



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:33 AM UTC

PDB ID : 2GO5 / pdb_00002go5
EMDB ID : EMD-1217
Title : Structure of signal recognition particle receptor (SR) in complex with signal recognition particle (SRP) and ribosome nascent chain complex
Authors : Halic, M.; Gartmann, M.; Schlenker, O.; Mielke, T.; Pool, M.R.; Sinning, I.; Beckmann, R.
Deposited on : 2006-04-12
Resolution : 7.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

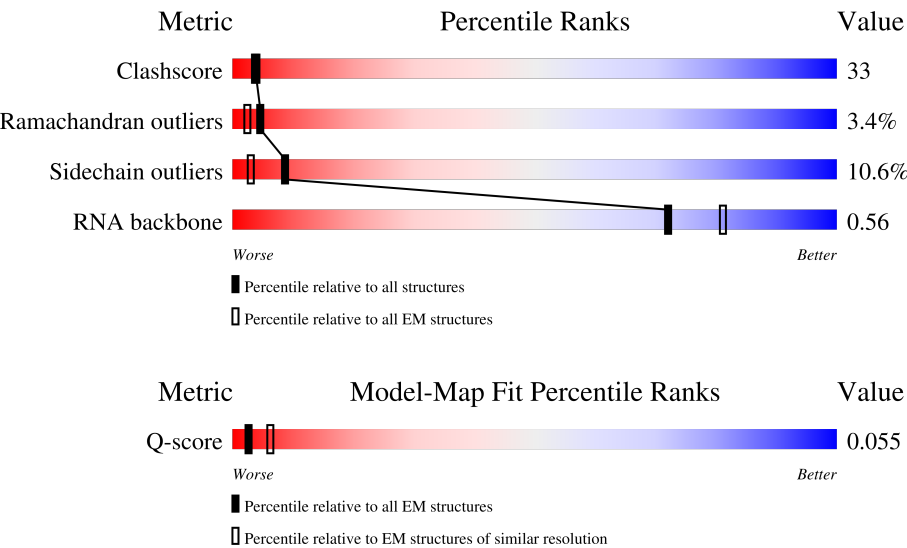
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.40 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	412 (6.90 - 7.90)

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	127	20% 33% 53% 13% .
2	9	90	28% 58% 12% .
3	B	108	49% 38% 49% 11% ..

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Mol	Chain	Length	Quality of chain
4	W	109	
5	1	185	
6	2	214	
7	5	124	
8	4	152	
9	6	123	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10724 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 RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	127	Total	C	N	O	P	0	0
			2728	1217	508	877	126		

- Molecule 2 is a RNA chain called ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	90	Total	C	N	O	P	0	0
			1935	863	364	618	90		

- Molecule 3 is a protein called Signal recognition particle 19 kDa protein (SRP19).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	107	Total	C	N	O	S	0	0
			870	549	159	156	6		

- Molecule 4 is a protein called Signal recognition particle 54 kDa protein (SRP54).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	109	Total	C	N	O	S	0	0
			865	540	150	164	11		

- Molecule 5 is a protein called Signal recognition particle receptor alpha subunit (SR a).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	125	Total	C	N	O	S	0	0
			1020	659	169	189	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-8	MET	-	cloning artifact	UNP P08240
1	-7	SER	-	cloning artifact	UNP P08240
1	-6	HIS	-	expression tag	UNP P08240

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-5	HIS	-	expression tag	UNP P08240
1	-4	HIS	-	expression tag	UNP P08240
1	-3	HIS	-	expression tag	UNP P08240
1	-2	HIS	-	expression tag	UNP P08240
1	-1	HIS	-	expression tag	UNP P08240
1	0	SER	-	cloning artifact	UNP P08240
1	1	MET	-	cloning artifact	UNP P08240
1	2	VAL	-	cloning artifact	UNP P08240

- Molecule 6 is a protein called Signal recognition particle receptor beta subunit (SR b).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	188	Total	C	N	O	S	0	0
			1479	940	256	278	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	56	MET	-	initiating methionine	UNP P47758
2	57	ALA	-	cloning artifact	UNP P47758

- Molecule 7 is a protein called ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	5	64	Total	C	N	O	0	0
			504	314	99	91		

- Molecule 8 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4	81	Total	C	N	O	S	0	0
			652	423	108	119	2		

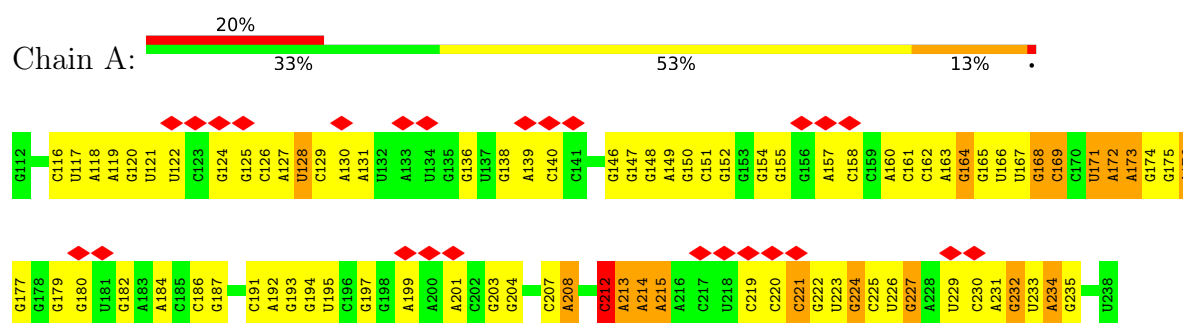
- Molecule 9 is a protein called ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	81	Total	C	N	O	S	0	0
			671	416	138	115	2		

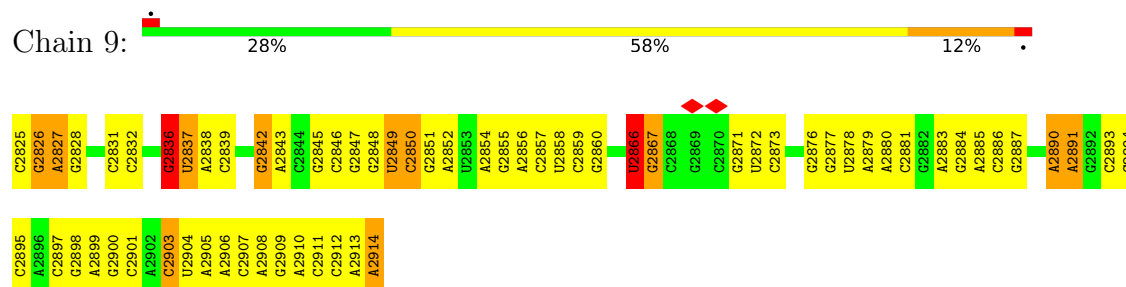
3 Residue-property plots

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

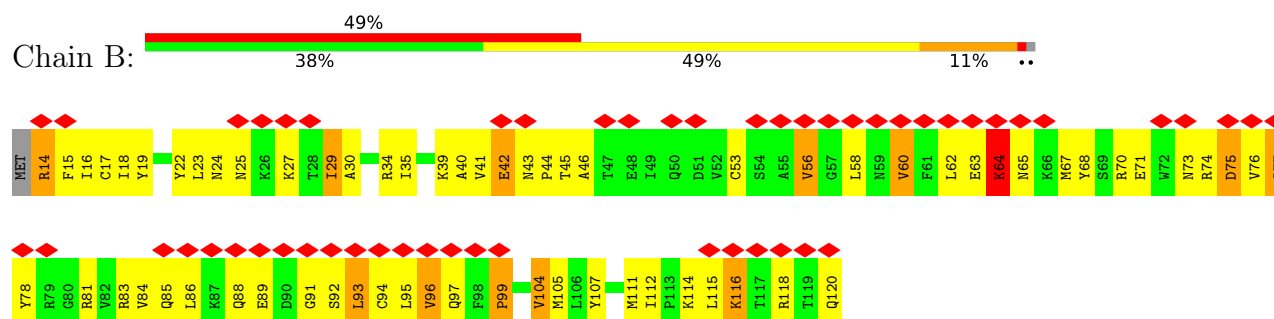
• Molecule 1: SRP RNA



• Molecule 2: ribosomal RNA

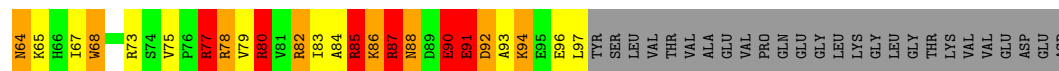


• Molecule 3: Signal recognition particle 19 kDa protein (SRP19)



• Molecule 4: Signal recognition particle 54 kDa protein (SRP54)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.546	Depositor
Minimum map value	-0.551	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.173	Depositor
Map size ($\text{\AA}$)	452.64, 452.64, 452.64	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.23, 1.23, 1.23	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	0.36	0/3053	0.69	1/4758 (0.0%)
2	9	0.39	0/2167	0.64	3/3379 (0.1%)
3	B	0.57	0/884	1.04	1/1188 (0.1%)
4	W	1.34	3/876 (0.3%)	1.82	9/1165 (0.8%)
5	1	0.67	0/1035	0.96	2/1389 (0.1%)
6	2	0.63	0/1496	1.04	5/2008 (0.2%)
7	5	2.24	9/506 (1.8%)	2.95	23/673 (3.4%)
8	4	1.87	16/660 (2.4%)	3.14	57/885 (6.4%)
9	6	1.79	12/680 (1.8%)	2.37	42/906 (4.6%)
All	All	0.97	40/11357 (0.4%)	1.40	143/16351 (0.9%)

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
2	9	0	2
4	W	0	5
7	5	2	2
8	4	3	7
9	6	0	11
All	All	5	30

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	345	PHE	C-N	-29.98	0.91	1.33
7	5	38	VAL	CA-C	22.19	1.80	1.52
4	W	362	LYS	C-N	21.41	1.64	1.33
7	5	38	VAL	C-N	19.77	1.61	1.33
7	5	39	ALA	N-CA	-17.05	1.24	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	97	ASP	N-CA	-14.07	1.28	1.45
8	4	96	VAL	C-N	9.11	1.46	1.33
8	4	97	ASP	CA-C	-8.74	1.41	1.53
8	4	125	ARG	CZ-NH2	8.71	1.44	1.33
7	5	43	SER	C-N	8.20	1.45	1.33
8	4	89	ASN	CA-C	-8.09	1.42	1.52
8	4	115	ILE	CA-C	-7.53	1.46	1.52
4	W	344	PRO	C-N	7.30	1.44	1.33
8	4	115	ILE	CA-CB	-7.28	1.45	1.54
7	5	38	VAL	CA-CB	7.25	1.64	1.54
8	4	145	VAL	CA-CB	-6.50	1.45	1.54
8	4	131	LYS	CD-CE	6.31	1.71	1.52
8	4	125	ARG	CD-NE	-6.30	1.37	1.46
8	4	101	ASP	C-N	6.28	1.42	1.34
7	5	41	SER	CA-C	-6.09	1.44	1.52
7	5	44	LYS	CA-CB	5.86	1.61	1.53
8	4	141	ASP	C-N	5.77	1.42	1.34
7	5	34	ARG	CZ-NH2	5.70	1.40	1.33
8	4	103	LYS	N-CA	-5.49	1.39	1.46
9	6	40	ALA	CA-C	-5.47	1.45	1.52
9	6	87	ARG	NE-CZ	5.46	1.39	1.33
9	6	85	ARG	CZ-NH1	5.44	1.40	1.32
9	6	78	ARG	NE-CZ	5.41	1.39	1.33
9	6	45	ARG	NE-CZ	5.39	1.39	1.33
8	4	98	LEU	N-CA	-5.34	1.40	1.46
8	4	135	LYS	CD-CE	5.31	1.68	1.52
9	6	73	ARG	NE-CZ	5.30	1.38	1.33
7	5	39	ALA	C-O	-5.28	1.17	1.24
9	6	27	ARG	CZ-NH1	5.19	1.40	1.32
9	6	85	ARG	CA-C	-5.14	1.46	1.52
9	6	58	ARG	CZ-NH2	5.09	1.40	1.33
8	4	102	LYS	CA-CB	5.04	1.61	1.53
9	6	58	ARG	NE-CZ	5.04	1.38	1.33
9	6	56	ASP	CA-C	-5.04	1.46	1.53
9	6	54	THR	N-CA	-5.03	1.40	1.46

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	125	ARG	NE-CZ-NH2	-39.23	83.89	119.20
7	5	39	ALA	N-CA-CB	-35.73	50.11	110.49
4	W	362	LYS	CA-C-N	-30.03	62.54	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	362	LYS	C-N-CA	-30.03	62.54	121.41
7	5	38	VAL	CA-C-O	-24.31	90.39	120.78
7	5	39	ALA	N-CA-C	-19.58	69.10	110.80
8	4	141	ASP	CA-C-N	19.27	149.60	120.31
8	4	141	ASP	C-N-CA	19.27	149.60	120.31
8	4	101	ASP	CA-C-N	17.42	145.37	120.28
8	4	101	ASP	C-N-CA	17.42	145.37	120.28
7	5	43	SER	CA-C-N	16.20	146.31	121.53
7	5	43	SER	C-N-CA	16.20	146.31	121.53
8	4	96	VAL	CA-C-O	-15.86	106.10	121.64
4	W	362	LYS	O-C-N	15.39	143.05	122.59
4	W	345	PHE	CA-C-N	15.35	150.86	121.54
4	W	345	PHE	C-N-CA	15.35	150.86	121.54
8	4	96	VAL	CA-C-N	-15.14	93.41	122.02
8	4	96	VAL	C-N-CA	-15.14	93.41	122.02
7	5	43	SER	N-CA-C	13.91	140.44	110.80
8	4	90	ASN	CB-CG-ND2	12.79	135.58	116.40
4	W	361	SER	O-C-N	12.45	137.39	123.33
7	5	43	SER	N-CA-CB	-11.72	90.69	110.49
7	5	38	VAL	N-CA-C	11.63	133.52	109.34
9	6	88	ASN	N-CA-C	-11.54	96.35	111.24
8	4	101	ASP	N-CA-C	11.34	134.96	110.80
7	5	34	ARG	NE-CZ-NH1	-11.34	110.16	121.50
9	6	92	ASP	CA-CB-CG	11.30	123.91	112.60
7	5	38	VAL	CA-C-N	-11.14	100.26	121.54
7	5	38	VAL	C-N-CA	-11.14	100.26	121.54
9	6	56	ASP	CA-CB-CG	11.09	123.69	112.60
7	5	44	LYS	N-CA-CB	11.08	125.09	111.79
8	4	90	ASN	CB-CG-OD1	-10.95	98.89	120.80
8	4	115	ILE	CA-CB-CG1	10.76	128.69	110.40
8	4	131	LYS	CG-CD-CE	10.69	135.88	111.30
8	4	125	ARG	NH1-CZ-NH2	10.65	133.15	119.30
9	6	57	VAL	CB-CA-C	10.05	127.77	111.29
8	4	97	ASP	CB-CA-C	9.92	133.60	111.78
9	6	87	ARG	N-CA-C	-9.56	101.62	113.28
8	4	115	ILE	CA-CB-CG2	-9.41	94.51	110.50
8	4	142	ALA	N-CA-C	9.40	122.73	111.82
9	6	96	GLU	N-CA-C	-9.28	96.15	110.17
9	6	80	ARG	N-CA-C	-9.18	93.94	108.90
7	5	38	VAL	CB-CA-C	9.09	126.20	111.29
8	4	97	ASP	N-CA-C	9.06	124.40	110.36
8	4	125	ARG	NE-CZ-NH1	9.05	130.55	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	39	ALA	O-C-N	-9.00	110.61	122.59
7	5	43	SER	O-C-N	8.62	134.06	122.59
8	4	135	LYS	CA-CB-CG	8.57	131.25	114.10
9	6	23	ASN	N-CA-C	-8.57	92.54	110.80
4	W	361	SER	CA-C-N	-8.47	105.37	121.54
4	W	361	SER	C-N-CA	-8.47	105.37	121.54
8	4	141	ASP	N-CA-C	8.43	128.75	110.80
9	6	90	GLU	CA-CB-CG	8.31	130.72	114.10
8	4	135	LYS	CB-CG-CD	8.29	130.37	111.30
8	4	115	ILE	CB-CA-C	-8.16	98.99	110.91
9	6	91	GLU	N-CA-C	7.89	120.51	110.33
8	4	142	ALA	CB-CA-C	-7.79	95.72	110.67
9	6	19	GLU	N-CA-C	-7.79	96.70	109.40
8	4	89	ASN	N-CA-C	-7.76	100.92	113.19
9	6	82	ARG	N-CA-C	-7.75	96.26	108.90
9	6	68	TRP	N-CA-C	-7.73	103.90	112.72
4	W	344	PRO	O-C-N	-7.68	112.27	122.64
9	6	52	MET	CG-SD-CE	-7.63	84.10	100.90
9	6	53	GLY	N-CA-C	-7.61	103.59	112.73
8	4	124	ILE	O-C-N	-7.42	114.13	122.36
7	5	38	VAL	N-CA-CB	-7.36	99.08	111.23
9	6	31	CYS	N-CA-C	-7.34	97.97	109.72
9	6	28	LEU	CB-CA-C	-7.30	96.11	110.27
8	4	141	ASP	O-C-N	7.27	132.26	122.59
8	4	145	VAL	CA-CB-CG2	-7.19	98.17	110.40
8	4	124	ILE	N-CA-C	-7.16	96.17	106.55
9	6	27	ARG	N-CA-C	-7.13	104.04	112.89
7	5	36	GLN	CA-C-O	-7.12	113.00	120.55
8	4	119	LYS	CG-CD-CE	6.96	127.31	111.30
9	6	18	ARG	NE-CZ-NH2	-6.93	112.96	119.20
8	4	131	LYS	CD-CE-NZ	6.88	133.93	111.90
9	6	55	ASN	OD1-CG-ND2	-6.75	115.85	122.60
8	4	97	ASP	CB-CG-OD1	6.74	133.90	118.40
9	6	93	ALA	N-CA-C	-6.71	97.64	109.06
9	6	90	GLU	N-CA-CB	6.70	121.82	110.49
9	6	33	PHE	CA-CB-CG	-6.68	107.11	113.80
8	4	89	ASN	CA-C-N	-6.67	113.33	125.66
8	4	89	ASN	C-N-CA	-6.67	113.33	125.66
6	2	131	LYS	N-CA-C	6.66	118.54	111.28
9	6	85	ARG	N-CA-CB	6.63	123.01	111.00
9	6	77	ARG	N-CA-C	-6.58	104.87	113.17
9	6	52	MET	N-CA-C	-6.57	96.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	85	ARG	CB-CA-C	-6.56	96.36	109.35
9	6	55	ASN	CA-C-N	6.49	132.49	120.95
9	6	55	ASN	C-N-CA	6.49	132.49	120.95
8	4	135	LYS	CG-CD-CE	6.45	126.12	111.30
7	5	38	VAL	CA-CB-CG2	6.34	121.18	110.40
8	4	102	LYS	CB-CA-C	-6.29	99.00	110.63
8	4	89	ASN	OD1-CG-ND2	-6.26	116.34	122.60
7	5	13	ASN	N-CA-C	-6.25	104.55	111.36
8	4	135	LYS	N-CA-C	-6.24	99.54	109.59
8	4	89	ASN	CB-CG-OD1	6.20	133.20	120.80
6	2	135	ARG	N-CA-C	-6.09	104.92	112.90
8	4	97	ASP	N-CA-CB	-6.08	101.19	110.49
9	6	39	ASN	CA-CB-CG	-6.01	106.59	112.60
7	5	34	ARG	NH1-CZ-NH2	5.95	127.03	119.30
2	9	2866	U	C2'-C3'-O3'	5.94	118.41	109.50
8	4	125	ARG	CB-CA-C	5.92	121.83	110.17
8	4	128	GLY	N-CA-C	-5.88	107.06	115.64
6	2	134	ALA	N-CA-C	5.85	119.06	109.76
9	6	62	LYS	N-CA-C	-5.81	105.03	111.36
8	4	96	VAL	O-C-N	5.78	129.36	122.95
8	4	90	ASN	O-C-N	-5.77	115.71	121.88
2	9	2914	A	C2'-C3'-O3'	5.74	122.31	113.70
8	4	125	ARG	N-CA-CB	5.73	120.57	110.37
6	2	183	ALA	N-CA-C	5.73	117.98	111.11
9	6	91	GLU	CB-CG-CD	-5.70	102.90	112.60
8	4	115	ILE	N-CA-C	5.68	115.46	108.53
8	4	101	ASP	N-CA-CB	5.67	120.07	110.49
7	5	57	ARG	NE-CZ-NH1	-5.67	115.83	121.50
8	4	91	THR	N-CA-C	5.66	118.80	110.59
9	6	85	ARG	CD-NE-CZ	-5.66	116.48	124.40
9	6	85	ARG	N-CA-C	-5.66	99.80	109.24
9	6	29	HIS	N-CA-C	-5.64	106.24	113.23
9	6	47	PHE	N-CA-C	-5.62	104.78	111.69
8	4	101	ASP	CA-CB-CG	5.61	118.21	112.60
9	6	94	LYS	N-CA-CB	5.61	120.92	110.99
8	4	96	VAL	CG1-CB-CG2	-5.58	98.52	110.80
9	6	52	MET	CA-CB-CG	5.57	125.24	114.10
8	4	90	ASN	N-CA-CB	-5.46	105.32	114.27
7	5	15	SER	CA-CB-OG	-5.45	100.20	111.10
7	5	36	GLN	N-CA-C	-5.42	105.37	111.28
1	A	212	C	C2'-C3'-O3'	5.40	117.60	109.50
8	4	125	ARG	CA-C-O	-5.29	112.92	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	18	ARG	NE-CZ-NH1	5.27	126.77	121.50
2	9	2836	G	C2'-C3'-O3'	5.26	117.39	109.50
8	4	95	ILE	CA-C-O	-5.25	114.95	120.57
5	1	126	GLU	N-CA-C	-5.22	106.97	113.55
8	4	135	LYS	CD-CE-NZ	5.21	128.56	111.90
9	6	64	ASN	N-CA-C	-5.21	105.69	111.36
3	B	60	VAL	N-CA-C	5.20	115.06	107.88
5	1	115	ASN	N-CA-C	5.20	116.63	111.07
9	6	56	ASP	N-CA-CB	5.13	117.27	110.29
8	4	103	LYS	N-CA-C	-5.12	105.59	111.07
6	2	173	LEU	N-CA-C	5.08	117.18	108.90
8	4	119	LYS	CD-CE-NZ	5.02	127.95	111.90
9	6	80	ARG	N-CA-CB	5.01	119.10	110.68
8	4	140	TYR	CE1-CZ-OH	5.01	134.92	119.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	5	38	VAL	CA
7	5	39	ALA	CA
8	4	97	ASP	CA
8	4	125	ARG	CA
8	4	141	ASP	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	4	101	ASP	Peptide,Mainchain
8	4	124	ILE	Peptide
8	4	125	ARG	Sidechain
8	4	140	TYR	Sidechain
8	4	141	ASP	Peptide
8	4	89	ASN	Peptide
7	5	38	VAL	Peptide
7	5	43	SER	Peptide
9	6	18	ARG	Sidechain
9	6	27	ARG	Sidechain
9	6	47	PHE	Sidechain
9	6	50	LYS	Peptide
9	6	51	ALA	Peptide
9	6	58	ARG	Sidechain
9	6	77	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	6	80	ARG	Sidechain
9	6	86	LYS	Peptide
9	6	87	ARG	Peptide,Sidechain
2	9	2842	G	Sidechain
2	9	2866	U	Sidechain
1	A	197	G	Sidechain
1	A	201	A	Sidechain
1	A	208	A	Sidechain
4	W	344	PRO	Peptide,Mainchain
4	W	361	SER	Peptide,Mainchain
4	W	362	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2728	0	1366	186	0
2	9	1935	0	977	103	0
3	B	870	0	901	83	0
4	W	865	0	871	36	0
5	1	1020	0	1019	54	0
6	2	1479	0	1533	33	0
7	5	504	0	553	62	0
8	4	652	0	708	87	0
9	6	671	0	705	91	0
All	All	10724	0	8633	643	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 33.

All (643) 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)
7:5:38:VAL:C	7:5:38:VAL:HA	1.20	1.53
2:9:2904:U:H4'	9:6:20:TYR:CD2	1.45	1.51
7:5:38:VAL:C	7:5:38:VAL:CA	1.80	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:A:C1'	1:A:224:G:C4'	1.87	1.45
2:9:2856:A:H4'	9:6:78:ARG:CG	1.40	1.44
5:1:0:SER:C	5:1:29:VAL:HG23	1.10	1.43
1:A:127:A:C1'	1:A:224:G:N2	1.72	1.41
1:A:127:A:C2'	1:A:224:G:C2	1.78	1.40
1:A:173:A:H1'	1:A:224:G:C4'	0.94	1.39
5:1:-1:HIS:CB	5:1:4:PHE:CD2	1.95	1.39
1:A:127:A:C3'	1:A:224:G:N2	1.88	1.37
1:A:173:A:C1'	1:A:224:G:H4'	1.50	1.36
1:A:173:A:H1'	1:A:224:G:C5'	1.60	1.32
1:A:125:G:C8	1:A:227:G:C6	2.12	1.31
2:9:2856:A:C4'	9:6:78:ARG:HG3	1.55	1.31
1:A:125:G:C8	1:A:227:G:O6	1.84	1.30
1:A:127:A:H2'	1:A:224:G:C2	1.38	1.30
1:A:172:A:C6	1:A:224:G:O2'	1.85	1.30
5:1:0:SER:C	5:1:29:VAL:CG2	2.04	1.29
1:A:172:A:N6	1:A:225:C:O4'	1.64	1.29
1:A:172:A:C5	1:A:224:G:O2'	1.74	1.27
6:2:204:VAL:HG11	9:6:17:THR:O	1.14	1.26
2:9:2856:A:O4'	9:6:23:ASN:ND2	1.68	1.26
1:A:234:A:OP2	5:1:49:HIS:HA	1.12	1.21
7:5:34:ARG:O	8:4:75:TYR:CD1	1.94	1.21
4:W:343:GLY:O	4:W:346:SER:HB2	1.05	1.19
2:9:2854:A:O2'	9:6:26:LYS:HE3	1.41	1.19
2:9:2854:A:O2'	9:6:26:LYS:CE	1.91	1.18
1:A:173:A:O2'	1:A:224:G:H5''	1.02	1.17
5:1:-1:HIS:HB2	5:1:4:PHE:CD2	1.79	1.16
2:9:2856:A:O2'	9:6:78:ARG:CD	1.96	1.14
4:W:361:SER:O	4:W:362:LYS:HG3	1.43	1.14
4:W:343:GLY:O	4:W:346:SER:CB	1.97	1.13
1:A:173:A:O2'	1:A:224:G:C5'	1.98	1.11
1:A:125:G:O2'	1:A:227:G:C1'	1.97	1.11
6:2:204:VAL:CG1	9:6:17:THR:O	1.99	1.10
8:4:140:TYR:CZ	8:4:145:VAL:HG21	1.88	1.09
1:A:172:A:C6	1:A:224:G:C2'	2.36	1.09
1:A:173:A:C2'	1:A:224:G:H5''	1.82	1.08
5:1:-1:HIS:HB3	5:1:4:PHE:CD2	1.73	1.07
1:A:173:A:C2	1:A:224:G:N3	2.18	1.06
2:9:2905:A:OP1	9:6:51:ALA:O	1.71	1.06
1:A:173:A:H1'	1:A:224:G:O4'	1.55	1.05
1:A:125:G:O2'	1:A:227:G:C8	2.08	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:34:ARG:O	8:4:75:TYR:CE1	2.08	1.05
1:A:127:A:N9	1:A:225:C:N3	2.05	1.04
2:9:2856:A:O2'	9:6:78:ARG:HD2	1.02	1.04
2:9:2904:U:C4'	9:6:20:TYR:CD2	2.40	1.03
8:4:119:LYS:HD3	8:4:135:LYS:HZ3	1.21	1.03
7:5:38:VAL:HA	7:5:38:VAL:O	1.56	1.03
1:A:234:A:OP2	5:1:49:HIS:CA	2.08	1.02
1:A:172:A:H61	1:A:225:C:C1'	1.73	1.01
5:1:0:SER:O	5:1:29:VAL:HG23	1.59	1.01
1:A:125:G:O2'	1:A:227:G:N9	1.56	1.01
7:5:38:VAL:CG2	8:4:76:PRO:O	2.10	1.00
7:5:38:VAL:C	8:4:75:TYR:OH	2.04	0.99
1:A:126:C:O2'	1:A:226:U:O4'	1.63	0.99
5:1:-1:HIS:HB2	5:1:4:PHE:HD2	1.09	0.98
2:9:2904:U:O2'	9:6:47:PHE:CZ	2.16	0.98
2:9:2856:A:HO2'	9:6:78:ARG:HD2	1.18	0.98
8:4:136:LEU:HD13	8:4:140:TYR:CE2	1.98	0.97
2:9:2904:U:H5''	9:6:20:TYR:HE2	1.26	0.97
2:9:2904:U:C4'	9:6:20:TYR:HD2	1.76	0.97
5:1:-1:HIS:CB	5:1:4:PHE:HD2	1.49	0.97
2:9:2904:U:H4'	9:6:20:TYR:CE2	1.99	0.96
1:A:220:C:H2'	1:A:221:C:H5''	1.45	0.96
7:5:34:ARG:HH12	7:5:48:ILE:HG23	1.29	0.95
5:1:-1:HIS:HB3	5:1:4:PHE:CE2	2.01	0.95
1:A:172:A:C6	1:A:225:C:O4'	1.96	0.95
3:B:60:VAL:HG23	3:B:83:ARG:O	1.67	0.94
1:A:172:A:C6	1:A:224:G:H2'	2.02	0.92
5:1:0:SER:CA	5:1:54:LEU:HD21	2.00	0.92
1:A:173:A:H1'	1:A:224:G:H4'	0.93	0.91
2:9:2906:A:P	9:6:50:LYS:HG2	2.11	0.91
1:A:127:A:C3'	1:A:224:G:H21	1.66	0.90
1:A:126:C:O2	1:A:226:U:C6	2.24	0.90
2:9:2904:U:H5''	9:6:20:TYR:CE2	2.06	0.90
2:9:2856:A:HO2'	9:6:21:THR:HG1	1.20	0.90
1:A:127:A:C8	1:A:225:C:N3	2.40	0.90
2:9:2905:A:O3'	9:6:50:LYS:HG2	1.71	0.89
1:A:127:A:C2'	1:A:128:U:H5''	2.02	0.89
1:A:221:C:N4	1:A:222:G:O6	2.05	0.89
3:B:64:LYS:HD3	3:B:64:LYS:N	1.88	0.89
9:6:52:MET:HE1	9:6:83:ILE:HD11	1.55	0.89
5:1:0:SER:HA	5:1:54:LEU:HD21	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:A:N7	1:A:224:G:O2'	2.06	0.88
1:A:126:C:C2	1:A:226:U:N1	2.17	0.88
6:2:204:VAL:HG12	9:6:18:ARG:CD	2.04	0.88
7:5:38:VAL:CA	7:5:38:VAL:O	2.18	0.87
1:A:124:G:C6	1:A:126:C:C5	2.62	0.87
2:9:2890:A:H5''	2:9:2890:A:H8	1.37	0.87
1:A:127:A:H2'	1:A:128:U:H5''	1.57	0.87
5:1:-1:HIS:ND1	5:1:68:VAL:O	2.06	0.87
1:A:127:A:C2'	1:A:224:G:N2	0.72	0.87
3:B:94:CYS:O	3:B:95:LEU:HD23	1.74	0.86
8:4:122:THR:HG23	8:4:130:LYS:HD3	1.56	0.86
1:A:173:A:C1'	1:A:224:G:O4'	2.05	0.86
5:1:0:SER:HB2	5:1:29:VAL:N	1.58	0.85
1:A:126:C:O2'	1:A:226:U:C4'	2.24	0.85
2:9:2906:A:OP1	9:6:50:LYS:HG2	1.77	0.84
1:A:184:A:N3	4:W:405:ARG:NH1	2.24	0.84
1:A:127:A:C2'	1:A:224:G:H21	0.59	0.84
1:A:126:C:O2	1:A:226:U:N1	2.08	0.84
4:W:344:PRO:C	4:W:346:SER:N	2.34	0.83
9:6:54:THR:HA	9:6:90:GLU:HB2	1.61	0.83
1:A:173:A:C1'	1:A:224:G:C5'	2.39	0.83
1:A:128:U:H5''	1:A:224:G:H21	1.44	0.82
7:5:27:LYS:HE3	7:5:27:LYS:O	1.80	0.82
1:A:127:A:O2'	1:A:224:G:N2	1.94	0.82
4:W:361:SER:O	4:W:362:LYS:CG	2.27	0.82
3:B:14:ARG:NH1	3:B:14:ARG:HB3	1.96	0.81
3:B:24:ASN:HD22	3:B:27:LYS:HG3	1.42	0.81
8:4:136:LEU:HD13	8:4:140:TYR:HE2	1.43	0.81
1:A:127:A:C3'	1:A:224:G:H22	1.66	0.81
7:5:12:TRP:HE1	7:5:61:VAL:HG22	1.45	0.81
1:A:172:A:N6	1:A:224:G:O2'	2.14	0.80
2:9:2855:G:C4	9:6:23:ASN:OD1	2.28	0.80
7:5:35:ILE:HA	8:4:75:TYR:HE1	1.46	0.80
2:9:2854:A:C2'	9:6:26:LYS:HE3	2.10	0.80
6:2:204:VAL:HG12	9:6:18:ARG:HD2	1.63	0.79
7:5:38:VAL:HG23	8:4:76:PRO:O	1.81	0.79
1:A:128:U:H5''	1:A:224:G:N2	1.96	0.79
7:5:16:LYS:HG3	7:5:67:ARG:C	2.08	0.79
8:4:115:ILE:HG21	8:4:140:TYR:OH	1.81	0.79
1:A:173:A:C1'	1:A:224:G:H5''	2.09	0.78
1:A:125:G:O2'	1:A:227:G:H1'	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:0:SER:CB	5:1:29:VAL:N	2.31	0.78
1:A:124:G:N1	1:A:126:C:C5	2.52	0.78
1:A:220:C:C2'	1:A:221:C:H5''	2.14	0.78
8:4:136:LEU:HD13	8:4:140:TYR:CD2	2.18	0.78
2:9:2856:A:C1'	9:6:23:ASN:HD21	1.97	0.78
2:9:2905:A:OP1	9:6:51:ALA:CB	2.32	0.78
6:2:204:VAL:CG1	9:6:18:ARG:HD3	2.14	0.77
4:W:344:PRO:O	4:W:346:SER:N	2.18	0.76
2:9:2904:U:C5'	9:6:20:TYR:CE2	2.69	0.76
7:5:35:ILE:HA	8:4:75:TYR:CE1	2.20	0.76
7:5:54:SER:HA	7:5:57:ARG:HE	1.51	0.76
1:A:175:G:H3'	1:A:176:A:H5'	1.68	0.75
1:A:127:A:H2'	1:A:128:U:C5'	2.17	0.75
8:4:115:ILE:HG21	8:4:140:TYR:CZ	2.21	0.75
1:A:127:A:C1'	1:A:225:C:N3	2.29	0.75
3:B:14:ARG:HB3	3:B:14:ARG:CZ	2.17	0.75
2:9:2878:U:H2'	2:9:2879:A:O4'	1.86	0.75
8:4:140:TYR:CE2	8:4:145:VAL:HG21	2.22	0.75
2:9:2904:U:C4'	9:6:20:TYR:CE2	2.66	0.75
1:A:173:A:C4	1:A:224:G:O2'	2.39	0.74
7:5:38:VAL:HG21	8:4:76:PRO:O	1.86	0.74
8:4:105:ILE:HD11	8:4:130:LYS:HE3	1.70	0.74
8:4:115:ILE:HG22	8:4:140:TYR:CE1	2.23	0.74
9:6:25:HIS:CE1	9:6:79:VAL:HG12	2.23	0.74
2:9:2906:A:OP1	9:6:50:LYS:CG	2.36	0.73
1:A:234:A:P	5:1:49:HIS:HA	2.28	0.73
5:1:-1:HIS:CB	5:1:4:PHE:CE2	2.67	0.73
7:5:35:ILE:CA	8:4:75:TYR:HE1	2.00	0.73
1:A:127:A:C2'	1:A:224:G:N3	2.47	0.73
1:A:117:U:H3	1:A:234:A:H61	1.37	0.73
5:1:-1:HIS:HD1	5:1:68:VAL:C	1.95	0.72
1:A:148:G:H4'	3:B:15:PHE:O	1.89	0.72
2:9:2903:C:H5'	2:9:2903:C:H6	1.55	0.72
5:1:-1:HIS:ND1	5:1:68:VAL:C	2.47	0.72
1:A:151:C:OP1	1:A:204:G:H4'	1.90	0.72
5:1:-1:HIS:C	5:1:54:LEU:HD11	2.14	0.72
5:1:0:SER:O	5:1:29:VAL:CG2	2.23	0.72
8:4:115:ILE:CG2	8:4:140:TYR:CZ	2.73	0.72
8:4:110:LYS:HG2	8:4:115:ILE:O	1.88	0.72
2:9:2851:G:O2'	2:9:2852:A:H5'	1.90	0.72
2:9:2866:U:H1'	2:9:2891:A:C4	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:G:C2'	1:A:227:G:C8	2.60	0.71
1:A:124:G:N1	1:A:126:C:C6	2.57	0.71
4:W:361:SER:C	4:W:362:LYS:HG3	2.13	0.71
9:6:83:ILE:HG22	9:6:94:LYS:HB2	1.71	0.71
2:9:2866:U:H4'	2:9:2867:G:H5'	1.71	0.71
7:5:34:ARG:NH1	7:5:48:ILE:HG23	2.06	0.71
8:4:119:LYS:HD3	8:4:135:LYS:NZ	2.02	0.71
3:B:73:ASN:ND2	3:B:75:ASP:H	1.89	0.71
1:A:130:A:H2'	1:A:131:A:C8	2.26	0.71
7:5:34:ARG:HH12	7:5:48:ILE:CG2	2.04	0.71
9:6:55:ASN:HD22	9:6:92:ASP:HB2	1.56	0.71
6:2:204:VAL:HG12	9:6:18:ARG:HD3	1.71	0.70
8:4:122:THR:O	8:4:123:LEU:HD12	1.91	0.70
8:4:140:TYR:CZ	8:4:145:VAL:CG2	2.71	0.70
2:9:2909:G:O2'	2:9:2910:A:H5'	1.91	0.70
2:9:2827:A:H2'	2:9:2828:G:O4'	1.92	0.70
5:1:-1:HIS:CE1	5:1:68:VAL:O	2.43	0.70
2:9:2904:U:C5'	9:6:20:TYR:HE2	2.00	0.69
6:2:63:ARG:HB2	6:2:135:ARG:HB2	1.75	0.69
8:4:103:LYS:HE3	8:4:103:LYS:O	1.93	0.69
7:5:38:VAL:HG11	8:4:76:PRO:HG2	1.75	0.68
3:B:60:VAL:HG23	3:B:83:ARG:C	2.18	0.68
1:A:154:G:O2'	1:A:155:G:H5'	1.93	0.68
9:6:25:HIS:HE1	9:6:79:VAL:HG12	1.58	0.68
1:A:127:A:C4	1:A:225:C:C4	2.82	0.68
3:B:93:LEU:HD23	3:B:93:LEU:N	2.08	0.68
8:4:119:LYS:HG3	8:4:135:LYS:HB2	1.75	0.68
5:1:20:GLY:C	5:1:22:SER:H	2.01	0.68
2:9:2895:C:OP1	9:6:77:ARG:NH1	2.27	0.67
8:4:119:LYS:HD2	8:4:119:LYS:C	2.18	0.67
7:5:44:LYS:NZ	7:5:44:LYS:HA	2.08	0.67
1:A:175:G:H1	1:A:221:C:H42	1.42	0.67
1:A:125:G:H8	1:A:227:G:C6	2.04	0.67
1:A:127:A:O2'	1:A:128:U:H5''	1.93	0.67
1:A:215:A:O5'	1:A:215:A:H8	1.78	0.67
9:6:22:VAL:HG12	9:6:23:ASN:O	1.95	0.67
2:9:2905:A:OP1	9:6:51:ALA:HB1	1.72	0.67
3:B:15:PHE:CE1	3:B:85:GLN:HB2	2.30	0.67
3:B:14:ARG:O	3:B:14:ARG:HG2	1.95	0.66
1:A:172:A:N6	1:A:224:G:C2'	2.59	0.66
9:6:37:ALA:HB1	9:6:68:TRP:CD1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:A:O4'	1:A:224:G:H4'	1.95	0.66
1:A:128:U:C5'	1:A:224:G:N2	2.58	0.66
4:W:361:SER:C	4:W:362:LYS:CG	2.66	0.66
1:A:127:A:O2'	1:A:224:G:C2	2.44	0.65
1:A:157:A:H2'	1:A:158:C:H6	1.62	0.65
1:A:233:U:O4'	5:1:40:GLU:HB3	1.68	0.65
6:2:202:LEU:O	6:2:206:ARG:HB2	1.96	0.65
7:5:16:LYS:HZ1	7:5:65:LYS:HE2	1.62	0.65
1:A:172:A:N6	1:A:224:G:H2'	2.11	0.65
8:4:119:LYS:HZ3	8:4:135:LYS:HD3	1.61	0.65
9:6:44:ILE:CD1	9:6:67:ILE:HD11	2.26	0.65
1:A:127:A:H3'	1:A:224:G:H22	1.58	0.65
9:6:67:ILE:HG23	9:6:75:VAL:HG23	1.77	0.65
4:W:349:LEU:HD22	4:W:359:PHE:HE2	1.62	0.64
6:2:159:GLN:CD	6:2:206:ARG:HH22	2.06	0.64
9:6:56:ASP:O	9:6:92:ASP:HB3	1.97	0.64
2:9:2890:A:H5''	2:9:2890:A:C8	2.26	0.64
2:9:2894:C:O2'	2:9:2895:C:H5'	1.97	0.64
5:1:0:SER:HA	5:1:28:PRO:HB2	1.78	0.64
2:9:2908:A:H2'	2:9:2909:G:O4'	1.98	0.64
8:4:125:ARG:HH22	8:4:131:LYS:HZ3	1.45	0.64
2:9:2856:A:C4'	9:6:78:ARG:CG	2.24	0.64
1:A:157:A:H2'	1:A:158:C:C6	2.32	0.63
2:9:2854:A:O2'	9:6:26:LYS:HE2	1.91	0.63
6:2:204:VAL:CG1	9:6:18:ARG:CD	2.74	0.63
1:A:148:G:O2'	3:B:83:ARG:NH2	2.31	0.63
5:1:0:SER:N	5:1:54:LEU:HD11	2.12	0.63
7:5:35:ILE:O	7:5:38:VAL:HG12	1.97	0.63
8:4:114:ASP:C	8:4:115:ILE:HG23	2.15	0.63
2:9:2904:U:H4'	9:6:20:TYR:HD2	0.88	0.63
1:A:124:G:O6	1:A:126:C:C5	2.51	0.63
4:W:344:PRO:O	4:W:346:SER:HB3	1.99	0.63
6:2:103:VAL:HG12	6:2:105:ASN:H	1.62	0.63
1:A:195:U:O4'	4:W:411:GLY:HA3	1.99	0.63
3:B:88:GLN:HE21	3:B:92:SER:HB2	1.63	0.63
1:A:139:A:H2'	1:A:140:C:H6	1.63	0.63
9:6:28:LEU:HD23	9:6:75:VAL:HG11	1.80	0.63
1:A:149:A:H4'	3:B:17:CYS:SG	2.39	0.62
5:1:0:SER:HB2	5:1:28:PRO:C	2.19	0.62
3:B:76:VAL:HG13	3:B:77:GLN:N	2.14	0.62
2:9:2849:U:O2'	2:9:2850:C:OP2	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:G:C6	1:A:126:C:H5	2.13	0.62
1:A:193:G:N1	4:W:409:GLY:O	2.32	0.62
3:B:107:TYR:CZ	3:B:111:MET:HG3	2.35	0.62
4:W:341:LYS:O	4:W:345:PHE:CD1	2.52	0.62
8:4:122:THR:HG23	8:4:130:LYS:CD	2.30	0.62
1:A:127:A:C2'	1:A:224:G:H22	1.27	0.62
8:4:119:LYS:NZ	8:4:135:LYS:HD3	2.14	0.62
1:A:139:A:H2'	1:A:140:C:C6	2.35	0.61
1:A:117:U:H3	1:A:234:A:N6	1.98	0.61
2:9:2855:G:N3	9:6:23:ASN:ND2	2.49	0.60
1:A:234:A:OP2	5:1:48:THR:O	2.19	0.60
1:A:173:A:H2	1:A:224:G:N3	1.55	0.60
1:A:120:G:N2	1:A:230:C:O2	2.32	0.60
3:B:73:ASN:HD21	3:B:75:ASP:H	1.50	0.60
8:4:110:LYS:HE3	8:4:110:LYS:O	2.01	0.60
4:W:344:PRO:O	4:W:346:SER:CB	2.50	0.60
5:1:0:SER:C	5:1:29:VAL:H	2.09	0.59
8:4:83:MET:HA	8:4:86:ILE:HG22	1.84	0.59
8:4:91:THR:HG22	8:4:135:LYS:HG3	1.83	0.59
7:5:27:LYS:HE3	7:5:27:LYS:C	2.28	0.59
5:1:-1:HIS:CG	5:1:69:GLY:CA	2.85	0.59
7:5:31:GLY:O	7:5:35:ILE:HG12	2.03	0.59
1:A:126:C:N3	1:A:226:U:N3	2.51	0.59
8:4:113:TYR:HB2	8:4:115:ILE:HD12	1.84	0.59
2:9:2900:G:H2'	2:9:2901:C:O4'	2.02	0.59
1:A:172:A:C5	1:A:224:G:C2'	2.77	0.59
2:9:2866:U:H4'	2:9:2867:G:C5'	2.32	0.58
3:B:73:ASN:ND2	3:B:75:ASP:N	2.51	0.58
8:4:125:ARG:HD3	8:4:127:ASP:HB3	1.84	0.58
1:A:212:C:H4'	1:A:213:A:OP1	2.03	0.58
3:B:73:ASN:HD21	3:B:75:ASP:CB	2.16	0.58
7:5:34:ARG:C	8:4:75:TYR:CD1	2.79	0.58
5:1:-1:HIS:N	5:1:4:PHE:CZ	2.52	0.58
1:A:214:A:H5'	1:A:215:A:P	2.43	0.58
1:A:233:U:H3'	1:A:234:A:H5'	1.86	0.58
1:A:233:U:H2'	1:A:234:A:H5''	1.84	0.58
2:9:2907:C:H2'	2:9:2908:A:O4'	2.04	0.57
1:A:128:U:H5'	1:A:128:U:H6	1.68	0.57
1:A:233:U:H1'	5:1:40:GLU:HA	1.84	0.57
7:5:44:LYS:HA	7:5:44:LYS:HZ2	1.69	0.57
8:4:115:ILE:CG2	8:4:140:TYR:CE1	2.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:ILE:HG23	3:B:115:LEU:HD12	1.87	0.57
1:A:163:A:O5'	1:A:163:A:H8	1.87	0.57
3:B:60:VAL:CG2	3:B:84:VAL:HG12	2.35	0.57
6:2:180:GLN:HG3	6:2:243:GLU:HB3	1.87	0.57
1:A:235:G:OP1	5:1:48:THR:N	2.37	0.57
2:9:2825:C:H4'	2:9:2826:G:O5'	2.05	0.57
3:B:112:ILE:C	3:B:114:LYS:H	2.13	0.57
4:W:391:ASP:HB3	4:W:394:LYS:HZ2	1.70	0.56
3:B:86:LEU:HD13	3:B:99:PRO:O	2.05	0.56
5:1:121:LEU:O	5:1:125:GLU:HG3	2.06	0.56
5:1:0:SER:CA	5:1:29:VAL:N	2.69	0.56
8:4:125:ARG:NH2	8:4:131:LYS:HZ3	2.03	0.56
8:4:114:ASP:C	8:4:115:ILE:CG2	2.75	0.56
8:4:96:VAL:HG23	8:4:130:LYS:HE2	1.87	0.56
1:A:127:A:C2'	1:A:128:U:C5'	2.79	0.56
1:A:173:A:C4	1:A:224:G:C2'	2.56	0.56
1:A:125:G:C4	1:A:226:U:O2	2.47	0.56
1:A:171:U:C3'	1:A:172:A:H5''	2.35	0.56
9:6:17:THR:HG22	9:6:82:ARG:HE	1.71	0.56
9:6:41:ILE:HD12	9:6:64:ASN:HD22	1.71	0.56
1:A:220:C:C3'	1:A:221:C:H5''	2.36	0.55
8:4:106:LYS:HG3	8:4:117:ALA:HB3	1.88	0.55
5:1:-1:HIS:CG	5:1:69:GLY:HA3	2.42	0.55
1:A:220:C:H2'	1:A:221:C:C5'	2.29	0.55
3:B:62:LEU:HD12	3:B:81:ARG:O	2.07	0.55
1:A:127:A:N9	1:A:225:C:C4	2.74	0.55
2:9:2856:A:H5'	9:6:23:ASN:HA	1.89	0.55
5:1:0:SER:CB	5:1:54:LEU:HD21	2.36	0.55
1:A:173:A:N1	1:A:224:G:N3	2.53	0.55
7:5:16:LYS:HZ1	7:5:65:LYS:CE	2.18	0.55
8:4:109:VAL:HG22	8:4:115:ILE:HD11	1.89	0.55
3:B:76:VAL:HG13	3:B:77:GLN:H	1.71	0.55
4:W:379:MET:HA	4:W:382:MET:HG3	1.87	0.55
4:W:429:GLN:O	4:W:432:LYS:HG2	2.06	0.55
1:A:125:G:N9	1:A:227:G:O6	2.10	0.55
2:9:2904:U:O2'	9:6:47:PHE:CE2	2.58	0.55
8:4:83:MET:O	8:4:86:ILE:HG22	2.07	0.54
2:9:2856:A:H5''	9:6:78:ARG:HB2	1.89	0.54
3:B:64:LYS:HZ3	3:B:65:ASN:HB2	1.71	0.54
3:B:77:GLN:O	3:B:77:GLN:HG2	2.05	0.54
8:4:73:LEU:HD23	8:4:96:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:60:VAL:HB	3:B:84:VAL:HG12	1.90	0.54
5:1:0:SER:N	5:1:54:LEU:HD21	2.23	0.54
2:9:2855:G:C4	9:6:23:ASN:CG	2.82	0.54
3:B:116:LYS:N	3:B:116:LYS:HD2	2.23	0.54
8:4:125:ARG:HG3	8:4:129:LYS:O	2.08	0.54
2:9:2909:G:O2'	2:9:2910:A:C5'	2.56	0.54
3:B:64:LYS:NZ	3:B:65:ASN:H	2.06	0.54
6:2:192:GLN:O	6:2:196:GLU:HG3	2.08	0.54
1:A:125:G:C4	1:A:227:G:N7	2.74	0.54
7:5:33:LEU:HD13	7:5:48:ILE:HG13	1.89	0.54
2:9:2904:U:C5'	9:6:20:TYR:CD2	2.91	0.53
1:A:233:U:H3'	1:A:234:A:C5'	2.39	0.53
3:B:73:ASN:HD21	3:B:75:ASP:N	2.05	0.53
7:5:14:LYS:HA	7:5:14:LYS:NZ	2.23	0.53
8:4:103:LYS:HE3	8:4:103:LYS:C	2.33	0.53
1:A:208:A:H1'	4:W:380:ASP:O	2.08	0.53
2:9:2856:A:H4'	9:6:78:ARG:CB	2.32	0.53
3:B:88:GLN:O	3:B:91:GLY:N	2.42	0.53
3:B:116:LYS:O	3:B:120:GLN:HG2	2.09	0.53
5:1:29:VAL:O	5:1:33:ILE:HD13	2.09	0.53
1:A:127:A:C4	1:A:225:C:N3	2.77	0.53
4:W:341:LYS:O	4:W:345:PHE:CE1	2.62	0.53
5:1:8:PHE:HB3	5:1:14:VAL:HA	1.91	0.53
6:2:245:SER:O	6:2:256:ALA:HB1	2.09	0.53
7:5:34:ARG:NH1	7:5:48:ILE:CG2	2.70	0.53
2:9:2866:U:O2'	2:9:2867:G:P	2.67	0.53
1:A:195:U:H4'	4:W:411:GLY:O	2.08	0.52
7:5:35:ILE:C	8:4:75:TYR:HE1	2.16	0.52
1:A:127:A:O2'	1:A:224:G:N3	2.34	0.52
1:A:172:A:N1	1:A:224:G:H2'	2.24	0.52
2:9:2912:C:H2'	2:9:2913:A:O4'	2.09	0.52
2:9:2855:G:N3	9:6:23:ASN:CG	2.68	0.52
3:B:71:GLU:OE2	3:B:78:TYR:HD2	1.92	0.52
2:9:2858:U:H2'	2:9:2859:C:C6	2.44	0.52
3:B:41:VAL:CG1	3:B:42:GLU:N	2.72	0.52
8:4:85:LYS:HB3	8:4:91:THR:OG1	2.10	0.52
1:A:164:G:OP2	1:A:164:G:H8	1.92	0.52
6:2:103:VAL:CG1	6:2:266:ALA:HA	2.40	0.52
2:9:2906:A:H5'	2:9:2907:C:O4'	2.10	0.52
5:1:53:THR:O	5:1:69:GLY:HA2	2.10	0.52
1:A:126:C:C2	1:A:226:U:C6	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:64:LYS:HD3	3:B:64:LYS:H	1.71	0.51
1:A:175:G:H1	1:A:221:C:N4	2.08	0.51
1:A:199:A:H8	1:A:199:A:OP1	1.93	0.51
3:B:15:PHE:CZ	3:B:85:GLN:HB2	2.45	0.51
7:5:35:ILE:CA	8:4:75:TYR:CE1	2.87	0.51
6:2:81:ARG:HD3	6:2:246:ALA:O	2.09	0.51
3:B:60:VAL:CG2	3:B:83:ARG:O	2.52	0.51
3:B:93:LEU:HD23	3:B:93:LEU:H	1.75	0.51
7:5:11:LEU:HD22	7:5:58:VAL:HG22	1.92	0.51
3:B:56:VAL:HG21	3:B:107:TYR:CE2	2.45	0.50
1:A:127:A:C5	1:A:225:C:N4	2.79	0.50
2:9:2905:A:O3'	9:6:50:LYS:HE2	2.06	0.50
8:4:96:VAL:HG21	8:4:130:LYS:HE3	1.94	0.50
8:4:125:ARG:CZ	8:4:131:LYS:CD	2.90	0.50
1:A:126:C:O2'	1:A:226:U:H4'	2.10	0.50
1:A:126:C:C2	1:A:226:U:N3	2.46	0.50
1:A:233:U:C4'	5:1:40:GLU:HB3	2.38	0.50
5:1:10:LYS:HG2	6:2:94:ILE:HD11	1.92	0.50
2:9:2857:C:H5'	9:6:78:ARG:NE	2.26	0.50
1:A:121:U:H2'	1:A:122:U:C6	2.46	0.50
1:A:233:U:H1'	5:1:40:GLU:CA	1.99	0.50
3:B:43:ASN:C	3:B:118:ARG:HH22	2.20	0.50
3:B:68:TYR:CE2	3:B:70:ARG:HB2	2.46	0.50
4:W:394:LYS:NZ	4:W:394:LYS:HB3	2.27	0.50
7:5:29:GLU:O	7:5:33:LEU:HG	2.11	0.50
8:4:119:LYS:CE	8:4:135:LYS:HD3	2.41	0.50
8:4:125:ARG:HB3	8:4:126:PRO:C	2.36	0.50
7:5:16:LYS:HE2	7:5:16:LYS:N	2.27	0.50
1:A:136:G:N3	1:A:214:A:H2	2.09	0.49
7:5:12:TRP:NE1	7:5:61:VAL:HG22	2.23	0.49
9:6:28:LEU:CD1	9:6:43:GLU:HG3	2.42	0.49
1:A:125:G:C8	1:A:227:G:N1	2.76	0.49
2:9:2856:A:OP1	9:6:77:ARG:HB3	2.12	0.49
3:B:24:ASN:ND2	3:B:27:LYS:HG3	2.22	0.49
5:1:20:GLY:C	5:1:22:SER:N	2.69	0.49
8:4:125:ARG:CZ	8:4:131:LYS:HG3	2.42	0.49
4:W:344:PRO:C	4:W:346:SER:CB	2.85	0.49
7:5:7:LYS:NZ	7:5:7:LYS:HA	2.27	0.49
7:5:37:LYS:C	7:5:39:ALA:O	2.55	0.49
1:A:231:A:H5''	1:A:232:G:OP2	2.12	0.49
1:A:127:A:H2'	1:A:224:G:N2	0.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:76:VAL:C	3:B:78:TYR:N	2.70	0.49
2:9:2885:A:H2'	2:9:2886:C:H6	1.78	0.49
1:A:130:A:H2'	1:A:131:A:H8	1.72	0.49
2:9:2842:G:H2'	2:9:2843:A:H5'	1.95	0.49
2:9:2856:A:H4'	9:6:78:ARG:HG3	0.59	0.49
2:9:2912:C:O2'	2:9:2913:A:H5'	2.12	0.49
3:B:45:THR:O	3:B:46:ALA:C	2.56	0.49
4:W:349:LEU:HD22	4:W:359:PHE:CE2	2.45	0.49
4:W:392:GLY:O	4:W:396:PHE:HD1	1.95	0.49
1:A:124:G:N7	1:A:125:G:N7	2.42	0.48
4:W:373:LYS:O	4:W:377:THR:HG23	2.13	0.48
7:5:36:GLN:O	7:5:39:ALA:O	2.31	0.48
8:4:110:LYS:HE3	8:4:110:LYS:C	2.37	0.48
1:A:160:A:H2'	1:A:161:C:C6	2.49	0.48
1:A:192:A:H2'	1:A:193:G:O4'	2.13	0.48
2:9:2903:C:O2'	2:9:2904:U:H5'	2.12	0.48
3:B:29:ILE:HG22	3:B:30:ALA:N	2.28	0.48
2:9:2886:C:O2'	2:9:2887:G:H5'	2.14	0.48
4:W:344:PRO:O	4:W:345:PHE:C	2.53	0.48
6:2:186:LYS:HD3	6:2:190:LEU:HD23	1.95	0.48
1:A:165:G:N7	1:A:176:A:C6	2.82	0.48
6:2:268:ILE:HD12	6:2:268:ILE:C	2.39	0.48
8:4:119:LYS:HD2	8:4:120:VAL:N	2.29	0.48
6:2:170:SER:HB3	6:2:237:LEU:HD23	1.95	0.48
5:1:13:LEU:HD11	5:1:107:LEU:HD21	1.96	0.48
8:4:140:TYR:OH	8:4:145:VAL:HG11	2.14	0.48
9:6:52:MET:HE2	9:6:85:ARG:HH21	1.79	0.48
9:6:54:THR:CA	9:6:90:GLU:HB2	2.39	0.48
1:A:224:G:H8	1:A:224:G:H5'	1.79	0.48
2:9:2883:A:H2'	2:9:2884:G:O4'	2.13	0.48
8:4:96:VAL:CG2	8:4:130:LYS:CE	2.92	0.47
5:1:37:LEU:HD12	5:1:37:LEU:C	2.38	0.47
3:B:94:CYS:C	3:B:95:LEU:HD23	2.38	0.47
8:4:125:ARG:HH22	8:4:131:LYS:NZ	2.11	0.47
1:A:125:G:H2'	1:A:126:C:C6	2.48	0.47
1:A:160:A:H2'	1:A:161:C:O4'	2.14	0.47
2:9:2842:G:C2'	2:9:2843:A:H5'	2.45	0.47
9:6:55:ASN:HD21	9:6:85:ARG:HB3	1.79	0.47
9:6:55:ASN:ND2	9:6:92:ASP:HB2	2.26	0.47
8:4:119:LYS:C	8:4:119:LYS:CD	2.85	0.47
8:4:125:ARG:CZ	8:4:125:ARG:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:A:C2'	1:A:224:G:C5'	2.64	0.47
2:9:2831:C:H2'	2:9:2832:C:H5'	1.96	0.47
2:9:2897:C:O2'	2:9:2898:G:H5'	2.15	0.47
1:A:167:U:H2'	1:A:168:G:O4'	2.15	0.47
2:9:2836:G:H4'	2:9:2837:U:OP1	2.15	0.47
3:B:62:LEU:HD12	3:B:63:GLU:N	2.30	0.47
2:9:2854:A:O2'	9:6:26:LYS:NZ	2.43	0.47
3:B:14:ARG:CZ	3:B:14:ARG:CB	2.88	0.47
3:B:73:ASN:HD21	3:B:75:ASP:HB3	1.80	0.47
8:4:91:THR:HG22	8:4:135:LYS:CG	2.44	0.47
1:A:171:U:H3'	1:A:172:A:H5''	1.96	0.47
5:1:0:SER:C	5:1:29:VAL:N	2.73	0.47
9:6:94:LYS:HB3	9:6:94:LYS:HZ2	1.79	0.47
7:5:35:ILE:HA	7:5:38:VAL:HG12	1.95	0.46
1:A:116:C:H2'	1:A:117:U:C6	2.50	0.46
2:9:2871:G:H2'	2:9:2872:U:C6	2.51	0.46
9:6:40:ALA:HB2	9:6:75:VAL:HG21	1.98	0.46
5:1:56:TYR:HA	5:1:66:PHE:O	2.15	0.46
2:9:2871:G:H2'	2:9:2872:U:H6	1.80	0.46
6:2:103:VAL:HG13	6:2:266:ALA:HA	1.97	0.46
7:5:53:LYS:O	7:5:57:ARG:HD3	2.15	0.46
8:4:144:ASP:OD1	8:4:145:VAL:HG23	2.14	0.46
7:5:5:LYS:NZ	7:5:47:ARG:HD2	2.31	0.46
8:4:110:LYS:HZ2	8:4:115:ILE:N	2.14	0.46
2:9:2911:C:O2'	2:9:2912:C:H5'	2.15	0.46
8:4:125:ARG:HD3	8:4:127:ASP:CB	2.45	0.46
9:6:28:LEU:HD11	9:6:40:ALA:HA	1.97	0.46
1:A:146:G:C6	1:A:147:G:C5	3.03	0.45
1:A:223:U:H2'	1:A:224:G:H5''	1.98	0.45
7:5:14:LYS:HB3	7:5:18:ASP:HB2	1.98	0.45
7:5:38:VAL:HG21	8:4:76:PRO:N	2.31	0.45
3:B:75:ASP:OD1	3:B:76:VAL:N	2.47	0.45
1:A:125:G:N3	1:A:227:G:N7	2.64	0.45
1:A:207:C:C4	1:A:208:A:N7	2.84	0.45
2:9:2856:A:C1'	9:6:23:ASN:ND2	2.58	0.45
4:W:427:PHE:O	4:W:431:VAL:HG23	2.17	0.45
5:1:0:SER:O	5:1:29:VAL:HG21	2.13	0.45
5:1:68:VAL:HG11	5:1:83:ILE:HD11	1.98	0.45
6:2:68:VAL:C	6:2:75:LYS:HD3	2.41	0.45
7:5:59:LEU:O	7:5:59:LEU:HD13	2.17	0.45
1:A:229:U:H2'	1:A:230:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:37:LYS:N	7:5:41:SER:HB3	2.32	0.45
7:5:65:LYS:O	7:5:66:GLN:HB3	2.16	0.45
8:4:122:THR:C	8:4:123:LEU:HD12	2.42	0.45
1:A:166:U:H2'	1:A:167:U:O4'	2.17	0.45
1:A:127:A:H2'	1:A:224:G:H22	1.14	0.44
1:A:168:G:H3'	1:A:169:C:H5'	1.99	0.44
2:9:2831:C:C2'	2:9:2832:C:H5'	2.46	0.44
3:B:116:LYS:N	3:B:116:LYS:CD	2.80	0.44
8:4:83:MET:CA	8:4:86:ILE:HG22	2.47	0.44
1:A:162:C:H2'	1:A:163:A:C8	2.52	0.44
3:B:76:VAL:C	3:B:78:TYR:H	2.25	0.44
3:B:76:VAL:O	3:B:78:TYR:N	2.50	0.44
3:B:35:ILE:HD11	3:B:40:ALA:HA	1.99	0.44
3:B:76:VAL:CG1	3:B:77:GLN:N	2.80	0.44
6:2:159:GLN:CD	6:2:206:ARG:NH2	2.74	0.44
9:6:25:HIS:CE1	9:6:79:VAL:CG1	2.99	0.44
2:9:2885:A:H2'	2:9:2886:C:C6	2.52	0.44
2:9:2905:A:OP1	9:6:51:ALA:C	2.54	0.44
3:B:104:VAL:O	3:B:105:MET:C	2.60	0.44
7:5:36:GLN:HB3	7:5:41:SER:HA	2.00	0.44
9:6:56:ASP:H	9:6:91:GLU:HA	1.83	0.44
1:A:163:A:H2'	1:A:164:G:N9	2.32	0.44
1:A:186:C:O5'	1:A:186:C:H6	2.01	0.44
2:9:2846:C:H2'	2:9:2847:G:H8	1.82	0.44
3:B:88:GLN:O	3:B:89:GLU:C	2.58	0.44
7:5:16:LYS:HG3	7:5:67:ARG:O	2.17	0.44
1:A:124:G:H1	1:A:125:G:H2'	1.31	0.44
6:2:82:LEU:HD23	6:2:258:ILE:HD12	2.00	0.44
7:5:66:GLN:O	7:5:66:GLN:HG2	2.18	0.44
1:A:138:G:H2'	1:A:139:A:H8	1.83	0.44
1:A:179:G:N2	1:A:180:G:H1'	2.33	0.44
2:9:2859:C:O2'	2:9:2860:G:H5'	2.18	0.44
3:B:88:GLN:HG3	3:B:92:SER:O	2.18	0.44
4:W:420:LEU:C	4:W:420:LEU:HD23	2.42	0.44
7:5:47:ARG:O	7:5:51:ILE:HG12	2.17	0.44
8:4:119:LYS:HE2	8:4:135:LYS:HD3	1.99	0.44
3:B:96:VAL:HG23	3:B:97:GLN:N	2.33	0.43
4:W:430:MET:HA	4:W:433:LYS:HB3	2.00	0.43
9:6:51:ALA:HB3	9:6:52:MET:HG3	1.99	0.43
2:9:2890:A:C2'	2:9:2891:A:OP2	2.65	0.43
6:2:120:GLU:CD	6:2:120:GLU:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:4:74:LYS:NZ	8:4:74:LYS:HA	2.33	0.43
8:4:125:ARG:HG3	8:4:129:LYS:C	2.43	0.43
9:6:83:ILE:C	9:6:83:ILE:HD12	2.44	0.43
1:A:162:C:O2'	1:A:213:A:N3	2.50	0.43
5:1:0:SER:C	5:1:29:VAL:CB	2.85	0.43
1:A:125:G:H2'	1:A:126:C:H6	1.81	0.43
1:A:221:C:N4	1:A:222:G:C6	2.82	0.43
3:B:15:PHE:O	3:B:83:ARG:NH2	2.52	0.43
3:B:116:LYS:HE3	3:B:116:LYS:H	1.83	0.43
7:5:65:LYS:O	7:5:66:GLN:CB	2.66	0.43
8:4:77:LEU:HD13	8:4:95:ILE:HD11	1.99	0.43
1:A:171:U:H3'	1:A:172:A:C5'	2.49	0.43
1:A:117:U:H2'	1:A:118:A:C8	2.53	0.43
2:9:2872:U:H2'	2:9:2873:C:H6	1.84	0.43
2:9:2899:A:O2'	2:9:2900:G:H5'	2.19	0.43
3:B:24:ASN:HD22	3:B:27:LYS:CG	2.22	0.43
3:B:53:CYS:O	3:B:58:LEU:HB2	2.19	0.43
1:A:150:G:O2'	1:A:203:G:N3	2.49	0.43
3:B:23:LEU:HB2	3:B:44:PRO:HG3	2.01	0.43
3:B:73:ASN:ND2	3:B:74:ARG:N	2.67	0.43
6:2:192:GLN:HG3	6:2:241:PHE:CE1	2.54	0.43
8:4:110:LYS:HZ1	8:4:114:ASP:HA	1.83	0.43
8:4:118:LYS:NZ	8:4:118:LYS:HA	2.33	0.43
2:9:2838:A:H2'	2:9:2839:C:C6	2.54	0.43
3:B:41:VAL:HG12	3:B:42:GLU:N	2.34	0.43
3:B:60:VAL:CB	3:B:84:VAL:HG12	2.49	0.43
7:5:62:ILE:HG23	7:5:67:ARG:HA	2.01	0.43
2:9:2885:A:O2'	2:9:2886:C:H5'	2.19	0.42
6:2:258:ILE:O	6:2:262:GLU:HG3	2.19	0.42
7:5:66:GLN:O	7:5:67:ARG:CB	2.67	0.42
8:4:119:LYS:CD	8:4:135:LYS:HZ3	2.11	0.42
4:W:347:GLN:O	4:W:351:MET:HG3	2.18	0.42
7:5:54:SER:CA	7:5:57:ARG:HE	2.26	0.42
8:4:125:ARG:NE	8:4:131:LYS:HG3	2.34	0.42
2:9:2847:G:O2'	2:9:2848:G:H5'	2.19	0.42
2:9:2909:G:H2'	2:9:2910:A:H8	1.83	0.42
1:A:195:U:C4'	4:W:411:GLY:HA3	2.50	0.42
7:5:23:LEU:HD23	7:5:23:LEU:C	2.44	0.42
3:B:19:TYR:CE2	3:B:81:ARG:HD3	2.55	0.42
3:B:42:GLU:HG3	3:B:43:ASN:N	2.34	0.42
3:B:112:ILE:C	3:B:114:LYS:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H2'	1:A:161:C:H6	1.84	0.42
4:W:344:PRO:HB2	4:W:345:PHE:H	1.69	0.42
8:4:98:LEU:HA	8:4:130:LYS:HB2	2.01	0.42
1:A:117:U:H2'	1:A:118:A:H8	1.83	0.42
1:A:173:A:O3'	1:A:223:U:O2'	2.38	0.42
2:9:2856:A:O2'	9:6:21:THR:OG1	2.08	0.42
3:B:16:ILE:HG12	3:B:84:VAL:HG22	2.02	0.42
3:B:56:VAL:O	3:B:56:VAL:HG12	2.20	0.42
3:B:93:LEU:N	3:B:93:LEU:CD2	2.77	0.42
6:2:87:TYR:O	6:2:88:ARG:HG2	2.19	0.42
9:6:48:ALA:O	9:6:52:MET:HB2	2.19	0.42
9:6:83:ILE:HG22	9:6:94:LYS:CB	2.44	0.42
1:A:149:A:C4'	3:B:17:CYS:SG	3.08	0.42
3:B:107:TYR:O	3:B:111:MET:HG2	2.19	0.42
7:5:30:LEU:C	7:5:30:LEU:HD23	2.44	0.42
1:A:233:U:C3'	1:A:234:A:C5'	2.98	0.41
3:B:18:ILE:HD12	3:B:105:MET:HG2	2.02	0.41
1:A:171:U:H5'	1:A:172:A:OP2	2.20	0.41
1:A:126:C:C4	1:A:226:U:C2	2.99	0.41
1:A:223:U:H2'	1:A:224:G:C5'	2.49	0.41
2:9:2836:G:O2'	2:9:2837:U:P	2.78	0.41
9:6:84:ALA:O	9:6:92:ASP:HA	2.19	0.41
3:B:22:TYR:CD1	3:B:34:ARG:HG3	2.56	0.41
3:B:67:MET:HE1	3:B:74:ARG:HG3	2.02	0.41
1:A:126:C:H2'	1:A:127:A:O4'	2.21	0.41
2:9:2858:U:H2'	2:9:2859:C:H6	1.85	0.41
7:5:36:GLN:O	7:5:41:SER:HA	2.20	0.41
8:4:125:ARG:HH22	8:4:131:LYS:CE	2.34	0.41
9:6:59:ILE:HG22	9:6:94:LYS:HD2	2.01	0.41
6:2:103:VAL:HG21	6:2:269:ALA:HB2	2.02	0.41
6:2:174:LEU:HD11	6:2:242:LEU:HG	2.03	0.41
7:5:5:LYS:HG3	7:5:6:VAL:HG23	2.03	0.41
7:5:35:ILE:C	7:5:38:VAL:HG12	2.44	0.41
1:A:151:C:H2'	1:A:152:G:H8	1.86	0.41
2:9:2893:C:O2'	2:9:2894:C:H5'	2.20	0.41
3:B:76:VAL:CG1	3:B:77:GLN:H	2.34	0.41
3:B:116:LYS:H	3:B:116:LYS:CE	2.34	0.41
1:A:124:G:N1	1:A:125:G:C4	2.50	0.41
1:A:193:G:H2'	1:A:194:G:O4'	2.21	0.41
2:9:2825:C:C2	2:9:2826:G:C5	3.09	0.41
2:9:2854:A:C2'	9:6:26:LYS:CE	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:2877:G:N2	2:9:2879:A:H3'	2.36	0.41
3:B:25:ASN:C	3:B:25:ASN:OD1	2.63	0.41
4:W:343:GLY:C	4:W:346:SER:HB2	2.14	0.41
8:4:100:ALA:O	8:4:104:LYS:HG3	2.21	0.41
9:6:52:MET:HE1	9:6:83:ILE:CD1	2.39	0.41
1:A:207:C:O2'	1:A:208:A:H5'	2.21	0.41
2:9:2906:A:P	9:6:50:LYS:HE2	2.61	0.41
9:6:51:ALA:HB3	9:6:52:MET:CG	2.51	0.41
2:9:2845:G:O2'	2:9:2846:C:H5'	2.20	0.40
6:2:71:CYS:O	6:2:72:ASP:HB2	2.19	0.40
6:2:88:ARG:HG2	6:2:88:ARG:HH11	1.85	0.40
8:4:119:LYS:HE2	8:4:135:LYS:CB	2.52	0.40
8:4:124:ILE:HD12	8:4:124:ILE:O	2.20	0.40
8:4:127:ASP:CG	8:4:129:LYS:HE3	2.46	0.40
1:A:118:A:H2'	1:A:119:A:H5'	2.03	0.40
1:A:127:A:H2'	1:A:128:U:H5'	1.99	0.40
1:A:164:G:OP2	1:A:164:G:C8	2.73	0.40
2:9:2880:A:H2'	2:9:2881:C:O4'	2.21	0.40
5:1:55:LYS:HB2	5:1:55:LYS:HE3	1.87	0.40
6:2:77:LEU:HG	6:2:246:ALA:HB1	2.02	0.40
4:W:344:PRO:C	4:W:346:SER:HB2	2.46	0.40
4:W:412:VAL:HG22	4:W:416:ASP:OD2	2.20	0.40
8:4:106:LYS:O	8:4:109:VAL:HG12	2.20	0.40
9:6:54:THR:HA	9:6:90:GLU:CB	2.41	0.40
1:A:182:G:H21	1:A:215:A:H62	1.68	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
3	B	105/108 (97%)	87 (83%)	11 (10%)	7 (7%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	W	107/109 (98%)	100 (94%)	2 (2%)	5 (5%)	2	16
5	1	115/185 (62%)	107 (93%)	7 (6%)	1 (1%)	14	51
6	2	182/214 (85%)	177 (97%)	5 (3%)	0	100	100
7	5	62/124 (50%)	55 (89%)	2 (3%)	5 (8%)	1	9
8	4	79/152 (52%)	71 (90%)	4 (5%)	4 (5%)	1	15
9	6	79/123 (64%)	66 (84%)	10 (13%)	3 (4%)	2	19
All	All	729/1015 (72%)	663 (91%)	41 (6%)	25 (3%)	4	21

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	42	GLU
3	B	75	ASP
4	W	344	PRO
4	W	345	PHE
4	W	362	LYS
7	5	39	ALA
7	5	45	LEU
8	4	101	ASP
8	4	125	ARG
9	6	24	LEU
9	6	52	MET
9	6	90	GLU
3	B	99	PRO
4	W	346	SER
7	5	66	GLN
8	4	127	ASP
8	4	141	ASP
7	5	38	VAL
7	5	43	SER
3	B	64	LYS
3	B	77	GLN
5	1	23	ASP
4	W	363	GLY
3	B	56	VAL
3	B	96	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	96/97 (99%)	89 (93%)	7 (7%)	13	34
4	W	96/96 (100%)	91 (95%)	5 (5%)	21	42
5	1	115/166 (69%)	110 (96%)	5 (4%)	26	47
6	2	164/182 (90%)	160 (98%)	4 (2%)	43	64
7	5	55/109 (50%)	44 (80%)	11 (20%)	1	7
8	4	72/128 (56%)	51 (71%)	21 (29%)	0	2
9	6	72/108 (67%)	54 (75%)	18 (25%)	0	4
All	All	670/886 (76%)	599 (89%)	71 (11%)	9	21

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	14	ARG
3	B	29	ILE
3	B	39	LYS
3	B	64	LYS
3	B	93	LEU
3	B	104	VAL
3	B	116	LYS
4	W	349	LEU
4	W	365	GLU
4	W	383	ASN
4	W	394	LYS
4	W	412	VAL
5	1	2	VAL
5	1	13	LEU
5	1	37	LEU
5	1	40	GLU
5	1	95	ARG
6	2	120	GLU
6	2	150	VAL
6	2	159	GLN

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Mol	Chain	Res	Type
6	2	186	LYS
7	5	7	LYS
7	5	14	LYS
7	5	16	LYS
7	5	21	LYS
7	5	25	GLU
7	5	27	LYS
7	5	37	LYS
7	5	38	VAL
7	5	44	LYS
7	5	46	ASN
7	5	63	ASN
8	4	70	TYR
8	4	74	LYS
8	4	85	LYS
8	4	87	GLU
8	4	90	ASN
8	4	97	ASP
8	4	99	LYS
8	4	101	ASP
8	4	103	LYS
8	4	104	LYS
8	4	106	LYS
8	4	110	LYS
8	4	115	ILE
8	4	118	LYS
8	4	119	LYS
8	4	125	ARG
8	4	129	LYS
8	4	130	LYS
8	4	135	LYS
8	4	141	ASP
8	4	147	ASN
9	6	18	ARG
9	6	23	ASN
9	6	27	ARG
9	6	28	LEU
9	6	52	MET
9	6	57	VAL
9	6	59	ILE
9	6	62	LYS
9	6	65	LYS

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Mol	Chain	Res	Type
9	6	77	ARG
9	6	80	ARG
9	6	85	ARG
9	6	86	LYS
9	6	87	ARG
9	6	88	ASN
9	6	90	GLU
9	6	91	GLU
9	6	97	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	59	ASN
3	B	73	ASN
3	B	88	GLN
4	W	383	ASN
4	W	385	GLN
4	W	399	GLN
4	W	429	GLN
5	1	49	HIS
5	1	61	GLN
5	1	99	GLN
6	2	91	GLN
6	2	178	ASN
6	2	194	GLN
7	5	22	GLN
7	5	49	HIS
7	5	63	ASN
7	5	66	GLN
8	4	71	GLN
9	6	64	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	125/127 (98%)	22 (17%)	1 (0%)
2	9	89/90 (98%)	10 (11%)	4 (4%)
All	All	214/217 (98%)	32 (14%)	5 (2%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	128	U
1	A	129	C
1	A	164	G
1	A	168	G
1	A	169	C
1	A	171	U
1	A	172	A
1	A	173	A
1	A	174	G
1	A	176	A
1	A	177	G
1	A	187	G
1	A	191	C
1	A	213	A
1	A	214	A
1	A	215	A
1	A	219	C
1	A	221	C
1	A	224	G
1	A	227	G
1	A	232	G
1	A	234	A
2	9	2826	G
2	9	2827	A
2	9	2837	U
2	9	2850	C
2	9	2867	G
2	9	2876	G
2	9	2890	A
2	9	2891	A
2	9	2903	C
2	9	2914	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	212	C
2	9	2836	G
2	9	2849	U
2	9	2866	U
2	9	2890	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	1	3
1	A	2
4	W	2
7	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	0:SER	C	1:MET	N	17.58
1	1	27:GLY	C	28:PRO	N	7.21
1	1	52:LEU	C	53:THR	N	5.58
1	A	124:G	O3'	125:G	P	4.22
1	A	221:C	O3'	222:G	P	3.26
1	W	362:LYS	C	363:GLY	N	1.64
1	5	38:VAL	C	39:ALA	N	1.61
1	W	345:PHE	C	346:SER	N	0.91

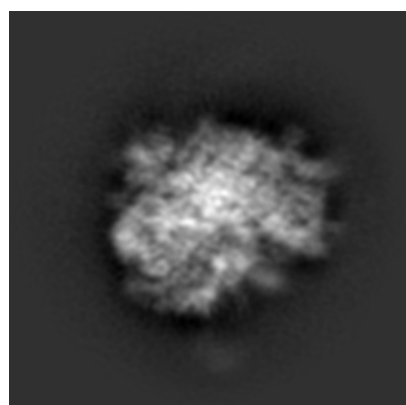
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1217. These allow visual inspection of the internal detail of the map and identification of artifacts.

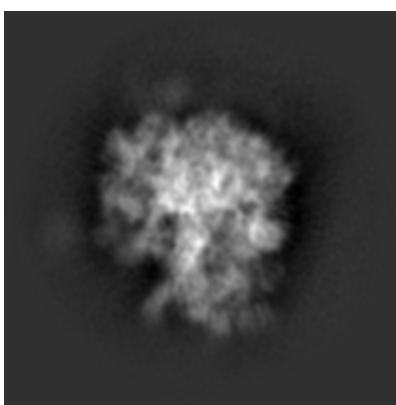
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

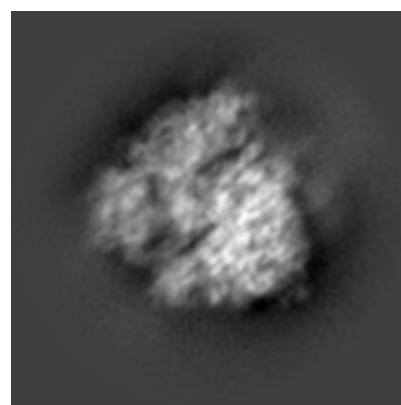
6.1.1 Primary map



X



Y

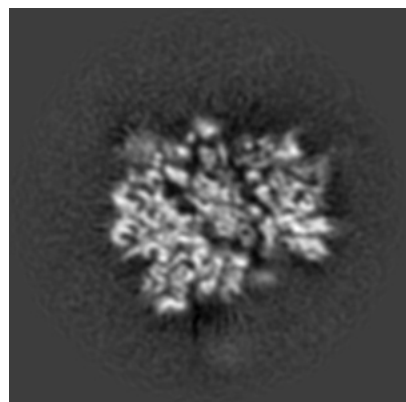


Z

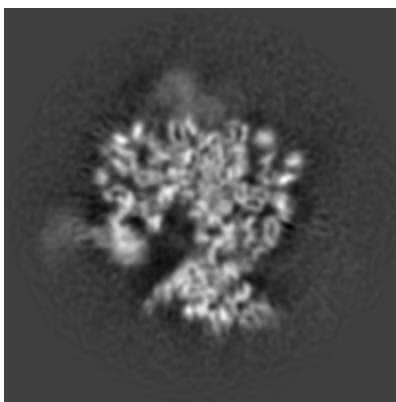
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

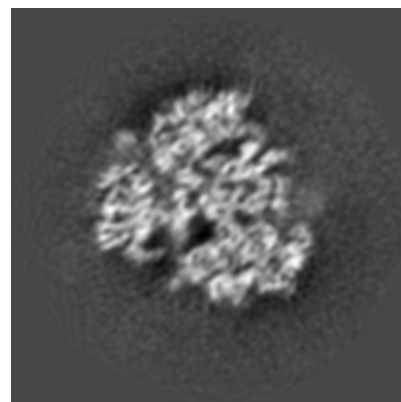
6.2.1 Primary map



X Index: 184



Y Index: 184

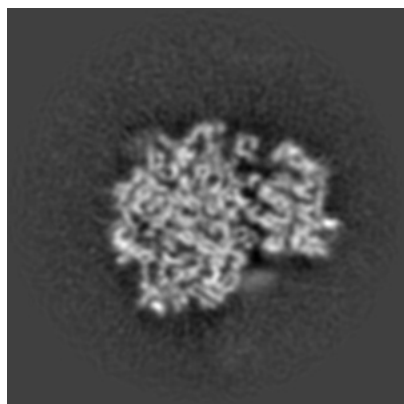


Z Index: 184

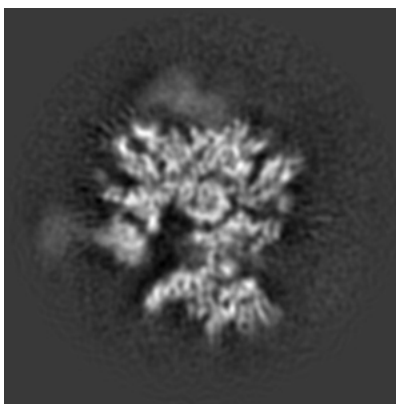
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

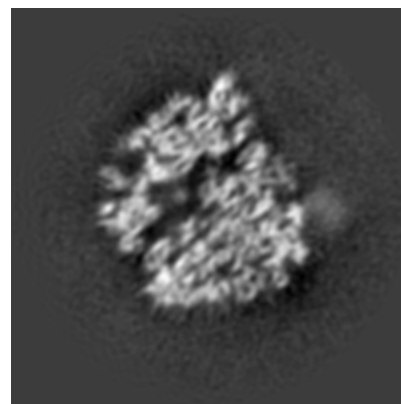
6.3.1 Primary map



X Index: 192



Y Index: 190

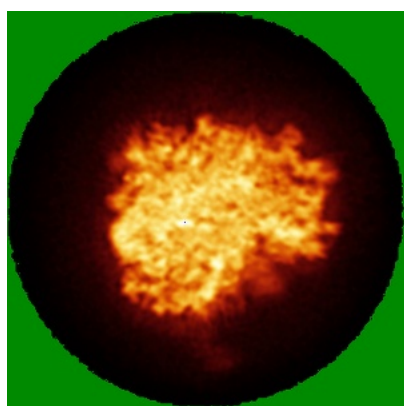


Z Index: 169

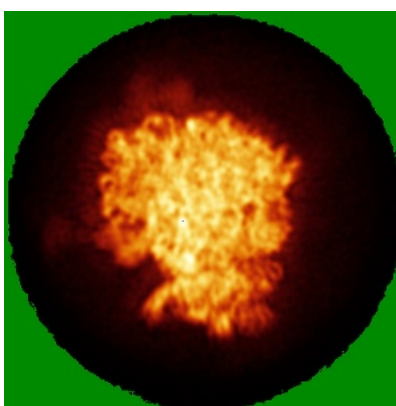
The images above show the largest variance slices of the map in three orthogonal directions.

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

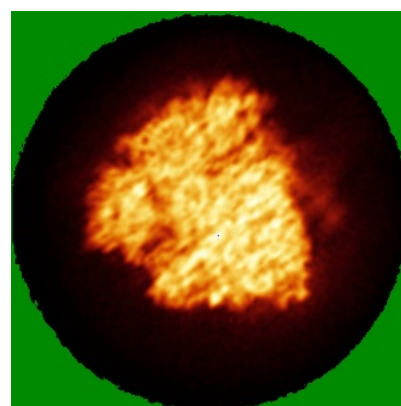
6.4.1 Primary map



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 0.173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

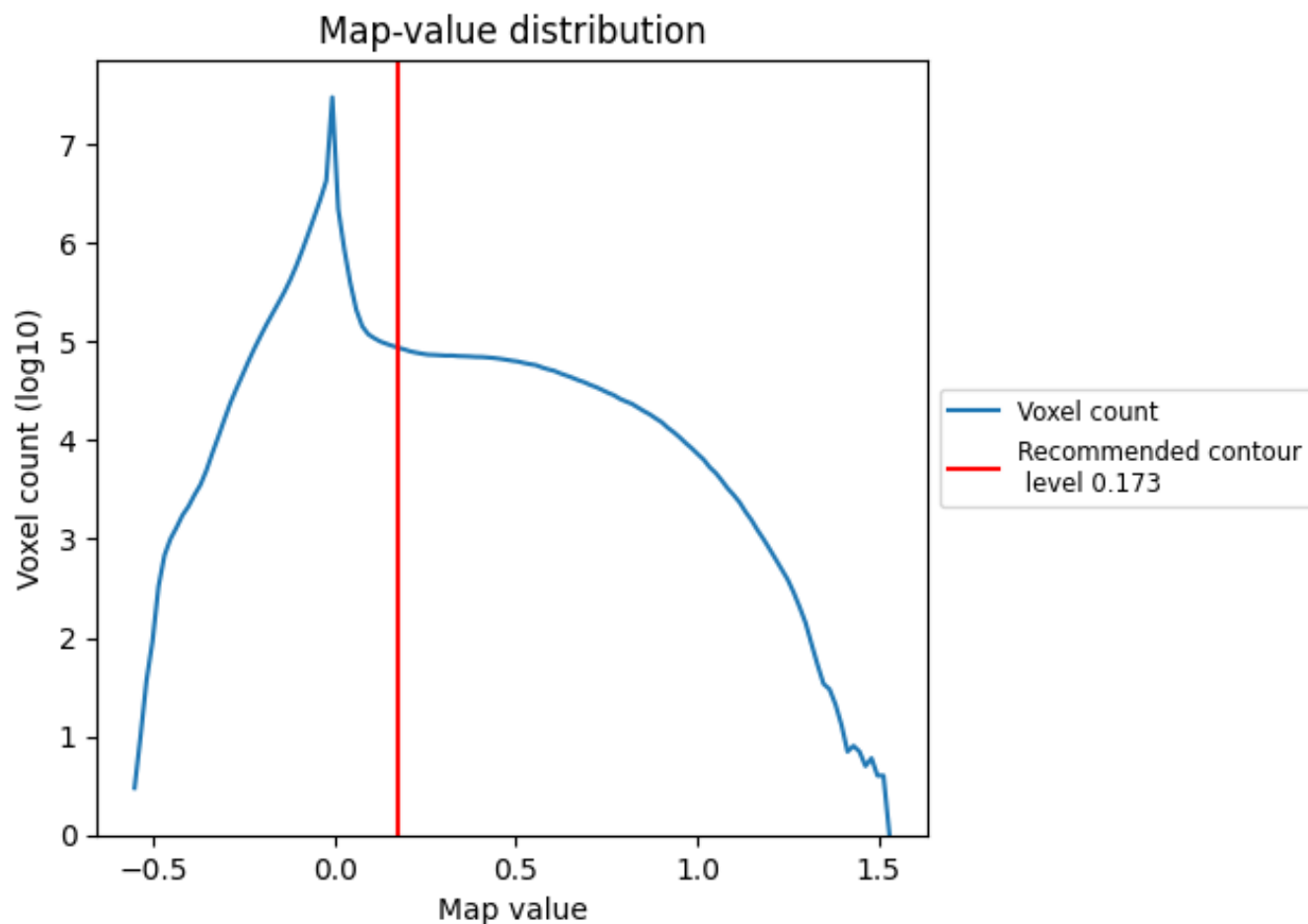
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

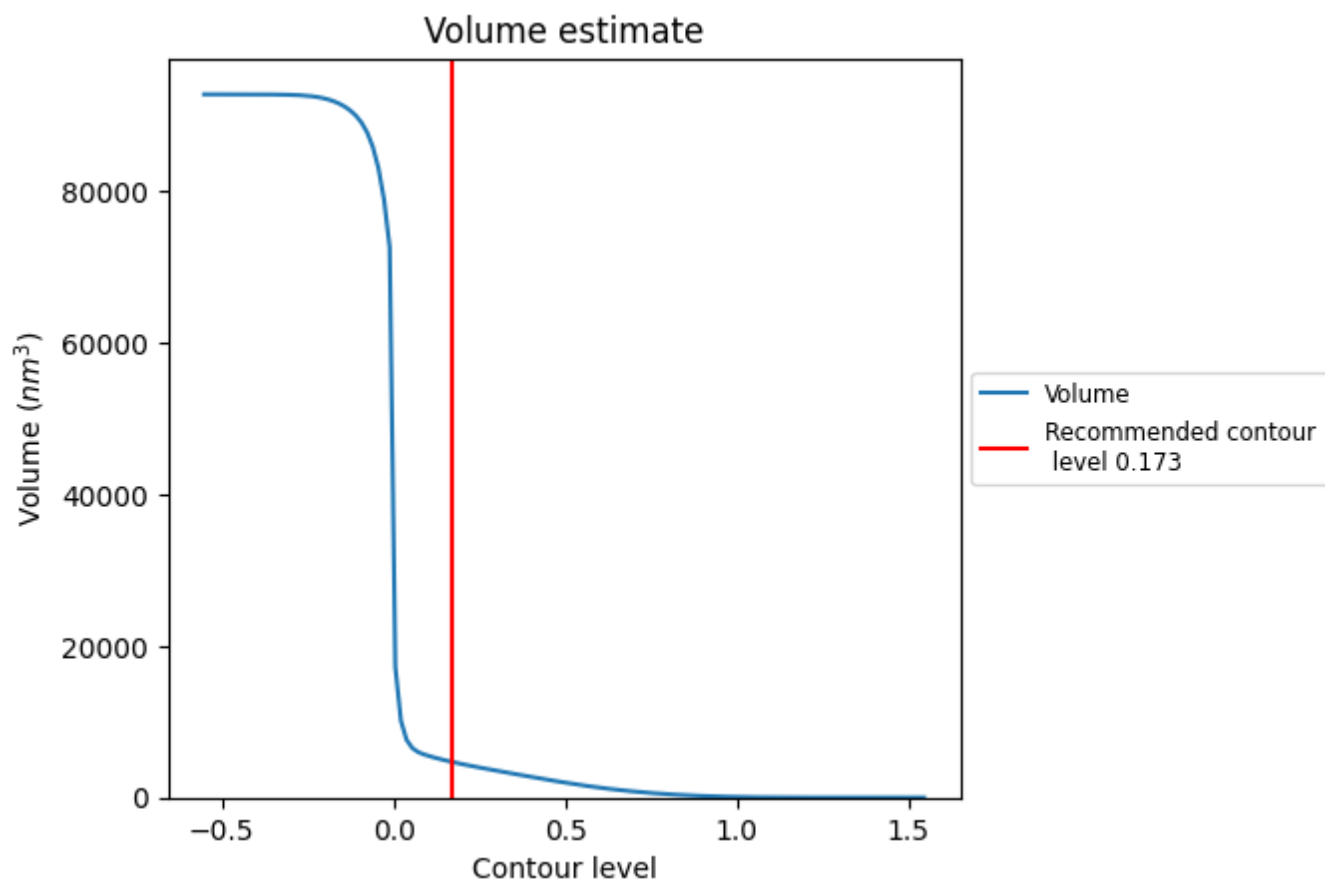
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

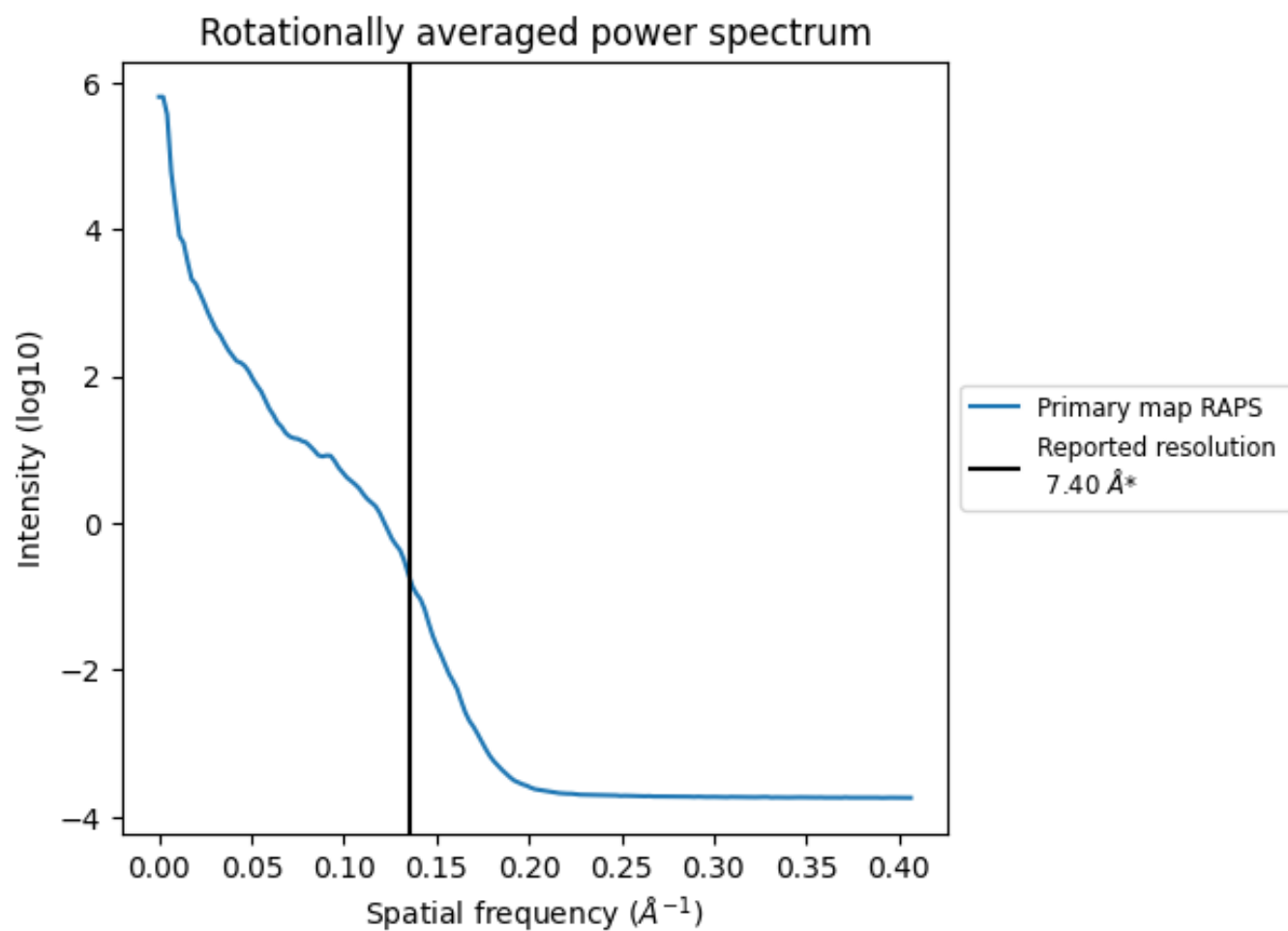
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4683 nm³; this corresponds to an approximate mass of 4230 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 0.135 Å⁻¹

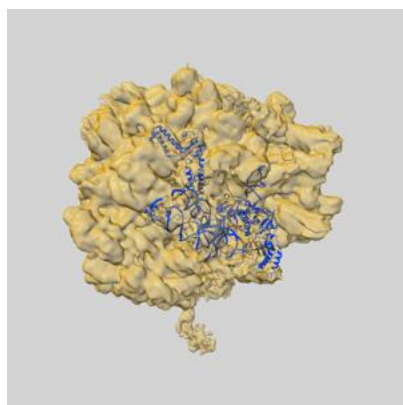
8 Fourier-Shell correlation

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

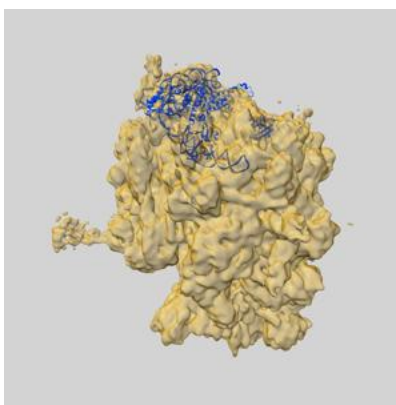
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1217 and PDB model 2GO5. Per-residue inclusion information can be found in section 3 on page 6.

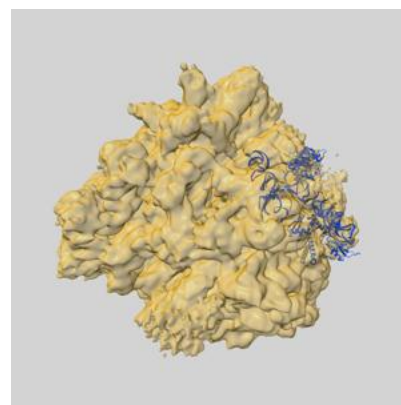
9.1 Map-model overlay [i](#)



X



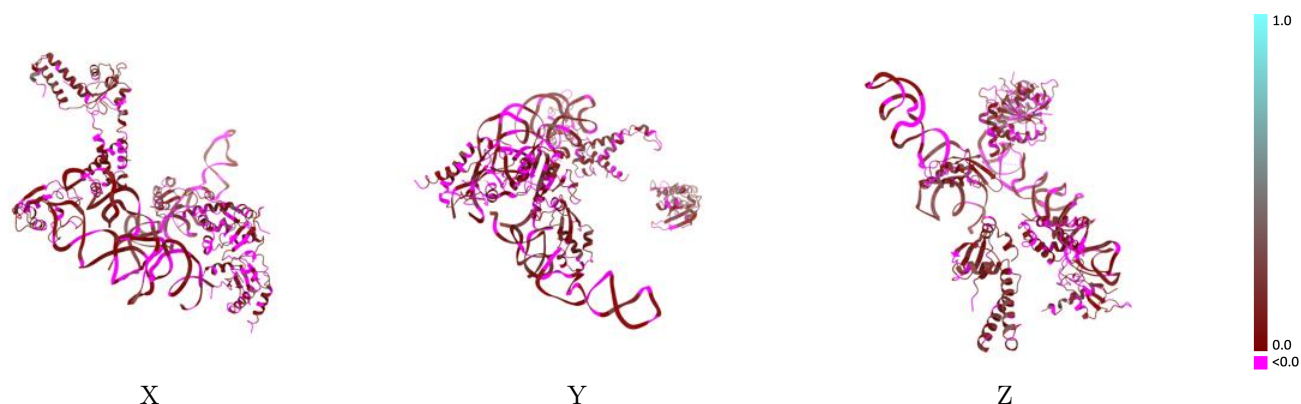
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.173 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](#)



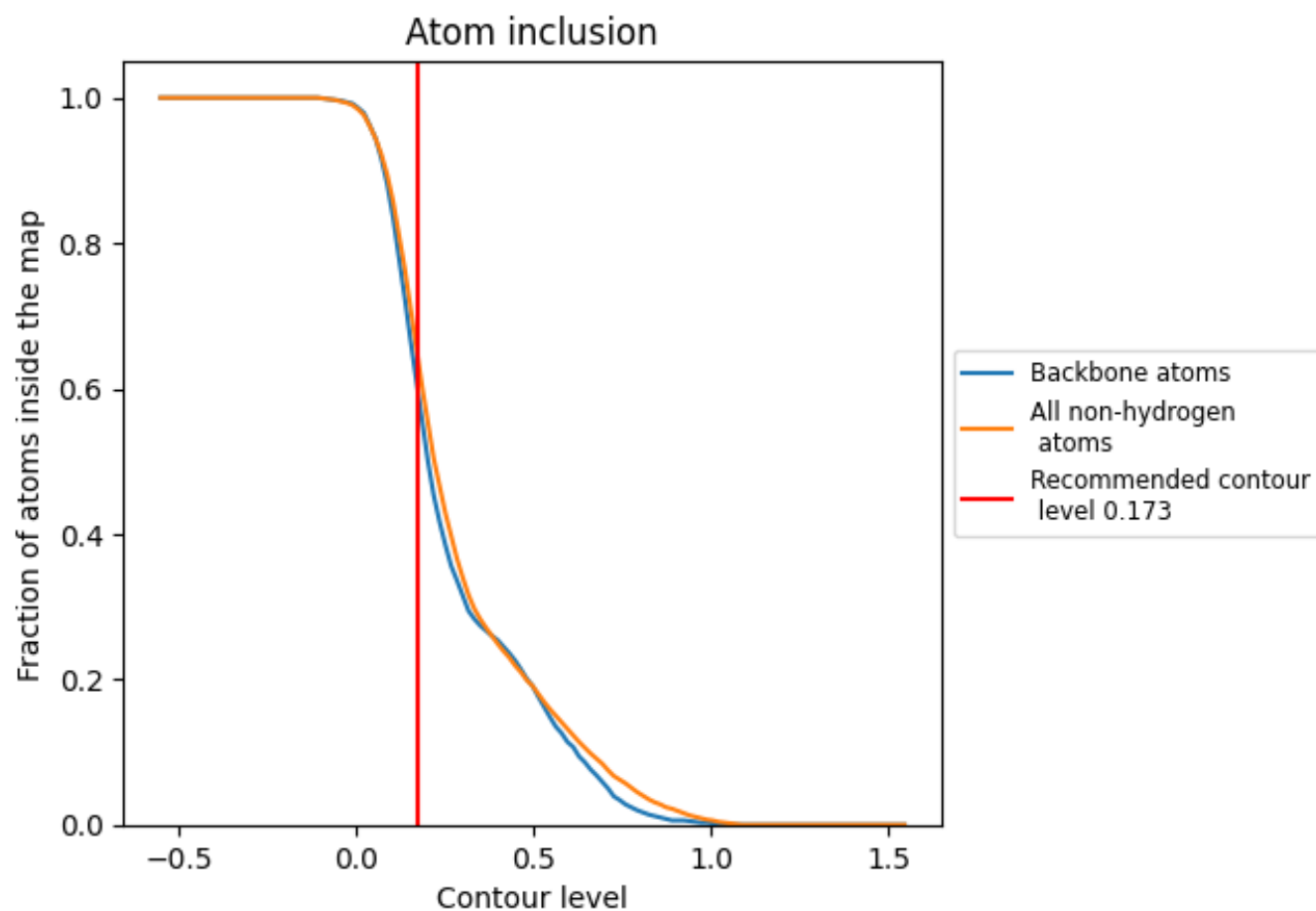
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.173).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 65% 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 (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6470	0.0550
1	0.1990	0.0270
2	0.2670	0.0220
4	0.9220	0.1230
5	0.9510	0.1440
6	0.9660	0.0990
9	0.9270	0.0550
A	0.7330	0.0490
B	0.4440	0.0560
W	0.4900	0.0300

1.0

0.0

<0.0