



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:06 AM UTC

PDB ID : 6UH5 / pdb_00006uh5
EMDB ID : EMD-20767
Title : Structural basis of COMPASS eCM recognition of the H2Bub nucleosome
Authors : Hsu, P.L.; Shi, H.; Zheng, N.
Deposited on : 2019-09-26
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

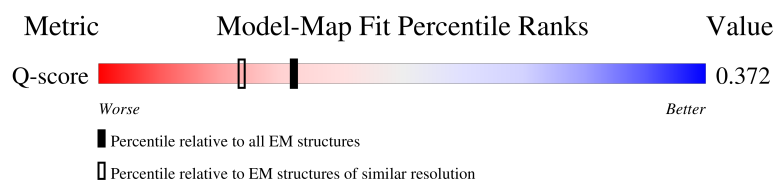
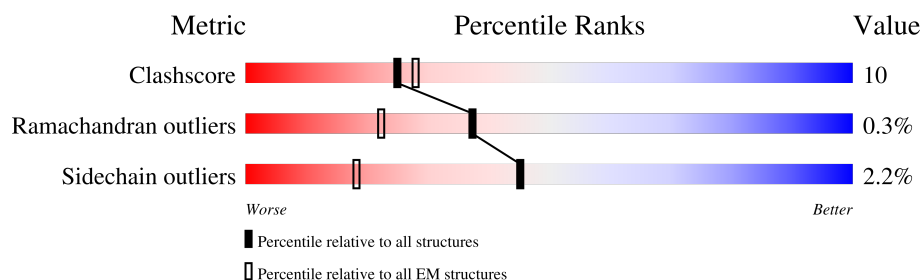
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	135	
1	E	135	
2	B	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
3	C	107	
3	G	107	
4	D	125	
5	H	125	
6	I	146	
7	J	146	
8	K	327	
9	M	275	
10	N	439	
11	Q	76	
12	R	8	
13	X	342	
14	L	405	
15	O	134	
15	P	134	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 24466 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			799	504	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			777	490	148	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	F	86	Total	C	N	O	S	0	0
			672	424	130	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			815	513	159	143		
3	G	107	Total	C	N	O	0	0
			815	513	159	143		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			722	454	129	137	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	7	PRO	ALA	conflict	UNP A0A1L8FQ56

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	93	Total	C	N	O	S	0	0
			723	454	129	137	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	7	PRO	ALA	conflict	UNP A0A1L8FQ56
H	117	CYS	LYS	conflict	UNP A0A1L8FQ56

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

- Molecule 7 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

- Molecule 8 is a protein called Swd3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	305	Total	C	N	O	S	0	0
			2365	1498	395	453	19		

- Molecule 9 is a protein called Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	222	Total	C	N	O	S	0	0
			1775	1119	317	331	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	761	GLU	ASP	conflict	UNP Q6CIT4

- Molecule 10 is a protein called Swd1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	408	Total	C	N	O	S	0	0
			3273	2095	539	622	17		

- Molecule 11 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	76	Total	C	N	O	S	0	0
			597	376	104	115	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	76	CYS	GLY	engineered mutation	UNP J3QS39

- Molecule 12 is a protein called H3 N-terminus.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	8	Total	C	N	O	S	0	0
			63	36	15	11	1		

- Molecule 13 is a protein called Spp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	73	Total	C	N	O	S	0	0
			604	379	108	117			

- Molecule 14 is a protein called Bre2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	382	Total	C	N	O	S	0	0
			3128	1985	519	609	15		

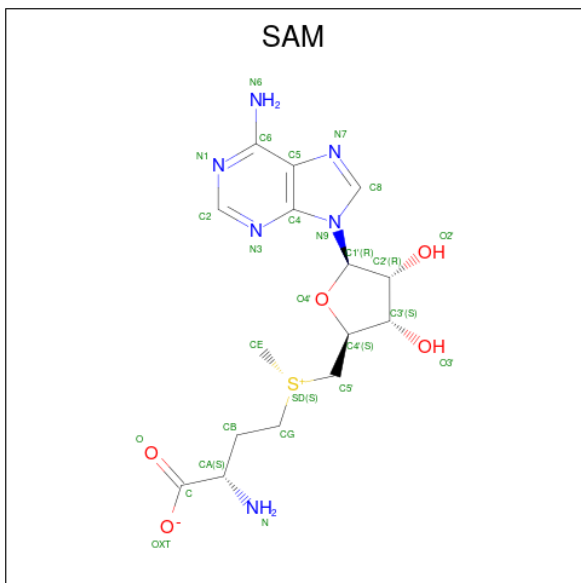
- Molecule 15 is a protein called Sdc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	42	Total	C	N	O	S	0	0
			342	216	63	62	1		
15	P	43	Total	C	N	O	S	0	0
			329	211	57	59	2		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	M	1	Total	Zn	0
			1	1	

- Molecule 17 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



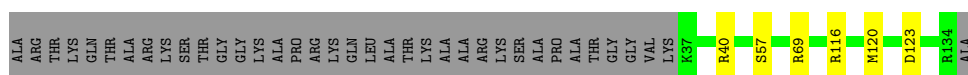
Mol	Chain	Residues	Atoms					AltConf
17	R	1	Total	C	N	O	S	0
			27	15	6	5	1	

3 Residue-property plots [i](#)

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

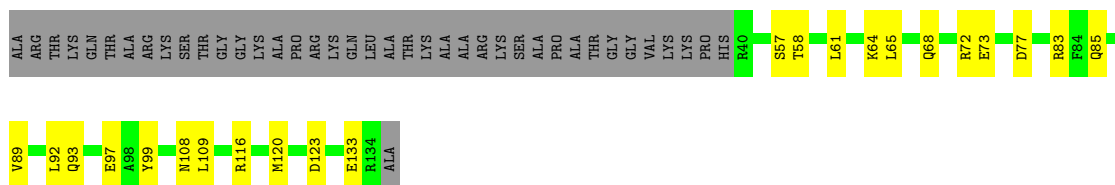
- Molecule 1: Histone H3

Chain A: 



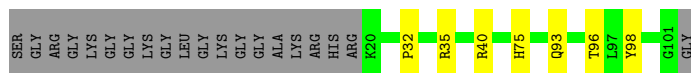
- Molecule 1: Histone H3

Chain E: 



- Molecule 2: Histone H4

Chain B: 



- Molecule 2: Histone H4

Chain F: 



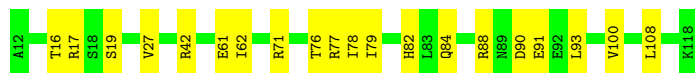
- Molecule 3: Histone H2A

Chain C: 



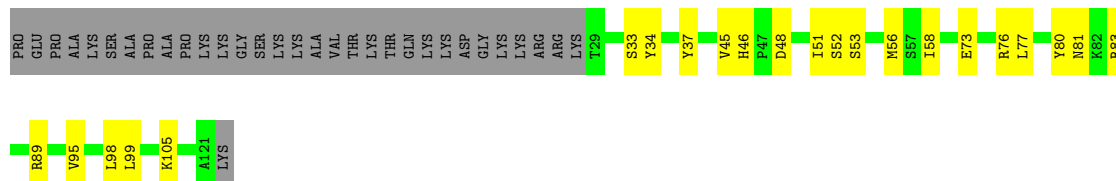
- Molecule 3: Histone H2A

Chain G:  81% 19%



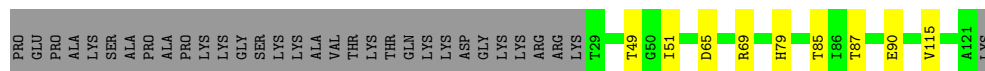
- Molecule 4: Histone H2B

Chain D:  57% 18% 26%



- Molecule 5: Histone H2B

Chain H:  67% 7% 26%



- Molecule 6: DNA (146-MER)

Chain I:  83% 17%



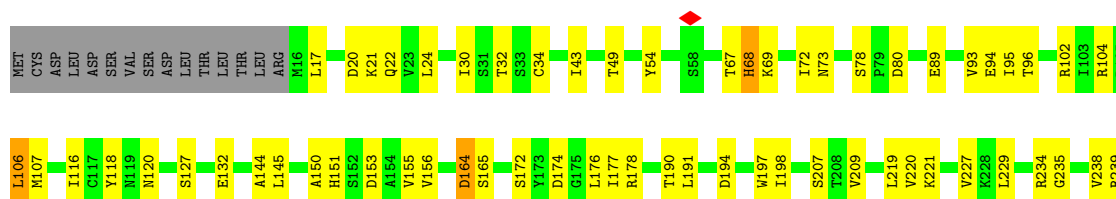
- Molecule 7: DNA (146-MER)

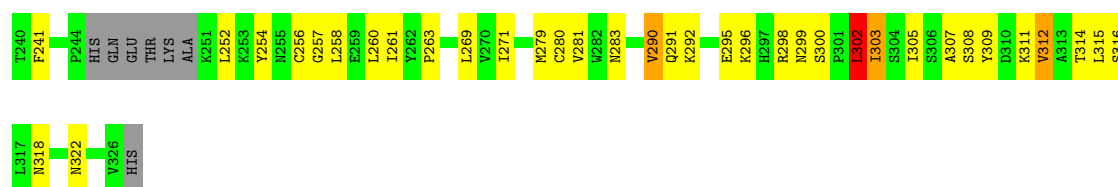
Chain J:  82% 18%



- Molecule 8: Swd3

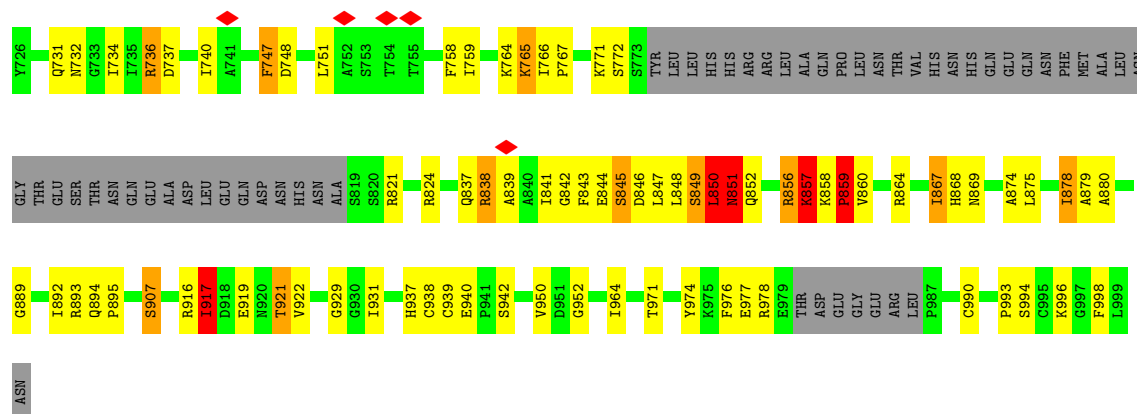
Chain K:  63% 28% 7%





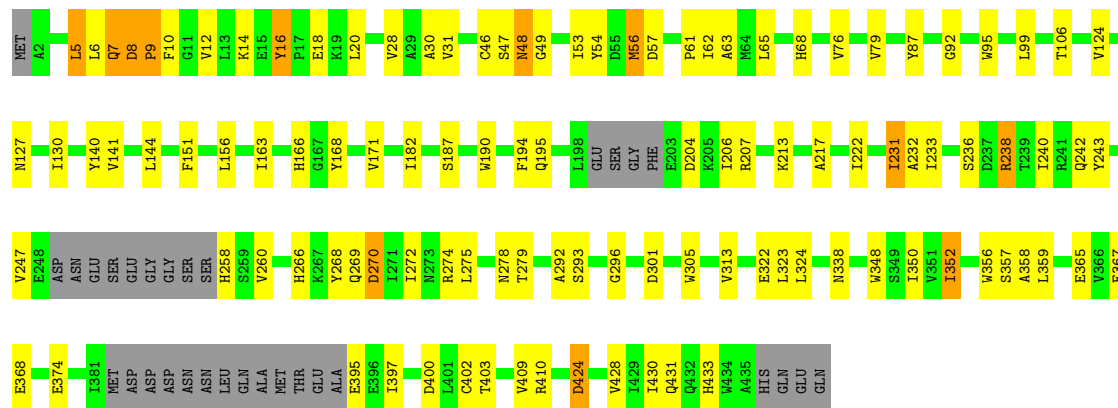
- Molecule 9: Histone-lysine N-methyltransferase, H3 lysine-4 specific

Chain M:



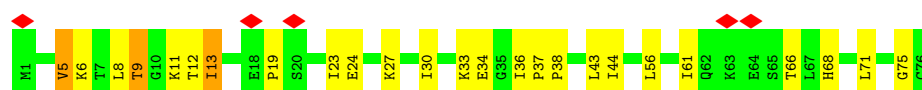
- Molecule 10: Swd1

Chain N:



- Molecule 11: Ubiquitin

Chain Q:



- Molecule 12: H3 N-terminus

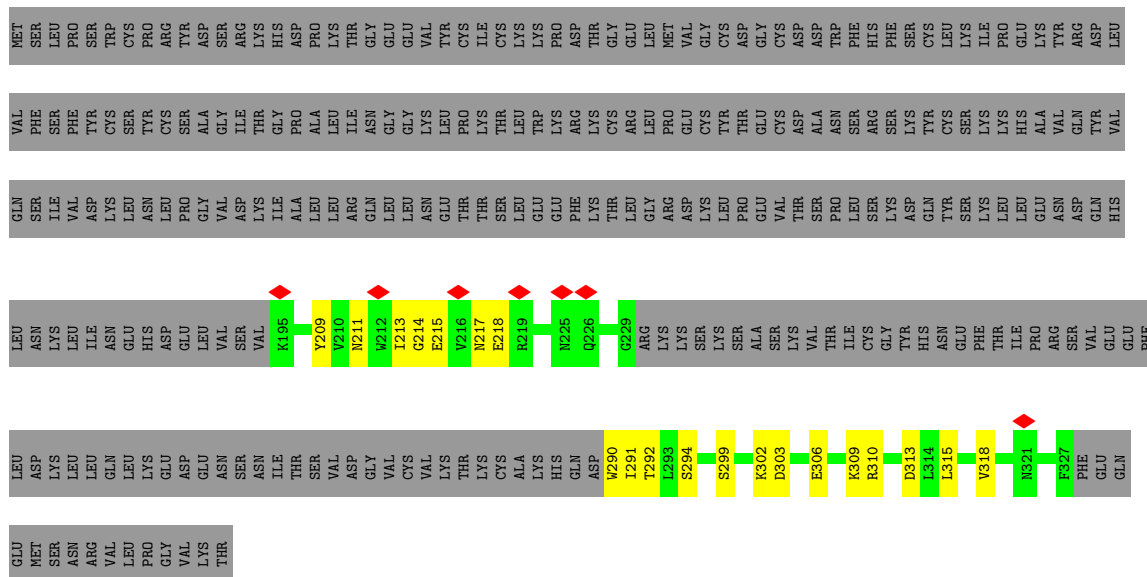
Chain R:





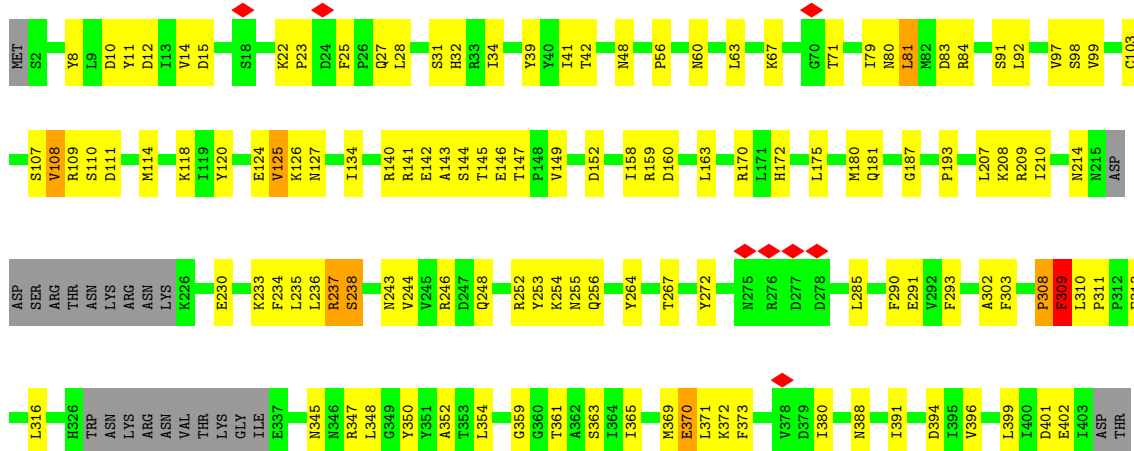
• Molecule 13: Spp1

Chain X: 15% 6% 79%



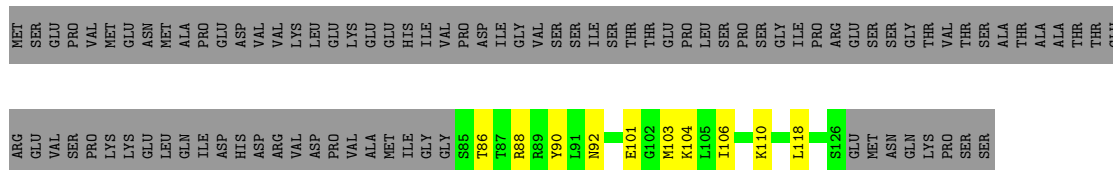
• Molecule 14: Bre2

Chain L: 63% 29% 6%

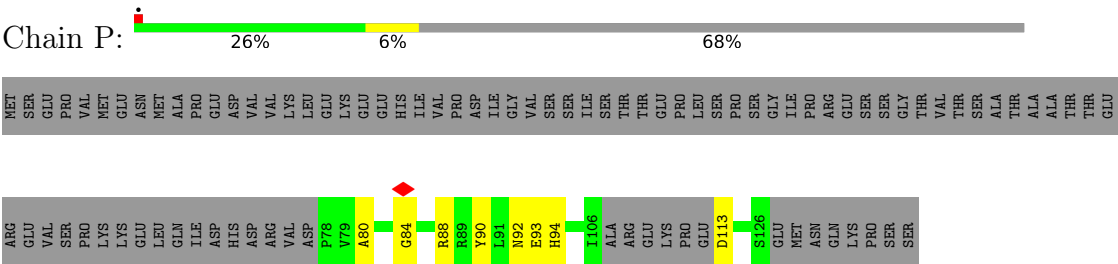


• Molecule 15: Sdc1

Chain O: 24% 7% 69%



● Molecule 15: Sdc1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	215199	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 ($e^-/\text{\AA}^2$)	74	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	342.144, 342.144, 342.144	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SAM, ZN

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	0.69	0/811	0.73	0/1089
1	E	0.68	0/787	0.77	0/1055
2	B	0.73	0/660	0.82	1/885 (0.1%)
2	F	0.71	0/680	1.46	7/912 (0.8%)
3	C	0.60	0/825	0.76	0/1116
3	G	0.72	0/825	0.79	0/1116
4	D	0.64	0/733	0.82	3/989 (0.3%)
5	H	0.78	0/734	0.83	2/990 (0.2%)
6	I	0.50	0/3333	0.54	0/5137
7	J	0.49	0/3381	0.53	0/5221
8	K	0.33	0/2410	0.92	17/3262 (0.5%)
9	M	0.42	0/1802	1.60	43/2415 (1.8%)
10	N	0.44	0/3360	0.98	23/4577 (0.5%)
11	Q	0.39	0/603	0.94	7/812 (0.9%)
12	R	0.51	0/62	0.99	0/81
13	X	0.34	0/612	0.68	0/825
14	L	0.28	0/3198	0.88	15/4323 (0.3%)
15	O	0.18	0/347	0.58	0/466
15	P	0.24	0/333	0.64	0/447
All	All	0.49	0/25496	0.88	118/35718 (0.3%)

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
8	K	0	1
9	M	0	4
10	N	0	1
14	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	857	LYS	N-CA-C	28.64	141.71	111.07
14	L	237	ARG	N-CA-C	-25.26	73.97	110.59
2	F	98	TYR	N-CA-C	24.70	140.59	112.93
2	F	95	ARG	N-CA-C	-20.97	71.57	108.69
9	M	952	GLY	N-CA-C	19.89	143.94	115.30
10	N	270	ASP	N-CA-C	-16.99	81.04	108.73
9	M	839	ALA	N-CA-C	16.40	128.86	111.14
10	N	57	ASP	N-CA-C	15.70	129.76	111.71
9	M	850	LEU	CA-C-N	15.39	150.94	121.54
9	M	850	LEU	C-N-CA	15.39	150.94	121.54
9	M	737	ASP	N-CA-C	14.33	126.98	111.36
9	M	850	LEU	CB-CA-C	-14.05	88.45	111.36
10	N	31	VAL	N-CA-C	13.69	123.29	110.42
9	M	837	GLN	N-CA-C	13.16	127.44	112.57
14	L	14	VAL	CB-CA-C	13.13	132.82	111.29
8	K	107	MET	N-CA-C	12.69	128.56	111.30
8	K	69	LYS	N-CA-C	12.35	129.08	112.90
14	L	238	SER	N-CA-CB	11.66	131.40	112.63
9	M	857	LYS	N-CA-CB	-11.64	93.13	110.01
8	K	302	LEU	CB-CA-C	-11.57	90.90	110.22
10	N	48	ASN	CB-CA-C	-10.86	91.50	110.72
4	D	45	VAL	CB-CA-C	10.69	124.42	111.80
2	F	98	TYR	CB-CA-C	-10.60	92.47	110.81
9	M	765	LYS	N-CA-C	-10.53	94.50	110.30
9	M	917	ILE	N-CA-C	10.45	121.17	111.45
10	N	56	MET	N-CA-C	10.40	125.86	112.34
10	N	124	VAL	N-CA-C	9.99	120.75	111.45
10	N	30	ALA	CB-CA-C	-9.86	91.85	109.70
9	M	839	ALA	CB-CA-C	-9.80	95.42	110.90
9	M	856	ARG	N-CA-C	9.57	124.86	112.41
9	M	765	LYS	CB-CA-C	9.44	123.18	110.06
9	M	838	ARG	N-CA-C	9.01	122.52	112.97
10	N	424	ASP	N-CA-C	-8.78	94.58	108.63
9	M	748	ASP	N-CA-C	8.62	123.98	113.38
8	K	302	LEU	N-CA-C	8.44	122.38	108.96
8	K	164	ASP	CB-CA-C	8.42	126.08	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	859	PRO	N-CA-C	8.20	124.11	114.03
14	L	371	LEU	CB-CA-C	-8.02	96.53	109.75
10	N	8	ASP	C-N-CD	8.01	138.22	120.60
2	F	95	ARG	CB-CA-C	7.93	123.53	109.65
10	N	16	TYR	CB-CA-C	7.83	122.11	109.97
2	F	95	ARG	CA-C-N	7.80	134.25	122.93
2	F	95	ARG	C-N-CA	7.80	134.25	122.93
9	M	867	ILE	CB-CA-C	-7.67	101.69	111.20
8	K	144	ALA	CB-CA-C	-7.59	97.54	110.22
8	K	234	ARG	CB-CA-C	-7.47	95.38	109.72
4	D	46	HIS	N-CA-CB	-7.42	98.98	111.30
9	M	851	ASN	CB-CA-C	7.35	125.04	110.42
8	K	145	LEU	N-CA-C	7.31	122.37	111.04
14	L	15	ASP	N-CA-C	-7.30	98.08	108.96
9	M	747	PHE	N-CA-C	7.27	121.67	107.57
14	L	309	PHE	N-CA-CB	-7.11	100.20	110.80
14	L	125	VAL	N-CA-C	7.09	118.56	107.28
14	L	125	VAL	CB-CA-C	-7.09	101.77	110.99
8	K	303	ILE	N-CA-C	7.08	123.71	113.16
9	M	859	PRO	CB-CA-C	-7.07	100.76	111.44
14	L	308	PRO	CB-CA-C	-6.99	102.93	111.11
4	D	45	VAL	N-CA-C	-6.95	105.07	111.67
2	F	101	GLY	N-CA-C	6.95	120.07	112.29
10	N	18	GLU	N-CA-C	6.93	122.83	113.97
14	L	15	ASP	N-CA-CB	6.67	122.09	111.56
9	M	952	GLY	CA-C-N	6.66	133.27	122.81
9	M	952	GLY	C-N-CA	6.66	133.27	122.81
10	N	124	VAL	CB-CA-C	-6.66	103.19	111.92
9	M	747	PHE	CB-CA-C	-6.66	100.56	111.68
10	N	49	GLY	N-CA-C	6.64	124.79	115.43
10	N	6	LEU	CB-CA-C	6.64	122.13	110.85
9	M	849	SER	CA-C-N	6.59	133.40	123.05
9	M	849	SER	C-N-CA	6.59	133.40	123.05
8	K	144	ALA	N-CA-C	6.56	119.39	108.96
11	Q	8	LEU	N-CA-C	6.55	124.76	110.80
11	Q	75	GLY	CA-C-N	6.48	133.36	121.70
11	Q	75	GLY	C-N-CA	6.48	133.36	121.70
9	M	907	SER	CB-CA-C	-6.47	97.82	110.11
10	N	270	ASP	CB-CA-C	6.40	120.56	110.19
10	N	8	ASP	N-CA-C	6.33	123.80	109.81
8	K	164	ASP	N-CA-C	-6.33	100.13	109.81
10	N	14	LYS	N-CA-C	6.30	124.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	8	LEU	CA-C-N	-6.27	111.07	121.92
11	Q	8	LEU	C-N-CA	-6.27	111.07	121.92
8	K	68	HIS	CB-CA-C	-6.08	99.23	109.50
14	L	309	PHE	N-CA-C	6.03	122.65	113.61
8	K	69	LYS	CB-CA-C	-5.97	97.67	109.67
9	M	748	ASP	N-CA-CB	-5.96	101.64	110.53
8	K	235	GLY	N-CA-C	5.94	123.52	115.32
11	Q	8	LEU	CB-CA-C	5.92	122.19	110.42
2	B	93	GLN	CB-CA-C	-5.90	100.61	110.81
5	H	79	HIS	N-CA-CB	-5.86	101.92	110.53
10	N	30	ALA	N-CA-C	5.79	118.55	108.76
5	H	79	HIS	N-CA-C	5.78	120.60	113.50
14	L	372	LYS	N-CA-C	5.77	120.45	113.41
9	M	838	ARG	N-CA-CB	-5.74	102.50	110.65
9	M	845	SER	N-CA-CB	5.73	120.17	110.49
14	L	126	LYS	N-CA-CB	-5.71	101.24	110.14
9	M	880	ALA	N-CA-C	5.70	117.98	111.02
9	M	917	ILE	CB-CA-C	-5.69	104.47	111.92
9	M	879	ALA	CA-C-N	5.66	128.66	120.79
9	M	879	ALA	C-N-CA	5.66	128.66	120.79
10	N	424	ASP	CB-CA-C	5.65	119.92	110.88
10	N	7	GLN	N-CA-CB	-5.62	101.93	111.20
8	K	234	ARG	N-CA-C	5.58	120.09	113.28
9	M	879	ALA	CB-CA-C	-5.56	100.49	111.60
10	N	7	GLN	N-CA-C	5.53	119.60	112.41
8	K	290	VAL	N-CA-C	-5.53	108.46	113.71
14	L	134	ILE	CB-CA-C	-5.47	101.33	111.18
9	M	856	ARG	CA-C-N	-5.29	113.56	120.44
9	M	856	ARG	C-N-CA	-5.29	113.56	120.44
10	N	31	VAL	N-CA-CB	-5.28	104.69	110.65
9	M	859	PRO	CA-C-N	5.22	127.50	120.50
9	M	859	PRO	C-N-CA	5.22	127.50	120.50
11	Q	9	THR	N-CA-C	-5.14	107.18	113.50
14	L	371	LEU	N-CA-C	5.13	117.61	109.24
9	M	736	ARG	CB-CA-C	5.09	119.89	109.55
9	M	845	SER	N-CA-C	5.08	121.63	110.80
9	M	751	LEU	N-CA-C	5.07	118.13	111.28
9	M	976	PHE	N-CA-C	-5.06	99.53	108.23
8	K	106	LEU	N-CA-C	5.05	119.91	113.55
10	N	269	GLN	CB-CA-C	-5.00	99.73	111.09

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	K	197	TRP	Peptide
14	L	309	PHE	Peptide
9	M	850	LEU	Peptide
9	M	851	ASN	Peptide
9	M	857	LYS	Peptide
9	M	859	PRO	Peptide
10	N	16	TYR	Peptide

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	799	0	827	6	0
1	E	777	0	811	18	0
2	B	653	0	695	7	0
2	F	672	0	698	13	0
3	C	815	0	860	15	0
3	G	815	0	860	15	0
4	D	722	0	736	15	0
5	H	723	0	738	7	0
6	I	2975	0	1639	19	0
7	J	3011	0	1639	21	0
8	K	2365	0	2376	61	0
9	M	1775	0	1795	66	0
10	N	3273	0	3136	75	0
11	Q	597	0	619	19	0
12	R	63	0	69	6	0
13	X	604	0	605	12	0
14	L	3128	0	3011	84	0
15	O	342	0	355	8	0
15	P	329	0	341	6	0
16	M	1	0	0	0	0
17	R	27	0	20	3	0
All	All	24466	0	21830	403	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 10.

All (403) 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)
10:N:424:ASP:O	10:N:428:VAL:HG13	1.25	1.25
10:N:8:ASP:OD2	10:N:352:ILE:HG12	1.51	1.10
9:M:850:LEU:HD12	9:M:850:LEU:O	1.52	1.06
14:L:253:TYR:CD2	14:L:254:LYS:HD3	1.90	1.06
10:N:238:ARG:NH1	10:N:274:ARG:HG2	1.72	1.04
9:M:844:GLU:OE2	11:Q:11:LYS:HD3	1.58	1.03
2:F:90:LEU:O	2:F:95:ARG:O	1.75	1.02
9:M:867:ILE:O	17:R:101:SAM:H2	1.66	0.93
9:M:850:LEU:O	9:M:850:LEU:CD1	2.18	0.92
10:N:238:ARG:HH12	10:N:274:ARG:HG2	1.32	0.92
10:N:56:MET:HE3	10:N:56:MET:O	1.71	0.91
9:M:977:GLU:HG2	12:R:8:ARG:HG2	1.54	0.90
10:N:368:GLU:OE1	11:Q:11:LYS:NZ	2.07	0.87
10:N:424:ASP:O	10:N:428:VAL:CG1	2.20	0.85
3:C:32:ARG:HD2	3:C:36:LYS:HZ1	1.40	0.85
10:N:238:ARG:H	10:N:238:ARG:HD3	1.42	0.83
14:L:253:TYR:CE2	14:L:254:LYS:HD3	2.14	0.82
14:L:308:PRO:O	14:L:313:PHE:CD2	2.33	0.82
10:N:238:ARG:HH12	10:N:274:ARG:CG	1.93	0.81
10:N:8:ASP:N	10:N:9:PRO:HA	1.93	0.81
10:N:8:ASP:OD2	10:N:352:ILE:CG1	2.29	0.79
9:M:977:GLU:CG	12:R:8:ARG:HG2	2.13	0.78
9:M:747:PHE:O	9:M:747:PHE:CD2	2.37	0.77
9:M:736:ARG:O	9:M:740:ILE:HG23	1.87	0.75
9:M:977:GLU:CD	12:R:8:ARG:HG2	2.11	0.74
9:M:838:ARG:NH2	9:M:842:GLY:O	2.21	0.73
3:C:32:ARG:HG3	3:C:36:LYS:HE3	1.72	0.72
10:N:238:ARG:NH1	10:N:274:ARG:CG	2.49	0.71
8:K:120:ASN:ND2	8:K:164:ASP:O	2.25	0.70
10:N:238:ARG:H	10:N:238:ARG:CD	2.04	0.70
8:K:49:THR:CG2	8:K:68:HIS:O	2.40	0.69
6:I:10:DC:H42	7:J:138:DG:H1	1.39	0.69
1:E:116:ARG:NH1	1:E:120:MET:SD	2.66	0.69
14:L:236:LEU:C	14:L:237:ARG:O	2.16	0.68
8:K:120:ASN:HD22	8:K:164:ASP:C	2.02	0.67
3:C:32:ARG:CG	3:C:36:LYS:HE3	2.25	0.67
14:L:109:ARG:NH2	14:L:143:ALA:O	2.27	0.67
8:K:198:ILE:O	9:M:907:SER:O	2.12	0.67
10:N:231:ILE:HG23	10:N:243:TYR:HB2	1.77	0.66
15:O:90:TYR:HH	15:P:113:ASP:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ARG:HH21	7:J:20:DC:H5'	1.61	0.65
5:H:115:VAL:HG11	10:N:272:ILE:HD11	1.78	0.65
9:M:844:GLU:OE2	11:Q:11:LYS:CD	2.40	0.65
8:K:49:THR:HG21	8:K:68:HIS:O	1.96	0.65
14:L:125:VAL:HG23	14:L:125:VAL:O	1.96	0.64
14:L:401:ASP:OD1	15:O:88:ARG:NH1	2.30	0.64
1:A:116:ARG:NH1	1:A:120:MET:SD	2.71	0.64
9:M:860:VAL:HG12	9:M:874:ALA:HA	1.77	0.64
8:K:261:ILE:HG23	8:K:263:PRO:HD3	1.80	0.64
11:Q:44:ILE:HB	11:Q:68:HIS:HB2	1.80	0.64
8:K:22:GLN:NE2	8:K:322:ASN:OD1	2.31	0.64
14:L:235:LEU:C	14:L:237:ARG:O	2.40	0.64
14:L:110:SER:HB3	14:L:352:ALA:HB3	1.80	0.62
9:M:736:ARG:O	9:M:740:ILE:CG2	2.46	0.62
9:M:864:ARG:NH2	9:M:869:ASN:OD1	2.32	0.62
3:G:61:GLU:OE2	9:M:821:ARG:NH1	2.31	0.62
8:K:150:ALA:O	8:K:178:ARG:NH1	2.33	0.62
3:G:78:ILE:HB	5:H:51:ILE:HG13	1.82	0.62
9:M:867:ILE:O	9:M:867:ILE:HG22	1.99	0.62
3:C:32:ARG:HD2	3:C:36:LYS:NZ	2.14	0.61
8:K:308:SER:OG	8:K:309:TYR:N	2.33	0.61
9:M:844:GLU:CD	11:Q:11:LYS:HD3	2.26	0.61
10:N:168:TYR:H	10:N:187:SER:H	1.49	0.61
8:K:209:VAL:HG12	8:K:220:VAL:HG12	1.82	0.61
3:G:61:GLU:OE2	9:M:824:ARG:NH1	2.34	0.61
14:L:80:ASN:HB3	14:L:111:ASP:HB3	1.82	0.60
8:K:32:THR:HG21	8:K:73:ASN:HA	1.82	0.60
8:K:95:ILE:HB	8:K:104:ARG:HB2	1.83	0.60
4:D:48:ASP:OD1	4:D:48:ASP:N	2.35	0.60
10:N:238:ARG:HD3	10:N:238:ARG:N	2.14	0.60
8:K:67:THR:HG21	8:K:102:ARG:HD2	1.84	0.59
14:L:81:LEU:HA	14:L:84:ARG:HE	1.67	0.59
8:K:238:VAL:O	10:N:395:GLU:N	2.34	0.59
14:L:71:THR:HG21	15:P:84:GLY:HA3	1.83	0.59
8:K:172:SER:OG	8:K:174:ASP:OD2	2.19	0.59
14:L:253:TYR:CE2	14:L:254:LYS:CE	2.86	0.59
14:L:396:VAL:HB	15:O:103:MET:HE2	1.82	0.59
9:M:916:ARG:HD2	9:M:919:GLU:HA	1.84	0.59
8:K:93:VAL:HB	8:K:106:LEU:HB2	1.85	0.59
9:M:747:PHE:O	9:M:747:PHE:CG	2.54	0.58
10:N:195:GLN:OE1	10:N:258:HIS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:242:GLN:HE21	10:N:266:HIS:HB2	1.68	0.58
2:F:90:LEU:C	2:F:95:ARG:O	2.47	0.58
6:I:132:DG:N2	7:J:17:DT:O2	2.36	0.58
8:K:305:ILE:HG22	8:K:314:THR:HA	1.85	0.58
10:N:278:ASN:ND2	10:N:322:GLU:OE2	2.32	0.58
14:L:83:ASP:OD2	14:L:141:ARG:NH1	2.36	0.58
14:L:309:PHE:HA	14:L:313:PHE:HB2	1.85	0.58
10:N:53:ILE:HG23	10:N:63:ALA:O	2.03	0.58
2:B:96:THR:HB	3:G:100:VAL:HG23	1.86	0.58
8:K:271:ILE:HD11	8:K:279:MET:HB3	1.86	0.57
14:L:180:MET:O	14:L:181:GLN:NE2	2.37	0.57
9:M:996:LYS:HD3	9:M:998:PHE:H	1.69	0.57
14:L:253:TYR:CE2	14:L:254:LYS:CD	2.86	0.57
8:K:295:GLU:O	8:K:298:ARG:NH2	2.31	0.56
11:Q:36:ILE:HG12	11:Q:71:LEU:HD22	1.87	0.56
8:K:49:THR:HG23	8:K:68:HIS:O	2.05	0.56
9:M:764:LYS:O	9:M:765:LYS:C	2.49	0.56
9:M:867:ILE:HG23	9:M:990:CYS:HA	1.87	0.56
4:D:95:VAL:HG13	4:D:99:LEU:HD12	1.86	0.56
10:N:163:ILE:HB	10:N:166:HIS:HB2	1.86	0.56
14:L:118:LYS:HB3	14:L:380:ILE:HD13	1.86	0.56
6:I:106:DA:H2"	6:I:107:DC:H5"	1.88	0.56
9:M:841:ILE:HG23	9:M:843:PHE:H	1.71	0.56
4:D:83:ARG:NH2	7:J:41:DG:OP2	2.38	0.56
8:K:307:ALA:HA	8:K:312:VAL:HA	1.88	0.56
14:L:170:ARG:HE	14:L:172:HIS:HE1	1.52	0.56
14:L:347:ARG:NH1	14:L:394:ASP:OD1	2.38	0.56
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.54	0.56
13:X:303:ASP:HA	13:X:306:GLU:HB2	1.87	0.56
10:N:275:LEU:HD13	10:N:296:GLY:H	1.70	0.56
9:M:849:SER:O	9:M:850:LEU:HG	2.06	0.55
9:M:938:CYS:HB3	9:M:971:THR:HB	1.89	0.55
3:G:16:THR:HG1	3:G:19:SER:HG	1.53	0.55
8:K:78:SER:OG	8:K:80:ASP:OD1	2.24	0.55
10:N:130:ILE:HG12	10:N:141:VAL:HG12	1.88	0.55
10:N:54:TYR:HA	10:N:61:PRO:HA	1.88	0.55
14:L:34:ILE:HD11	14:L:98:SER:HB3	1.89	0.54
9:M:850:LEU:HB2	11:Q:9:THR:HG21	1.90	0.54
10:N:8:ASP:OD2	10:N:352:ILE:CD1	2.55	0.54
14:L:12:ASP:HA	14:L:22:LYS:HE3	1.88	0.54
2:B:75:HIS:O	4:D:89:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:316:LEU:HD21	14:L:345:ASN:HD22	1.73	0.54
8:K:194:ASP:OD1	8:K:194:ASP:N	2.41	0.54
9:M:878:ILE:HG23	9:M:964:ILE:HB	1.91	0.53
10:N:240:ILE:HB	10:N:268:TYR:HB2	1.90	0.53
14:L:11:TYR:OH	14:L:252:ARG:NH1	2.42	0.53
4:D:52:SER:OG	4:D:53:SER:N	2.40	0.53
4:D:58:ILE:HA	2:F:98:TYR:O	2.07	0.53
14:L:209:ARG:HB3	14:L:236:LEU:HD21	1.91	0.53
14:L:99:VAL:HB	14:L:103:CYS:HB2	1.90	0.53
3:C:32:ARG:CD	3:C:36:LYS:HZ1	2.18	0.53
9:M:940:GLU:OE2	9:M:994:SER:OG	2.26	0.53
10:N:76:VAL:HA	10:N:92:GLY:HA2	1.91	0.53
14:L:97:VAL:HG11	14:L:108:VAL:HG11	1.91	0.53
14:L:308:PRO:O	14:L:313:PHE:CG	2.62	0.53
10:N:5:LEU:HD13	10:N:409:VAL:HG22	1.90	0.53
13:X:209:TYR:HA	13:X:213:ILE:HB	1.90	0.53
14:L:244:VAL:HG11	14:L:246:ARG:HE	1.73	0.53
14:L:42:THR:OG1	14:L:84:ARG:NH2	2.42	0.52
1:E:61:LEU:O	2:F:36:ARG:NH2	2.36	0.52
8:K:252:LEU:HG	8:K:254:TYR:H	1.73	0.52
10:N:7:GLN:C	10:N:9:PRO:HA	2.34	0.52
14:L:365:ILE:HG23	14:L:370:GLU:HG3	1.92	0.52
14:L:79:ILE:HA	14:L:110:SER:HA	1.90	0.52
4:D:51:ILE:HG21	4:D:56:MET:HE2	1.92	0.52
1:E:83:ARG:HB2	2:F:80:THR:HG22	1.90	0.52
14:L:10:ASP:OD1	14:L:10:ASP:N	2.41	0.52
1:A:116:ARG:NH2	1:A:123:ASP:OD1	2.43	0.52
10:N:53:ILE:CG2	10:N:63:ALA:O	2.57	0.52
13:X:217:ASN:ND2	13:X:306:GLU:OE1	2.43	0.52
14:L:158:ILE:HD12	14:L:163:LEU:HD22	1.90	0.52
6:I:34:DG:O6	7:J:113:DA:N6	2.43	0.51
3:G:76:THR:O	5:H:49:THR:OG1	2.25	0.51
10:N:56:MET:O	10:N:56:MET:CE	2.51	0.51
5:H:87:THR:N	5:H:90:GLU:OE1	2.39	0.51
13:X:309:LYS:NZ	13:X:313:ASP:OD2	2.43	0.51
8:K:22:GLN:OE1	8:K:24:LEU:N	2.38	0.51
8:K:116:ILE:HG22	8:K:127:SER:HA	1.92	0.51
9:M:841:ILE:CG2	9:M:843:PHE:H	2.24	0.51
9:M:937:HIS:NE2	9:M:939:CYS:SG	2.74	0.51
10:N:204:ASP:N	10:N:204:ASP:OD1	2.41	0.51
13:X:290:TRP:CD1	13:X:294:SER:HG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:235:LEU:O	14:L:237:ARG:O	2.27	0.51
10:N:20:LEU:HA	10:N:348:TRP:HA	1.92	0.51
14:L:83:ASP:HB2	14:L:145:THR:HG21	1.93	0.51
14:L:233:LYS:O	14:L:237:ARG:N	2.43	0.51
13:X:214:GLY:O	13:X:218:GLU:N	2.43	0.51
14:L:124:GLU:N	14:L:363:SER:O	2.44	0.51
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.29	0.51
13:X:217:ASN:ND2	13:X:303:ASP:OD1	2.44	0.51
8:K:229:LEU:HB3	8:K:239:ARG:HB2	1.93	0.50
8:K:302:LEU:HA	8:K:316:SER:HA	1.92	0.50
9:M:850:LEU:O	9:M:850:LEU:CG	2.50	0.50
10:N:238:ARG:CD	10:N:238:ARG:N	2.73	0.50
14:L:187:GLY:H	14:L:293:PHE:HB2	1.75	0.50
8:K:176:LEU:HD11	8:K:194:ASP:HB3	1.93	0.50
8:K:256:CYS:SG	8:K:257:GLY:N	2.85	0.50
10:N:238:ARG:HH12	10:N:274:ARG:CD	2.24	0.50
10:N:357:SER:N	10:N:365:GLU:OE2	2.38	0.50
2:B:98:TYR:CZ	3:G:100:VAL:HG21	2.47	0.50
9:M:771:LYS:NZ	9:M:772:SER:O	2.36	0.50
10:N:95:TRP:HE1	13:X:291:ILE:HD11	1.75	0.50
10:N:127:ASN:HB2	10:N:144:LEU:HB3	1.94	0.50
14:L:107:SER:HB2	14:L:145:THR:HA	1.93	0.50
14:L:388:ASN:HA	14:L:391:ILE:HD12	1.94	0.50
6:I:41:DA:N6	7:J:106:DG:O6	2.45	0.49
8:K:283:ASN:HB2	8:K:290:VAL:HG13	1.94	0.49
14:L:208:LYS:HE2	14:L:272:TYR:HD2	1.77	0.49
9:M:851:ASN:ND2	9:M:852:GLN:O	2.46	0.49
14:L:25:PHE:O	14:L:27:GLN:NE2	2.46	0.49
3:C:32:ARG:CD	3:C:36:LYS:NZ	2.75	0.49
8:K:316:SER:OG	8:K:318:ASN:O	2.29	0.49
2:F:39:ARG:NH1	2:F:43:VAL:O	2.44	0.49
8:K:34:CYS:HB3	8:K:315:LEU:HD13	1.95	0.49
9:M:893:ARG:NH1	10:N:374:GLU:OE1	2.46	0.49
14:L:114:MET:N	14:L:350:TYR:O	2.40	0.49
7:J:77:DC:H2"	7:J:78:DG:C8	2.48	0.49
8:K:190:THR:OG1	10:N:358:ALA:O	2.25	0.49
9:M:844:GLU:CG	11:Q:11:LYS:HD3	2.42	0.49
8:K:280:CYS:HA	8:K:292:LYS:HA	1.95	0.48
1:E:61:LEU:N	1:E:97:GLU:OE2	2.45	0.48
8:K:73:ASN:HD21	9:M:758:PHE:HB2	1.77	0.48
3:C:32:ARG:NH1	7:J:30:DG:OP1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:80:ALA:HB2	15:P:93:GLU:HB2	1.94	0.48
14:L:254:LYS:HD2	14:L:254:LYS:N	2.27	0.48
9:M:867:ILE:O	17:R:101:SAM:C2	2.52	0.48
10:N:357:SER:HB2	10:N:365:GLU:HG3	1.94	0.48
10:N:409:VAL:HG23	10:N:410:ARG:HD2	1.94	0.48
3:C:16:THR:HG22	3:C:18:SER:H	1.79	0.48
8:K:227:VAL:HB	8:K:241:PHE:HB2	1.96	0.48
14:L:60:ASN:HD21	15:P:92:ASN:HD21	1.62	0.48
3:G:71:ARG:HH22	9:M:856:ARG:HH21	1.62	0.48
6:I:85:DG:O6	7:J:62:DA:N6	2.47	0.48
9:M:859:PRO:HB2	9:M:875:LEU:HB2	1.95	0.48
14:L:108:VAL:HG13	14:L:354:LEU:HB3	1.96	0.48
8:K:73:ASN:ND2	8:K:89:GLU:OE2	2.44	0.47
10:N:87:TYR:HB3	10:N:99:LEU:HD11	1.96	0.47
10:N:247:VAL:HB	10:N:260:VAL:HG23	1.96	0.47
4:D:33:SER:OG	4:D:34:TYR:N	2.47	0.47
14:L:253:TYR:CZ	14:L:254:LYS:HE2	2.50	0.47
10:N:238:ARG:HB3	10:N:275:LEU:O	2.14	0.47
10:N:217:ALA:HB1	10:N:236:SER:H	1.79	0.47
14:L:142:GLU:HG3	14:L:264:TYR:HB2	1.95	0.47
10:N:324:LEU:HD12	10:N:338:ASN:HD21	1.80	0.47
14:L:63:LEU:HD22	14:L:402:GLU:HG3	1.97	0.47
14:L:193:PRO:HG3	14:L:285:LEU:HD22	1.97	0.47
9:M:766:ILE:HD12	9:M:767:PRO:HD2	1.97	0.47
9:M:895:PRO:HG3	14:L:146:GLU:HB3	1.96	0.47
9:M:844:GLU:HG3	9:M:848:LEU:HD13	1.97	0.46
10:N:130:ILE:HD13	10:N:182:ILE:HG21	1.97	0.46
8:K:269:LEU:HD23	8:K:281:VAL:HB	1.98	0.46
10:N:424:ASP:N	10:N:424:ASP:OD1	2.48	0.46
14:L:31:SER:OG	14:L:32:HIS:N	2.49	0.46
14:L:159:ARG:NH1	14:L:160:ASP:OD1	2.48	0.46
9:M:841:ILE:HA	9:M:842:GLY:HA3	1.61	0.46
1:E:68:GLN:HG3	1:E:89:VAL:HG11	1.98	0.46
8:K:30:ILE:HG21	9:M:759:ILE:HG13	1.97	0.46
1:A:69:ARG:NH2	6:I:91:DA:OP1	2.49	0.46
6:I:29:DA:N6	7:J:118:DT:O4	2.49	0.46
6:I:122:DG:N2	7:J:27:DC:O2	2.48	0.46
14:L:236:LEU:CA	14:L:237:ARG:O	2.64	0.46
15:O:101:GLU:HA	15:O:104:LYS:HE2	1.98	0.46
3:C:112:GLN:OE1	1:E:108:ASN:ND2	2.49	0.46
9:M:977:GLU:OE1	12:R:8:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:93:DC:H2"	7:J:94:DG:C8	2.51	0.46
8:K:151:HIS:O	9:M:864:ARG:NH1	2.48	0.46
14:L:255:ASN:HB3	14:L:256:GLN:NE2	2.30	0.46
8:K:165:SER:O	8:K:165:SER:OG	2.32	0.46
9:M:942:SER:N	9:M:971:THR:OG1	2.47	0.46
11:Q:19:PRO:HA	11:Q:56:LEU:HB2	1.97	0.46
6:I:104:DT:O4	7:J:43:DA:N6	2.48	0.45
8:K:219:LEU:HD11	8:K:260:LEU:HD12	1.98	0.45
1:A:40:ARG:HH22	7:J:66:DG:H21	1.64	0.45
3:C:79:ILE:HG12	3:C:82:HIS:ND1	2.31	0.45
4:D:76:ARG:NH1	4:D:80:TYR:OH	2.49	0.45
14:L:290:PHE:HB3	14:L:303:PHE:H	1.81	0.45
9:M:917:ILE:HG13	9:M:921:THR:HG23	1.99	0.45
10:N:232:ALA:HA	10:N:242:GLN:HA	1.99	0.45
9:M:894:GLN:OE1	9:M:916:ARG:NH1	2.47	0.45
14:L:144:SER:HB2	14:L:147:THR:HG22	1.97	0.45
10:N:12:VAL:HG23	10:N:350:ILE:HG21	1.99	0.45
7:J:129:DC:H2"	7:J:130:DG:N7	2.32	0.45
8:K:49:THR:HG23	8:K:68:HIS:HB2	1.98	0.45
11:Q:23:ILE:HG23	11:Q:43:LEU:HD12	1.98	0.45
11:Q:56:LEU:HA	11:Q:61:ILE:HD12	1.98	0.45
14:L:175:LEU:HD11	14:L:302:ALA:HB2	1.98	0.45
1:E:120:MET:N	1:E:123:ASP:OD2	2.46	0.44
8:K:156:VAL:HG22	8:K:172:SER:HA	2.00	0.44
10:N:293:SER:OG	10:N:323:LEU:O	2.28	0.44
14:L:48:ASN:HD22	14:L:83:ASP:HB3	1.82	0.44
4:D:37:TYR:OH	6:I:122:DG:OP1	2.29	0.44
5:H:65:ASP:OD2	5:H:69:ARG:NH2	2.48	0.44
8:K:20:ASP:HB3	8:K:21:LYS:HZ2	1.82	0.44
9:M:846:ASP:HA	11:Q:11:LYS:HD2	1.98	0.44
9:M:977:GLU:HG2	12:R:8:ARG:C	2.42	0.44
15:O:106:ILE:HD13	15:O:118:LEU:HD21	1.98	0.44
1:A:57:SER:O	2:B:40:ARG:NH2	2.51	0.44
4:D:73:GLU:HG3	4:D:98:LEU:HD21	1.99	0.44
1:A:116:ARG:HH12	1:A:120:MET:HB2	1.83	0.44
3:C:34:LEU:HB3	3:C:43:VAL:HG21	2.00	0.44
1:E:109:LEU:HD23	1:E:109:LEU:HA	1.83	0.44
2:F:22:LEU:HD22	2:F:25:ASN:HD21	1.83	0.44
8:K:311:LYS:HA	8:K:311:LYS:HD3	1.82	0.44
9:M:844:GLU:O	9:M:846:ASP:N	2.51	0.44
10:N:68:HIS:ND1	10:N:106:THR:OG1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.50	0.44
7:J:87:DT:H2''	7:J:88:DT:C6	2.53	0.44
7:J:95:DG:H1'	7:J:96:DT:H5'	1.99	0.44
11:Q:24:GLU:HA	11:Q:27:LYS:HB2	1.99	0.44
1:E:57:SER:OG	1:E:58:THR:N	2.50	0.44
3:G:77:ARG:HE	3:G:77:ARG:HB3	1.45	0.44
6:I:125:DC:H2''	6:I:126:DG:C8	2.52	0.44
9:M:937:HIS:HB2	9:M:974:TYR:CZ	2.53	0.44
6:I:76:DG:O6	7:J:71:DA:N6	2.51	0.43
9:M:977:GLU:OE1	12:R:8:ARG:HG2	2.17	0.43
10:N:48:ASN:OD1	10:N:48:ASN:C	2.61	0.43
14:L:254:LYS:O	14:L:255:ASN:HB3	2.18	0.43
10:N:301:ASP:OD1	10:N:301:ASP:N	2.51	0.43
13:X:211:ASN:O	13:X:215:GLU:N	2.42	0.43
8:K:177:ILE:HB	8:K:191:LEU:HB2	2.00	0.43
9:M:892:ILE:HG13	9:M:922:VAL:HG23	2.01	0.43
10:N:428:VAL:HA	10:N:431:GLN:HB2	2.00	0.43
13:X:299:SER:HA	13:X:302:LYS:HB3	1.99	0.43
3:C:90:ASP:OD2	3:C:91:GLU:N	2.51	0.43
9:M:868:HIS:NE2	17:R:101:SAM:O2'	2.51	0.43
2:B:32:PRO:HA	2:B:35:ARG:HG2	2.01	0.43
1:E:97:GLU:HG2	2:F:37:LEU:HD21	2.00	0.43
7:J:138:DG:H2''	7:J:139:DA:C8	2.54	0.43
1:E:85:GLN:HB3	2:F:82:THR:HA	1.99	0.43
14:L:109:ARG:NE	14:L:140:ARG:O	2.52	0.43
14:L:369:MET:HE2	14:L:369:MET:HB3	1.86	0.43
2:B:98:TYR:OH	5:H:65:ASP:OD2	2.30	0.43
2:F:37:LEU:HD23	2:F:37:LEU:HA	1.87	0.43
6:I:99:DG:H4'	6:I:100:DG:H5'	2.01	0.43
8:K:207:SER:OG	8:K:221:LYS:O	2.34	0.43
10:N:9:PRO:HB2	10:N:10:PHE:H	1.58	0.43
15:O:110:LYS:HD3	15:P:90:TYR:CZ	2.54	0.43
1:E:64:LYS:HA	1:E:93:GLN:HE22	1.84	0.43
8:K:17:LEU:O	8:K:291:GLN:NE2	2.35	0.43
10:N:356:TRP:N	10:N:365:GLU:OE2	2.52	0.43
2:F:73:THR:HG21	2:F:81:VAL:HA	2.01	0.42
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.54	0.42
9:M:731:GLN:HA	9:M:734:ILE:HG12	2.00	0.42
14:L:39:TYR:HA	14:L:91:SER:HB2	2.01	0.42
14:L:83:ASP:OD2	14:L:109:ARG:NH1	2.48	0.42
14:L:209:ARG:O	14:L:214:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:396:VAL:HA	14:L:399:LEU:HD12	2.00	0.42
8:K:132:GLU:HG2	8:K:153:ASP:N	2.34	0.42
10:N:400:ASP:OD1	10:N:400:ASP:N	2.53	0.42
1:E:77:ASP:OD1	1:E:77:ASP:N	2.52	0.42
13:X:315:LEU:HA	13:X:318:VAL:HB	2.01	0.42
8:K:32:THR:HA	8:K:303:ILE:HD13	2.01	0.42
8:K:219:LEU:HD13	8:K:258:LEU:HD21	1.99	0.42
9:M:931:ILE:HG12	10:N:356:TRP:CD1	2.55	0.42
14:L:120:TYR:OH	14:L:373:PHE:O	2.34	0.42
14:L:127:ASN:N	14:L:361:THR:OG1	2.50	0.42
14:L:207:LEU:HD13	14:L:210:ILE:HD11	2.01	0.42
14:L:290:PHE:HD2	14:L:302:ALA:HB3	1.84	0.42
6:I:3:DC:H2''	6:I:4:DG:C8	2.54	0.42
10:N:190:TRP:CE2	10:N:213:LYS:HB2	2.55	0.42
11:Q:30:ILE:O	11:Q:34:GLU:N	2.49	0.42
4:D:73:GLU:OE2	4:D:76:ARG:NH2	2.52	0.42
4:D:105:LYS:HA	4:D:105:LYS:HD2	1.87	0.42
3:G:62:ILE:HD13	3:G:93:LEU:HD13	2.01	0.42
10:N:166:HIS:HB3	10:N:190:TRP:HB2	2.02	0.42
4:D:77:LEU:O	4:D:81:ASN:ND2	2.53	0.42
2:F:35:ARG:NH2	2:F:51:TYR:OH	2.53	0.42
8:K:261:ILE:N	8:K:269:LEU:O	2.50	0.42
9:M:977:GLU:HA	9:M:978:ARG:HA	1.54	0.42
10:N:292:ALA:HB3	10:N:305:TRP:HZ3	1.85	0.42
14:L:244:VAL:H	15:O:88:ARG:HH21	1.68	0.42
8:K:296:LYS:HA	8:K:296:LYS:HD3	1.85	0.42
10:N:207:ARG:HH22	10:N:258:HIS:HA	1.85	0.42
9:M:889:GLY:HA2	9:M:929:GLY:HA2	2.02	0.41
11:Q:43:LEU:HD23	11:Q:43:LEU:HA	1.91	0.41
6:I:46:DT:H1'	6:I:47:DC:H5'	2.02	0.41
10:N:279:THR:OG1	10:N:324:LEU:O	2.37	0.41
11:Q:37:PRO:HA	11:Q:38:PRO:HD3	1.89	0.41
10:N:46:CYS:SG	10:N:47:SER:N	2.94	0.41
10:N:144:LEU:HA	10:N:151:PHE:CD1	2.56	0.41
2:B:98:TYR:CE2	3:G:100:VAL:HG21	2.56	0.41
9:M:850:LEU:HD12	9:M:850:LEU:C	2.35	0.41
10:N:270:ASP:HB3	10:N:275:LEU:H	1.85	0.41
14:L:152:ASP:OD2	14:L:152:ASP:N	2.51	0.41
14:L:391:ILE:HD13	15:P:88:ARG:HB2	2.02	0.41
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.89	0.41
3:C:102:ILE:HG23	4:D:58:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:155:VAL:HG13	8:K:172:SER:HB3	2.03	0.41
14:L:8:TYR:OH	14:L:67:LYS:O	2.29	0.41
14:L:310:LEU:HA	14:L:348:LEU:HD21	2.02	0.41
3:G:90:ASP:OD1	3:G:91:GLU:N	2.53	0.41
6:I:68:DT:H2"	6:I:69:DA:C8	2.55	0.41
9:M:843:PHE:O	9:M:844:GLU:C	2.64	0.41
11:Q:5:VAL:HB	11:Q:13:ILE:HD12	2.01	0.41
11:Q:6:LYS:HG3	11:Q:12:THR:HG22	2.03	0.41
14:L:28:LEU:HD23	14:L:28:LEU:HA	1.92	0.41
3:G:84:GLN:HE21	3:G:88:ARG:HG3	1.86	0.41
6:I:39:DA:N6	7:J:108:DC:N3	2.68	0.41
8:K:96:THR:HG22	8:K:102:ARG:HA	2.03	0.41
10:N:156:LEU:HG	10:N:194:PHE:HD2	1.86	0.41
10:N:222:ILE:HG12	10:N:233:ILE:HG23	2.02	0.41
10:N:359:LEU:HD13	10:N:359:LEU:HA	1.87	0.41
10:N:430:ILE:O	10:N:433:HIS:N	2.50	0.41
14:L:243:ASN:HA	15:O:92:ASN:HD21	1.86	0.41
6:I:78:DC:H2"	6:I:79:DC:C5	2.56	0.41
8:K:227:VAL:O	8:K:241:PHE:N	2.54	0.41
9:M:838:ARG:HD2	9:M:847:LEU:HB3	2.02	0.41
9:M:841:ILE:HG21	11:Q:33:LYS:O	2.21	0.41
3:G:42:ARG:HB2	5:H:85:THR:HG22	2.01	0.40
13:X:209:TYR:HE2	13:X:310:ARG:HD2	1.86	0.40
14:L:99:VAL:HG23	14:L:359:GLY:H	1.86	0.40
1:E:65:LEU:HD23	1:E:65:LEU:HA	1.87	0.40
8:K:68:HIS:CE1	8:K:94:GLU:HB2	2.55	0.40
8:K:299:ASN:OD1	8:K:300:SER:N	2.54	0.40
14:L:246:ARG:HB2	14:L:248:GLN:HG3	2.03	0.40
7:J:106:DG:H2"	7:J:107:DT:H5"	2.04	0.40
8:K:43:ILE:HD12	8:K:54:TYR:HD1	1.85	0.40
14:L:230:GLU:O	14:L:234:PHE:N	2.44	0.40
14:L:236:LEU:N	14:L:237:ARG:O	2.54	0.40
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.80	0.40
10:N:402:CYS:SG	10:N:403:THR:N	2.94	0.40
14:L:23:PRO:HB3	14:L:56:PRO:HB2	2.03	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	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
2	B	80/102 (78%)	77 (96%)	3 (4%)	0	100	100
2	F	84/102 (82%)	82 (98%)	2 (2%)	0	100	100
3	C	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	G	105/107 (98%)	101 (96%)	3 (3%)	1 (1%)	12	44
4	D	91/125 (73%)	86 (94%)	5 (6%)	0	100	100
5	H	91/125 (73%)	89 (98%)	2 (2%)	0	100	100
8	K	301/327 (92%)	282 (94%)	19 (6%)	0	100	100
9	M	216/275 (78%)	196 (91%)	16 (7%)	4 (2%)	6	33
10	N	400/439 (91%)	369 (92%)	30 (8%)	1 (0%)	36	67
11	Q	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
12	R	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
13	X	69/342 (20%)	62 (90%)	7 (10%)	0	100	100
14	L	376/405 (93%)	359 (96%)	16 (4%)	1 (0%)	36	67
15	O	40/134 (30%)	40 (100%)	0	0	100	100
15	P	39/134 (29%)	37 (95%)	2 (5%)	0	100	100
All	All	2266/3078 (74%)	2141 (94%)	118 (5%)	7 (0%)	37	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	M	845	SER
9	M	858	LYS
10	N	9	PRO
9	M	851	ASN
3	G	17	ARG

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Mol	Chain	Res	Type
14	L	311	PRO
9	M	993	PRO

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	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	82 (100%)	0	100	100
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	67/78 (86%)	65 (97%)	2 (3%)	36	60
3	C	82/84 (98%)	80 (98%)	2 (2%)	43	64
3	G	82/84 (98%)	80 (98%)	2 (2%)	43	64
4	D	78/105 (74%)	78 (100%)	0	100	100
5	H	79/105 (75%)	79 (100%)	0	100	100
8	K	275/298 (92%)	271 (98%)	4 (2%)	57	71
9	M	191/238 (80%)	185 (97%)	6 (3%)	35	59
10	N	360/387 (93%)	346 (96%)	14 (4%)	28	54
11	Q	67/69 (97%)	64 (96%)	3 (4%)	24	50
12	R	6/6 (100%)	6 (100%)	0	100	100
13	X	70/319 (22%)	69 (99%)	1 (1%)	59	71
14	L	352/375 (94%)	343 (97%)	9 (3%)	40	62
15	O	38/120 (32%)	37 (97%)	1 (3%)	40	62
15	P	36/120 (30%)	35 (97%)	1 (3%)	38	61
All	All	2016/2686 (75%)	1971 (98%)	45 (2%)	45	65

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	51	LEU

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Mol	Chain	Res	Type
3	C	72	ASP
2	F	21	VAL
2	F	30	THR
3	G	27	VAL
3	G	108	LEU
8	K	72	ILE
8	K	118	TYR
8	K	302	LEU
8	K	312	VAL
9	M	732	ASN
9	M	857	LYS
9	M	878	ILE
9	M	917	ILE
9	M	921	THR
9	M	950	VAL
10	N	5	LEU
10	N	28	VAL
10	N	62	ILE
10	N	65	LEU
10	N	79	VAL
10	N	140	TYR
10	N	171	VAL
10	N	206	ILE
10	N	231	ILE
10	N	238	ARG
10	N	313	VAL
10	N	352	ILE
10	N	367	GLU
10	N	397	ILE
11	Q	5	VAL
11	Q	13	ILE
11	Q	66	THR
13	X	292	THR
14	L	41	ILE
14	L	81	LEU
14	L	92	LEU
14	L	108	VAL
14	L	149	VAL
14	L	238	SER
14	L	267	THR
14	L	291	GLU
14	L	370	GLU

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Mol	Chain	Res	Type
15	O	86	THR
15	P	94	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	ASN
4	D	81	ASN
4	D	106	HIS
1	E	68	GLN
2	F	25	ASN
3	G	24	GLN
3	G	94	ASN
5	H	46	HIS
5	H	81	ASN
8	K	48	ASN
8	K	73	ASN
8	K	120	ASN
8	K	255	ASN
9	M	731	GLN
9	M	743	ASN
9	M	837	GLN
9	M	852	GLN
10	N	149	ASN
10	N	175	HIS
10	N	242	GLN
10	N	244	GLN
10	N	258	HIS
10	N	273	ASN
10	N	412	ASN
10	N	432	GLN
10	N	433	HIS
11	Q	2	GLN
11	Q	41	GLN
11	Q	68	HIS
13	X	200	ASN
13	X	217	ASN
13	X	321	ASN
13	X	322	GLN
14	L	27	GLN
14	L	55	GLN
14	L	172	HIS

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Mol	Chain	Res	Type
14	L	181	GLN
14	L	214	ASN
14	L	228	ASN
14	L	255	ASN
14	L	344	ASN
14	L	346	ASN
14	L	388	ASN
15	O	92	ASN
15	P	92	ASN
15	P	94	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	SAM	R	101	-	27,29,29	1.15	3 (11%)	34,42,42	1.90	9 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SAM	R	101	-	-	9/17/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	101	SAM	C2-N1	2.61	1.38	1.33
17	R	101	SAM	C5-N7	-2.57	1.34	1.39
17	R	101	SAM	OXT-C	-2.15	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	101	SAM	N3-C2-N1	-5.03	120.97	128.58
17	R	101	SAM	C5-C4-N3	-4.04	121.15	126.72
17	R	101	SAM	N9-C8-N7	-3.83	108.50	113.94
17	R	101	SAM	C2-N3-C4	3.22	119.70	111.83
17	R	101	SAM	C5-N7-C8	3.05	108.24	103.45
17	R	101	SAM	OXT-C-O	-2.83	117.66	124.08
17	R	101	SAM	N3-C4-N9	2.39	131.23	127.17
17	R	101	SAM	C3'-C2'-C1'	2.30	105.81	101.46
17	R	101	SAM	C4-C5-N7	-2.27	107.99	110.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

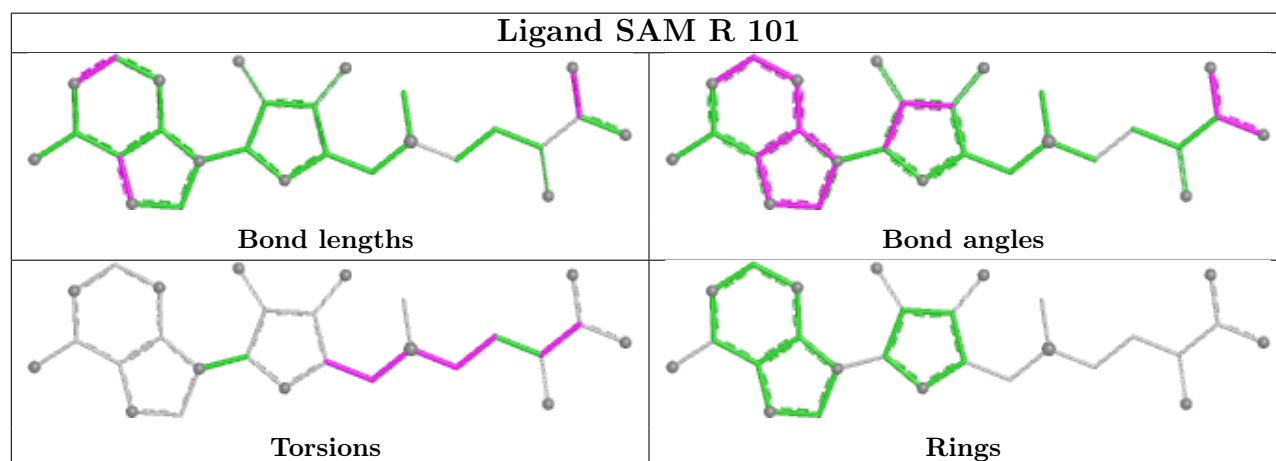
Mol	Chain	Res	Type	Atoms
17	R	101	SAM	C4'-C5'-SD-CG
17	R	101	SAM	C4'-C5'-SD-CE
17	R	101	SAM	O4'-C4'-C5'-SD
17	R	101	SAM	C3'-C4'-C5'-SD
17	R	101	SAM	CB-CG-SD-CE
17	R	101	SAM	OXT-C-CA-CB
17	R	101	SAM	CA-CB-CG-SD
17	R	101	SAM	CB-CG-SD-C5'
17	R	101	SAM	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	R	101	SAM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

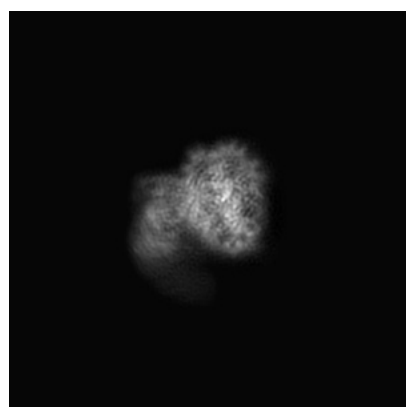
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20767. These allow visual inspection of the internal detail of the map and identification of artifacts.

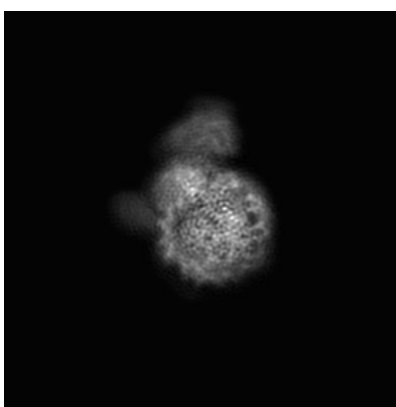
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

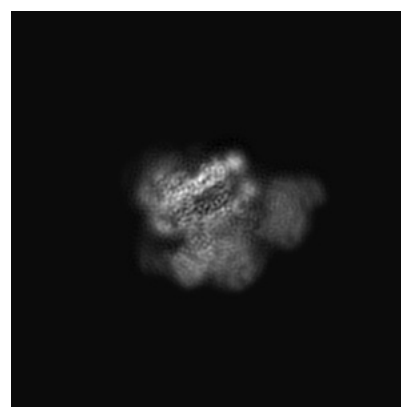
6.1.1 Primary map



X



Y

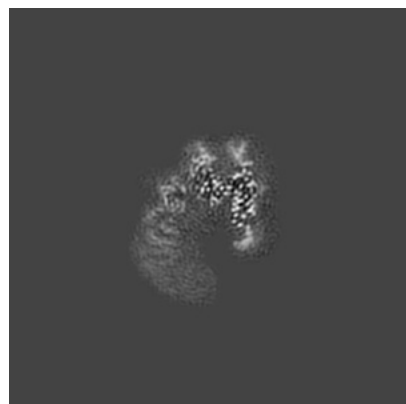


Z

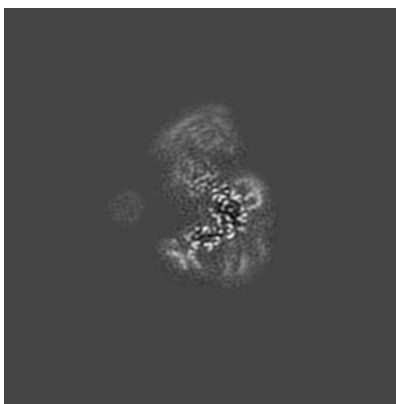
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

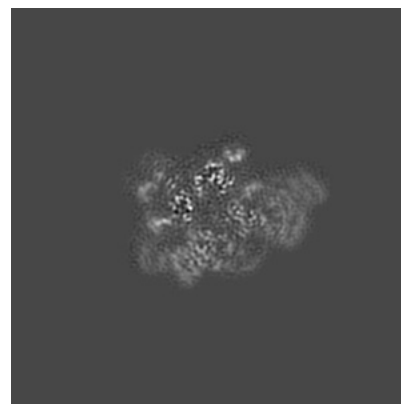
6.2.1 Primary map



X Index: 162



Y Index: 162

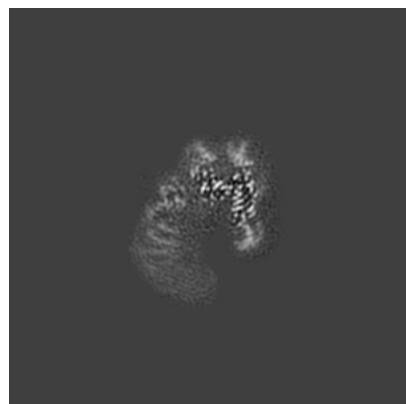


Z Index: 162

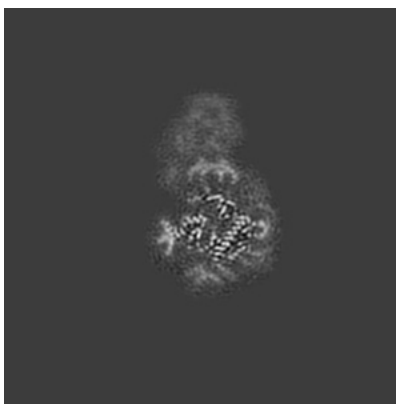
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

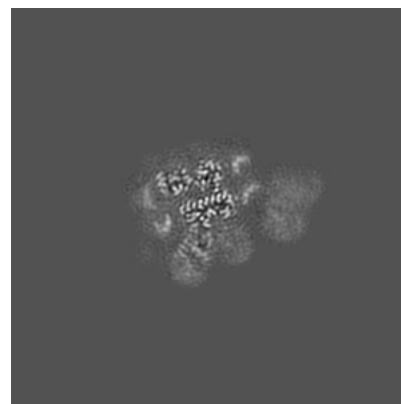
6.3.1 Primary map



X Index: 163



Y Index: 177

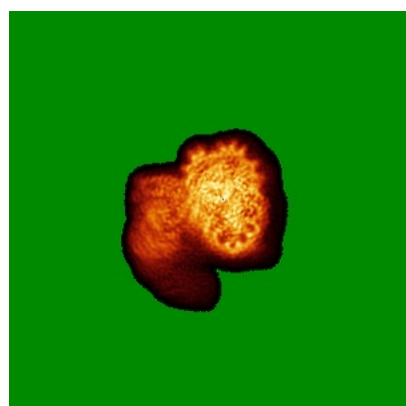


Z Index: 181

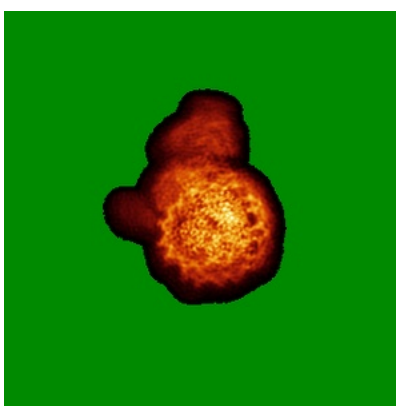
The images above show the largest variance slices of the map in three orthogonal directions.

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

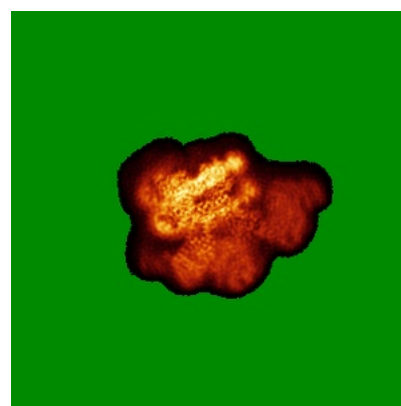
6.4.1 Primary map



X



Y

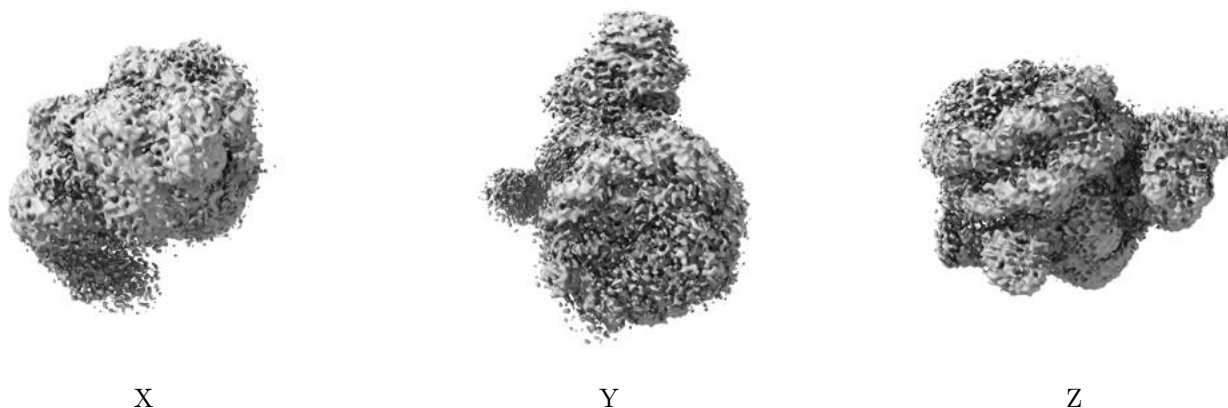


Z

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

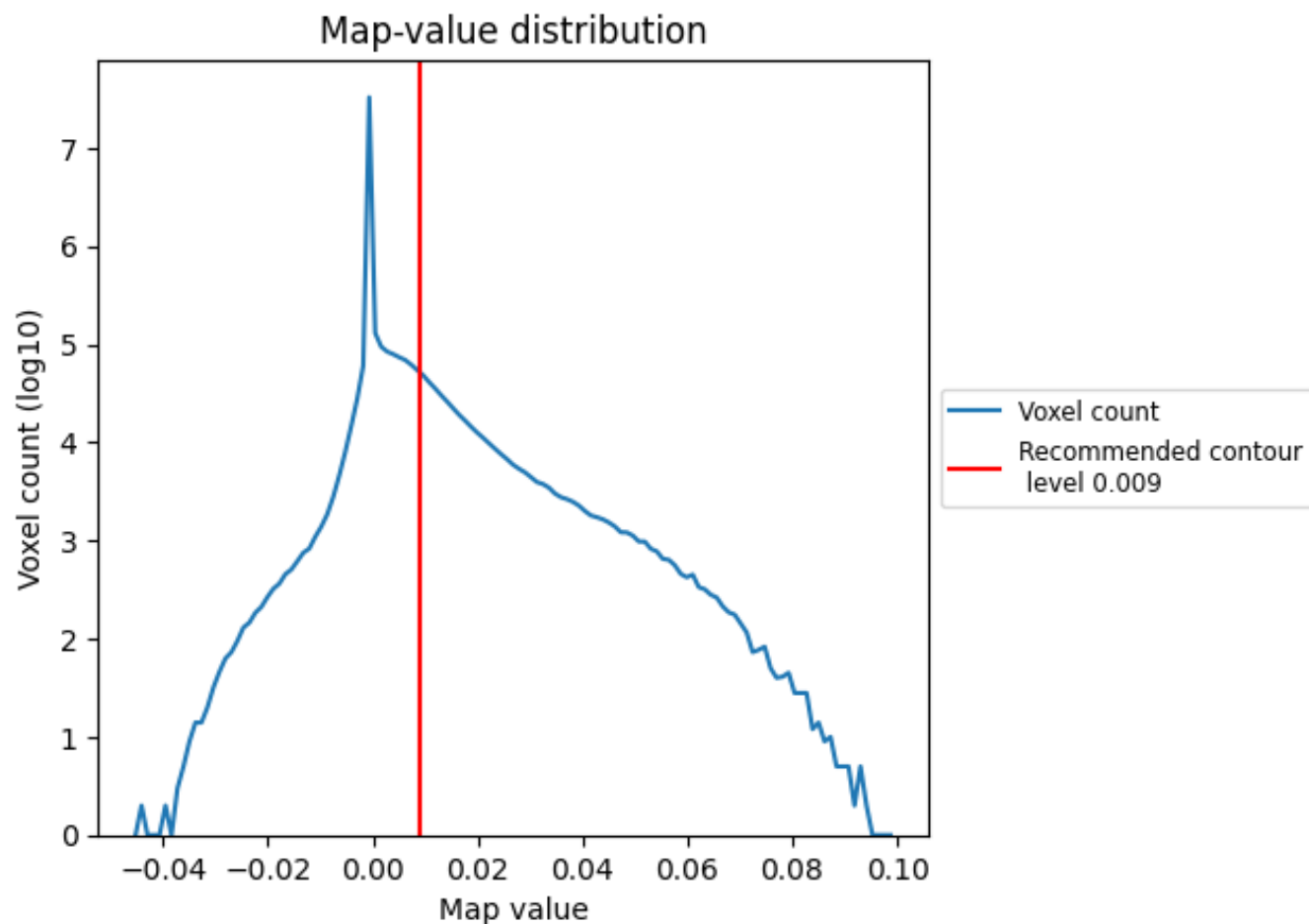
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

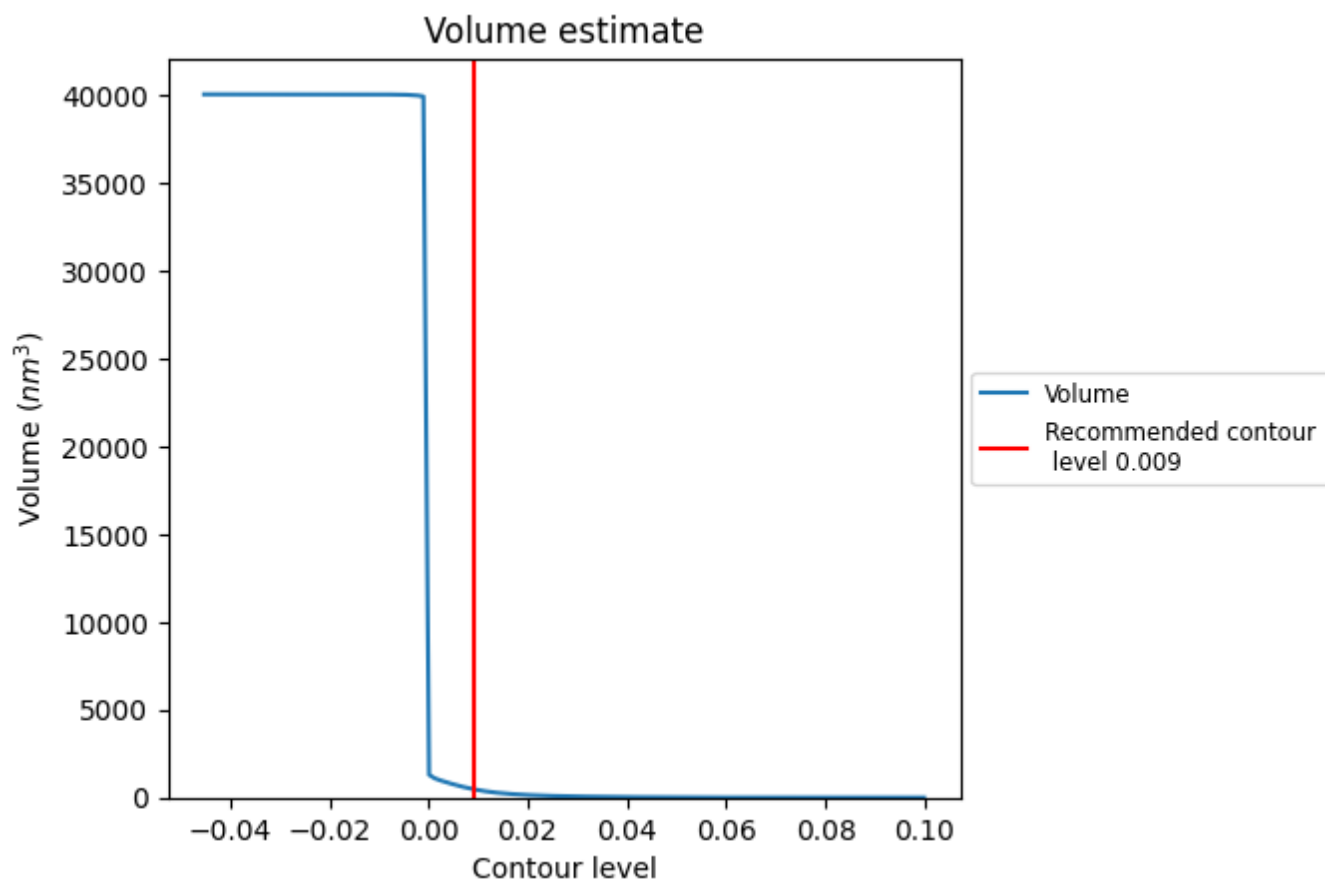
This section contains the results of statistical analysis of the map.

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.

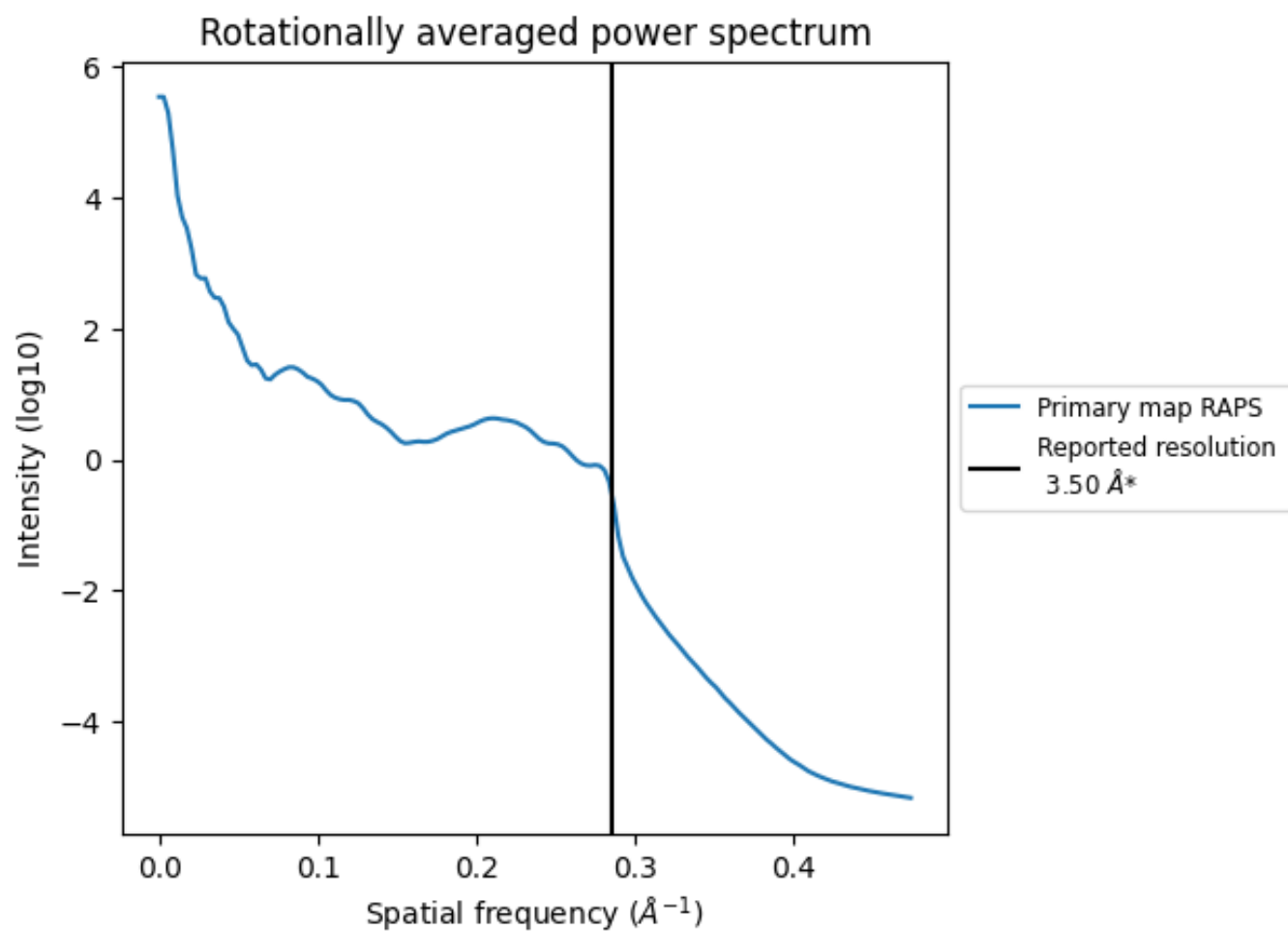
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm^3 ; this corresponds to an approximate mass of 434 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 0.286 Å⁻¹

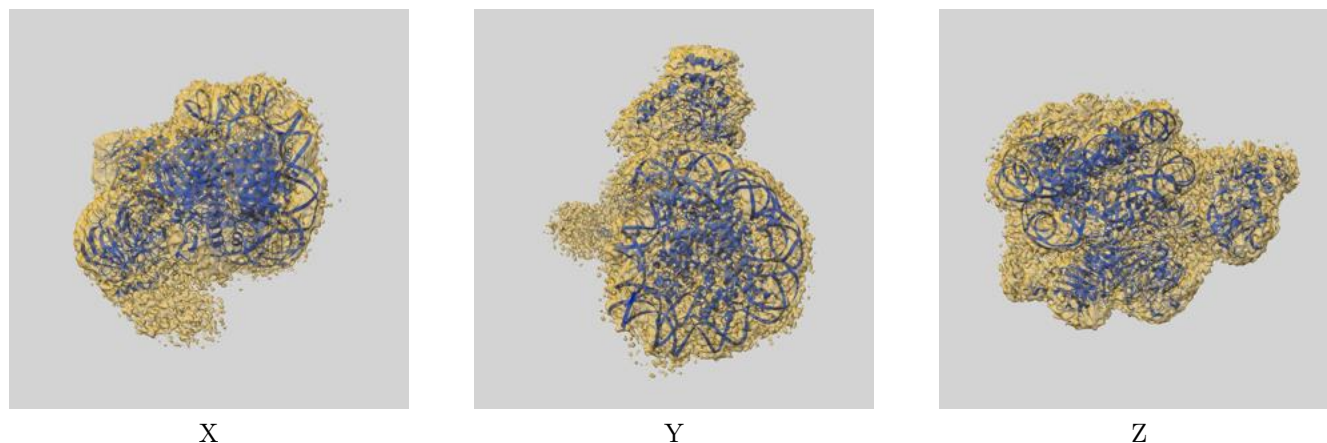
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

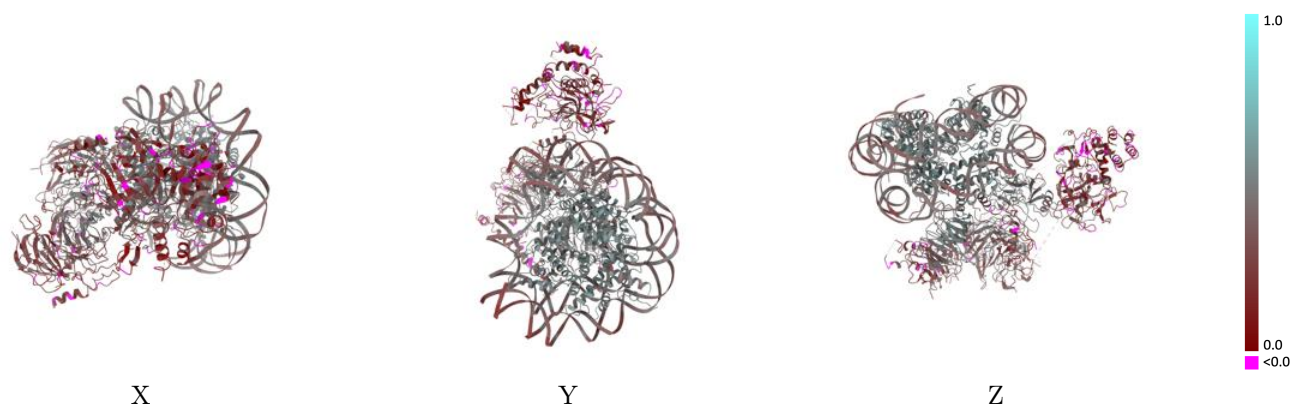
This section contains information regarding the fit between EMDB map EMD-20767 and PDB model 6UH5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.009 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](#)



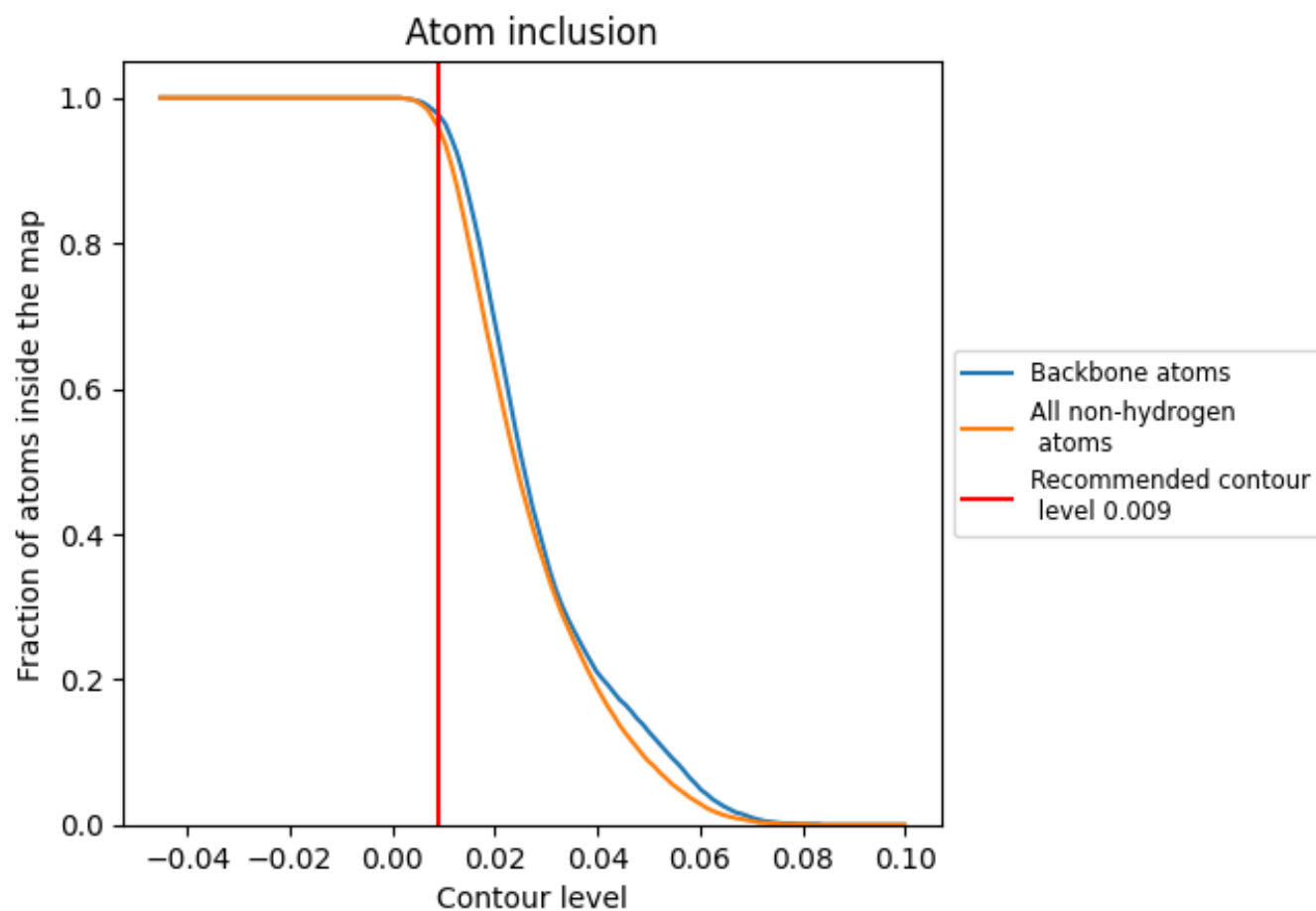
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.3720
A	 0.9870	 0.5190
B	 0.9890	 0.5110
C	 0.9820	 0.5080
D	 0.9900	 0.5020
E	 0.9890	 0.5180
F	 0.9630	 0.5080
G	 0.9700	 0.5120
H	 0.9920	 0.5180
I	 0.9960	 0.3900
J	 0.9900	 0.3860
K	 0.9760	 0.3300
L	 0.9120	 0.2050
M	 0.9180	 0.3660
N	 0.9700	 0.3900
O	 0.9010	 0.1380
P	 0.9040	 0.1520
Q	 0.8200	 0.2330
R	 0.9770	 0.4290
X	 0.8160	 0.1410

