
2	H	156	LYS
2	H	160	LYS
2	H	172	GLN
3	I	22	LEU
3	I	152	GLU
3	I	154	TRP
3	I	156	ASP
3	I	241	LYS
3	I	285	PHE
3	I	298	ILE
3	I	304	GLN

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Mol	Chain	Res	Type
3	I	324	ASP
3	I	326	LYS
3	I	349	GLN
3	I	359	LYS
3	I	377	ARG
3	I	381	TYR
3	I	416	ASP
3	I	418	GLU
3	I	461	PHE
3	I	479	PHE
3	I	547	VAL
3	I	686	ASP
3	I	721	ASP
3	I	870	GLU
3	I	871	GLN
3	I	936	LEU
4	J	33	LEU
4	J	75	ARG
4	J	102	THR
4	J	106	ASP
4	J	121	GLU
4	K	3	GLU
4	K	15	TYR
4	K	25	LYS
4	K	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	218	HIS
1	B	10	GLN
1	B	43	ASN
1	B	171	HIS
1	C	10	GLN
1	C	20	HIS
1	C	218	HIS
1	D	68	GLN
1	D	218	HIS
1	E	148	ASN
1	G	218	HIS
2	H	57	ASN

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Mol	Chain	Res	Type
3	I	261	ASN
3	I	651	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	Z	42/43 (97%)	9 (21%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	Z	9	G
7	Z	15	U
7	Z	20	C
7	Z	21	C
7	Z	26	C
7	Z	27	G
7	Z	33	U
7	Z	38	A
7	Z	39	U

There are no RNA pucker outliers to report.

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)

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

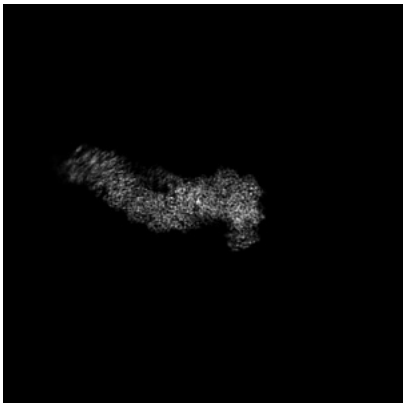
This section contains visualisations of the EMDB entry EMD-24974. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

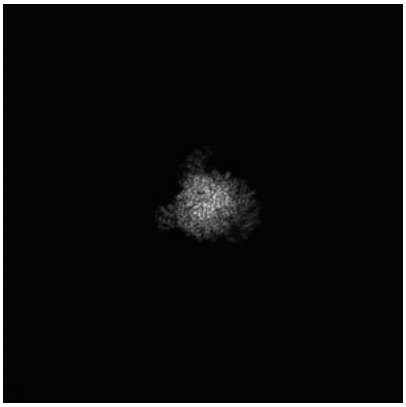
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

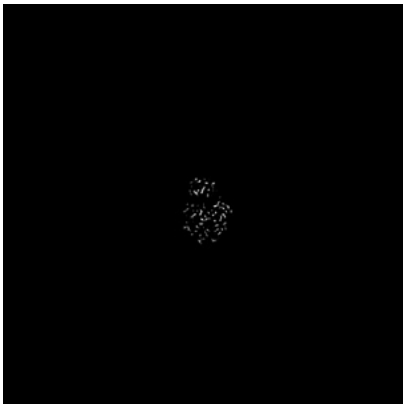
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 220

Y Index: 220



Z Index: 220

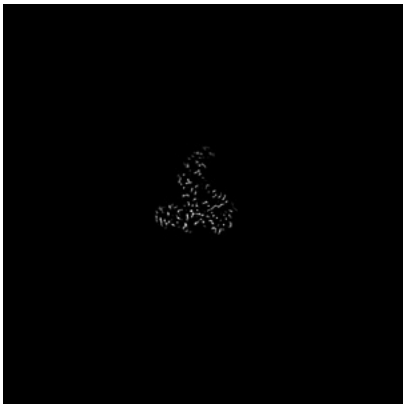
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 225

Y Index: 217



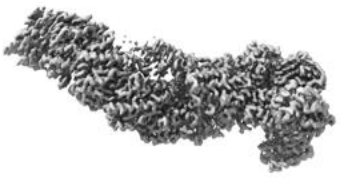
Z Index: 257

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

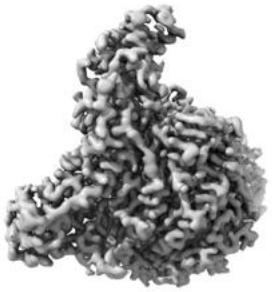
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

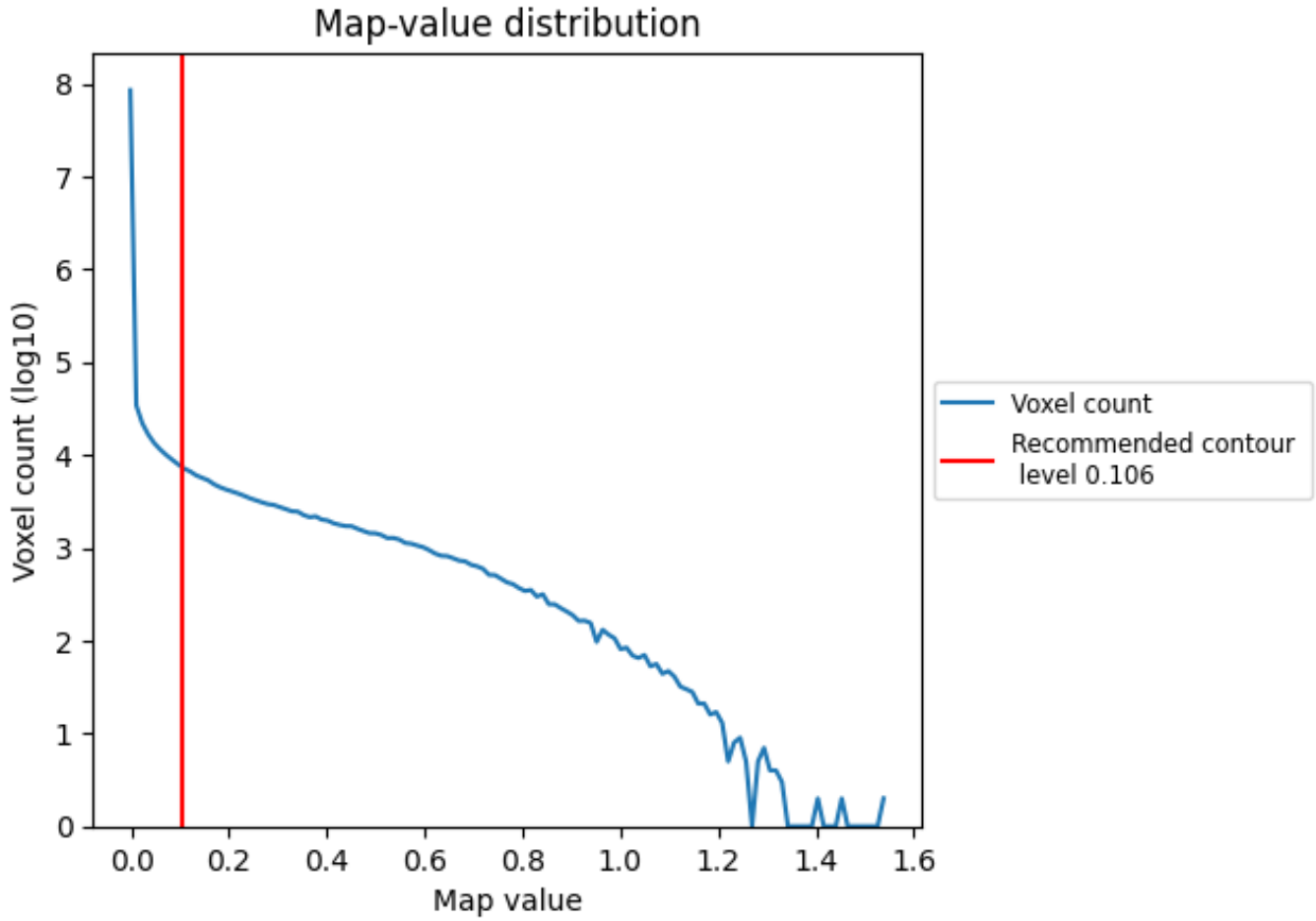
6.5 Mask visualisation (i)

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

7 Map analysis

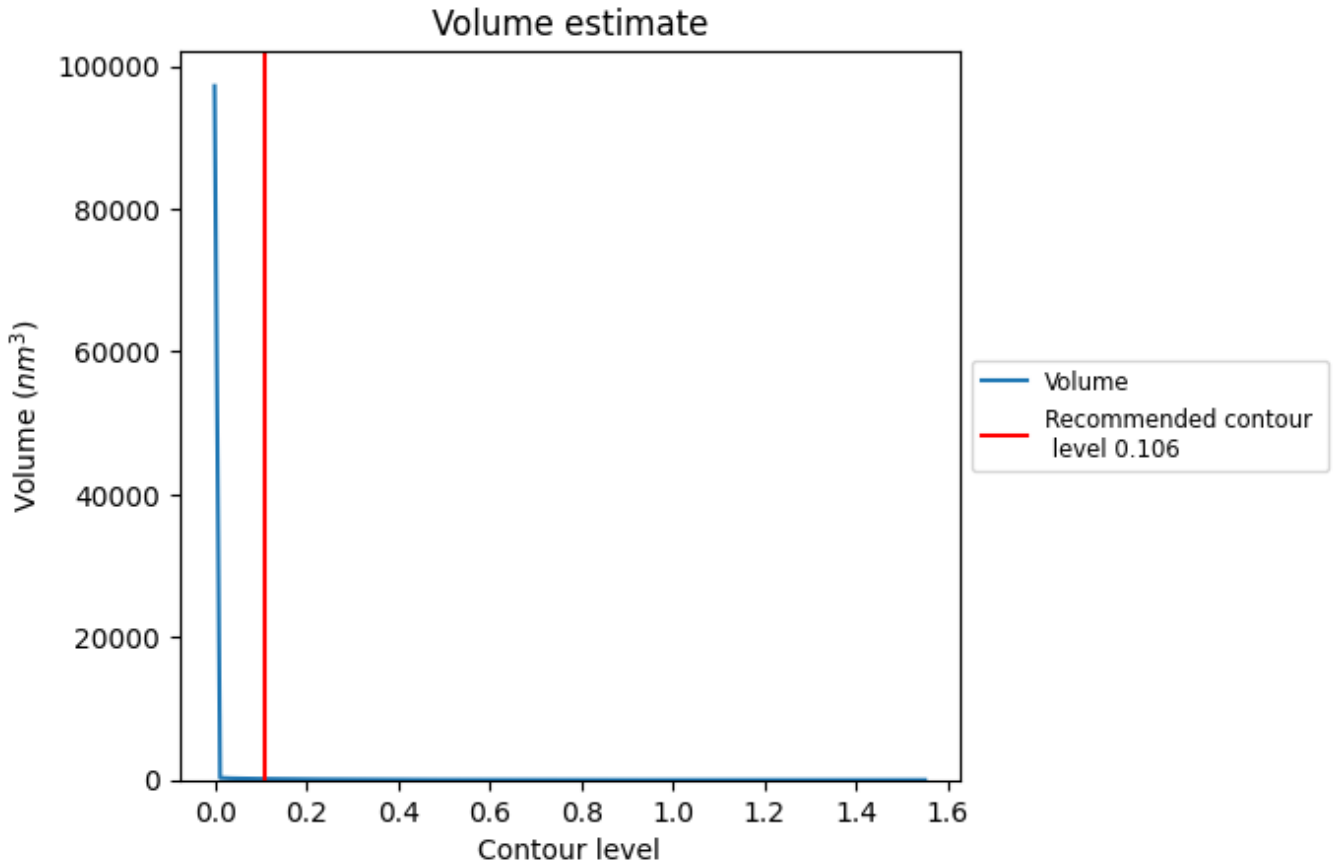
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

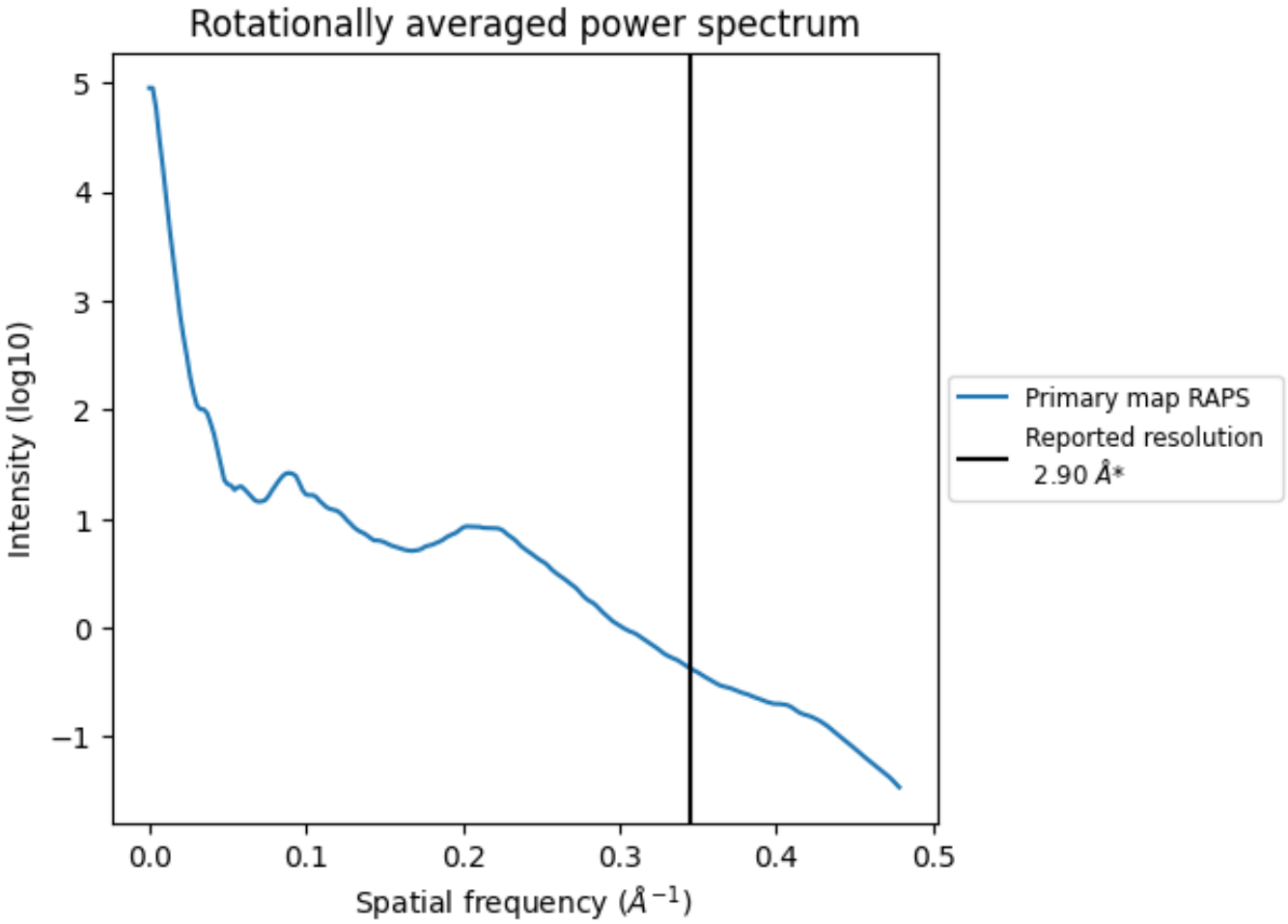
7.2 Volume estimate



The volume at the recommended contour level is 149 nm^3; this corresponds to an approximate mass of 135 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)

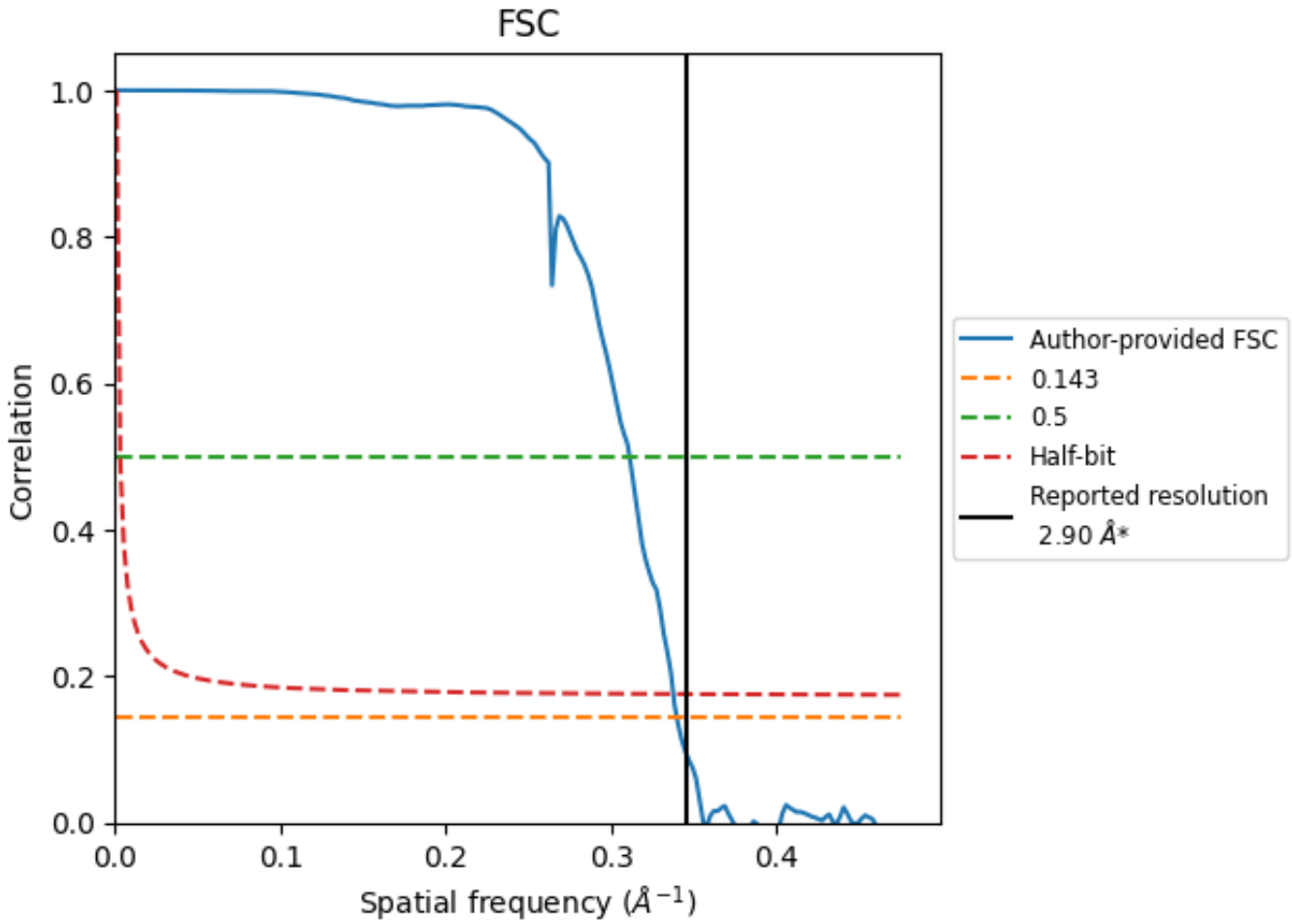


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

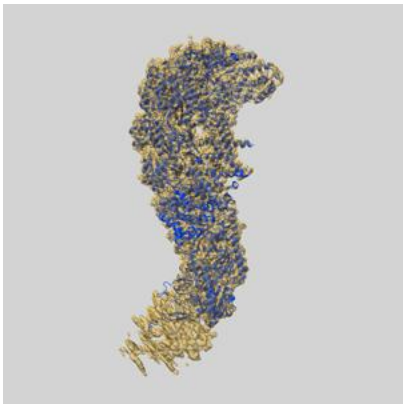
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.22	2.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

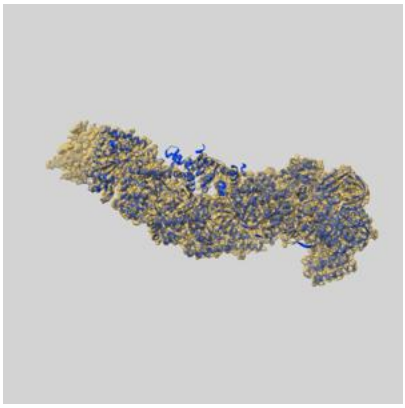
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24974 and PDB model 7SBA. Per-residue inclusion information can be found in section 3 on page 6.

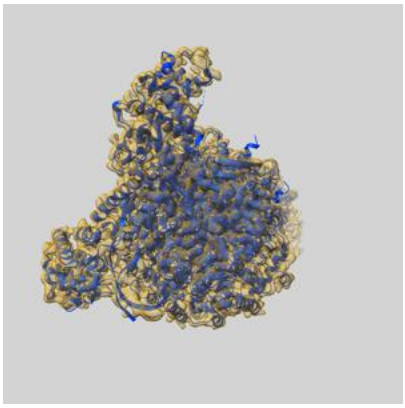
9.1 Map-model overlay



X



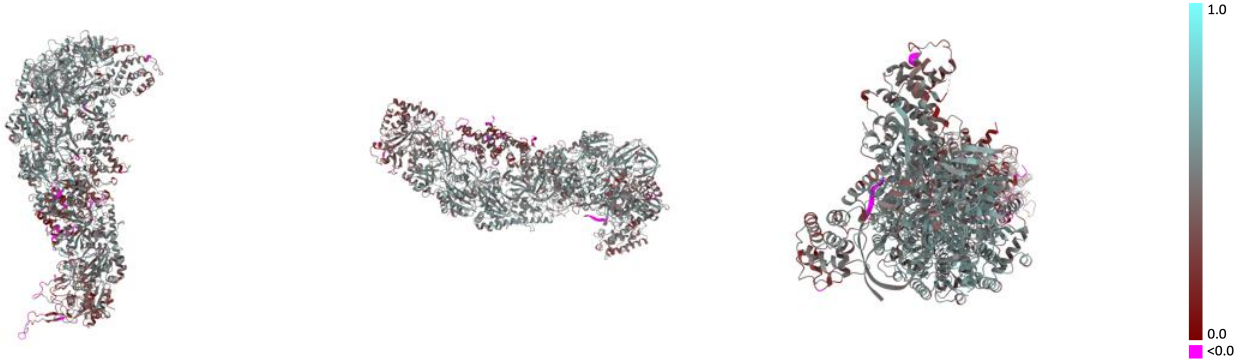
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106 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.

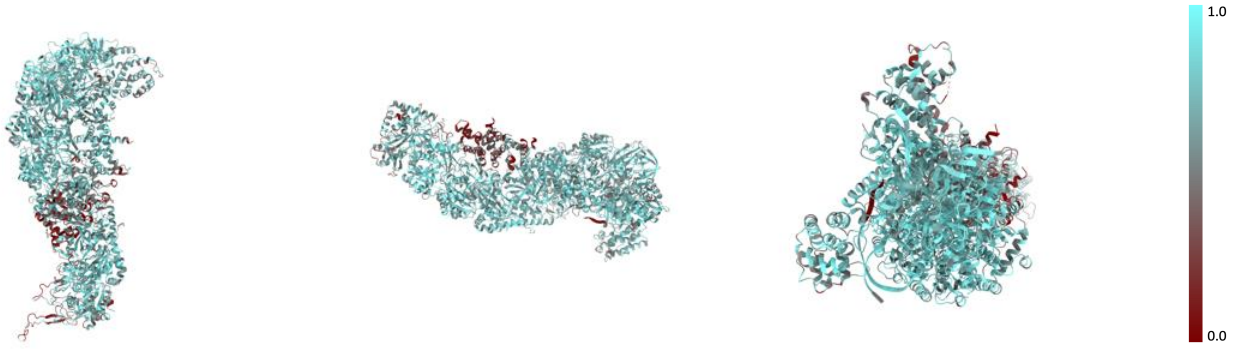
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

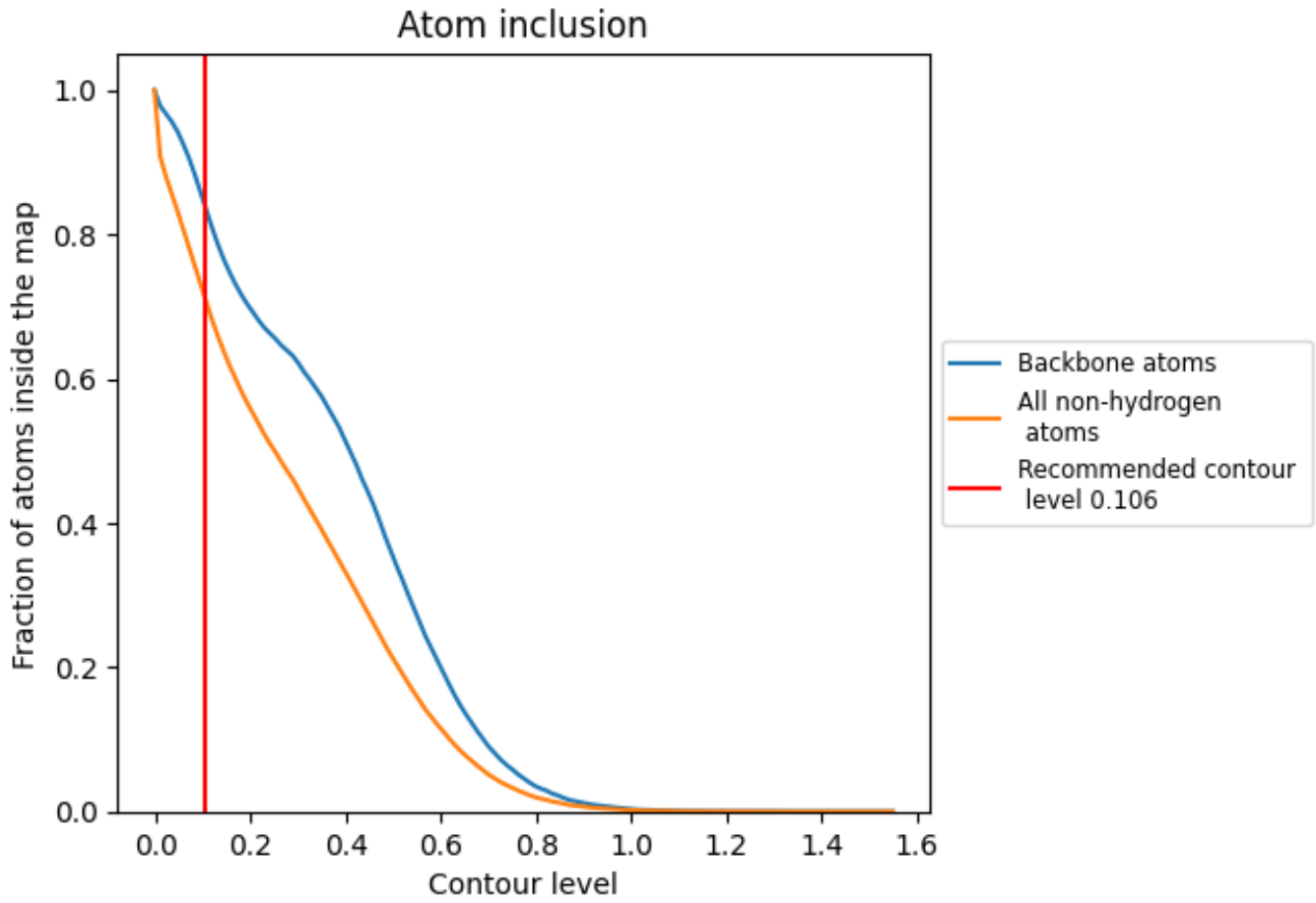
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 71% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7089	0.4530
A	0.7536	0.5060
B	0.7723	0.5140
C	0.8024	0.5130
D	0.7808	0.5060
E	0.7198	0.4780
F	0.7336	0.4440
G	0.5893	0.3300
H	0.8007	0.5250
I	0.7186	0.4470
J	0.5017	0.3320
K	0.2264	0.2140
X	0.6708	0.4650
Y	0.5134	0.2700
Z	0.8838	0.5320