



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:40 AM UTC

PDB ID : 7SBB / pdb_00007sbb
EMDB ID : EMD-24976
Title : Structure of type I-D Cascade bound to a ssRNA target
Authors : Schwartz, E.A.; Taylor, D.W.
Deposited on : 2021-09-24
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

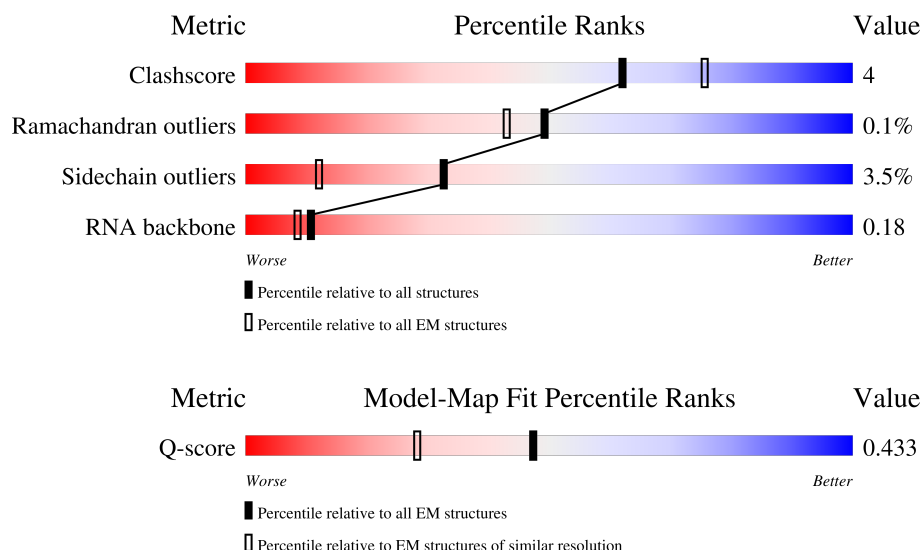
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	329	
1	B	329	
1	C	329	

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Mol	Chain	Length	Quality of chain
1	D	329	87% 10%
1	E	329	84% 12%
1	F	329	83% 13%
1	G	329	12% 88% 8%
2	H	254	75% 13% 12%
3	I	975	6% 61% 8% 30%
4	J	146	7% 83% 15%
4	K	146	17% 91% 8%
5	X	33	6% 52% 33% 9%
6	Z	43	37% 42% 14% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28938 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	223	Total	C	N	O	S	0	0
			1819	1178	309	327	5		

- Molecule 3 is a protein called Cas10d.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	680	Total	C	N	O	S	0	0
			5593	3608	947	1024	14		

- 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 RNA chain called ssRNA target.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	33	Total	C	N	O	P	0	0
			713	319	141	220	33		

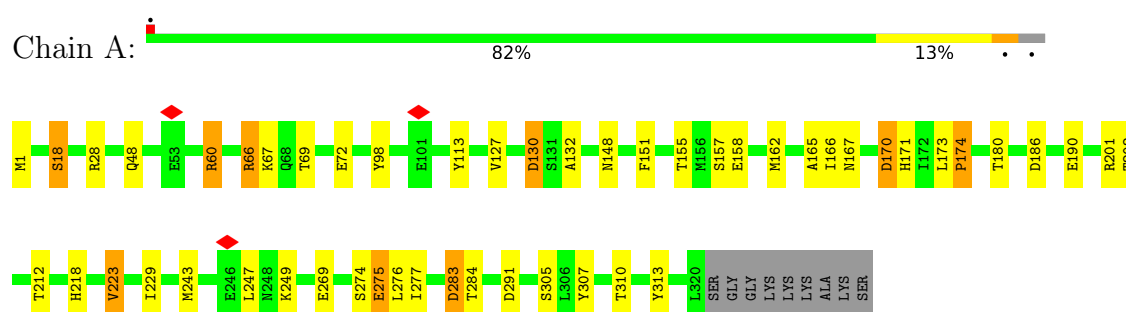
- Molecule 6 is a RNA chain called crRNA.

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

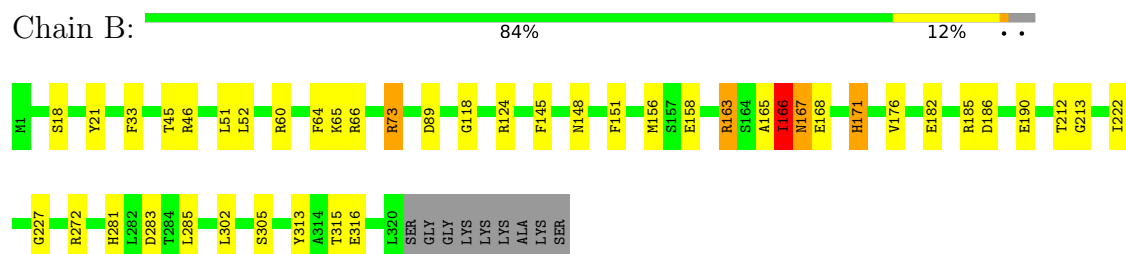
3 Residue-property plots [i](#)

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.

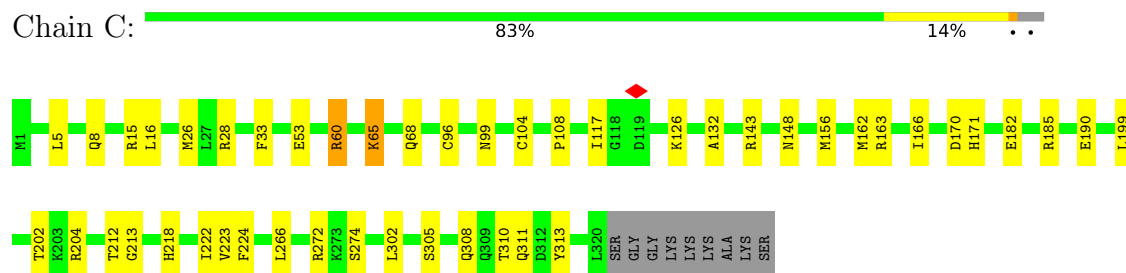
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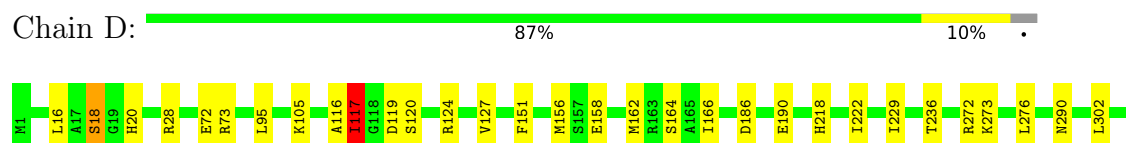
• Molecule 1: Cas7d

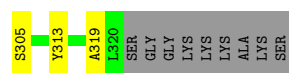


• Molecule 1: Cas7d

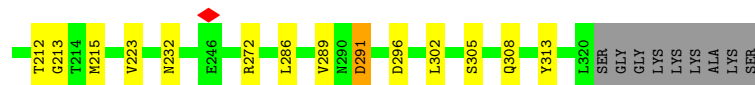
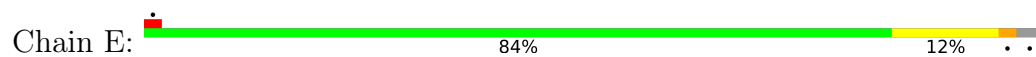


• Molecule 1: Cas7d

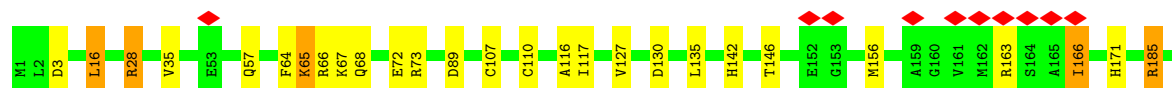
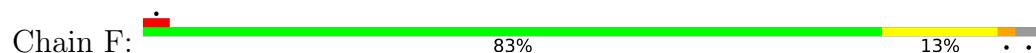




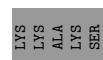
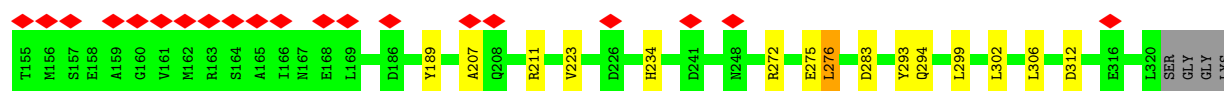
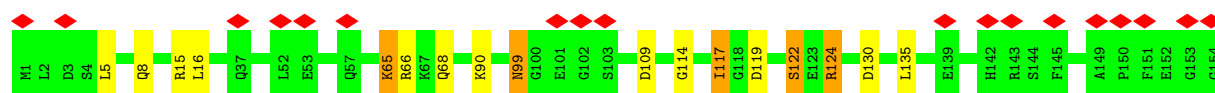
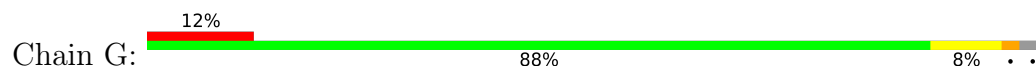
• Molecule 1: Cas7d



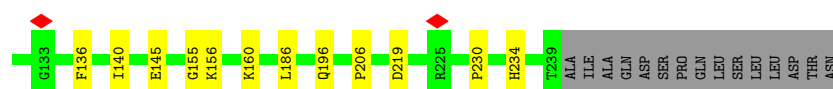
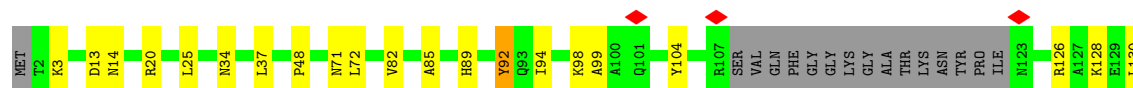
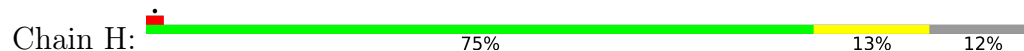
• Molecule 1: Cas7d

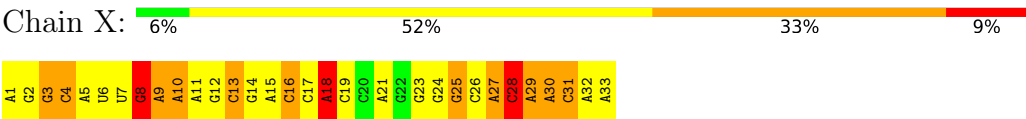


• Molecule 1: Cas7d

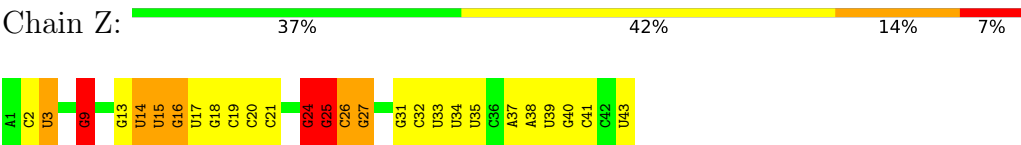


• Molecule 2: Cas5d





• Molecule 6: crRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.627	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	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

5.1 Standard geometry

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	0.82	2/2549 (0.1%)	1.43	17/3442 (0.5%)
1	B	0.87	3/2549 (0.1%)	1.46	18/3442 (0.5%)
1	C	0.84	2/2549 (0.1%)	1.43	12/3442 (0.3%)
1	D	0.87	2/2549 (0.1%)	1.42	10/3442 (0.3%)
1	E	0.82	2/2549 (0.1%)	1.44	14/3442 (0.4%)
1	F	0.90	2/2549 (0.1%)	1.50	22/3442 (0.6%)
1	G	0.90	4/2549 (0.2%)	1.48	13/3442 (0.4%)
2	H	0.91	5/1874 (0.3%)	1.40	17/2551 (0.7%)
3	I	0.79	0/5718	1.45	42/7756 (0.5%)
4	J	0.80	1/1209 (0.1%)	1.47	8/1624 (0.5%)
4	K	0.78	0/1209	1.49	4/1624 (0.2%)
5	X	0.51	0/800	0.93	5/1246 (0.4%)
6	Z	0.82	0/1007	1.30	9/1566 (0.6%)
All	All	0.84	23/29660 (0.1%)	1.43	191/40461 (0.5%)

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	3
1	B	0	5
1	C	0	4
1	D	0	2
1	E	0	3
1	F	0	3
1	G	0	2
2	H	0	1
3	I	0	5
4	J	0	3
6	Z	0	10
All	All	0	41

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	313	TYR	C-O	-8.00	1.14	1.24
1	F	313	TYR	C-O	-7.88	1.15	1.24
1	D	313	TYR	C-O	-7.88	1.15	1.24
1	C	313	TYR	C-O	-7.41	1.15	1.24
2	H	71	ASN	CA-C	-7.15	1.44	1.52
1	A	313	TYR	C-O	-6.31	1.16	1.24
1	A	223	VAL	C-O	-6.29	1.17	1.24
1	B	165	ALA	CA-CB	-6.27	1.48	1.53
2	H	37	LEU	C-O	-5.89	1.17	1.24
1	B	148	ASN	CA-C	-5.74	1.45	1.52
1	B	313	TYR	C-O	-5.70	1.17	1.24
1	E	223	VAL	C-O	-5.68	1.17	1.24
2	H	104	TYR	C-O	-5.68	1.17	1.24
1	G	124	ARG	CA-C	-5.59	1.45	1.53
2	H	34	ASN	C-O	-5.53	1.17	1.24
1	G	223	VAL	C-O	-5.40	1.18	1.24
2	H	186	LEU	C-O	-5.37	1.17	1.23
1	G	306	LEU	C-O	-5.10	1.18	1.24
4	J	123	ARG	CA-C	-5.04	1.45	1.52
1	C	311	GLN	CA-C	-5.03	1.46	1.52
1	G	66	ARG	C-O	-5.03	1.17	1.24
1	D	117	ILE	CA-C	-5.01	1.46	1.52
1	F	306	LEU	CA-C	-5.00	1.46	1.52

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	285	PHE	N-CA-C	-11.94	91.34	110.32
1	F	130	ASP	CA-CB-CG	9.88	122.48	112.60
1	G	114	GLY	N-CA-C	9.67	123.12	112.29
3	I	640	ASP	CA-CB-CG	9.62	122.22	112.60
1	A	130	ASP	CA-CB-CG	9.06	121.67	112.60
1	E	163	ARG	N-CA-C	-8.47	95.43	109.24
1	F	269	GLU	CB-CA-C	8.21	120.01	108.76
2	H	13	ASP	CA-CB-CG	8.15	120.75	112.60
1	B	163	ARG	N-CA-C	8.06	123.28	112.88
1	F	67	LYS	CA-C-N	8.04	133.46	120.60
1	F	67	LYS	C-N-CA	8.04	133.46	120.60
3	I	743	ASP	CA-CB-CG	7.98	120.58	112.60
3	I	271	ASP	CA-CB-CG	7.90	120.50	112.60
1	B	65	LYS	N-CA-CB	-7.78	98.35	109.94
1	A	173	LEU	CA-C-N	7.75	129.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	LEU	C-N-CA	7.75	129.53	119.84
5	X	28	C	C2'-C3'-O3'	7.57	125.05	113.70
6	Z	16	G	O3'-P-O5'	-7.36	92.96	104.00
1	B	182	GLU	CB-CA-C	7.33	121.63	109.53
1	B	89	ASP	CA-CB-CG	7.32	119.92	112.60
1	C	65	LYS	N-CA-C	7.26	119.83	111.11
1	E	291	ASP	CA-CB-CG	7.26	119.86	112.60
5	X	18	A	C2'-C3'-O3'	7.20	124.49	113.70
1	G	312	ASP	N-CA-C	-7.19	103.53	111.36
1	B	73	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	D	16	LEU	N-CA-C	-7.08	98.55	109.52
1	A	283	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	170	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	18	SER	N-CA-C	6.83	122.04	113.43
1	C	99	ASN	CB-CA-C	6.83	121.76	111.80
3	I	898	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	B	272	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	64	PHE	CA-C-N	6.75	129.66	120.54
1	B	64	PHE	C-N-CA	6.75	129.66	120.54
1	E	72	GLU	CA-CB-CG	6.74	127.59	114.10
1	F	185	ARG	CD-NE-CZ	6.73	133.82	124.40
1	C	171	HIS	CB-CG-CD2	-6.72	122.46	131.20
1	F	185	ARG	NE-CZ-NH2	6.72	125.25	119.20
3	I	507	HIS	CB-CG-CD2	-6.69	122.50	131.20
3	I	686	ASP	CA-CB-CG	6.69	119.29	112.60
4	K	22	GLU	CB-CA-C	6.68	120.29	110.26
1	F	65	LYS	N-CA-C	6.68	121.02	112.34
1	C	222	ILE	N-CA-C	-6.61	98.61	108.46
3	I	717	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	G	117	ILE	N-CA-C	6.56	122.99	109.34
3	I	720	GLN	CB-CA-C	6.51	119.12	109.29
4	J	70	GLN	CA-C-N	6.47	129.90	120.71
4	J	70	GLN	C-N-CA	6.47	129.90	120.71
1	G	272	ARG	NE-CZ-NH2	6.44	124.99	119.20
1	C	185	ARG	NE-CZ-NH2	6.37	124.94	119.20
3	I	506	ASP	CA-CB-CG	6.31	118.91	112.60
1	F	171	HIS	CB-CG-CD2	-6.31	123.00	131.20
3	I	719	ASP	CA-CB-CG	6.26	118.86	112.60
1	E	148	ASN	OD1-CG-ND2	-6.26	116.34	122.60
2	H	219	ASP	CA-CB-CG	6.25	118.85	112.60
5	X	5	A	C1'-C2'-O2'	-6.25	99.03	108.40
3	I	107	LEU	CB-CA-C	6.23	122.64	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	3	U	O4'-C1'-N1	6.22	117.83	108.50
1	G	294	GLN	OE1-CD-NE2	-6.16	116.44	122.60
3	I	858	THR	N-CA-C	-6.16	104.67	111.82
2	H	20	ARG	CD-NE-CZ	6.15	133.01	124.40
1	E	3	ASP	CA-CB-CG	6.14	118.74	112.60
1	G	99	ASN	CA-CB-CG	6.07	118.67	112.60
2	H	85	ALA	N-CA-C	6.05	118.38	108.52
1	G	65	LYS	N-CA-C	6.00	119.69	112.38
1	G	114	GLY	CA-C-O	-5.99	118.10	122.23
6	Z	9	G	O3'-P-O5'	-5.97	95.04	104.00
1	F	290	ASN	CA-CB-CG	5.92	118.52	112.60
3	I	683	THR	N-CA-C	5.89	119.13	110.59
2	H	155	GLY	CA-C-N	5.88	130.10	120.63
2	H	155	GLY	C-N-CA	5.88	130.10	120.63
4	J	68	ASP	CA-CB-CG	5.88	118.48	112.60
3	I	807	ARG	NE-CZ-NH2	5.86	124.48	119.20
3	I	940	MET	CB-CA-C	5.86	120.15	110.90
1	B	73	ARG	NE-CZ-NH2	5.83	124.45	119.20
3	I	310	LEU	CA-C-N	5.83	126.58	119.99
3	I	310	LEU	C-N-CA	5.83	126.58	119.99
1	F	28	ARG	CD-NE-CZ	5.83	132.56	124.40
1	F	57	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	D	73	ARG	NE-CZ-NH1	-5.81	115.69	121.50
6	Z	3	U	C3'-C2'-C1'	5.81	107.11	101.30
4	J	8	THR	N-CA-C	5.79	117.59	111.28
6	Z	17	U	C5'-C4'-C3'	-5.78	107.33	116.00
6	Z	25	G	O4'-C1'-N9	5.76	116.84	108.20
3	I	629	ASP	CA-CB-CG	5.75	118.35	112.60
1	F	68	GLN	N-CA-CB	-5.73	100.58	110.32
1	B	222	ILE	N-CA-C	-5.72	99.88	108.12
4	J	25	LYS	CA-C-N	5.71	128.99	122.83
4	J	25	LYS	C-N-CA	5.71	128.99	122.83
1	D	272	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	D	186	ASP	N-CA-C	5.68	119.03	111.30
1	B	166	ILE	CB-CA-C	-5.67	101.99	111.29
1	G	283	ASP	CA-CB-CG	5.67	118.27	112.60
1	E	66	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	G	122	SER	N-CA-C	-5.61	98.85	110.80
1	F	127	VAL	CA-C-N	5.60	129.87	122.42
1	F	127	VAL	C-N-CA	5.60	129.87	122.42
5	X	8	G	C4'-C3'-O3'	5.60	121.39	113.00
3	I	815	GLU	CB-CG-CD	5.56	122.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	777	ASP	CA-CB-CG	5.56	118.16	112.60
3	I	770	PRO	N-CA-C	5.54	117.46	110.70
1	C	148	ASN	CA-CB-CG	5.53	118.13	112.60
3	I	16	GLN	CA-C-N	5.52	129.97	122.07
3	I	16	GLN	C-N-CA	5.52	129.97	122.07
1	A	60	ARG	CD-NE-CZ	5.50	132.10	124.40
5	X	28	C	C3'-C2'-O2'	5.50	118.96	110.70
3	I	246	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	H	20	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	H	14	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	145	PHE	O-C-N	-5.47	116.08	123.19
1	B	186	ASP	N-CA-C	5.47	118.98	111.54
3	I	228	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	272	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	C	99	ASN	OD1-CG-ND2	-5.45	117.15	122.60
6	Z	24	G	C2'-C3'-O3'	5.44	117.66	109.50
1	E	170	ASP	CA-CB-CG	5.42	118.02	112.60
3	I	713	VAL	CA-C-N	5.41	125.61	120.31
3	I	713	VAL	C-N-CA	5.41	125.61	120.31
4	K	16	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	222	ILE	N-CA-C	-5.40	99.73	107.78
3	I	722	PHE	CA-CB-CG	5.39	119.19	113.80
3	I	718	SER	CA-C-N	5.38	129.30	120.63
3	I	718	SER	C-N-CA	5.38	129.30	120.63
1	G	234	HIS	CA-CB-CG	5.38	119.18	113.80
2	H	89	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	F	205	TYR	N-CA-C	5.37	119.84	113.12
4	J	146	ASN	CA-CB-CG	5.37	117.97	112.60
1	G	119	ASP	N-CA-C	-5.36	102.34	110.28
1	C	60	ARG	CD-NE-CZ	5.36	131.90	124.40
1	A	66	ARG	CD-NE-CZ	5.36	131.90	124.40
1	F	272	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	F	283	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	127	VAL	CA-C-N	5.33	130.51	123.05
1	D	127	VAL	C-N-CA	5.33	130.51	123.05
1	A	98	TYR	N-CA-C	5.33	117.09	111.28
2	H	48	PRO	CA-C-O	-5.33	115.38	121.56
1	B	51	LEU	N-CA-C	5.32	116.77	110.97
1	B	66	ARG	N-CA-C	5.32	118.94	112.23
1	D	73	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	A	171	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	E	162	MET	N-CA-C	5.30	117.91	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	ASP	CA-CB-CG	5.30	117.90	112.60
1	E	72	GLU	CB-CG-CD	5.30	121.61	112.60
2	H	99	ALA	CA-C-N	5.29	128.38	120.87
2	H	99	ALA	C-N-CA	5.29	128.38	120.87
2	H	206	PRO	N-CA-CB	5.28	105.97	103.22
4	K	30	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	E	73	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	274	SER	N-CA-C	5.26	117.01	111.28
2	H	230	PRO	CA-C-O	-5.26	115.61	121.23
3	I	685	THR	N-CA-C	-5.25	105.64	111.36
2	H	98	LYS	N-CA-C	5.24	116.95	109.14
1	E	72	GLU	CA-C-N	5.22	127.58	120.54
1	E	72	GLU	C-N-CA	5.22	127.58	120.54
3	I	247	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	F	73	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	I	763	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	269	GLU	CB-CA-C	5.20	116.91	109.26
1	G	90	LYS	N-CA-C	5.19	118.40	111.75
3	I	147	ARG	CB-CG-CD	5.19	123.25	111.30
4	J	30	HIS	CB-CG-CD2	-5.19	124.45	131.20
3	I	819	PHE	CA-CB-CG	5.17	118.97	113.80
3	I	286	ALA	CA-C-N	-5.16	114.64	119.85
3	I	286	ALA	C-N-CA	-5.16	114.64	119.85
1	A	66	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	148	ASN	CA-CB-CG	5.15	117.75	112.60
1	F	16	LEU	N-CA-C	-5.12	101.58	109.52
1	A	165	ALA	N-CA-C	5.12	116.94	107.73
1	F	226	ASP	CA-CB-CG	5.11	117.71	112.60
4	K	29	THR	CA-CB-CG2	5.11	119.18	110.50
1	E	148	ASN	CA-CB-CG	5.09	117.69	112.60
6	Z	27	G	O3'-P-O5'	-5.09	96.36	104.00
1	B	171	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	224	PHE	N-CA-C	-5.08	101.03	109.46
1	D	290	ASN	CA-CB-CG	5.08	117.68	112.60
1	F	3	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	283	ASP	CA-CB-CG	5.08	117.67	112.60
3	I	507	HIS	CA-CB-CG	5.07	118.87	113.80
1	A	48	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	281	HIS	CB-CG-CD2	-5.06	124.63	131.20
2	H	234	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	C	28	ARG	CD-NE-CZ	5.04	131.45	124.40
1	E	208	GLN	OE1-CD-NE2	-5.04	117.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	876	PRO	N-CA-CB	5.03	107.79	103.31
6	Z	15	U	O3'-P-O5'	-5.03	96.45	104.00
1	C	170	ASP	CA-CB-CG	5.03	117.63	112.60
3	I	909	ASP	CA-CB-CG	5.03	117.63	112.60
3	I	115	HIS	N-CA-C	5.03	118.51	112.38
1	D	73	ARG	CD-NE-CZ	5.01	131.41	124.40
1	A	269	GLU	N-CA-C	5.01	116.14	109.93
2	H	196	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	60	ARG	Sidechain
1	B	124	ARG	Sidechain
1	B	185	ARG	Sidechain
1	B	46	ARG	Sidechain
1	B	60	ARG	Sidechain
1	B	73	ARG	Sidechain
1	C	143	ARG	Sidechain
1	C	163	ARG	Sidechain
1	C	204	ARG	Sidechain
1	C	60	ARG	Sidechain
1	D	124	ARG	Sidechain
1	D	28	ARG	Sidechain
1	E	15	ARG	Sidechain
1	E	205	TYR	Sidechain
1	E	272	ARG	Sidechain
1	F	204	ARG	Sidechain
1	F	28	ARG	Sidechain
1	F	293	TYR	Sidechain
1	G	189	TYR	Sidechain
1	G	293	TYR	Sidechain
2	H	92	TYR	Sidechain
3	I	487	ARG	Sidechain
3	I	497	TYR	Sidechain
3	I	507	HIS	Sidechain
3	I	607	TYR	Sidechain
3	I	917	ARG	Sidechain
4	J	10	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	J	15	TYR	Sidechain
4	J	88	ARG	Sidechain
6	Z	14	U	Sidechain
6	Z	16	G	Sidechain
6	Z	18	G	Sidechain
6	Z	19	C	Sidechain
6	Z	2	C	Sidechain
6	Z	25	G	Sidechain
6	Z	26	C	Sidechain
6	Z	3	U	Sidechain
6	Z	31	G	Sidechain
6	Z	34	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2503	0	2454	30	0
1	B	2503	0	2454	20	0
1	C	2503	0	2454	29	0
1	D	2503	0	2454	13	0
1	E	2503	0	2454	37	0
1	F	2503	0	2454	23	0
1	G	2503	0	2454	20	0
2	H	1819	0	1765	13	0
3	I	5593	0	5592	47	0
4	J	1194	0	1219	14	0
4	K	1194	0	1219	9	0
5	X	713	0	362	59	0
6	Z	904	0	460	8	0
All	All	28938	0	27795	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (239) 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:E:144:SER:HB3	1:E:170:ASP:OD1	1.25	1.33
1:E:33:PHE:O	1:E:212:THR:HG21	1.41	1.18
1:F:146:THR:CG2	1:F:166:ILE:HD11	1.73	1.17
3:I:836:LEU:HD23	3:I:940:MET:SD	1.85	1.16
1:C:162:MET:HG3	5:X:16:C:O2'	1.52	1.09
1:D:162:MET:HG3	5:X:10:A:O2'	1.52	1.07
1:E:144:SER:CB	1:E:170:ASP:OD1	2.03	1.07
1:A:1:MET:HG3	1:A:284:THR:HG23	1.34	1.06
3:I:833:LYS:HG3	3:I:940:MET:HE1	1.07	1.05
3:I:221:LEU:HD13	3:I:283:ILE:CD1	1.86	1.04
1:F:146:THR:HG22	1:F:166:ILE:HD11	1.38	1.01
1:E:212:THR:HG22	1:E:213:GLY:N	1.75	1.01
1:A:162:MET:CB	5:X:29:A:H5'	1.93	0.98
3:I:833:LYS:HG3	3:I:940:MET:CE	1.94	0.97
1:E:36:PHE:CZ	1:E:63:MET:HE2	2.02	0.95
1:G:15:ARG:O	1:G:16:LEU:HD12	1.67	0.94
1:A:1:MET:HG3	1:A:284:THR:CG2	1.97	0.94
1:D:162:MET:CG	5:X:10:A:O2'	2.16	0.93
1:B:212:THR:HG22	1:B:213:GLY:N	1.82	0.92
3:I:833:LYS:CG	3:I:940:MET:HE1	1.97	0.92
1:C:33:PHE:O	1:C:212:THR:HG21	1.68	0.92
1:C:212:THR:HG22	1:C:213:GLY:N	1.82	0.91
1:D:164:SER:HA	5:X:11:A:O2'	1.71	0.89
1:A:162:MET:HB2	5:X:29:A:H5'	1.54	0.88
1:E:212:THR:CG2	1:E:213:GLY:N	2.37	0.88
2:H:25:LEU:HD12	2:H:126:ARG:O	1.74	0.88
3:I:221:LEU:HD13	3:I:283:ILE:HD11	1.55	0.86
1:C:166:ILE:HG22	5:X:17:C:O2'	1.74	0.86
1:D:162:MET:SD	5:X:10:A:O2'	2.34	0.85
3:I:833:LYS:HE2	3:I:940:MET:HE3	1.58	0.84
3:I:221:LEU:CD1	3:I:283:ILE:HD13	2.07	0.84
4:K:28:SER:CB	5:X:10:A:H5'	2.07	0.84
3:I:221:LEU:HD13	3:I:283:ILE:HD13	1.60	0.81
1:E:151:PHE:CZ	1:G:16:LEU:HD11	2.14	0.81
1:B:33:PHE:O	1:B:212:THR:HG21	1.80	0.81
2:H:3:LYS:HE2	2:H:145:GLU:CG	2.12	0.80
1:E:33:PHE:C	1:E:212:THR:HG21	2.09	0.77
1:F:146:THR:CG2	1:F:166:ILE:CD1	2.59	0.77
3:I:221:LEU:CD1	3:I:283:ILE:CD1	2.60	0.77
2:H:3:LYS:HE2	2:H:145:GLU:HG3	1.67	0.77
1:B:212:THR:CG2	1:B:213:GLY:N	2.47	0.76
1:G:15:ARG:C	1:G:16:LEU:HD12	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:GLN:NE2	1:G:275:GLU:OE1	2.19	0.76
1:C:212:THR:CG2	1:C:213:GLY:N	2.48	0.75
4:J:29:THR:HG22	5:X:17:C:OP2	1.87	0.75
1:E:212:THR:CG2	1:E:213:GLY:H	1.98	0.74
1:C:166:ILE:CG2	5:X:17:C:O2'	2.35	0.74
1:F:212:THR:HG21	1:G:65:LYS:HZ3	1.53	0.73
3:I:215:LEU:HD13	3:I:221:LEU:CD1	2.19	0.73
1:E:32:SER:O	1:E:212:THR:HG23	1.89	0.73
1:C:162:MET:CG	5:X:16:C:O2'	2.33	0.72
1:G:15:ARG:HG2	1:G:16:LEU:HD13	1.72	0.72
3:I:633:HIS:CB	3:I:647:LEU:HD11	2.19	0.72
3:I:221:LEU:CD2	3:I:283:ILE:HD13	2.19	0.71
4:K:28:SER:CB	5:X:10:A:C5'	2.67	0.71
4:K:28:SER:HB2	5:X:10:A:C5'	2.20	0.71
1:A:130:ASP:OD1	2:H:160:LYS:HG3	1.91	0.71
1:B:212:THR:OG1	1:C:65:LYS:HD2	1.91	0.70
5:X:31:C:H2'	5:X:32:A:H8	1.56	0.70
1:E:152:GLU:HG3	1:G:16:LEU:HD21	1.74	0.70
1:G:15:ARG:HG2	1:G:16:LEU:CD1	2.23	0.69
1:C:117:ILE:HG22	5:X:27:A:H1'	1.74	0.69
1:A:162:MET:HB2	5:X:29:A:C5'	2.22	0.69
4:K:28:SER:HB3	5:X:10:A:H5'	1.75	0.69
1:E:152:GLU:HG3	1:G:16:LEU:CD2	2.24	0.68
3:I:833:LYS:HE2	3:I:940:MET:CE	2.24	0.68
1:E:35:VAL:CG2	1:E:171:HIS:ND1	2.57	0.67
4:J:69:ARG:NH2	5:X:13:C:H5'	2.10	0.67
1:B:33:PHE:O	1:B:212:THR:CG2	2.43	0.66
3:I:836:LEU:CD2	3:I:940:MET:SD	2.75	0.65
1:G:5:LEU:HD12	1:G:275:GLU:OE1	1.96	0.65
1:E:155:THR:HG22	6:Z:41:C:O4'	1.97	0.64
1:C:190:GLU:HG2	1:C:305:SER:OG	1.97	0.64
1:C:33:PHE:O	1:C:212:THR:CG2	2.43	0.63
3:I:221:LEU:HD22	3:I:283:ILE:HD13	1.78	0.63
1:C:162:MET:HE3	5:X:16:C:H1'	1.80	0.63
1:F:146:THR:HG23	1:F:166:ILE:HD11	1.77	0.63
4:K:28:SER:HB2	5:X:10:A:H5''	1.82	0.62
1:F:163:ARG:NH1	1:G:99:ASN:OD1	2.33	0.62
3:I:633:HIS:HB3	3:I:647:LEU:HD11	1.82	0.61
1:A:162:MET:CB	5:X:29:A:C5'	2.75	0.61
1:E:35:VAL:HG23	1:E:171:HIS:ND1	2.14	0.61
4:J:28:SER:CB	5:X:16:C:H5'	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:PHE:CZ	1:E:63:MET:CE	2.82	0.60
1:F:212:THR:HG21	1:G:65:LYS:NZ	2.15	0.60
3:I:898:ARG:HH11	5:X:18:A:H5'	1.65	0.60
3:I:215:LEU:HD13	3:I:221:LEU:HD11	1.83	0.60
1:A:162:MET:HG3	5:X:28:C:O2'	2.01	0.59
1:D:273:LYS:HB3	1:D:276:LEU:HD11	1.85	0.59
4:K:28:SER:HB2	5:X:10:A:H5'	1.79	0.59
1:F:117:ILE:HG12	5:X:8:G:H21	1.68	0.59
4:K:29:THR:HG22	5:X:11:A:P	2.42	0.59
1:D:120:SER:HB2	1:D:319:ALA:HB1	1.84	0.59
1:F:223:VAL:HG13	1:F:276:LEU:HD23	1.83	0.59
2:H:3:LYS:HE2	2:H:145:GLU:HG2	1.86	0.58
1:A:130:ASP:CG	2:H:160:LYS:HG3	2.28	0.58
3:I:215:LEU:HD13	3:I:221:LEU:HD12	1.84	0.58
3:I:631:ARG:HB2	3:I:761:THR:HG22	1.86	0.58
5:X:3:G:H3'	5:X:4:C:H5''	1.85	0.58
1:F:163:ARG:CZ	1:G:99:ASN:OD1	2.52	0.57
1:A:162:MET:HE2	5:X:28:C:O2'	2.03	0.57
1:E:36:PHE:CE2	1:E:63:MET:CE	2.88	0.57
4:J:28:SER:HB2	5:X:16:C:H5'	1.86	0.56
1:E:151:PHE:HZ	1:G:16:LEU:HD11	1.69	0.56
3:I:240:GLU:O	3:I:241:LYS:HD3	2.07	0.55
1:A:162:MET:HB3	5:X:29:A:H5'	1.84	0.55
1:B:118:GLY:CA	5:X:33:A:O2'	2.54	0.55
1:B:212:THR:CG2	1:B:213:GLY:H	2.20	0.55
5:X:1:A:H2'	5:X:2:G:O4'	2.06	0.55
1:E:35:VAL:CG1	1:E:37:GLN:HG3	2.37	0.54
1:C:162:MET:HE3	5:X:16:C:O2'	2.08	0.54
3:I:142:LEU:CD2	3:I:158:ARG:HG3	2.37	0.54
2:H:25:LEU:CD1	2:H:126:ARG:O	2.54	0.53
1:E:36:PHE:CE2	1:E:63:MET:HE2	2.44	0.53
5:X:29:A:H2'	5:X:30:A:C8	2.44	0.52
1:A:1:MET:CG	1:A:284:THR:CG2	2.81	0.52
1:E:33:PHE:C	1:E:212:THR:CG2	2.80	0.52
1:F:116:ALA:O	5:X:9:A:C2	2.63	0.52
1:A:1:MET:CG	1:A:284:THR:HG23	2.25	0.51
1:E:36:PHE:CE2	1:E:63:MET:HE3	2.45	0.51
1:F:117:ILE:CG1	5:X:8:G:H21	2.23	0.51
1:A:190:GLU:HG2	1:A:305:SER:OG	2.09	0.51
1:G:275:GLU:HG2	1:G:276:LEU:N	2.26	0.51
1:F:116:ALA:O	5:X:9:A:H2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:THR:HG22	6:Z:41:C:C1'	2.41	0.51
1:F:146:THR:HG23	1:F:166:ILE:CD1	2.37	0.51
1:F:273:LYS:HD2	1:F:276:LEU:HD21	1.92	0.51
3:I:221:LEU:HD23	3:I:243:PHE:HB3	1.93	0.51
3:I:221:LEU:HD21	3:I:283:ILE:HG21	1.91	0.50
1:E:212:THR:HG23	1:E:213:GLY:H	1.75	0.50
4:J:29:THR:CG2	5:X:17:C:OP2	2.57	0.50
3:I:221:LEU:CD2	3:I:283:ILE:HG21	2.42	0.49
1:E:32:SER:O	1:E:212:THR:CG2	2.60	0.49
1:C:212:THR:CG2	1:C:213:GLY:H	2.21	0.49
1:C:26:MET:HE3	1:C:199:LEU:HD22	1.93	0.49
1:F:64:PHE:CZ	1:F:65:LYS:HE3	2.47	0.49
4:K:139:LEU:HD12	4:K:143:GLN:HG2	1.94	0.49
1:D:156:MET:SD	1:D:166:ILE:HD11	2.52	0.49
3:I:215:LEU:CD1	3:I:221:LEU:HD11	2.43	0.49
1:C:117:ILE:HG22	5:X:27:A:C1'	2.40	0.49
4:J:69:ARG:HH22	5:X:13:C:H5'	1.74	0.49
1:A:162:MET:CG	5:X:29:A:H5'	2.43	0.48
5:X:9:A:N1	6:Z:35:U:C5	2.81	0.48
1:E:35:VAL:HG13	1:E:37:GLN:HG3	1.96	0.48
1:C:108:PRO:HA	1:C:310:THR:HG21	1.96	0.48
1:B:156:MET:HE1	1:B:166:ILE:HG12	1.96	0.48
3:I:935:ASP:O	3:I:940:MET:HG2	2.14	0.47
1:A:130:ASP:OD2	2:H:160:LYS:HG3	2.14	0.47
1:A:275:GLU:C	1:A:276:LEU:HD22	2.39	0.47
4:J:107:LEU:HD12	4:J:111:MET:HE2	1.97	0.47
3:I:683:THR:HG22	3:I:686:ASP:HB3	1.95	0.47
1:D:151:PHE:CZ	1:F:16:LEU:HD21	2.50	0.47
1:E:302:LEU:O	1:E:305:SER:OG	2.21	0.47
4:J:28:SER:CB	5:X:16:C:C5'	2.93	0.47
1:A:151:PHE:CZ	1:C:16:LEU:HD21	2.51	0.46
4:J:28:SER:HB3	5:X:16:C:H5'	1.97	0.46
1:E:152:GLU:HG3	1:G:16:LEU:HD23	1.97	0.46
3:I:631:ARG:CB	3:I:761:THR:HG22	2.45	0.46
3:I:261:ASN:ND2	3:I:265:ARG:NH1	2.64	0.46
4:J:30:HIS:CD2	5:X:16:C:C5	3.04	0.46
4:J:107:LEU:CD1	4:J:111:MET:HE2	2.45	0.46
1:F:156:MET:SD	1:G:207:ALA:HB1	2.56	0.46
1:B:118:GLY:N	5:X:33:A:O2'	2.48	0.45
1:C:162:MET:HB2	5:X:17:C:C5'	2.46	0.45
1:F:163:ARG:NH2	1:G:99:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:OG1	1:C:65:LYS:CD	2.62	0.45
1:C:162:MET:HB2	5:X:17:C:H5'	1.99	0.45
1:C:302:LEU:O	1:C:305:SER:OG	2.27	0.45
1:B:167:ASN:HD21	5:X:25:G:H5''	1.81	0.45
1:A:158:GLU:OE2	1:C:15:ARG:NH1	2.49	0.45
3:I:142:LEU:HD21	3:I:158:ARG:HG3	1.99	0.45
1:D:302:LEU:O	1:D:305:SER:OG	2.31	0.45
1:E:286:LEU:HA	1:E:289:VAL:HG12	1.99	0.45
4:K:124:ASN:HB3	5:X:13:C:OP2	2.17	0.45
1:B:302:LEU:O	1:B:305:SER:OG	2.27	0.44
6:Z:24:G:N3	6:Z:24:G:H2'	2.31	0.44
3:I:633:HIS:HB2	3:I:647:LEU:HD11	1.99	0.44
2:H:92:TYR:CE1	2:H:128:LYS:HE2	2.53	0.44
1:B:118:GLY:C	5:X:33:A:O2'	2.61	0.44
3:I:776:GLN:HB2	5:X:30:A:OP2	2.17	0.44
1:A:132:ALA:HB2	1:A:180:THR:HG22	2.00	0.44
1:G:5:LEU:CD1	1:G:275:GLU:OE1	2.63	0.44
1:B:166:ILE:HG23	1:B:166:ILE:HD13	1.61	0.44
1:A:307:TYR:HA	1:A:310:THR:HG22	2.01	0.43
1:D:18:SER:HB2	1:D:20:HIS:CE1	2.53	0.43
1:A:155:THR:HG22	1:A:157:SER:H	1.84	0.43
1:E:144:SER:HB2	1:E:170:ASP:OD1	2.09	0.43
1:E:143:ARG:NH1	1:E:173:LEU:HD21	2.34	0.43
3:I:898:ARG:NH1	5:X:18:A:H5'	2.32	0.43
1:A:18:SER:HB2	1:A:186:ASP:OD1	2.19	0.43
3:I:240:GLU:O	3:I:241:LYS:CD	2.66	0.43
4:J:67:LEU:HD21	4:J:96:ILE:HD11	2.01	0.43
1:E:155:THR:HG22	6:Z:41:C:C4'	2.49	0.43
1:A:291:ASP:OD1	1:A:291:ASP:O	2.36	0.43
1:F:190:GLU:HG2	1:F:305:SER:OG	2.18	0.43
3:I:645:LYS:HE2	3:I:700:TYR:CZ	2.54	0.43
1:A:113:TYR:CE2	1:A:127:VAL:HG11	2.53	0.43
1:E:35:VAL:CG2	1:E:171:HIS:CE1	3.01	0.43
2:H:130:LEU:HD13	2:H:136:PHE:CZ	2.54	0.43
1:E:212:THR:OG1	1:F:65:LYS:HE2	2.19	0.42
3:I:266:THR:HG21	3:I:301:ILE:HG21	2.01	0.42
1:C:68:GLN:HE22	1:C:132:ALA:CB	2.32	0.42
1:C:96:CYS:SG	1:C:104:CYS:HB3	2.59	0.42
1:E:181:VAL:H	1:E:232:ASN:ND2	2.17	0.42
3:I:767:ARG:HH22	5:X:28:C:N4	2.17	0.42
3:I:604:ALA:HA	3:I:705:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HG13	1:A:276:LEU:HD13	2.02	0.42
2:H:25:LEU:HD21	2:H:94:ILE:HD13	2.01	0.42
4:J:127:LYS:HB2	4:J:127:LYS:HE2	1.54	0.42
1:C:223:VAL:HG21	1:C:266:LEU:HD11	2.02	0.42
3:I:875:VAL:HG21	3:I:887:GLN:NE2	2.34	0.42
4:J:123:ARG:HE	4:J:123:ARG:HB3	1.59	0.42
1:D:190:GLU:HG2	1:D:305:SER:OG	2.19	0.42
1:E:63:MET:HE1	1:E:215:MET:SD	2.60	0.42
1:A:67:LYS:HZ2	6:Z:9:G:P	2.41	0.42
1:C:162:MET:SD	5:X:16:C:O2'	2.78	0.42
1:E:152:GLU:CD	1:G:16:LEU:HD23	2.45	0.42
1:F:135:LEU:HD21	1:F:243:MET:HE1	2.02	0.42
2:H:25:LEU:HD13	2:H:126:ARG:CB	2.50	0.42
1:C:8:GLN:HE22	1:C:274:SER:HB3	1.84	0.41
1:B:21:TYR:CE1	1:B:227:GLY:HA2	2.55	0.41
1:B:118:GLY:O	5:X:33:A:O2'	2.38	0.41
1:B:190:GLU:HG2	1:B:305:SER:OG	2.21	0.41
3:I:875:VAL:HG13	3:I:879:TRP:CE3	2.55	0.41
3:I:802:ARG:C	3:I:804:LYS:H	2.28	0.41
3:I:208:PHE:CD2	3:I:233:LEU:HD11	2.55	0.41
1:A:174:PRO:CG	1:B:45:THR:HG21	2.51	0.41
1:A:243:MET:HE3	1:A:249:LYS:HD2	2.03	0.41
1:C:166:ILE:CG2	5:X:17:C:C2'	2.99	0.41
1:F:107:CYS:HG	1:F:110:CYS:HG	1.66	0.41
3:I:240:GLU:O	3:I:241:LYS:HG2	2.21	0.41
1:B:285:LEU:HD23	1:B:285:LEU:C	2.45	0.41
3:I:841:VAL:HG23	3:I:844:TYR:CZ	2.56	0.41
1:A:66:ARG:HH11	6:Z:9:G:P	2.44	0.40
1:B:166:ILE:HD12	1:B:166:ILE:HG21	1.59	0.40
1:D:116:ALA:HB3	6:Z:24:G:C8	2.56	0.40
1:D:117:ILE:H	1:D:117:ILE:HG12	1.70	0.40
3:I:841:VAL:HA	3:I:844:TYR:CD2	2.56	0.40
2:H:82:VAL:HG23	2:H:140:ILE:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/329 (97%)	306 (96%)	10 (3%)	2 (1%)	21	52
1	B	318/329 (97%)	299 (94%)	19 (6%)	0	100	100
1	C	318/329 (97%)	306 (96%)	12 (4%)	0	100	100
1	D	318/329 (97%)	302 (95%)	15 (5%)	1 (0%)	36	67
1	E	318/329 (97%)	304 (96%)	13 (4%)	1 (0%)	36	67
1	F	318/329 (97%)	301 (95%)	16 (5%)	1 (0%)	36	67
1	G	318/329 (97%)	289 (91%)	29 (9%)	0	100	100
2	H	219/254 (86%)	214 (98%)	5 (2%)	0	100	100
3	I	666/975 (68%)	644 (97%)	22 (3%)	0	100	100
4	J	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
4	K	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
All	All	3399/3824 (89%)	3236 (95%)	158 (5%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

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

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	273/279 (98%)	261 (96%)	12 (4%)	25	56
1	B	273/279 (98%)	261 (96%)	12 (4%)	25	56
1	C	273/279 (98%)	265 (97%)	8 (3%)	37	66
1	D	273/279 (98%)	264 (97%)	9 (3%)	33	63
1	E	273/279 (98%)	263 (96%)	10 (4%)	30	61
1	F	273/279 (98%)	264 (97%)	9 (3%)	33	63
1	G	273/279 (98%)	262 (96%)	11 (4%)	28	60
2	H	194/219 (89%)	192 (99%)	2 (1%)	68	79
3	I	606/855 (71%)	589 (97%)	17 (3%)	38	66
4	J	130/130 (100%)	121 (93%)	9 (7%)	14	41
4	K	130/130 (100%)	124 (95%)	6 (5%)	24	55
All	All	2971/3287 (90%)	2866 (96%)	105 (4%)	32	62

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	72	GLU
1	A	166	ILE
1	A	167	ASN
1	A	170	ASP
1	A	202	THR
1	A	212	THR
1	A	218	HIS
1	A	247	LEU
1	A	275	GLU
1	A	277	ILE
1	A	283	ASP
1	B	18	SER
1	B	52	LEU
1	B	151	PHE
1	B	158	GLU
1	B	163	ARG
1	B	166	ILE
1	B	167	ASN
1	B	168	GLU
1	B	171	HIS

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	315	THR
1	B	316	GLU
1	C	5	LEU
1	C	53	GLU
1	C	126	LYS
1	C	156	MET
1	C	182	GLU
1	C	202	THR
1	C	218	HIS
1	C	308	GLN
1	D	18	SER
1	D	72	GLU
1	D	95	LEU
1	D	105	LYS
1	D	117	ILE
1	D	119	ASP
1	D	158	GLU
1	D	218	HIS
1	D	236	THR
1	E	72	GLU
1	E	104	CYS
1	E	161	VAL
1	E	162	MET
1	E	166	ILE
1	E	167	ASN
1	E	202	THR
1	E	291	ASP
1	E	296	ASP
1	E	308	GLN
1	F	35	VAL
1	F	66	ARG
1	F	72	GLU
1	F	142	HIS
1	F	166	ILE
1	F	185	ARG
1	F	232	ASN
1	F	271	VAL
1	F	274	SER
1	G	68	GLN
1	G	109	ASP
1	G	117	ILE

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Mol	Chain	Res	Type
1	G	122	SER
1	G	124	ARG
1	G	130	ASP
1	G	135	LEU
1	G	211	ARG
1	G	276	LEU
1	G	299	LEU
1	G	302	LEU
2	H	72	LEU
2	H	156	LYS
3	I	240	GLU
3	I	244	VAL
3	I	270	LEU
3	I	487	ARG
3	I	508	GLN
3	I	641	LEU
3	I	683	THR
3	I	685	THR
3	I	686	ASP
3	I	780	LYS
3	I	802	ARG
3	I	871	GLN
3	I	900	GLU
3	I	915	GLU
3	I	950	GLU
3	I	952	ARG
3	I	954	ARG
4	J	63	LEU
4	J	102	THR
4	J	105	ARG
4	J	110	GLU
4	J	122	GLN
4	J	123	ARG
4	J	127	LYS
4	J	128	SER
4	J	143	GLN
4	K	8	THR
4	K	22	GLU
4	K	23	LEU
4	K	71	GLU
4	K	92	GLU
4	K	142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	43	ASN
1	A	48	GLN
1	A	82	ASN
1	A	167	ASN
1	A	198	ASN
1	A	218	HIS
1	A	311	GLN
1	B	167	ASN
1	B	171	HIS
1	B	217	ASN
1	B	309	GLN
1	C	8	GLN
1	C	140	GLN
1	C	198	ASN
1	C	218	HIS
1	C	290	ASN
1	D	99	ASN
1	D	290	ASN
1	E	8	GLN
1	E	10	GLN
1	E	20	HIS
1	E	37	GLN
1	E	208	GLN
1	E	232	ASN
1	E	281	HIS
1	F	8	GLN
1	F	57	GLN
1	F	106	GLN
1	F	218	HIS
1	F	281	HIS
1	G	10	GLN
1	G	48	GLN
1	G	68	GLN
1	G	217	ASN
1	G	218	HIS
1	G	237	GLN
1	G	248	ASN
1	G	281	HIS
1	G	294	GLN
2	H	14	ASN

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Mol	Chain	Res	Type
2	H	59	GLN
2	H	86	GLN
2	H	93	GLN
2	H	95	ASN
2	H	196	GLN
2	H	217	GLN
3	I	81	HIS
3	I	169	GLN
3	I	219	HIS
3	I	280	GLN
3	I	512	GLN
3	I	516	ASN
3	I	595	GLN
3	I	798	GLN
3	I	849	GLN
3	I	891	GLN
4	J	30	HIS
4	J	70	GLN
4	J	144	ASN
4	K	20	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	X	32/33 (96%)	23 (71%)	5 (15%)
6	Z	42/43 (97%)	15 (35%)	2 (4%)
All	All	74/76 (97%)	38 (51%)	7 (9%)

All (38) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	X	3	G
5	X	4	C
5	X	6	U
5	X	7	U
5	X	9	A
5	X	10	A
5	X	12	G
5	X	13	C
5	X	14	G
5	X	15	A

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Mol	Chain	Res	Type
5	X	16	C
5	X	18	A
5	X	19	C
5	X	21	A
5	X	23	G
5	X	24	G
5	X	25	G
5	X	26	C
5	X	27	A
5	X	28	C
5	X	29	A
5	X	30	A
5	X	31	C
6	Z	9	G
6	Z	14	U
6	Z	15	U
6	Z	20	C
6	Z	21	C
6	Z	24	G
6	Z	25	G
6	Z	26	C
6	Z	27	G
6	Z	32	C
6	Z	33	U
6	Z	38	A
6	Z	39	U
6	Z	40	G
6	Z	43	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	X	8	G
5	X	18	A
5	X	25	G
5	X	28	C
5	X	30	A
6	Z	13	G
6	Z	37	A

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-24976. These allow visual inspection of the internal detail of the map and identification of artifacts.

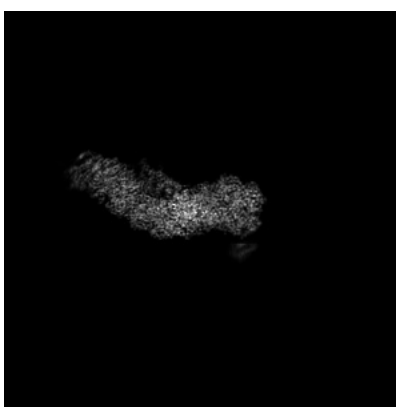
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

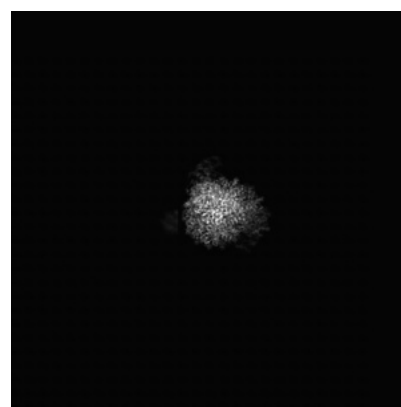
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

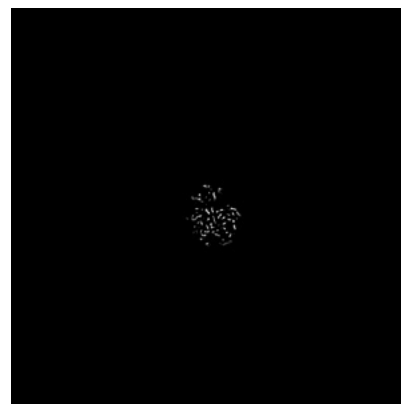
6.2.1 Primary map



X Index: 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](#)

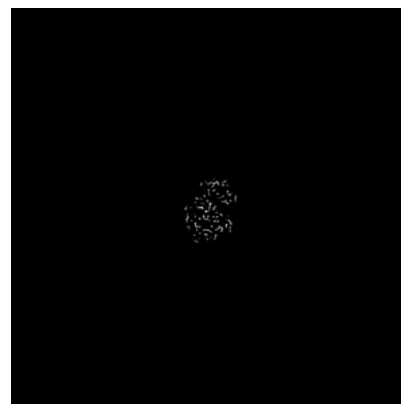
6.3.1 Primary map



X Index: 226



Y Index: 219



Z Index: 198

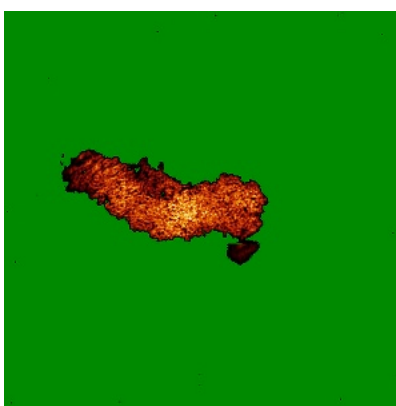
The images above show the largest variance slices of the map in three orthogonal directions.

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

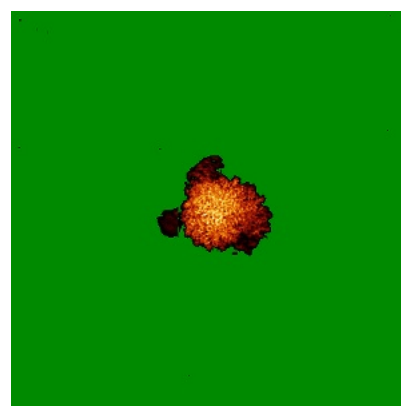
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

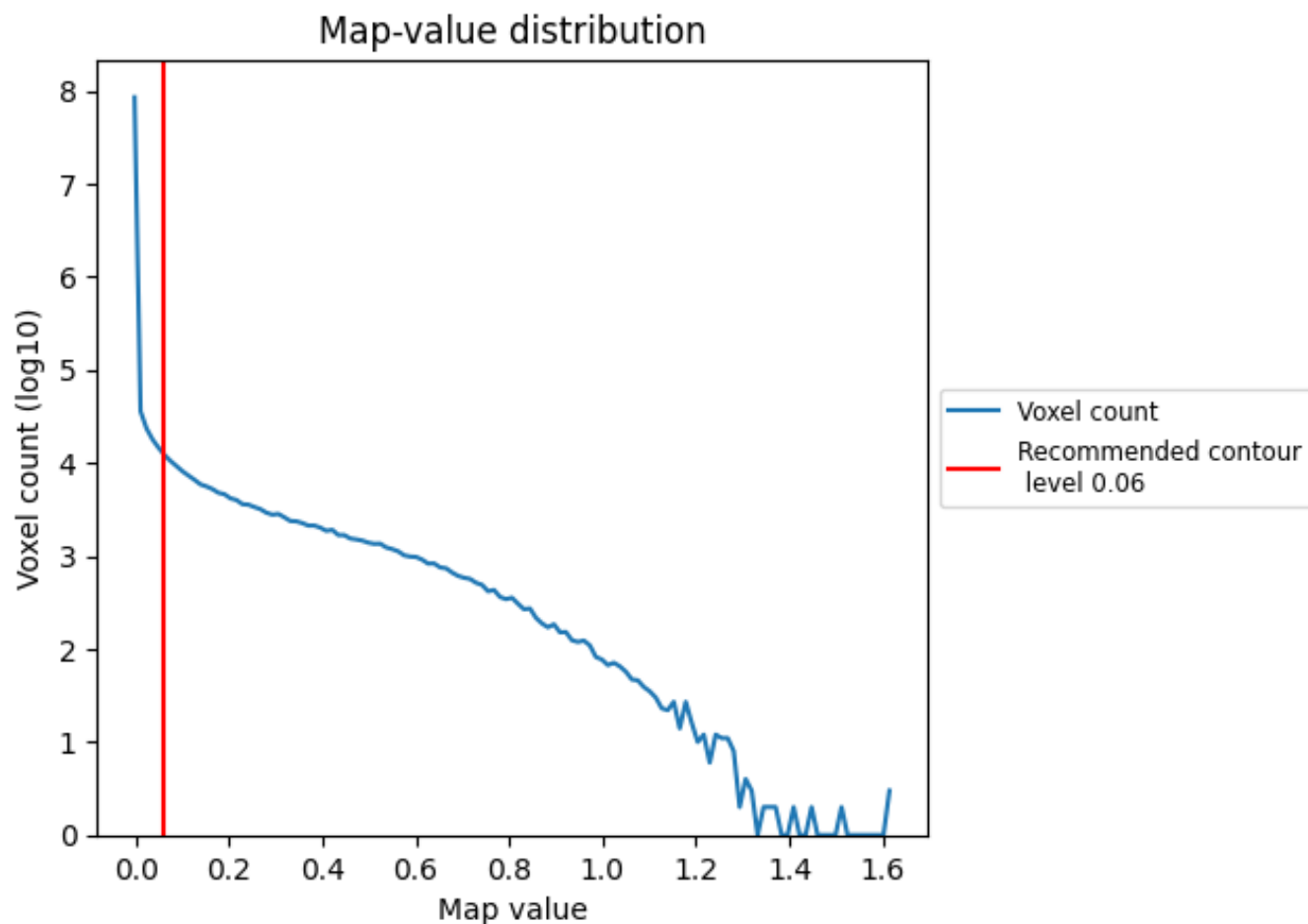
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

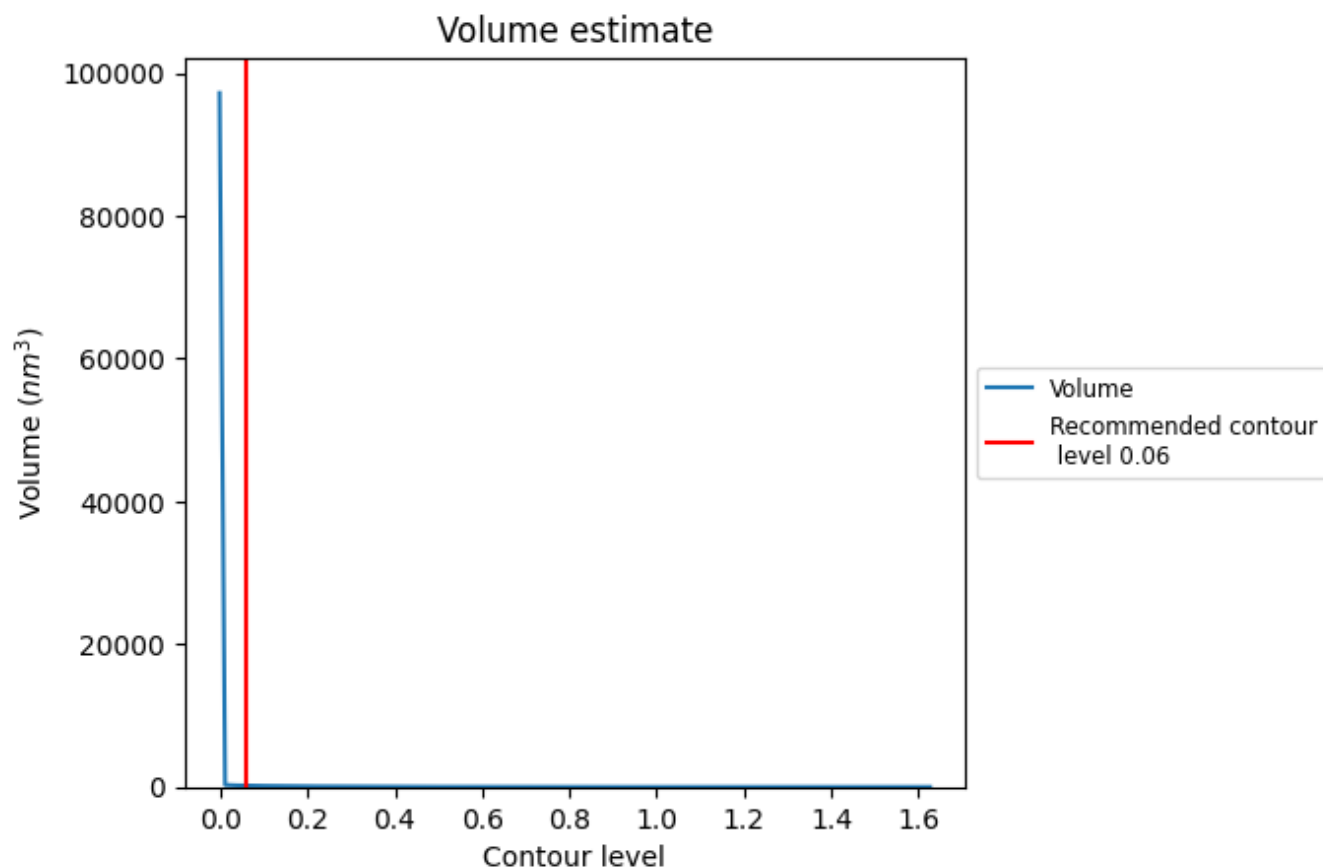
This section contains the results of statistical analysis of the map.

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.

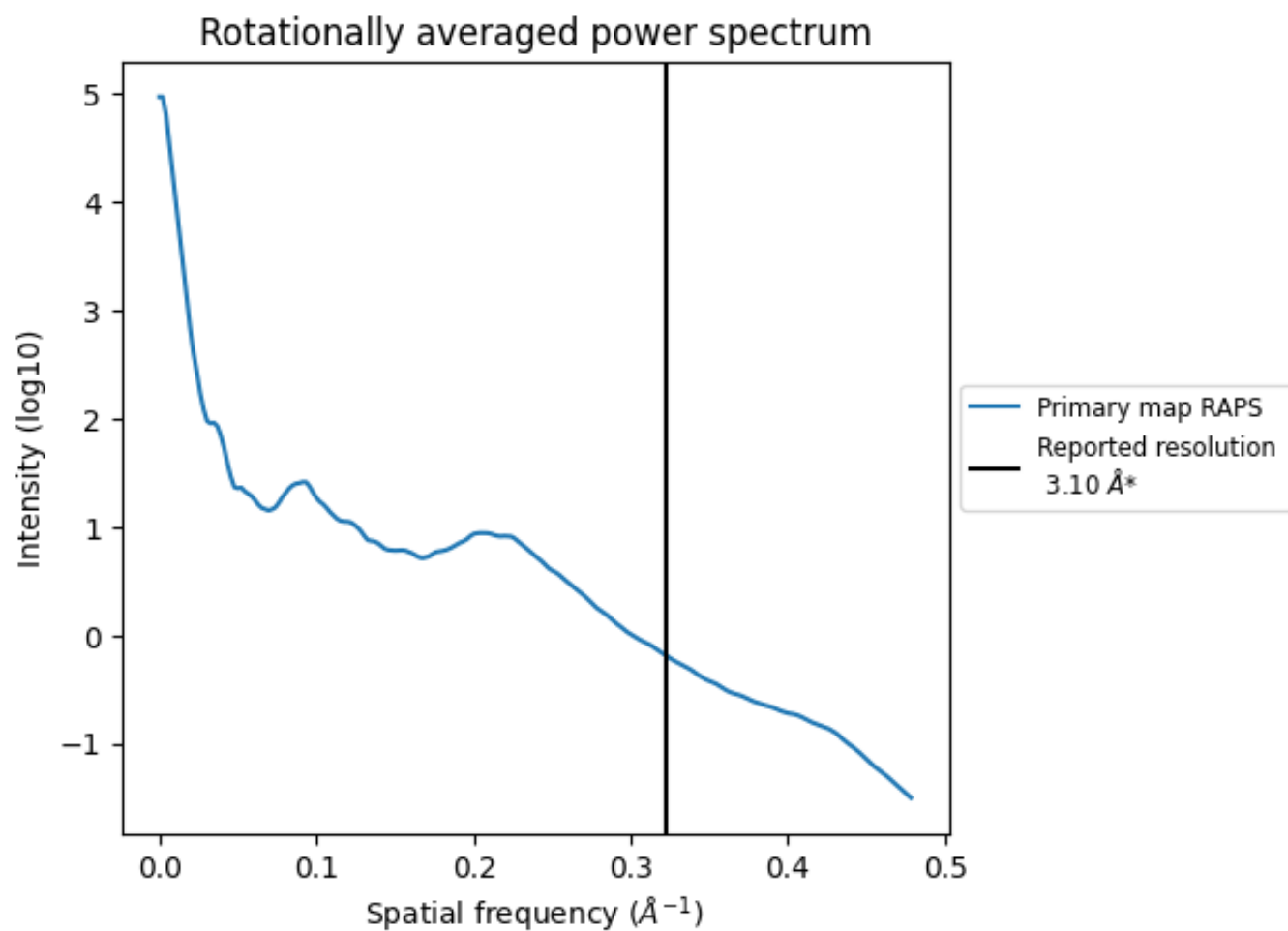
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 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 ⓘ

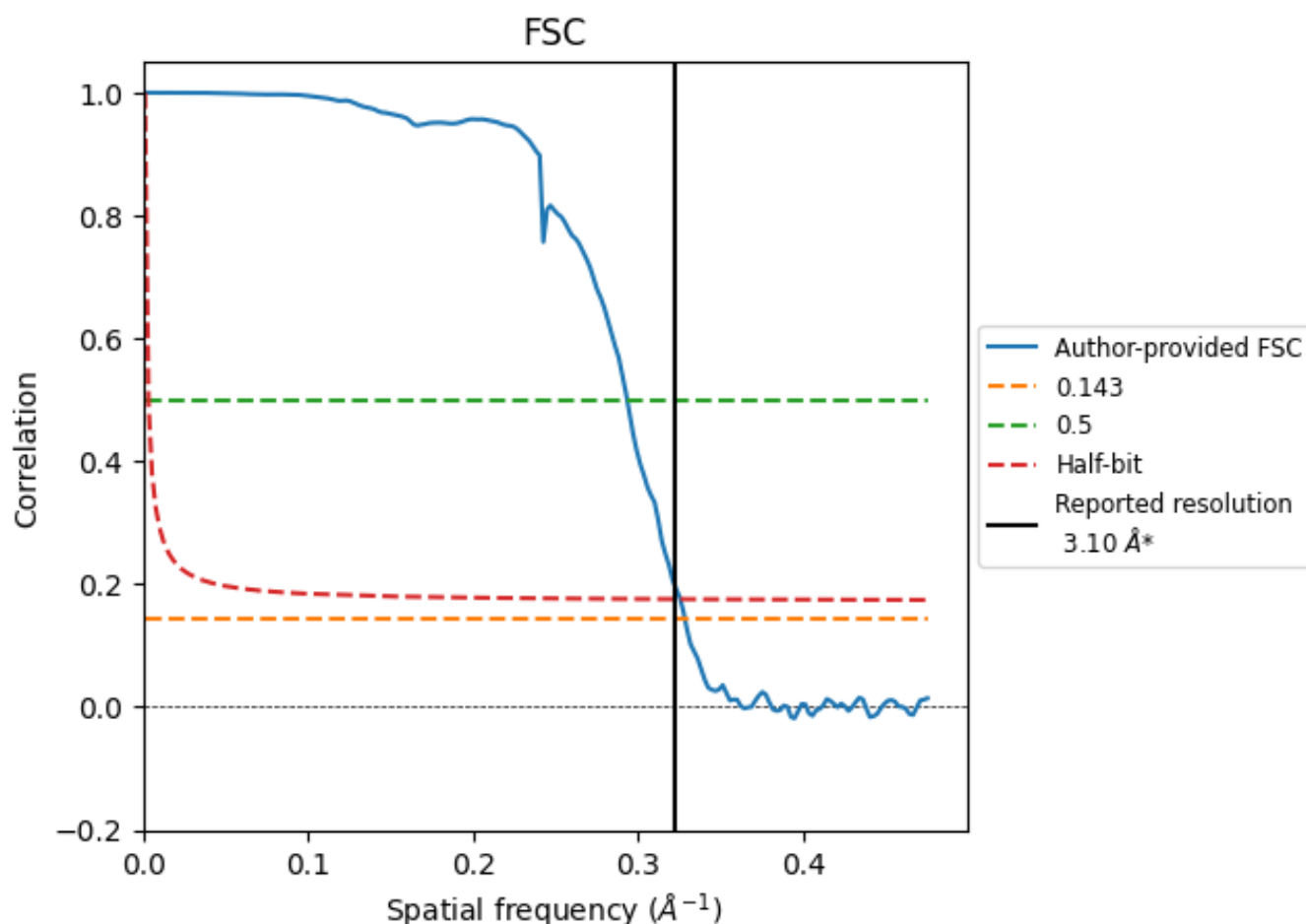


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

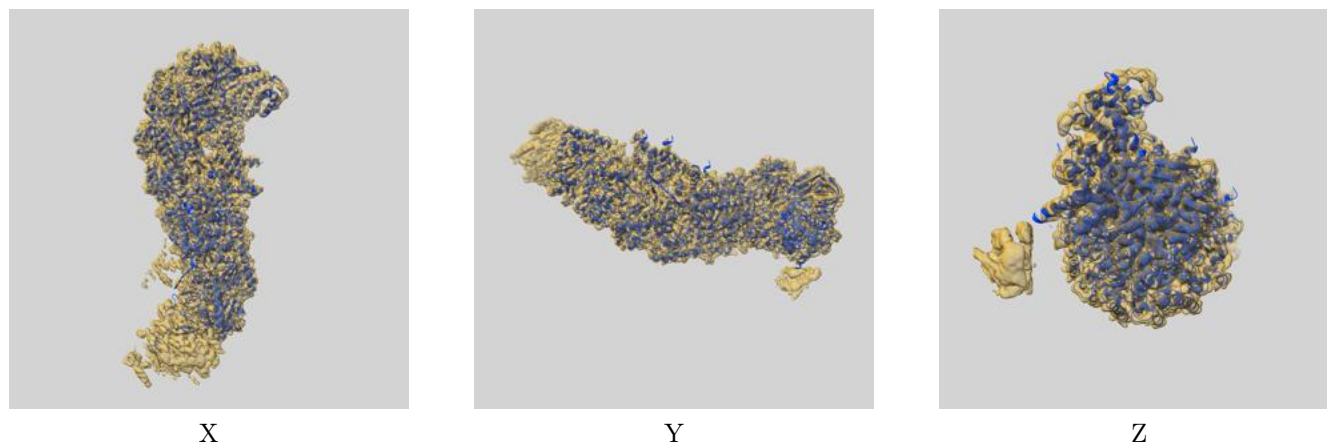
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.41	3.07
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

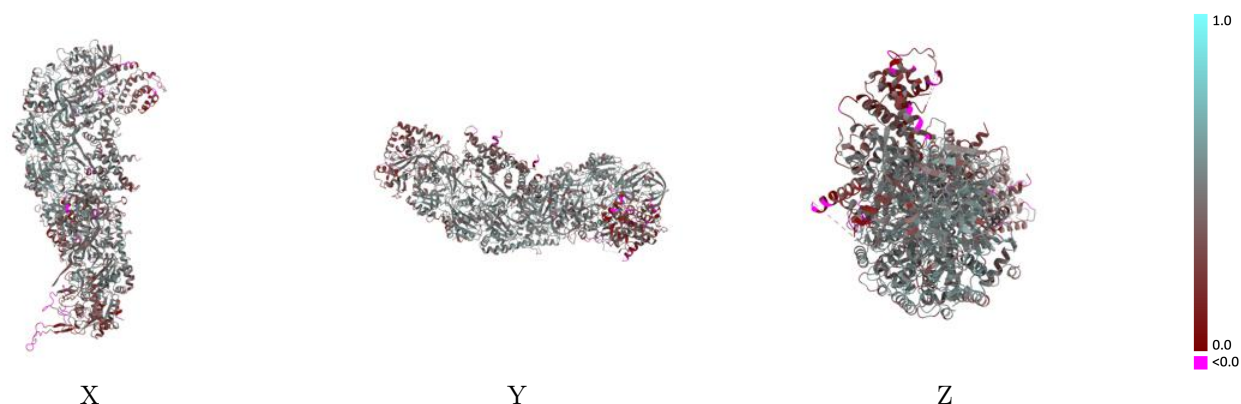
This section contains information regarding the fit between EMDB map EMD-24976 and PDB model 7SBB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



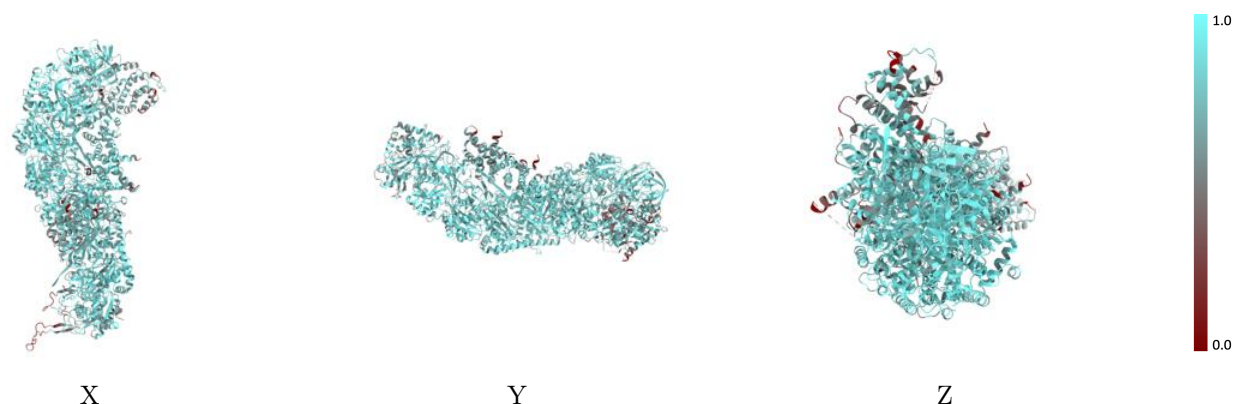
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



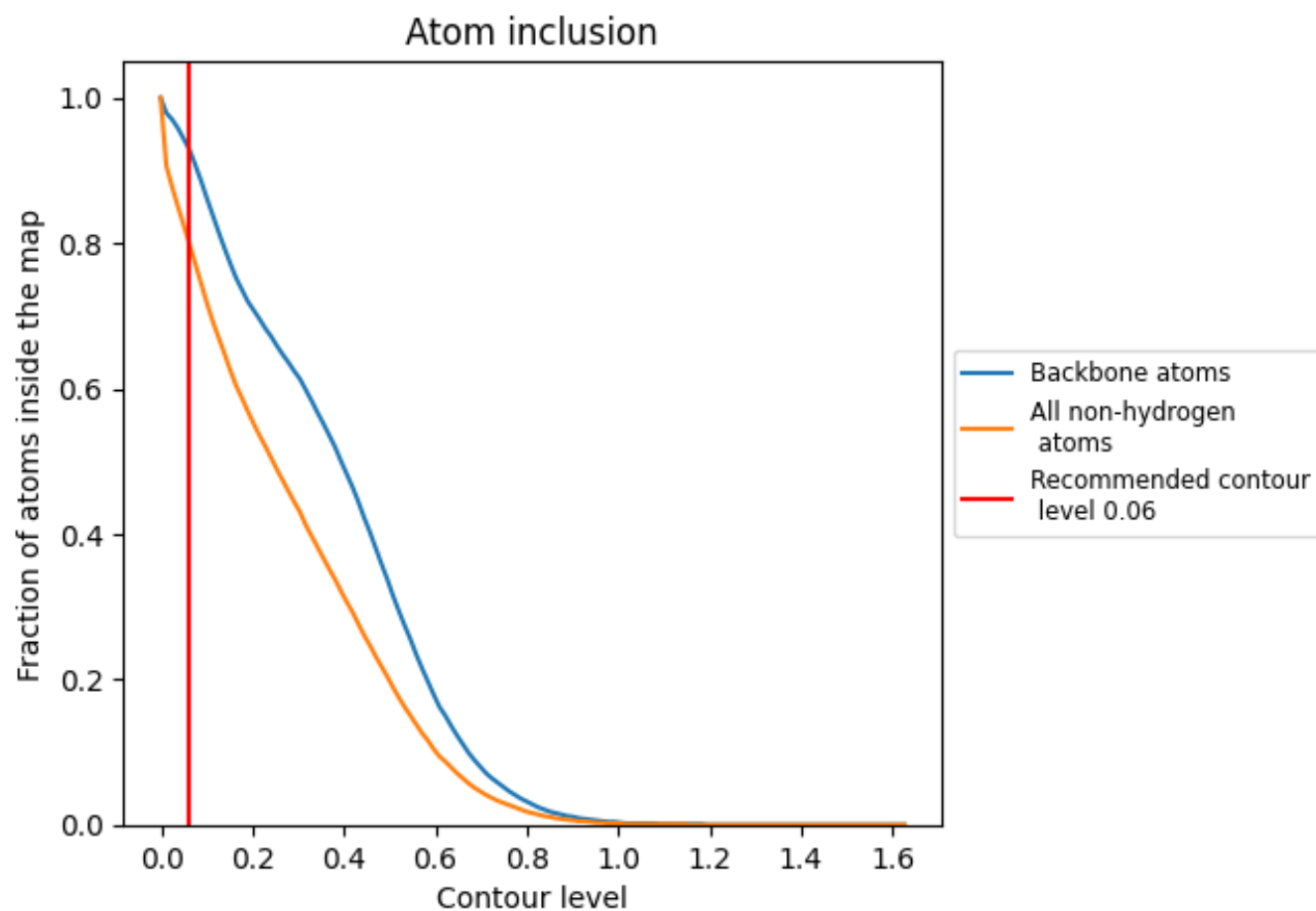
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 80% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.4330
A	 0.8520	 0.4830
B	 0.8710	 0.4960
C	 0.8900	 0.4980
D	 0.8730	 0.4990
E	 0.8350	 0.4720
F	 0.8180	 0.4400
G	 0.6870	 0.3120
H	 0.8400	 0.4650
I	 0.7270	 0.3620
J	 0.7380	 0.3990
K	 0.5940	 0.3190
X	 0.8220	 0.4530
Z	 0.9450	 0.5160

