



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 8W9E / pdb_00008w9e
EMDB ID : EMD-37366
Title : Cryo-EM structure of the Rpd3S-nucleosome complex from budding yeast in State 2
Authors : Wang, C.; Zhan, X.
Deposited on : 2023-09-05
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

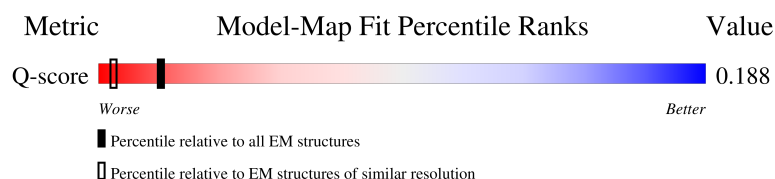
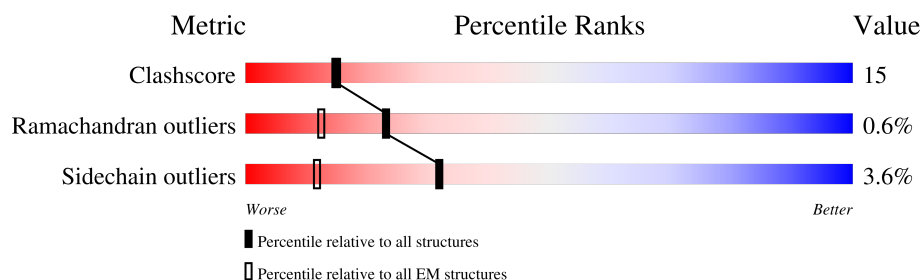
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



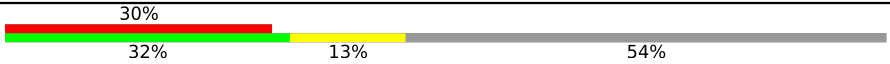
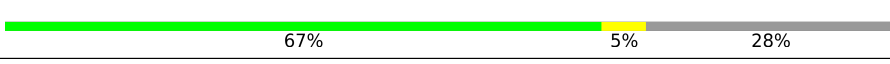
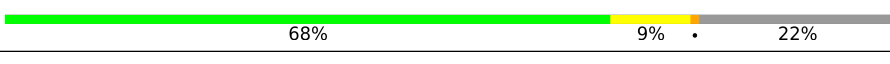
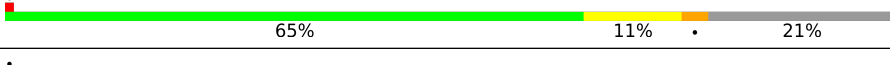
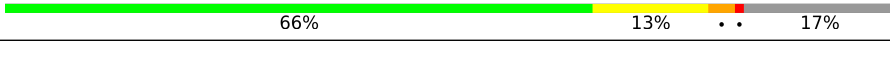
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1536	29% 26% 14% 61%
2	E	684	44% 28% 18% 48%
2	F	684	22% 14% 9% 77%
3	B	433	34% 60% 27% 11%

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Mol	Chain	Length	Quality of chain
4	C	401	
4	D	401	
4	G	401	
5	a	136	
5	e	136	
6	b	103	
6	f	103	
7	c	130	
7	g	130	
8	d	126	
8	h	126	
9	i	147	
10	j	147	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 27886 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			5066	3253	860	938	15		

- Molecule 2 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	353	Total	C	N	O	S	0	0
			2884	1837	493	536	18		
2	F	156	Total	C	N	O	S	0	0
			1282	822	211	239	10		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 4 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	183	Total	C	N	O	S	0	0
			1483	950	239	285	9		
4	D	185	Total	C	N	O	S	0	0
			1497	959	241	288	9		
4	G	69	Total	C	N	O	S	0	0
			570	371	98	97	4		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	98	Total	C	N	O	S	0	0
			807	508	156	139	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	98	Total	C	N	O	S	0	0
			810	511	157	138	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
6	f	81	Total	C	N	O	S	0	0
			648	410	126	111	1		

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	107	Total	C	N	O		0	0
			817	516	158	143			
7	g	108	Total	C	N	O		0	0
			828	522	162	144			

- Molecule 8 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	94	Total	C	N	O	S	0	0
			735	461	134	138	2		
8	h	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

- Molecule 9 is a DNA chain called 5-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	147	Total	C	N	O	P	0	0
			3011	1440	546	879	146		

- Molecule 10 is a DNA chain called 3-DNA.

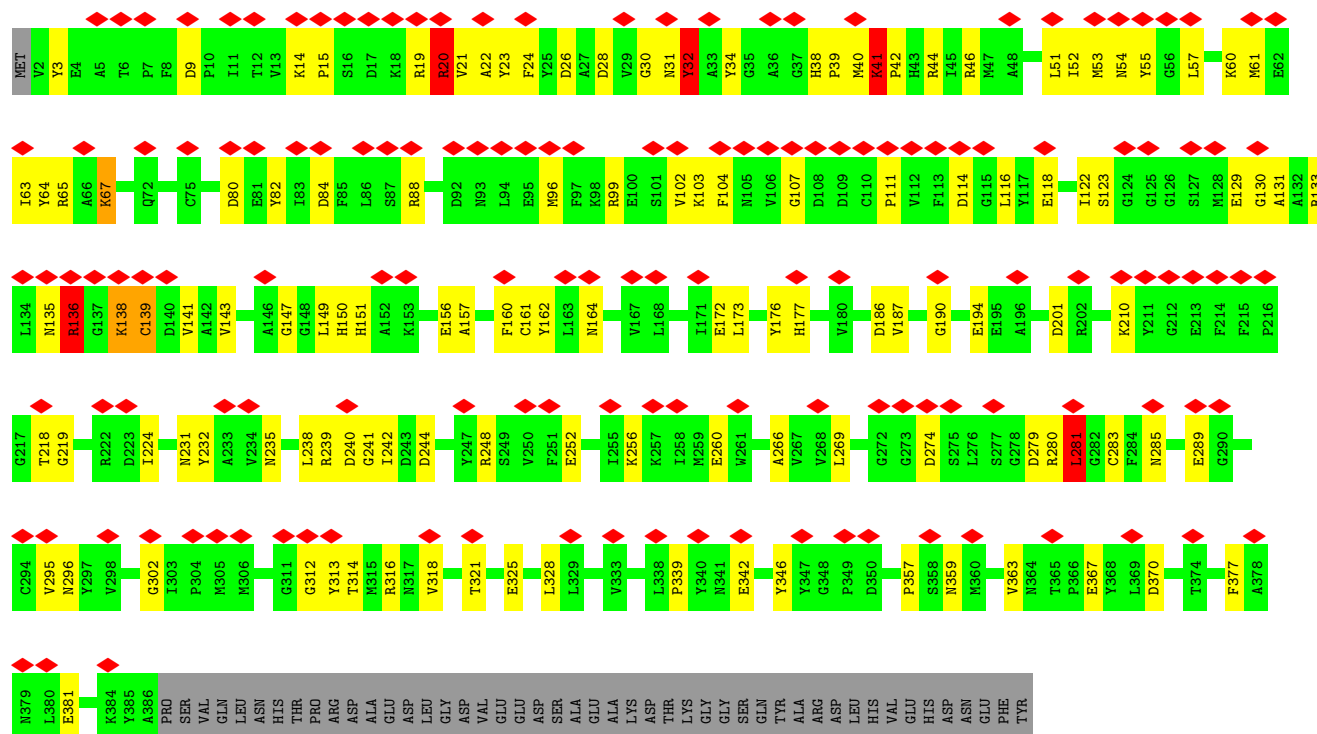
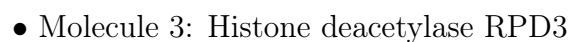
Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	147	Total	C	N	O	P	0	0
			3010	1440	543	881	146		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

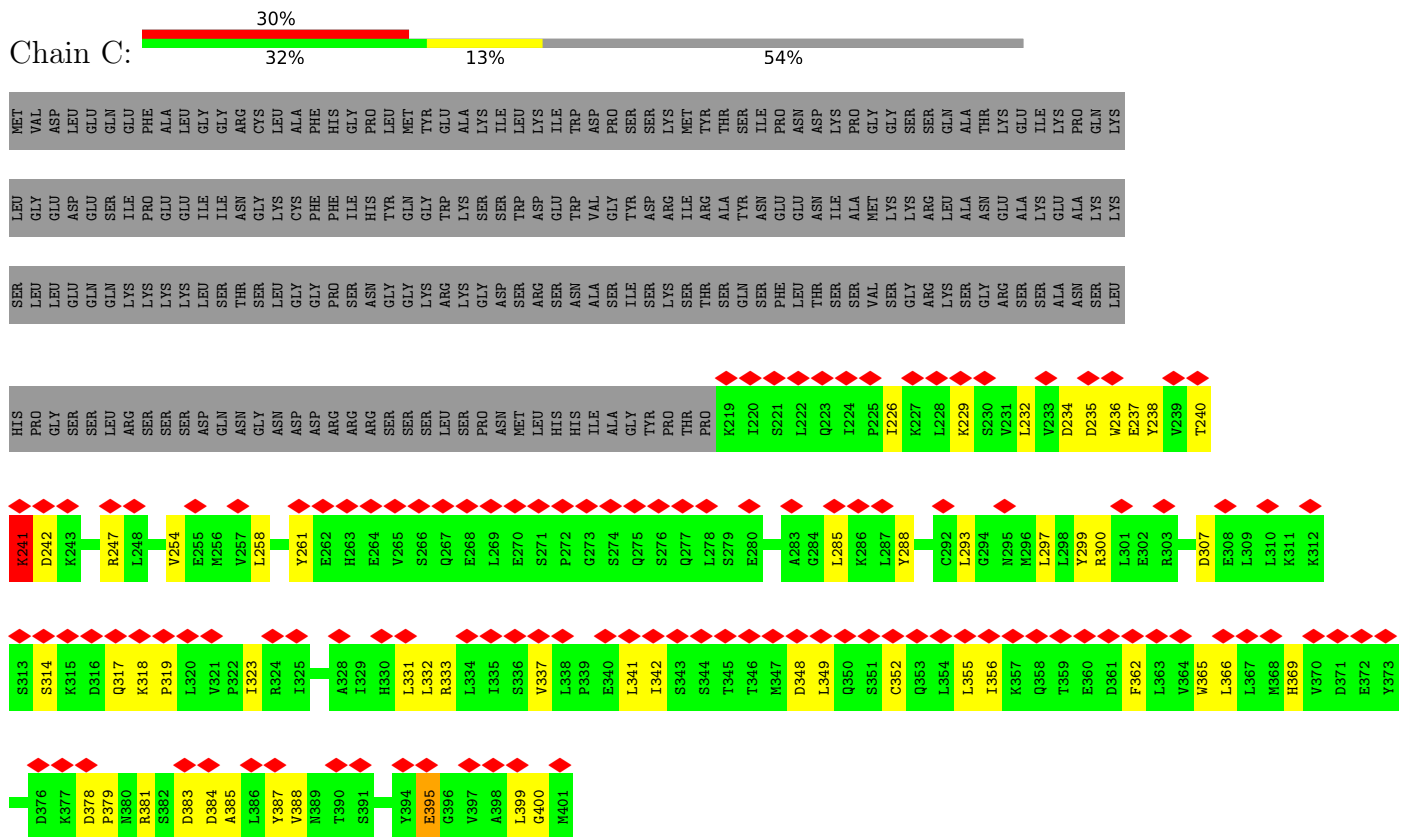
Mol	Chain	Residues	Atoms		AltConf
11	E	4	Total 4	Zn 4	0
11	B	1	Total 1	Zn 1	0
11	F	2	Total 2	Zn 2	0

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

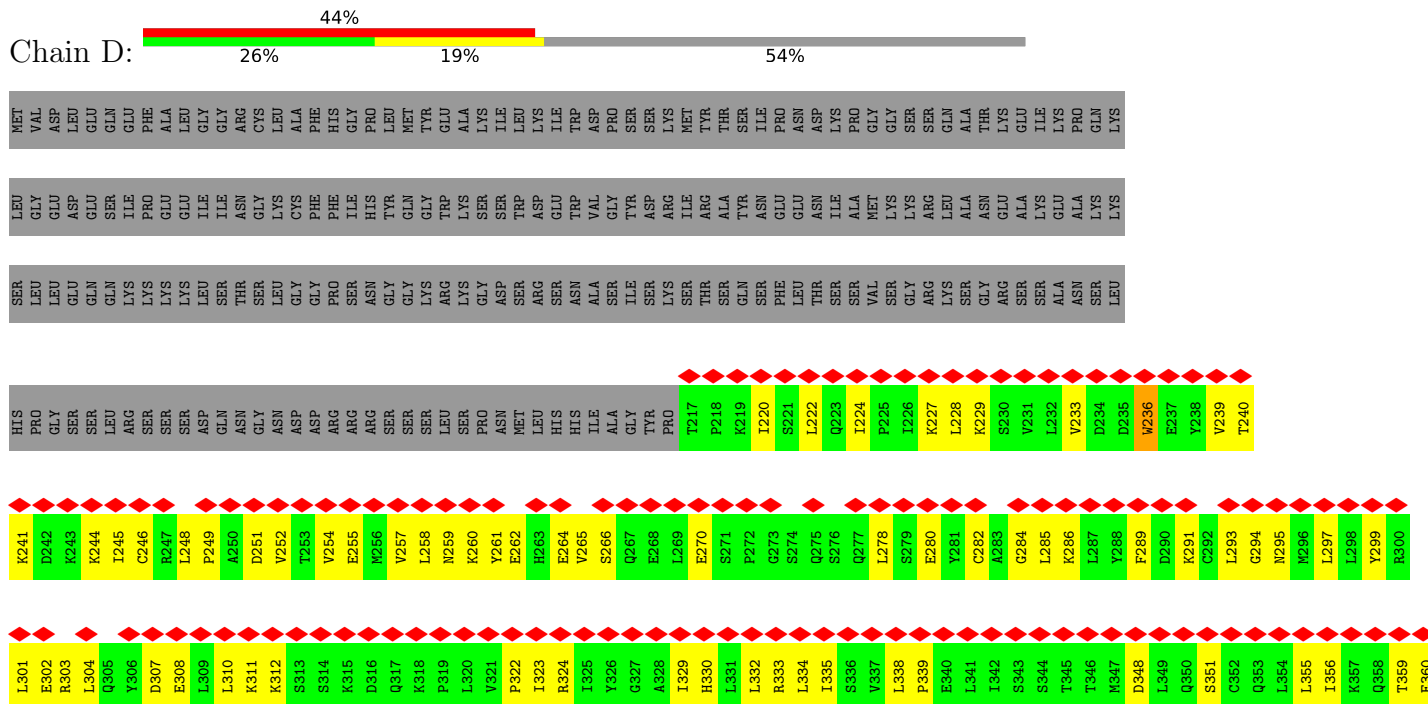
Mol	Chain	Residues	Atoms		AltConf
12	B	1	Total 1	K 1	0

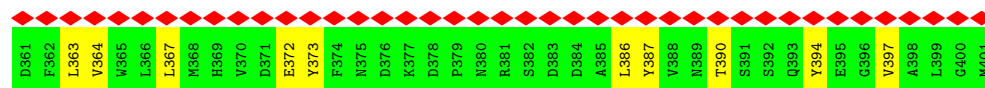


Chain C:

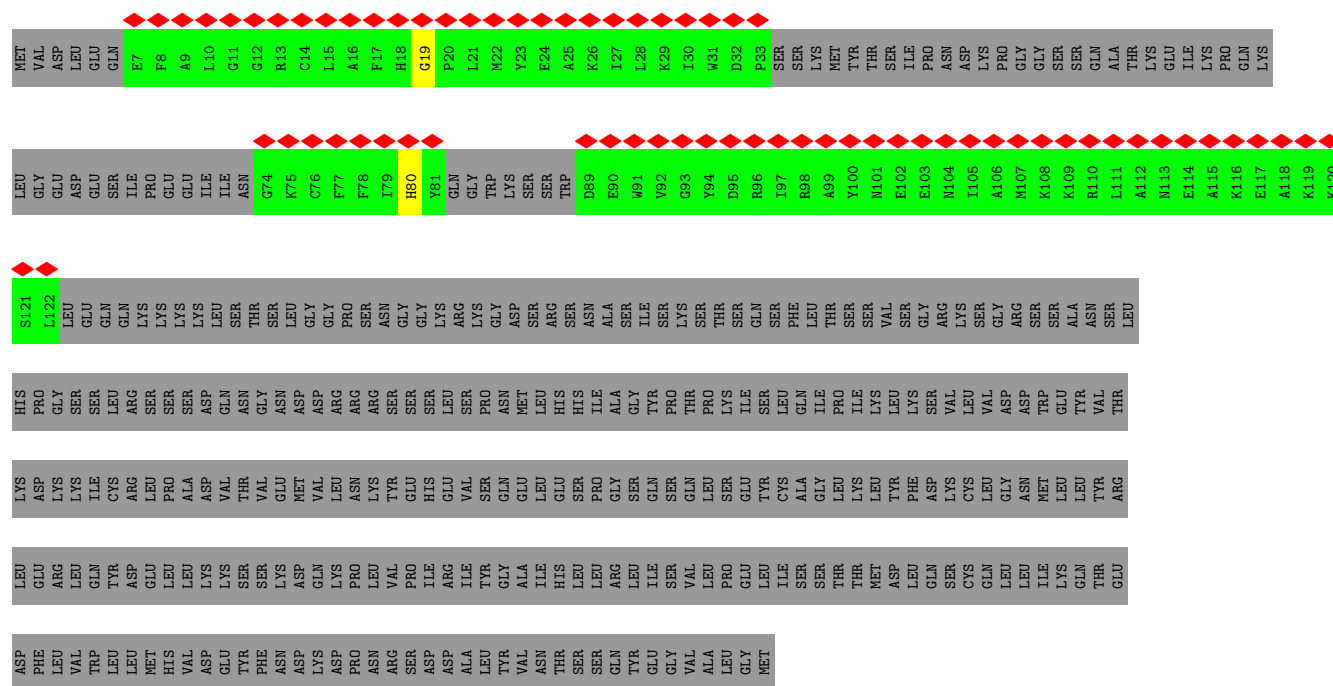


Chain D:

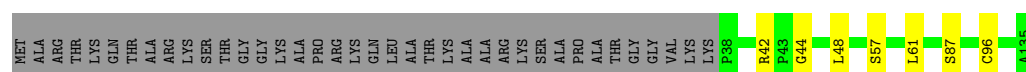




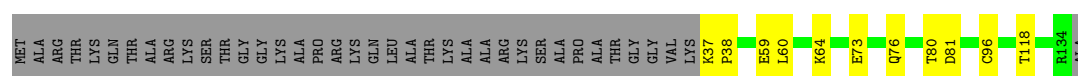
• Molecule 4: Chromatin modification-related protein EAF3



• Molecule 5: Histone H3.1



• Molecule 5: Histone H3.1



• Molecule 6: Histone H4



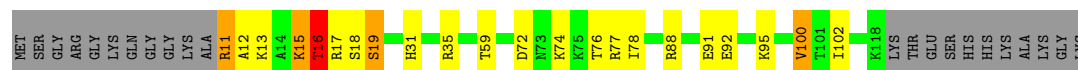
• Molecule 6: Histone H4



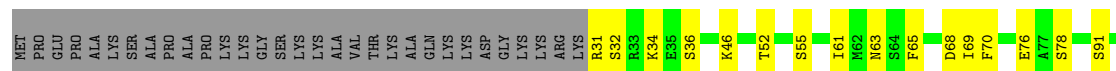
- Molecule 7: Histone H2A type 1-B/E



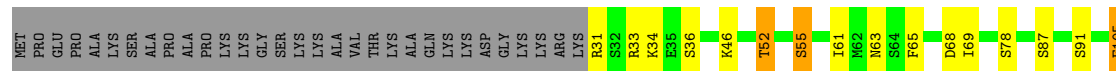
- Molecule 7: Histone H2A type 1-B/E



- Molecule 8: Histone H2B type 1-K



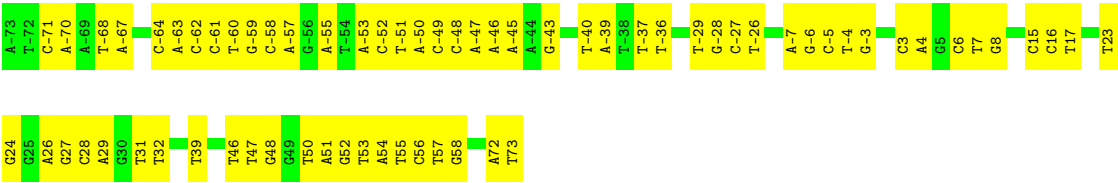
- Molecule 8: Histone H2B type 1-K



- Molecule 9: 5-DNA



● Molecule 10: 3-DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	327408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/5180	0.47	0/6984
2	E	0.80	14/2952 (0.5%)	1.14	40/3978 (1.0%)
2	F	1.54	3/1313 (0.2%)	0.56	2/1763 (0.1%)
3	B	0.50	2/3137 (0.1%)	0.77	12/4246 (0.3%)
4	C	0.29	0/1509	0.53	0/2039
4	D	1.23	6/1524 (0.4%)	0.47	1/2061 (0.0%)
4	G	0.70	0/583	1.13	0/777
5	a	0.33	0/819	0.42	0/1097
5	e	0.38	0/822	0.47	0/1102
6	b	0.47	0/645	0.67	1/862 (0.1%)
6	f	0.38	0/655	0.53	1/878 (0.1%)
7	c	0.56	2/827 (0.2%)	0.62	1/1116 (0.1%)
7	g	0.48	1/838 (0.1%)	0.71	3/1130 (0.3%)
8	d	0.36	0/746	0.49	0/1003
8	h	0.37	0/746	0.47	0/1003
9	i	0.31	0/3378	0.45	0/5212
10	j	0.32	0/3376	0.44	0/5209
All	All	0.61	28/29050 (0.1%)	0.64	61/40460 (0.2%)

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	2
2	E	0	4
3	B	0	1
4	C	0	1
7	g	0	1
All	All	0	9

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	372	TYR	CB-CG	54.46	2.71	1.51
4	D	236	TRP	CE3-CZ3	29.28	2.26	1.38
4	D	236	TRP	CE2-CZ2	20.73	1.83	1.39
4	D	236	TRP	CZ3-CH2	18.36	1.86	1.40
2	E	380	PRO	N-CA	17.60	1.69	1.47
4	D	236	TRP	CD2-CE2	15.07	1.67	1.41
4	D	236	TRP	CZ2-CH2	14.62	1.65	1.37
4	D	236	TRP	CD2-CE3	13.70	1.62	1.40
7	c	15	LYS	C-O	-9.07	1.12	1.23
2	E	177	GLU	C-O	-8.24	1.14	1.24
7	c	16	THR	C-O	-7.83	1.13	1.23
2	E	184	THR	C-O	-7.75	1.14	1.23
2	E	114	PRO	C-O	-7.75	1.14	1.23
3	B	67	LYS	C-N	7.40	1.51	1.33
7	g	15	LYS	C-O	-7.35	1.15	1.23
2	E	179	SER	CA-CB	-7.26	1.43	1.53
2	E	182	ARG	C-O	-7.00	1.15	1.24
2	F	372	TYR	CG-CD1	6.98	1.54	1.39
2	E	111	THR	C-O	-6.31	1.16	1.24
2	E	178	GLU	C-O	-6.18	1.16	1.23
2	F	372	TYR	CG-CD2	6.16	1.52	1.39
2	E	109	SER	C-O	-5.88	1.16	1.24
2	E	123	ILE	C-O	-5.66	1.17	1.24
3	B	41	LYS	C-O	-5.61	1.17	1.24
2	E	110	VAL	C-O	-5.53	1.17	1.24
2	E	108	VAL	C-O	-5.31	1.17	1.24
2	E	128	LEU	C-O	-5.07	1.19	1.24
2	E	109	SER	CA-CB	-5.05	1.45	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	379	ILE	CA-C-N	14.92	138.49	119.84
2	E	379	ILE	C-N-CA	14.92	138.49	119.84
2	F	372	TYR	CA-CB-CG	13.03	137.36	113.90
3	B	67	LYS	CA-C-N	12.69	135.70	119.84
3	B	67	LYS	C-N-CA	12.69	135.70	119.84
7	c	16	THR	CB-CA-C	-8.54	92.67	111.71
2	E	181	ILE	N-CA-C	-8.53	104.13	113.43
2	F	372	TYR	CD1-CG-CD2	-8.44	105.44	118.10
2	E	182	ARG	CB-CG-CD	-8.25	92.32	111.30
2	E	184	THR	OG1-CB-CG2	-8.05	93.20	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	LYS	CA-C-N	7.95	130.93	120.28
2	E	500	LYS	C-N-CA	7.95	130.93	120.28
7	g	15	LYS	CA-C-O	-7.84	111.98	120.92
2	E	380	PRO	CA-N-CD	-7.73	101.18	112.00
2	E	172	THR	CA-CB-OG1	7.56	120.95	109.60
2	E	169	THR	CB-CA-C	7.34	122.95	111.13
6	b	25	ASN	N-CA-C	-7.25	104.01	112.92
2	E	180	ASN	CA-C-N	7.19	131.22	122.16
2	E	180	ASN	C-N-CA	7.19	131.22	122.16
2	E	123	ILE	N-CA-CB	6.68	119.13	110.57
7	g	11	ARG	CA-C-N	6.62	134.18	121.54
7	g	11	ARG	C-N-CA	6.62	134.18	121.54
2	E	170	PHE	CA-C-N	6.58	134.10	121.54
2	E	170	PHE	C-N-CA	6.58	134.10	121.54
2	E	169	THR	CA-C-N	6.55	129.06	120.28
2	E	169	THR	C-N-CA	6.55	129.06	120.28
2	E	499	ASN	CA-C-N	6.54	134.03	121.54
2	E	499	ASN	C-N-CA	6.54	134.03	121.54
2	E	125	ARG	CB-CA-C	-6.44	97.61	110.42
2	E	181	ILE	N-CA-CB	-6.44	105.13	112.21
3	B	32	TYR	CB-CA-C	6.32	122.99	110.42
3	B	136	ARG	CA-C-N	-6.25	114.00	122.63
3	B	136	ARG	C-N-CA	-6.25	114.00	122.63
3	B	32	TYR	CA-CB-CG	-6.17	102.79	113.90
2	E	129	TRP	N-CA-C	-6.11	105.73	113.43
4	D	236	TRP	CE3-CZ3-CH2	-6.08	113.19	121.10
2	E	114	PRO	N-CA-CB	-6.04	98.25	103.32
2	E	499	ASN	O-C-N	5.84	129.51	122.85
2	E	379	ILE	O-C-N	-5.71	114.59	121.10
2	E	184	THR	CA-C-O	-5.67	114.84	122.44
2	E	185	ILE	CA-C-N	5.65	126.22	120.00
2	E	185	ILE	C-N-CA	5.65	126.22	120.00
2	E	405	THR	N-CA-C	-5.62	106.58	113.50
2	E	499	ASN	CB-CA-C	5.58	120.87	109.76
2	E	126	GLU	CA-C-N	5.50	130.76	122.67
2	E	126	GLU	C-N-CA	5.50	130.76	122.67
3	B	139	CYS	CA-C-O	-5.50	114.79	120.89
3	B	139	CYS	CA-C-N	5.39	130.02	121.44
3	B	139	CYS	C-N-CA	5.39	130.02	121.44
6	f	23	ARG	CA-C-O	-5.29	114.25	120.60
2	E	182	ARG	CB-CA-C	-5.19	100.08	110.42
2	E	110	VAL	CA-C-N	5.19	128.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	110	VAL	C-N-CA	5.19	128.90	120.60
2	E	380	PRO	N-CD-CG	5.17	110.96	103.20
2	E	169	THR	OG1-CB-CG2	5.14	119.57	109.30
3	B	281	LEU	CA-C-N	5.14	126.33	120.53
3	B	281	LEU	C-N-CA	5.14	126.33	120.53
2	E	108	VAL	CA-C-O	-5.10	116.48	121.58
2	E	174	ASN	CB-CA-C	-5.08	100.32	110.42
3	B	32	TYR	CA-C-O	-5.06	113.28	120.51
2	E	178	GLU	CB-CA-C	-5.05	100.58	109.62

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1232	TYR	Peptide
1	A	930	HIS	Peptide
3	B	20	ARG	Mainchain
4	C	241	LYS	Peptide
2	E	428	TRP	Peptide
2	E	469	HIS	Peptide
2	E	470	SER	Peptide
2	E	471	PRO	Peptide
7	g	16	THR	Mainchain

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	5066	0	5024	190	0
2	E	2884	0	2831	178	0
2	F	1282	0	1243	78	0
3	B	3057	0	2934	134	0
4	C	1483	0	1510	45	0
4	D	1497	0	1524	97	0
4	G	570	0	563	8	0
5	a	807	0	844	5	0
5	e	810	0	851	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	b	638	0	676	9	0
6	f	648	0	693	19	0
7	c	817	0	872	7	0
7	g	828	0	885	12	0
8	d	735	0	756	17	0
8	h	735	0	756	19	0
9	i	3011	0	1662	63	0
10	j	3010	0	1663	50	0
11	B	1	0	0	0	0
11	E	4	0	0	0	0
11	F	2	0	0	0	0
12	B	1	0	0	0	0
All	All	27886	0	25287	793	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 15.

All (793) 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)
4:D:236:TRP:CE2	4:D:236:TRP:CZ2	1.83	1.65
4:D:236:TRP:CH2	4:D:236:TRP:CZ3	1.86	1.62
1:A:918:GLU:CD	2:E:128:LEU:HD12	1.44	1.35
1:A:918:GLU:OE1	2:E:128:LEU:CD1	1.73	1.35
4:D:236:TRP:CZ3	2:F:372:TYR:CG	2.16	1.33
2:E:380:PRO:N	2:E:380:PRO:CA	1.69	1.32
1:A:918:GLU:OE1	2:E:128:LEU:HD12	1.23	1.31
1:A:813:GLU:OE2	2:E:111:THR:HA	1.18	1.31
4:D:236:TRP:CE3	2:F:372:TYR:CG	2.18	1.31
4:D:236:TRP:CE3	2:F:372:TYR:CB	2.16	1.28
2:E:379:ILE:HG13	2:E:380:PRO:CD	1.61	1.27
4:D:236:TRP:CE3	2:F:372:TYR:HB3	1.72	1.24
4:D:236:TRP:CZ3	4:D:236:TRP:CE3	2.26	1.23
4:D:236:TRP:CZ3	2:F:372:TYR:CB	2.23	1.22
4:D:236:TRP:CE2	2:F:372:TYR:HB2	1.75	1.21
4:D:236:TRP:CH2	2:F:372:TYR:CG	2.29	1.21
4:D:236:TRP:CD2	2:F:372:TYR:CG	2.28	1.20
4:D:236:TRP:CE2	2:F:372:TYR:CB	2.24	1.20
3:B:135:ASN:OD1	3:B:176:TYR:CD2	1.95	1.20
4:D:236:TRP:CD2	2:F:372:TYR:CB	2.25	1.20
2:E:379:ILE:CG1	2:E:380:PRO:HD2	1.71	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:TRP:CE2	2:F:372:TYR:CG	2.31	1.19
3:B:40:MET:HG3	3:B:44:ARG:HH21	1.11	1.16
8:d:65:PHE:CE1	8:d:69:ILE:HD11	1.82	1.14
8:h:65:PHE:CE1	8:h:69:ILE:HD11	1.82	1.13
3:B:38:HIS:ND1	3:B:160:PHE:HE1	1.45	1.12
4:D:236:TRP:CZ2	2:F:372:TYR:CG	2.37	1.12
1:A:799:ARG:HH12	2:E:389:THR:HA	1.14	1.11
1:A:813:GLU:OE1	2:E:111:THR:OG1	1.72	1.08
2:E:181:ILE:HG21	3:B:133:ARG:HG2	1.38	1.06
4:D:236:TRP:CZ2	2:F:372:TYR:CB	2.39	1.06
1:A:904:GLU:OE2	2:E:116:ASN:HB2	1.56	1.05
4:D:236:TRP:CZ3	2:F:372:TYR:CD1	2.46	1.04
5:e:37:LYS:N	5:e:38:PRO:HD2	1.71	1.04
4:D:236:TRP:CH2	2:F:372:TYR:CB	2.44	1.01
4:D:236:TRP:CE2	2:F:372:TYR:CD2	2.48	1.00
1:A:813:GLU:CD	2:E:111:THR:HA	1.88	0.99
3:B:38:HIS:ND1	3:B:160:PHE:CE1	2.24	0.99
2:E:179:SER:OG	3:B:133:ARG:NH1	1.96	0.98
8:d:65:PHE:CZ	8:d:69:ILE:HD11	2.00	0.97
8:h:65:PHE:CZ	8:h:69:ILE:HD11	2.00	0.95
1:A:813:GLU:OE2	2:E:111:THR:CA	2.14	0.94
4:D:236:TRP:CZ2	2:F:372:TYR:CD2	2.56	0.93
1:A:918:GLU:CD	2:E:128:LEU:CD1	2.12	0.92
5:e:37:LYS:N	5:e:38:PRO:CD	2.30	0.90
1:A:904:GLU:OE2	2:E:116:ASN:ND2	2.03	0.90
8:h:65:PHE:CZ	8:h:69:ILE:CD1	2.54	0.90
8:d:65:PHE:CZ	8:d:69:ILE:CD1	2.55	0.90
5:e:96:CYS:SG	6:f:62:LEU:HD21	2.11	0.89
4:D:236:TRP:CE3	2:F:372:TYR:CD1	2.60	0.89
3:B:40:MET:HG3	3:B:44:ARG:NH2	1.88	0.89
3:B:38:HIS:CE1	3:B:160:PHE:HE1	1.91	0.88
2:E:503:GLN:HE22	2:E:539:ILE:CG2	1.86	0.88
5:e:76:GLN:OE1	6:f:21:VAL:CG2	2.22	0.88
3:B:274:ASP:HA	3:B:279:ASP:OD2	1.75	0.87
5:e:37:LYS:NZ	4:G:19:GLY:CA	2.38	0.87
2:E:385:GLN:O	2:E:385:GLN:NE2	2.08	0.87
4:D:335:ILE:HG21	4:D:363:LEU:HD21	1.58	0.86
1:A:1300:MET:O	1:A:1317:ILE:HB	1.75	0.85
5:a:96:CYS:SG	6:b:62:LEU:HD21	2.17	0.84
3:B:135:ASN:OD1	3:B:176:TYR:HD2	1.53	0.83
2:E:503:GLN:HE22	2:E:539:ILE:HG21	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:504:LEU:HD12	2:E:504:LEU:H	1.40	0.83
5:e:76:GLN:OE1	6:f:21:VAL:HG22	1.76	0.83
4:C:240:THR:O	4:C:242:ASP:N	2.12	0.83
3:B:136:ARG:HB3	3:B:136:ARG:NH2	1.94	0.82
1:A:1009:ARG:HH12	1:A:1071:ARG:HG2	1.45	0.81
2:E:503:GLN:NE2	2:E:539:ILE:HG22	1.96	0.81
8:h:65:PHE:CE1	8:h:69:ILE:CD1	2.64	0.81
2:E:503:GLN:NE2	2:E:539:ILE:CG2	2.44	0.80
1:A:799:ARG:NH1	2:E:389:THR:HA	1.94	0.80
5:e:37:LYS:HZ3	4:G:19:GLY:HA3	1.46	0.80
5:e:37:LYS:NZ	4:G:19:GLY:HA3	1.97	0.80
1:A:827:THR:HG21	1:A:866:VAL:HG11	1.64	0.79
3:B:149:LEU:HB3	3:B:161:CYS:HB2	1.62	0.79
1:A:918:GLU:OE1	2:E:128:LEU:HD11	1.79	0.79
3:B:269:LEU:HD21	3:B:295:VAL:HG22	1.65	0.78
1:A:904:GLU:CD	2:E:116:ASN:HB2	2.07	0.78
1:A:929:ASP:OD1	3:B:359:ASN:ND2	2.17	0.78
3:B:138:LYS:HD3	3:B:138:LYS:N	1.97	0.78
3:B:296:ASN:HB2	3:B:328:LEU:HD21	1.66	0.78
2:F:544:GLU:HA	2:F:547:ILE:HD12	1.64	0.78
1:A:904:GLU:OE2	2:E:116:ASN:CB	2.29	0.78
8:d:65:PHE:CE1	8:d:69:ILE:CD1	2.64	0.78
4:C:378:ASP:OD2	4:C:381:ARG:NH2	2.17	0.77
3:B:40:MET:CG	3:B:44:ARG:HH21	1.95	0.76
3:B:150:HIS:HD2	3:B:190:GLY:HA2	1.50	0.76
7:g:15:LYS:HE2	7:g:19:SER:OG	1.86	0.76
4:C:258:LEU:HD11	4:C:285:LEU:HD22	1.66	0.76
6:f:22:LEU:HD12	6:f:22:LEU:H	1.51	0.76
3:B:136:ARG:HB3	3:B:136:ARG:HH21	1.47	0.76
4:C:232:LEU:HD21	4:C:332:LEU:HB3	1.67	0.75
1:A:851:LEU:HD12	1:A:852:PRO:HD2	1.68	0.75
1:A:860:MET:O	1:A:864:LYS:NZ	2.18	0.75
3:B:38:HIS:CE1	3:B:160:PHE:CE1	2.73	0.74
2:F:372:TYR:CG	2:F:372:TYR:CB	2.71	0.74
3:B:28:ASP:O	3:B:31:ASN:ND2	2.19	0.74
1:A:1190:GLN:HG3	2:E:129:TRP:CZ3	2.23	0.73
4:D:236:TRP:CD2	2:F:372:TYR:HB2	2.08	0.73
1:A:1179:THR:HA	1:A:1182:LYS:HG2	1.70	0.73
1:A:799:ARG:HH12	2:E:389:THR:CA	1.98	0.72
2:E:414:PHE:HB3	2:E:423:THR:HG21	1.70	0.72
3:B:23:TYR:HB3	3:B:63:ILE:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:ILE:HG21	3:B:133:ARG:CG	2.18	0.71
2:E:383:ASP:HA	2:E:386:LEU:HD22	1.72	0.71
3:B:20:ARG:HH11	3:B:20:ARG:CG	2.04	0.71
4:D:297:LEU:HD11	4:D:334:LEU:HD13	1.73	0.71
4:D:329:ILE:HD11	4:D:386:LEU:HD13	1.73	0.71
2:E:167:LEU:HD13	3:B:342:GLU:CD	2.16	0.71
3:B:135:ASN:OD1	3:B:176:TYR:CG	2.43	0.71
10:j:-51:DT:O4	10:j:-50:DA:N6	2.23	0.71
2:E:113:LEU:HD12	2:E:113:LEU:N	2.06	0.70
1:A:1302:ARG:NH1	1:A:1323:THR:O	2.24	0.70
2:E:543:ASP:O	2:E:546:SER:OG	2.10	0.70
1:A:1145:TYR:HB2	1:A:1301:PHE:CE2	2.27	0.70
1:A:794:GLY:HA2	2:E:460:LEU:HD13	1.72	0.70
4:D:229:LYS:HD3	2:F:357:ILE:HA	1.74	0.69
2:E:504:LEU:HD12	2:E:504:LEU:N	2.07	0.69
3:B:30:GLY:O	3:B:46:ARG:NH2	2.22	0.69
6:f:31:LYS:HE2	6:f:35:ARG:HH21	1.58	0.69
3:B:312:GLY:HA2	3:B:318:VAL:HG21	1.74	0.68
2:E:187:TRP:HE3	2:E:187:TRP:N	1.91	0.68
1:A:1009:ARG:HG2	1:A:1074:TYR:CZ	2.29	0.67
2:E:455:ALA:HB1	3:B:239:ARG:HE	1.58	0.67
1:A:813:GLU:CD	2:E:111:THR:CA	2.63	0.67
2:E:379:ILE:CG1	2:E:380:PRO:CD	2.50	0.67
1:A:813:GLU:OE1	2:E:111:THR:CB	2.43	0.66
4:D:348:ASP:OD1	4:D:351:SER:OG	2.13	0.66
2:E:167:LEU:HD13	3:B:342:GLU:HG3	1.78	0.66
2:E:179:SER:O	3:B:129:GLU:OE2	2.14	0.66
1:A:799:ARG:HG2	2:E:393:GLN:OE1	1.96	0.66
2:E:283:HIS:CE1	4:C:300:ARG:HH12	2.14	0.66
2:E:180:ASN:HB2	2:E:185:ILE:HD12	1.78	0.66
1:A:977:PHE:O	1:A:1311:HIS:ND1	2.28	0.65
3:B:30:GLY:HA2	3:B:42:PRO:O	1.97	0.65
1:A:690:ASN:ND2	2:E:520:ILE:HG13	2.11	0.65
4:D:236:TRP:CE2	2:F:372:TYR:HD2	2.08	0.65
1:A:667:THR:HA	1:A:670:GLU:HG2	1.78	0.65
5:e:96:CYS:SG	6:f:62:LEU:CD2	2.84	0.65
3:B:135:ASN:CG	3:B:176:TYR:HD2	2.03	0.65
3:B:40:MET:HE3	3:B:44:ARG:HH22	1.62	0.65
4:D:236:TRP:CH2	2:F:372:TYR:CA	2.80	0.65
4:D:294:GLY:O	4:D:303:ARG:NH1	2.27	0.65
5:e:37:LYS:HZ3	4:G:19:GLY:CA	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:180:ASN:C	2:E:180:ASN:HD22	2.00	0.64
3:B:20:ARG:N	3:B:20:ARG:HD3	2.11	0.64
1:A:765:MET:HE3	1:A:766:PRO:HD2	1.79	0.64
4:C:314:SER:O	4:C:317:GLN:NE2	2.31	0.64
5:e:76:GLN:NE2	6:f:21:VAL:HG23	2.13	0.64
1:A:1322:LEU:HD22	1:A:1336:TYR:HE2	1.63	0.64
9:i:-52:DC:H2'	9:i:-51:DT:H71	1.80	0.64
2:E:542:ILE:HG12	2:E:546:SER:OG	1.98	0.64
3:B:136:ARG:HA	3:B:136:ARG:CZ	2.28	0.64
2:E:374:ASP:O	2:E:375:GLU:HG3	1.98	0.64
4:D:260:LYS:NZ	4:D:372:GLU:OE2	2.31	0.64
2:E:124:LYS:O	2:E:124:LYS:HG3	1.98	0.63
2:E:379:ILE:HG13	2:E:380:PRO:HD2	0.75	0.63
5:e:76:GLN:CD	6:f:21:VAL:HG23	2.22	0.63
2:E:380:PRO:N	2:E:380:PRO:C	2.54	0.63
4:D:245:ILE:O	4:D:387:TYR:HA	1.97	0.63
4:D:351:SER:O	4:D:355:LEU:HG	1.99	0.63
1:A:973:SER:OG	1:A:1315:GLN:NE2	2.30	0.63
10:j:-48:DC:H2''	10:j:-47:DA:N7	2.13	0.63
2:E:517:ASN:ND2	2:E:519:ASN:OD1	2.31	0.63
9:i:-22:DT:H2''	9:i:-21:DC:H5''	1.81	0.63
2:E:121:GLU:O	2:E:125:ARG:HG2	1.98	0.63
1:A:678:ASN:HB3	1:A:681:LEU:HD13	1.80	0.63
5:e:96:CYS:HG	6:f:62:LEU:HD21	1.62	0.63
1:A:918:GLU:OE1	2:E:128:LEU:CG	2.38	0.63
2:E:386:LEU:N	2:E:386:LEU:HD13	2.14	0.63
1:A:978:ASP:OD1	1:A:1311:HIS:ND1	2.31	0.62
1:A:821:ILE:HD11	1:A:905:TRP:HB3	1.81	0.62
4:D:224:ILE:HG21	4:D:228:LEU:HD22	1.81	0.62
7:g:35:ARG:NH2	9:i:39:DT:OP2	2.21	0.62
1:A:974:GLN:HE21	1:A:1316:TYR:H	1.48	0.62
3:B:149:LEU:O	3:B:164:ASN:ND2	2.31	0.62
1:A:975:LEU:HD13	1:A:1149:ARG:HH22	1.63	0.62
2:E:293:PRO:HD2	3:B:99:ARG:HH21	1.64	0.62
1:A:788:TRP:HZ2	4:C:395:GLU:HG3	1.65	0.61
1:A:977:PHE:HZ	1:A:1149:ARG:HH12	1.46	0.61
2:E:384:ARG:HA	2:E:387:PHE:HB2	1.81	0.61
2:E:182:ARG:NH2	3:B:67:LYS:O	2.31	0.61
9:i:-5:DC:H2''	9:i:-4:DT:H71	1.82	0.61
1:A:1007:LYS:O	1:A:1011:LYS:HG3	2.00	0.61
4:C:236:TRP:CD1	4:C:299:TYR:HH	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ASP:HB2	3:B:248:ARG:HH12	1.66	0.61
2:E:419:LYS:HD3	2:E:451:CYS:HB3	1.83	0.61
10:j:-29:DT:H2''	10:j:-28:DG:C8	2.36	0.60
10:j:72:DA:H2''	10:j:73:DT:H5''	1.83	0.60
2:F:263:CYS:O	2:F:267:ASN:N	2.35	0.60
3:B:84:ASP:OD2	3:B:88:ARG:NH1	2.32	0.60
9:i:-51:DT:O4	9:i:-50:DA:N6	2.35	0.60
4:D:252:VAL:HG11	4:D:373:TYR:HE1	1.67	0.60
1:A:952:ILE:HD12	1:A:975:LEU:HD12	1.83	0.60
10:j:-60:DT:H2''	10:j:-59:DG:N7	2.17	0.60
8:d:115:THR:O	8:d:119:THR:HG23	2.02	0.60
7:g:78:ILE:O	8:h:55:SER:OG	2.20	0.60
2:F:305:GLU:HG3	2:F:346:HIS:HA	1.84	0.59
3:B:21:VAL:HG12	3:B:141:VAL:HB	1.83	0.59
3:B:135:ASN:CG	3:B:176:TYR:CD2	2.76	0.59
5:e:37:LYS:NZ	4:G:19:GLY:HA2	2.17	0.59
8:h:115:THR:O	8:h:119:THR:HG23	2.02	0.59
1:A:694:GLN:NE2	2:E:515:GLN:O	2.36	0.59
2:E:167:LEU:HD13	3:B:342:GLU:CG	2.32	0.59
3:B:39:PRO:HB3	3:B:313:TYR:CD1	2.37	0.59
2:F:287:LEU:HB2	2:F:290:PRO:HA	1.85	0.59
9:i:-15:DG:H1	10:j:15:DC:H42	1.47	0.59
2:E:180:ASN:ND2	2:E:180:ASN:O	2.35	0.59
4:C:236:TRP:HD1	4:C:299:TYR:HH	1.51	0.59
1:A:921:GLN:NE2	1:A:1186:LEU:O	2.36	0.59
1:A:1145:TYR:HB2	1:A:1301:PHE:CZ	2.38	0.59
3:B:135:ASN:OD1	3:B:176:TYR:HB2	2.03	0.59
9:i:6:DC:H2''	9:i:7:DT:H71	1.85	0.59
2:E:187:TRP:N	2:E:187:TRP:CE3	2.71	0.58
1:A:831:LEU:HD21	1:A:894:VAL:HG13	1.84	0.58
3:B:82:TYR:OH	3:B:157:ALA:HB2	2.03	0.58
2:F:302:HIS:O	2:F:307:LYS:NZ	2.36	0.58
4:C:235:ASP:OD1	4:C:387:TYR:OH	2.18	0.58
4:D:297:LEU:O	4:D:333:ARG:NH1	2.29	0.58
3:B:186:ASP:OD1	3:B:187:VAL:N	2.37	0.58
1:A:1315:GLN:HE22	1:A:1325:LYS:HD3	1.69	0.58
2:E:171:LEU:O	2:E:173:GLU:N	2.36	0.58
9:i:-29:DT:H2''	9:i:-28:DG:C8	2.39	0.58
9:i:-54:DT:H1'	9:i:-53:DA:H5'	1.85	0.58
4:C:236:TRP:O	4:C:240:THR:OG1	2.15	0.58
6:b:24:ASP:N	6:b:24:ASP:OD1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:80:THR:OG1	5:e:81:ASP:OD2	2.22	0.57
2:E:107:LYS:HG3	2:E:107:LYS:O	2.05	0.57
2:E:260:GLU:HG2	2:E:279:PRO:O	2.04	0.57
1:A:904:GLU:OE2	2:E:116:ASN:CG	2.47	0.57
6:f:22:LEU:HD12	6:f:22:LEU:N	2.18	0.57
2:F:303:CYS:SG	2:F:347:ASN:ND2	2.76	0.57
2:E:350:GLN:NE2	2:E:352:GLN:OE1	2.37	0.57
2:E:521:GLN:HB2	2:E:539:ILE:HD11	1.87	0.57
4:D:233:VAL:HG21	2:F:364:VAL:HG11	1.86	0.57
10:j:-68:DT:H2"	10:j:-67:DA:C8	2.40	0.57
10:j:23:DT:H2"	10:j:24:DG:H5"	1.86	0.57
3:B:321:THR:O	3:B:325:GLU:HG2	2.05	0.56
4:D:254:VAL:HB	4:D:323:ILE:HG13	1.85	0.56
4:D:236:TRP:CZ2	2:F:372:TYR:HB2	2.35	0.56
4:D:293:LEU:HA	4:D:297:LEU:HD12	1.87	0.56
9:i:-27:DC:H2"	9:i:-26:DT:H71	1.86	0.56
2:E:505:TYR:CD2	2:E:505:TYR:N	2.72	0.56
4:D:236:TRP:CZ3	2:F:372:TYR:CA	2.88	0.56
4:D:258:LEU:HD11	4:D:285:LEU:HD23	1.87	0.56
4:D:260:LYS:O	4:D:264:GLU:HG2	2.05	0.56
2:F:355:ASN:HA	2:F:358:LYS:HZ3	1.71	0.56
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.87	0.56
3:B:151:HIS:HB2	3:B:161:CYS:SG	2.46	0.56
3:B:285:ASN:ND2	3:B:285:ASN:O	2.39	0.56
5:a:44:GLY:O	5:a:48:LEU:HD12	2.05	0.56
9:i:-36:DT:H2"	9:i:-35:DG:N7	2.21	0.56
1:A:696:ILE:HD13	2:E:493:LYS:HG2	1.87	0.56
5:a:42:ARG:NH1	9:i:72:DA:OP1	2.39	0.55
10:j:6:DC:H2"	10:j:7:DT:H72	1.89	0.55
1:A:1245:VAL:O	1:A:1248:SER:HB3	2.06	0.55
4:D:295:ASN:ND2	2:F:288:ASP:OD1	2.39	0.55
9:i:51:DA:H2"	9:i:52:DG:H5"	1.89	0.55
3:B:26:ASP:OD2	3:B:65:ARG:NE	2.40	0.55
5:e:37:LYS:HZ1	4:G:19:GLY:CA	2.18	0.55
3:B:239:ARG:HD2	3:B:363:VAL:HG12	1.87	0.55
2:F:260:GLU:HG3	2:F:262:PHE:H	1.72	0.55
6:b:50:ILE:O	6:b:54:THR:HG23	2.07	0.55
2:E:562:GLN:O	2:E:566:LEU:HG	2.07	0.55
3:B:28:ASP:OD1	3:B:31:ASN:ND2	2.39	0.55
4:C:332:LEU:HD21	4:C:366:LEU:HD21	1.89	0.55
2:F:305:GLU:OE1	2:F:347:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:PRO:HG3	2:E:499:ASN:HB2	1.89	0.55
3:B:39:PRO:O	3:B:313:TYR:HA	2.07	0.55
4:D:236:TRP:CH2	2:F:372:TYR:HA	2.41	0.54
2:E:179:SER:C	3:B:129:GLU:CD	2.72	0.54
2:E:465:LYS:HE3	2:E:469:HIS:HB2	1.89	0.54
3:B:40:MET:HE3	3:B:44:ARG:NH2	2.21	0.54
1:A:799:ARG:NH1	2:E:388:ASN:O	2.40	0.54
1:A:785:HIS:HB3	1:A:788:TRP:CZ3	2.42	0.54
1:A:1281:LYS:HA	1:A:1284:ILE:HD12	1.89	0.54
2:E:440:CYS:SG	2:E:441:ASP:N	2.80	0.54
3:B:150:HIS:CD2	3:B:190:GLY:HA2	2.38	0.54
2:E:184:THR:O	2:E:184:THR:OG1	2.15	0.54
2:E:402:ASN:OD1	2:E:405:THR:HB	2.07	0.54
4:C:383:ASP:OD1	4:C:384:ASP:N	2.41	0.54
2:E:511:LYS:NZ	4:D:280:GLU:OE1	2.40	0.54
2:E:510:GLN:HE22	2:E:513:GLY:H	1.54	0.54
1:A:664:GLU:O	1:A:667:THR:OG1	2.19	0.54
1:A:675:TYR:CE2	1:A:713:ASN:HB2	2.43	0.54
2:E:327:ILE:HG22	2:E:337:ALA:HB1	1.90	0.54
4:D:236:TRP:CZ3	2:F:372:TYR:HD1	2.20	0.54
5:a:96:CYS:SG	6:b:62:LEU:CD2	2.92	0.54
5:e:76:GLN:CD	6:f:21:VAL:CG2	2.81	0.54
1:A:813:GLU:OE1	2:E:111:THR:CA	2.55	0.54
1:A:874:GLU:HG3	1:A:875:ARG:H	1.72	0.54
1:A:1181:ALA:HB1	1:A:1186:LEU:HB2	1.88	0.54
1:A:1324:LEU:HD12	1:A:1325:LYS:H	1.73	0.53
2:E:167:LEU:CD1	3:B:342:GLU:HG3	2.37	0.53
8:h:36:SER:HB2	8:h:63:ASN:ND2	2.23	0.53
1:A:972:LYS:NZ	1:A:976:ASP:OD2	2.41	0.53
1:A:1145:TYR:OH	1:A:1149:ARG:NH2	2.27	0.53
1:A:1260:ALA:O	1:A:1264:GLU:HG2	2.07	0.53
2:E:106:SER:O	2:E:106:SER:OG	2.18	0.53
8:d:65:PHE:CZ	8:d:69:ILE:HD12	2.41	0.53
5:e:73:GLU:HB2	6:f:22:LEU:HD13	1.89	0.53
2:E:273:LEU:O	2:E:281:SER:OG	2.21	0.53
4:C:300:ARG:NH2	4:C:399:LEU:O	2.38	0.53
4:C:342:ILE:HD11	4:C:355:LEU:HD23	1.90	0.53
3:B:55:TYR:CE1	3:B:339:PRO:HD3	2.43	0.53
1:A:1219:LEU:HD11	1:A:1224:PHE:HB2	1.90	0.53
2:E:333:VAL:HG11	2:E:340:LEU:HD11	1.91	0.53
1:A:822:GLU:HG2	3:B:46:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:360:GLU:O	4:D:364:VAL:HG23	2.09	0.53
2:F:353:LEU:HB2	2:F:372:TYR:CZ	2.44	0.53
1:A:1139:PHE:HB2	1:A:1286:TYR:HE2	1.74	0.53
2:E:339:LEU:HB3	4:C:288:TYR:CZ	2.43	0.53
4:D:293:LEU:HD23	4:D:322:PRO:HB3	1.91	0.53
8:d:36:SER:HB2	8:d:63:ASN:ND2	2.23	0.53
9:i:28:DC:H2''	9:i:29:DA:C8	2.43	0.53
7:g:102:ILE:HG23	8:h:61:ILE:HD12	1.89	0.53
2:E:126:GLU:O	2:E:126:GLU:HG3	2.09	0.53
3:B:103:LYS:HD2	3:B:104:PHE:CE1	2.44	0.53
4:C:241:LYS:HD2	4:C:241:LYS:O	2.09	0.53
1:A:1066:LEU:HG	1:A:1270:VAL:HG11	1.91	0.53
2:E:266:CYS:SG	4:C:300:ARG:NH1	2.82	0.53
2:F:559:LYS:O	2:F:563:LYS:HG2	2.09	0.53
5:e:118:THR:OG1	6:f:45:ARG:NH1	2.40	0.52
9:i:-60:DT:H2''	9:i:-59:DG:N7	2.24	0.52
1:A:785:HIS:ND1	1:A:787:VAL:HG22	2.24	0.52
1:A:826:ARG:HD2	1:A:829:GLN:NE2	2.24	0.52
2:E:402:ASN:N	2:E:403:PRO:HD3	2.24	0.52
3:B:19:ARG:NH2	3:B:302:GLY:HA2	2.24	0.52
3:B:39:PRO:HB3	3:B:313:TYR:HD1	1.74	0.52
2:E:335:ILE:HG13	2:E:336:PHE:H	1.74	0.52
2:E:339:LEU:HB3	4:C:288:TYR:CE1	2.44	0.52
3:B:19:ARG:HH22	3:B:302:GLY:HA2	1.75	0.52
5:e:73:GLU:HG3	6:f:23:ARG:HH12	1.73	0.52
1:A:1232:TYR:O	1:A:1234:ASN:N	2.42	0.52
4:D:227:LYS:HB3	4:D:367:LEU:HD11	1.92	0.52
1:A:974:GLN:NE2	1:A:1316:TYR:H	2.07	0.52
1:A:1202:ASP:OD2	1:A:1205:LYS:NZ	2.42	0.52
3:B:20:ARG:N	3:B:20:ARG:CD	2.70	0.52
2:E:516:ASN:OD1	2:E:517:ASN:N	2.43	0.52
3:B:177:HIS:CD2	3:B:266:ALA:HB2	2.45	0.52
10:j:52:DG:C5	10:j:53:DT:C4	2.97	0.52
1:A:700:ASP:O	1:A:704:GLU:HG3	2.10	0.52
1:A:846:LYS:HE3	1:A:888:ALA:HB1	1.90	0.52
1:A:1266:MET:O	1:A:1270:VAL:HG23	2.09	0.52
3:B:367:GLU:OE1	3:B:367:GLU:N	2.41	0.52
4:C:333:ARG:O	4:C:337:VAL:HG23	2.09	0.52
10:j:-40:DT:H2''	10:j:-39:DA:C8	2.45	0.52
2:E:452:VAL:HG11	2:E:464:TRP:CH2	2.45	0.52
8:h:65:PHE:CZ	8:h:69:ILE:HD12	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:51:DA:H1'	10:j:52:DG:H5'	1.92	0.52
3:B:218:THR:HG22	3:B:219:GLY:H	1.75	0.52
3:B:238:LEU:HD23	3:B:242:ILE:HD12	1.91	0.52
3:B:14:LYS:HD2	3:B:15:PRO:HD2	1.92	0.51
3:B:210:LYS:HD2	3:B:283:CYS:SG	2.50	0.51
9:i:-71:DC:H2''	9:i:-70:DA:C8	2.45	0.51
1:A:1165:ASN:ND2	1:A:1202:ASP:OD1	2.40	0.51
6:f:30:THR:HB	6:f:32:PRO:HD2	1.92	0.51
3:B:52:ILE:HG23	3:B:57:LEU:HD12	1.92	0.51
5:e:73:GLU:OE1	6:f:25:ASN:ND2	2.32	0.51
10:j:-62:DC:H1'	10:j:-61:DC:H5'	1.90	0.51
1:A:917:ARG:CZ	1:A:1186:LEU:HD22	2.40	0.51
2:E:432:GLU:OE1	2:E:432:GLU:N	2.41	0.51
3:B:279:ASP:OD1	3:B:314:THR:HG22	2.10	0.51
10:j:50:DT:H1'	10:j:51:DA:H5'	1.92	0.51
1:A:1141:ASN:HB3	1:A:1294:MET:SD	2.51	0.51
3:B:177:HIS:HD2	3:B:266:ALA:HB2	1.74	0.51
10:j:7:DT:H2''	10:j:8:DG:C8	2.45	0.51
1:A:1345:HIS:CD2	1:A:1346:PRO:HD2	2.46	0.51
4:C:254:VAL:HB	4:C:323:ILE:HG13	1.92	0.51
4:C:348:ASP:OD2	4:C:349:LEU:N	2.43	0.51
10:j:-51:DT:C4	10:j:-50:DA:N6	2.78	0.51
1:A:1190:GLN:CA	1:A:1190:GLN:HE21	2.24	0.51
4:D:222:LEU:HD13	4:D:339:PRO:HG3	1.93	0.51
9:i:-60:DT:H2''	9:i:-59:DG:C8	2.46	0.51
9:i:-27:DC:H2''	9:i:-26:DT:C7	2.41	0.51
1:A:663:ASN:ND2	1:A:664:GLU:H	2.09	0.51
1:A:1281:LYS:NZ	1:A:1285:ILE:HD11	2.26	0.51
2:E:263:CYS:O	2:E:267:ASN:N	2.36	0.51
4:C:293:LEU:HA	4:C:297:LEU:HD12	1.93	0.51
9:i:-47:DA:H2''	9:i:-46:DA:C8	2.46	0.51
10:j:51:DA:C6	10:j:52:DG:C6	2.99	0.51
2:E:265:ALA:HB1	2:E:349:LYS:HA	1.93	0.50
3:B:194:GLU:OE2	3:B:235:ASN:ND2	2.37	0.50
3:B:244:ASP:OD1	3:B:244:ASP:N	2.44	0.50
9:i:59:DC:H2''	9:i:60:DA:N7	2.26	0.50
2:E:440:CYS:HB2	2:E:466:CYS:SG	2.50	0.50
10:j:46:DT:H2''	10:j:47:DT:C6	2.46	0.50
1:A:1294:MET:HB2	1:A:1298:GLU:HG3	1.92	0.50
2:E:505:TYR:H	2:E:505:TYR:HD2	1.59	0.50
10:j:31:DT:H1'	10:j:32:DT:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ASP:OD1	1:A:773:MET:N	2.44	0.50
4:C:285:LEU:HD21	4:C:331:LEU:HD11	1.93	0.50
4:D:310:LEU:HD23	4:D:311:LYS:HD3	1.93	0.50
1:A:785:HIS:HD2	3:B:156:GLU:OE2	1.95	0.50
1:A:857:HIS:CD2	1:A:858:THR:H	2.30	0.50
1:A:1148:PHE:CZ	1:A:1312:VAL:HG11	2.47	0.50
1:A:1190:GLN:HE21	1:A:1190:GLN:HA	1.76	0.50
2:E:510:GLN:NE2	2:E:512:ILE:H	2.10	0.50
4:D:228:LEU:HG	4:D:332:LEU:HD21	1.92	0.50
4:D:236:TRP:CZ2	2:F:372:TYR:HD2	2.24	0.50
9:i:50:DT:H1'	9:i:51:DA:H5'	1.94	0.50
1:A:952:ILE:HG13	1:A:974:GLN:HB3	1.94	0.50
2:E:111:THR:HG22	2:E:113:LEU:H	1.77	0.50
2:E:306:CYS:O	2:E:310:ILE:HG12	2.11	0.50
2:F:555:ILE:O	2:F:559:LYS:HG3	2.12	0.50
1:A:757:ARG:NH2	4:C:379:PRO:O	2.45	0.49
1:A:1066:LEU:HD23	1:A:1069:LEU:HD23	1.94	0.49
3:B:135:ASN:ND2	3:B:172:GLU:O	2.44	0.49
4:D:304:LEU:HD23	4:D:394:TYR:CD1	2.46	0.49
1:A:749:GLU:N	1:A:749:GLU:OE2	2.44	0.49
1:A:1191:LEU:O	1:A:1196:LEU:N	2.44	0.49
1:A:1322:LEU:HD22	1:A:1336:TYR:CE2	2.46	0.49
8:h:46:LYS:NZ	8:h:52:THR:O	2.40	0.49
9:i:-28:DG:H2''	9:i:-27:DC:C6	2.47	0.49
9:i:-26:DT:H2''	9:i:-25:DC:C5	2.47	0.49
9:i:7:DT:H2''	9:i:8:DG:C8	2.47	0.49
10:j:-64:DC:C2	10:j:-63:DA:N7	2.80	0.49
4:C:318:LYS:HD2	4:C:319:PRO:HD2	1.93	0.49
8:h:111:VAL:O	8:h:115:THR:OG1	2.29	0.49
1:A:877:PHE:HA	1:A:880:ILE:HG22	1.94	0.49
9:i:-49:DC:H2''	9:i:-48:DC:C6	2.46	0.49
2:E:494:LYS:HA	2:E:519:ASN:HD21	1.78	0.49
3:B:24:PHE:HE1	3:B:64:TYR:HD2	1.60	0.49
8:d:68:ASP:OD2	6:f:98:TYR:OH	2.30	0.49
10:j:-4:DT:H2''	10:j:-3:DG:C8	2.47	0.49
9:i:-58:DC:H2''	9:i:-57:DA:N7	2.28	0.49
9:i:-16:DG:H2''	9:i:-15:DG:N7	2.27	0.49
2:F:264:SER:N	2:F:281:SER:O	2.33	0.49
3:B:23:TYR:HD2	3:B:143:VAL:HG23	1.78	0.49
2:F:353:LEU:HB2	2:F:372:TYR:OH	2.13	0.49
9:i:51:DA:C6	9:i:52:DG:C6	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:TYR:HB3	1:A:927:SER:HB2	1.95	0.48
2:E:502:ASN:OD1	4:C:226:ILE:HD11	2.12	0.48
1:A:874:GLU:HG3	1:A:875:ARG:N	2.28	0.48
2:F:300:ASP:HB3	2:F:302:HIS:CE1	2.47	0.48
3:B:39:PRO:CB	3:B:313:TYR:HD1	2.27	0.48
4:D:239:VAL:O	4:D:301:LEU:HD21	2.13	0.48
2:F:258:GLU:OE1	2:F:259:ASN:N	2.46	0.48
4:D:310:LEU:HD13	2:F:290:PRO:HG2	1.96	0.48
2:F:570:GLN:O	2:F:574:ILE:HG12	2.12	0.48
1:A:785:HIS:CG	1:A:786:PRO:HD2	2.48	0.48
1:A:802:GLN:O	1:A:805:GLU:HG2	2.12	0.48
7:g:16:THR:HA	10:j:-43:DG:H5''	1.96	0.48
3:B:57:LEU:HD23	3:B:60:LYS:HG3	1.95	0.48
4:C:261:TYR:HD2	4:C:365:TRP:CE3	2.32	0.48
4:D:246:CYS:SG	4:D:330:HIS:NE2	2.87	0.48
1:A:785:HIS:CD2	1:A:786:PRO:HD2	2.48	0.48
2:E:427:SER:O	2:E:430:HIS:N	2.39	0.48
10:j:3:DC:H2''	10:j:4:DA:C8	2.49	0.48
1:A:1127:GLN:HB2	1:A:1335:LYS:HE2	1.96	0.48
2:E:523:ILE:HG13	2:E:543:ASP:OD1	2.14	0.48
3:B:20:ARG:CG	3:B:20:ARG:NH1	2.70	0.48
3:B:224:ILE:HG12	3:B:231:ASN:HA	1.95	0.48
4:D:236:TRP:CD1	4:D:240:THR:HG1	2.32	0.48
1:A:853:PRO:HA	1:A:884:HIS:CE1	2.48	0.48
4:C:247:ARG:HB2	4:C:388:VAL:HG13	1.96	0.48
4:D:241:LYS:NZ	2:F:371:GLN:HB2	2.29	0.48
4:D:329:ILE:HG21	4:D:387:TYR:OH	2.14	0.48
7:c:102:ILE:HG23	8:d:61:ILE:HD12	1.96	0.48
2:E:177:GLU:H	2:E:177:GLU:HG2	1.52	0.47
2:E:180:ASN:ND2	2:E:180:ASN:N	2.59	0.47
3:B:135:ASN:OD1	3:B:176:TYR:CB	2.61	0.47
5:e:37:LYS:HZ1	4:G:19:GLY:HA2	1.76	0.47
10:j:-46:DA:H2''	10:j:-45:DA:C8	2.49	0.47
10:j:28:DC:H2''	10:j:29:DA:C8	2.49	0.47
9:i:-73:DA:H1'	9:i:-72:DT:H5'	1.95	0.47
2:E:494:LYS:HA	2:E:519:ASN:ND2	2.29	0.47
4:D:335:ILE:HA	4:D:338:LEU:HG	1.97	0.47
6:b:98:TYR:CZ	7:g:100:VAL:HG11	2.49	0.47
8:d:36:SER:HB2	8:d:63:ASN:HD21	1.79	0.47
9:i:-51:DT:C4	9:i:-50:DA:N6	2.82	0.47
1:A:885:GLU:HG3	1:A:886:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:102:VAL:HG11	4:C:400:GLY:O	2.14	0.47
3:B:131:ALA:O	3:B:135:ASN:HB2	2.14	0.47
4:D:390:THR:HB	4:D:394:TYR:HB2	1.96	0.47
1:A:1287:ARG:HD2	1:A:1323:THR:HG22	1.96	0.47
2:E:376:ASN:ND2	2:E:442:TYR:OH	2.46	0.47
4:D:236:TRP:CZ3	2:F:372:TYR:HA	2.50	0.47
8:h:113:GLU:HA	8:h:113:GLU:OE1	2.15	0.47
1:A:872:ASP:HB3	1:A:875:ARG:HD2	1.96	0.47
3:B:111:PRO:O	3:B:162:TYR:OH	2.32	0.47
7:c:35:ARG:NH2	10:j:39:DT:OP2	2.31	0.47
8:h:36:SER:HB2	8:h:63:ASN:HD21	1.80	0.47
1:A:853:PRO:HA	1:A:884:HIS:HE1	1.80	0.47
2:E:179:SER:O	3:B:129:GLU:CD	2.58	0.47
3:B:20:ARG:HH11	3:B:20:ARG:HG2	1.78	0.47
3:B:39:PRO:CB	3:B:313:TYR:CD1	2.98	0.47
4:D:280:GLU:HG2	2:F:335:ILE:HD12	1.96	0.47
2:F:284:PHE:HE1	2:F:296:LEU:HD21	1.78	0.47
3:B:218:THR:HG22	3:B:219:GLY:N	2.30	0.47
2:E:179:SER:HG	3:B:133:ARG:NH1	2.07	0.47
2:E:380:PRO:O	2:E:380:PRO:HG2	2.15	0.47
4:D:258:LEU:HA	4:D:258:LEU:HD23	1.79	0.47
10:j:55:DT:H2''	10:j:56:DC:C6	2.50	0.47
1:A:863:TYR:HA	1:A:866:VAL:HG12	1.97	0.47
2:E:462:SER:OG	2:E:463:LYS:N	2.47	0.47
4:D:307:ASP:O	4:D:310:LEU:HB3	2.14	0.47
2:F:354:PRO:HD2	2:F:357:ILE:HD12	1.96	0.47
9:i:51:DA:C4	9:i:52:DG:C5	3.03	0.47
10:j:53:DT:C2	10:j:54:DA:C8	3.03	0.47
1:A:765:MET:HB3	1:A:766:PRO:HD2	1.96	0.46
1:A:835:VAL:HA	1:A:838:ILE:HG22	1.97	0.46
5:e:60:LEU:HD12	5:e:64:LYS:HE2	1.97	0.46
9:i:-52:DC:H42	10:j:51:DA:N6	2.12	0.46
2:E:452:VAL:O	2:E:454:ARG:N	2.49	0.46
3:B:256:LYS:O	3:B:260:GLU:HG2	2.15	0.46
10:j:-5:DC:H2''	10:j:-4:DT:H71	1.98	0.46
1:A:1267:ALA:O	1:A:1271:LYS:HG2	2.15	0.46
3:B:23:TYR:O	3:B:63:ILE:HA	2.15	0.46
4:D:246:CYS:HG	4:D:330:HIS:CE1	2.33	0.46
9:i:-45:DA:H2''	9:i:-44:DA:C8	2.50	0.46
1:A:1120:LEU:O	1:A:1123:GLU:HG2	2.14	0.46
7:g:77:ARG:CZ	10:j:-55:DA:H4'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:383:ASP:O	4:C:385:ALA:N	2.49	0.46
8:d:113:GLU:OE1	8:d:113:GLU:HA	2.15	0.46
4:D:284:GLY:HA3	2:F:336:PHE:CD2	2.50	0.46
1:A:1076:LYS:O	1:A:1080:SER:OG	2.28	0.46
3:B:239:ARG:HG2	3:B:240:ASP:H	1.80	0.46
2:F:361:PHE:HD2	2:F:364:VAL:HG13	1.81	0.46
9:i:16:DC:H2''	9:i:17:DT:C7	2.46	0.46
4:C:365:TRP:O	4:C:369:HIS:ND1	2.44	0.46
6:f:95:ARG:HE	6:f:95:ARG:HB3	1.58	0.46
9:i:-39:DA:H1'	9:i:-38:DT:H5'	1.98	0.46
1:A:872:ASP:O	1:A:875:ARG:N	2.47	0.46
1:A:1336:TYR:HA	1:A:1339:THR:HG22	1.98	0.46
1:A:872:ASP:O	1:A:874:GLU:N	2.49	0.45
2:E:290:PRO:HG2	4:C:307:ASP:OD1	2.15	0.45
10:j:56:DC:H2''	10:j:57:DT:C6	2.52	0.45
2:E:500:LYS:HB2	2:E:500:LYS:HE3	1.33	0.45
4:D:220:ILE:HD12	4:D:356:ILE:HD11	1.98	0.45
10:j:-58:DC:H2''	10:j:-57:DA:N7	2.31	0.45
1:A:992:ALA:O	1:A:996:ILE:HG12	2.17	0.45
1:A:1034:TYR:O	1:A:1038:GLN:HG3	2.16	0.45
1:A:1233:ASN:OD1	1:A:1234:ASN:N	2.47	0.45
2:E:363:ALA:HB3	2:E:497:LEU:HD13	1.98	0.45
2:E:381:LEU:HD12	2:E:381:LEU:HA	1.58	0.45
3:B:316:ARG:HD2	3:B:346:TYR:O	2.15	0.45
7:g:17:ARG:HH22	7:g:31:HIS:HD2	1.64	0.45
9:i:-4:DT:H2''	9:i:-3:DG:C8	2.51	0.45
3:B:30:GLY:C	3:B:46:ARG:HH21	2.19	0.45
8:h:31:ARG:HH12	10:j:-48:DC:H5''	1.82	0.45
1:A:959:GLN:NE2	1:A:972:LYS:O	2.44	0.45
1:A:1196:LEU:HD11	1:A:1223:TRP:HB3	1.98	0.45
2:E:384:ARG:HA	2:E:387:PHE:CD1	2.51	0.45
2:E:386:LEU:N	2:E:386:LEU:CD1	2.79	0.45
4:D:248:LEU:HD12	4:D:249:PRO:HA	1.98	0.45
9:i:49:DG:H2''	9:i:50:DT:H72	1.98	0.45
10:j:-71:DC:H2''	10:j:-70:DA:C8	2.52	0.45
1:A:1191:LEU:HD23	1:A:1191:LEU:H	1.80	0.45
3:B:136:ARG:NH2	3:B:136:ARG:CB	2.73	0.45
4:C:238:TYR:HD1	4:C:387:TYR:CE2	2.34	0.45
4:D:289:PHE:CE2	4:D:293:LEU:HD13	2.51	0.45
7:c:17:ARG:HH22	7:c:31:HIS:HD2	1.63	0.45
1:A:843:GLU:HA	1:A:846:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:TRP:CD2	2:F:372:TYR:HB3	2.21	0.45
1:A:996:ILE:HD11	1:A:1011:LYS:HG2	1.99	0.45
1:A:1189:SER:O	1:A:1193:GLU:N	2.46	0.45
2:E:494:LYS:HG2	2:E:495:GLN:O	2.17	0.45
4:D:261:TYR:O	4:D:265:VAL:HG23	2.17	0.45
4:D:266:SER:HB2	4:D:278:LEU:HD23	1.98	0.45
1:A:871:TYR:OH	1:A:897:ARG:HD3	2.17	0.45
1:A:1147:PHE:HE2	1:A:1253:ALA:HB2	1.81	0.45
2:E:565:LYS:O	2:E:568:GLN:HG3	2.17	0.45
4:D:299:TYR:O	4:D:303:ARG:HG3	2.17	0.45
2:F:570:GLN:OE1	2:F:573:LEU:HD21	2.17	0.45
7:c:92:GLU:OE1	8:d:105:GLU:HB2	2.17	0.45
1:A:1020:LEU:O	1:A:1023:SER:N	2.47	0.44
1:A:715:GLU:HG3	1:A:716:LEU:N	2.32	0.44
1:A:830:CYS:HA	1:A:833:THR:HG22	1.99	0.44
4:C:234:ASP:O	4:C:237:GLU:HG2	2.16	0.44
2:F:288:ASP:OD1	2:F:348:PRO:HB3	2.18	0.44
9:i:-5:DC:H2"	9:i:-4:DT:C7	2.45	0.44
9:i:15:DC:H2"	9:i:16:DC:C5	2.52	0.44
1:A:768:SER:HB2	3:B:80:ASP:OD1	2.17	0.44
1:A:813:GLU:HB3	1:A:916:TRP:HZ2	1.82	0.44
3:B:20:ARG:HH11	3:B:20:ARG:HG3	1.80	0.44
3:B:239:ARG:HH11	3:B:363:VAL:HG12	1.82	0.44
3:B:248:ARG:NE	3:B:252:GLU:OE1	2.51	0.44
1:A:886:HIS:HB3	1:A:889:VAL:HG12	1.98	0.44
1:A:1148:PHE:HZ	1:A:1312:VAL:HG11	1.82	0.44
1:A:1303:ILE:HG12	1:A:1314:ILE:HG12	2.00	0.44
2:E:125:ARG:HD3	2:E:125:ARG:HA	1.31	0.44
2:E:168:LYS:CB	3:B:53:MET:O	2.65	0.44
2:E:335:ILE:HG13	2:E:336:PHE:N	2.33	0.44
9:i:3:DC:H2"	9:i:4:DA:C8	2.51	0.44
1:A:866:VAL:O	1:A:870:VAL:HG23	2.18	0.44
1:A:922:LYS:HG3	1:A:923:VAL:HG23	1.98	0.44
1:A:1138:LEU:HD13	1:A:1269:PHE:CD1	2.53	0.44
2:E:519:ASN:O	2:E:539:ILE:HG13	2.18	0.44
1:A:918:GLU:OE1	2:E:128:LEU:HG	2.07	0.44
3:B:23:TYR:HB2	3:B:61:MET:HE3	1.99	0.44
10:j:57:DT:H2"	10:j:58:DG:N7	2.32	0.44
1:A:1003:SER:OG	1:A:1005:PRO:HD2	2.18	0.44
1:A:1289:GLN:O	1:A:1292:SER:OG	2.30	0.44
1:A:786:PRO:HB2	1:A:795:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:HD12	1:A:880:ILE:HD13	2.00	0.44
2:E:504:LEU:H	2:E:504:LEU:CD1	2.20	0.44
4:D:258:LEU:HB3	4:D:286:LYS:HE2	1.99	0.44
7:g:92:GLU:OE1	8:h:105:GLU:HB2	2.18	0.44
1:A:1003:SER:OG	1:A:1004:ASN:N	2.51	0.44
2:F:554:LYS:HD2	2:F:554:LYS:HA	1.80	0.44
9:i:23:DT:H2"	9:i:24:DG:C8	2.53	0.44
2:E:402:ASN:OD1	2:E:406:HIS:HD2	2.01	0.43
3:B:22:ALA:HB2	3:B:139:CYS:SG	2.58	0.43
3:B:123:SER:HB2	3:B:147:GLY:HA2	1.99	0.43
2:E:180:ASN:ND2	2:E:180:ASN:H	2.16	0.43
2:E:357:ILE:HG23	4:C:229:LYS:HD3	2.00	0.43
2:E:417:CYS:HA	2:E:446:PRO:O	2.18	0.43
3:B:118:GLU:O	3:B:122:ILE:HG13	2.18	0.43
2:F:320:LYS:HA	2:F:323:GLU:HG3	1.98	0.43
7:g:88:ARG:HA	7:g:88:ARG:HD3	1.85	0.43
10:j:16:DC:H2"	10:j:17:DT:H72	1.99	0.43
1:A:881:ASP:O	1:A:885:GLU:HG2	2.18	0.43
2:E:175:MET:HB3	2:E:175:MET:HE2	1.59	0.43
2:E:293:PRO:HD2	3:B:99:ARG:NH2	2.32	0.43
8:d:46:LYS:HA	8:d:46:LYS:HD3	1.54	0.43
9:i:16:DC:H2"	9:i:17:DT:H71	2.00	0.43
2:E:384:ARG:HE	2:E:384:ARG:HB2	1.54	0.43
1:A:1151:TRP:O	1:A:1154:ILE:HG22	2.18	0.43
4:D:241:LYS:HA	4:D:241:LYS:HD3	1.83	0.43
9:i:70:DT:H2"	9:i:71:DG:C8	2.54	0.43
1:A:689:LEU:HD23	1:A:689:LEU:HA	1.83	0.43
1:A:965:HIS:HE1	1:A:967:LEU:HB3	1.83	0.43
1:A:1078:LYS:O	1:A:1081:ASN:ND2	2.52	0.43
2:E:560:MET:HG2	2:F:557:LYS:NZ	2.33	0.43
2:F:361:PHE:CE2	2:F:363:ALA:HB3	2.54	0.43
1:A:799:ARG:HG2	2:E:393:GLN:HG2	2.01	0.43
2:E:168:LYS:H	3:B:54:ASN:ND2	2.16	0.43
2:E:465:LYS:HG2	2:E:466:CYS:O	2.19	0.43
3:B:32:TYR:HD1	3:B:32:TYR:HA	1.69	0.43
4:D:244:LYS:HB3	4:D:387:TYR:HB3	2.01	0.43
9:i:-7:DA:H2"	9:i:-6:DG:C8	2.54	0.43
3:B:39:PRO:HB3	3:B:281:LEU:HD21	1.99	0.43
5:a:61:LEU:HD12	6:b:37:LEU:HD23	2.01	0.43
1:A:1005:PRO:O	1:A:1009:ARG:HG3	2.19	0.43
2:E:113:LEU:HD12	2:E:113:LEU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:409:SER:OG	2:E:410:ASN:N	2.51	0.43
2:E:455:ALA:HB1	3:B:239:ARG:NE	2.32	0.43
2:E:498:ILE:HD13	4:C:226:ILE:HG21	2.00	0.43
3:B:24:PHE:HE2	3:B:130:GLY:CA	2.30	0.43
3:B:96:MET:HE3	3:B:96:MET:HB3	1.85	0.43
2:F:280:LYS:HB3	2:F:282:PHE:CZ	2.53	0.43
9:i:-48:DC:H2''	9:i:-47:DA:C8	2.54	0.43
10:j:-5:DC:H2''	10:j:-4:DT:C7	2.49	0.43
10:j:47:DT:H2''	10:j:48:DG:C8	2.53	0.43
4:D:304:LEU:HD22	4:D:397:VAL:HG21	2.00	0.42
10:j:-49:DC:H2''	10:j:-48:DC:C6	2.54	0.42
1:A:813:GLU:HB3	1:A:916:TRP:CZ2	2.53	0.42
2:E:517:ASN:OD1	2:E:518:GLY:N	2.48	0.42
4:C:337:VAL:HG12	4:C:341:LEU:HG	2.01	0.42
10:j:-53:DA:H1'	10:j:-52:DC:H5'	2.01	0.42
1:A:1234:ASN:ND2	3:B:357:PRO:O	2.52	0.42
4:D:259:ASN:O	4:D:262:GLU:HG3	2.19	0.42
6:b:98:TYR:OH	8:h:68:ASP:OD2	2.31	0.42
9:i:-40:DT:H2''	9:i:-39:DA:C8	2.54	0.42
2:E:179:SER:HG	3:B:133:ARG:HH11	1.58	0.42
3:B:240:ASP:OD1	3:B:241:GLY:N	2.52	0.42
2:F:266:CYS:SG	2:F:268:GLN:HB2	2.58	0.42
9:i:-48:DC:H2''	9:i:-47:DA:N7	2.34	0.42
1:A:723:PHE:CZ	2:E:555:ILE:HG21	2.55	0.42
1:A:799:ARG:HB2	2:E:395:ILE:HD13	2.00	0.42
2:E:317:ALA:O	2:E:320:LYS:HG3	2.19	0.42
2:E:452:VAL:HG11	2:E:464:TRP:CZ2	2.55	0.42
2:F:309:LYS:HE3	2:F:309:LYS:HB3	1.86	0.42
1:A:754:SER:OG	3:B:218:THR:HG23	2.19	0.42
4:D:236:TRP:CZ3	2:F:372:TYR:HB3	2.39	0.42
4:D:308:GLU:O	4:D:312:LYS:HG2	2.20	0.42
8:h:31:ARG:NH1	10:j:-48:DC:H5''	2.35	0.42
10:j:-27:DC:H2''	10:j:-26:DT:C7	2.50	0.42
1:A:868:ARG:HD3	1:A:877:PHE:CE1	2.54	0.42
1:A:1268:LEU:O	1:A:1286:TYR:HE1	2.03	0.42
2:E:384:ARG:O	2:E:388:ASN:N	2.52	0.42
3:B:239:ARG:HD2	3:B:363:VAL:CG1	2.48	0.42
4:C:235:ASP:O	4:C:238:TYR:N	2.53	0.42
4:C:352:CYS:O	4:C:356:ILE:HG12	2.20	0.42
7:c:16:THR:HA	9:i:-43:DG:H5''	2.02	0.42
9:i:12:DA:OP1	4:G:80:HIS:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:TYR:HD2	1:A:916:TRP:HH2	1.68	0.42
4:D:251:ASP:OD1	4:D:252:VAL:HG23	2.19	0.42
4:D:255:GLU:HB3	4:D:324:ARG:HH11	1.84	0.42
8:d:111:VAL:O	8:d:115:THR:OG1	2.29	0.42
10:j:-64:DC:H2''	10:j:-63:DA:H8	1.85	0.42
10:j:-37:DT:H2''	10:j:-36:DT:C6	2.55	0.42
4:C:293:LEU:HD12	4:C:297:LEU:HB2	2.02	0.42
4:D:299:TYR:HD2	4:D:333:ARG:HH22	1.68	0.42
8:h:87:SER:O	8:h:87:SER:OG	2.38	0.42
1:A:972:LYS:HD2	1:A:973:SER:H	1.84	0.42
2:E:168:LYS:HB3	3:B:53:MET:O	2.20	0.42
3:B:280:ARG:HE	3:B:280:ARG:HB3	1.49	0.42
4:C:232:LEU:HD23	4:C:232:LEU:HA	1.86	0.42
4:C:261:TYR:CE2	4:C:362:PHE:HA	2.55	0.42
4:C:288:TYR:HE2	4:C:341:LEU:HD13	1.85	0.42
4:D:355:LEU:O	4:D:359:THR:HG23	2.20	0.42
7:c:30:VAL:HG13	8:d:70:PHE:HE1	1.84	0.42
1:A:912:TRP:CZ3	2:E:119:PRO:HA	2.55	0.41
2:E:477:LYS:HA	2:E:477:LYS:HD3	1.89	0.41
3:B:377:PHE:O	3:B:381:GLU:HG2	2.19	0.41
4:D:280:GLU:OE2	2:F:334:LYS:N	2.52	0.41
2:F:273:LEU:HG	2:F:301:TRP:CE3	2.55	0.41
1:A:690:ASN:HD21	2:E:520:ILE:HG13	1.82	0.41
1:A:692:TYR:CG	1:A:702:LEU:HD22	2.55	0.41
1:A:865:LYS:N	1:A:868:ARG:HH21	2.18	0.41
2:E:443:CYS:SG	2:E:445:THR:HG22	2.59	0.41
3:B:38:HIS:HA	3:B:39:PRO:HD3	1.94	0.41
9:i:-50:DA:C5	9:i:-49:DC:C4	3.08	0.41
9:i:-21:DC:H2''	9:i:-20:DA:H8	1.85	0.41
10:j:-50:DA:H2''	10:j:-49:DC:C6	2.55	0.41
1:A:1129:ILE:HG23	1:A:1279:SER:HB3	2.01	0.41
1:A:1142:THR:HA	1:A:1301:PHE:CZ	2.55	0.41
1:A:1265:ILE:HG23	1:A:1290:VAL:HG13	2.01	0.41
2:E:107:LYS:NZ	2:E:107:LYS:HB2	2.35	0.41
9:i:-35:DG:H2''	9:i:-34:DG:C8	2.55	0.41
9:i:-6:DG:H2''	9:i:-5:DC:C6	2.55	0.41
10:j:-49:DC:H2''	10:j:-48:DC:C5	2.55	0.41
1:A:1198:PHE:HE1	1:A:1232:TYR:HE2	1.67	0.41
2:E:107:LYS:HB2	2:E:107:LYS:HZ2	1.85	0.41
2:E:381:LEU:HB3	2:E:384:ARG:HB3	2.02	0.41
6:b:62:LEU:HD23	6:b:62:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:31:ARG:HD2	8:d:31:ARG:HA	1.88	0.41
9:i:33:DT:H5'	9:i:33:DT:C6	2.56	0.41
4:D:291:LYS:HA	4:D:291:LYS:HD3	1.85	0.41
2:F:287:LEU:HD11	2:F:301:TRP:HZ2	1.84	0.41
2:F:552:PHE:HA	2:F:555:ILE:HG22	2.01	0.41
2:E:292:ASP:CG	3:B:99:ARG:HH22	2.28	0.41
2:E:510:GLN:HE22	2:E:513:GLY:N	2.16	0.41
3:B:201:ASP:HA	3:B:232:TYR:HD1	1.86	0.41
4:D:254:VAL:HA	4:D:257:VAL:HG12	2.03	0.41
10:j:-7:DA:H2''	10:j:-6:DG:C8	2.55	0.41
10:j:26:DA:H2''	10:j:27:DG:C8	2.55	0.41
1:A:1139:PHE:HB2	1:A:1286:TYR:CE2	2.53	0.41
1:A:1190:GLN:HG3	2:E:129:TRP:CE3	2.55	0.41
2:E:353:LEU:HD23	2:E:353:LEU:HA	1.95	0.41
2:E:399:ASP:O	2:E:400:SER:OG	2.31	0.41
6:b:92:ARG:NH2	8:d:76:GLU:OE2	2.40	0.41
7:g:35:ARG:HH12	9:i:39:DT:P	2.43	0.41
1:A:904:GLU:CG	2:E:116:ASN:HB2	2.49	0.41
1:A:1074:TYR:OH	1:A:1078:LYS:NZ	2.47	0.41
3:B:51:LEU:HD23	3:B:51:LEU:HA	1.85	0.41
3:B:114:ASP:C	3:B:116:LEU:N	2.78	0.41
4:C:261:TYR:HD2	4:C:365:TRP:CD2	2.38	0.41
2:F:303:CYS:O	2:F:307:LYS:HG2	2.19	0.41
5:e:73:GLU:HG3	6:f:23:ARG:NH1	2.35	0.41
9:i:57:DT:H1'	9:i:58:DG:C5	2.56	0.41
1:A:946:LYS:O	1:A:950:SER:OG	2.30	0.41
1:A:1333:LYS:HA	1:A:1333:LYS:HD2	1.84	0.41
2:E:408:ASP:OD1	2:E:409:SER:N	2.54	0.41
2:E:516:ASN:O	2:E:517:ASN:HB2	2.20	0.41
3:B:3:TYR:N	3:B:370:ASP:OD2	2.54	0.41
3:B:289:GLU:N	3:B:289:GLU:OE1	2.54	0.41
4:D:303:ARG:O	2:F:285:LEU:HD11	2.20	0.41
9:i:-70:DA:H2''	9:i:-69:DA:C8	2.56	0.41
9:i:-52:DC:N4	10:j:51:DA:N6	2.69	0.41
9:i:46:DT:H2''	9:i:47:DT:C6	2.55	0.41
1:A:785:HIS:HE1	1:A:787:VAL:HG13	1.86	0.41
1:A:1287:ARG:CD	1:A:1323:THR:HG22	2.51	0.41
2:E:495:GLN:HG3	2:E:519:ASN:OD1	2.21	0.41
2:E:558:SER:HA	2:E:561:VAL:HG22	2.02	0.41
4:D:220:ILE:CD1	4:D:356:ILE:HD11	2.51	0.41
4:D:236:TRP:CD2	2:F:372:TYR:CD2	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:363:ALA:O	2:F:375:GLU:HG2	2.21	0.41
8:h:46:LYS:HA	8:h:46:LYS:HD3	1.54	0.41
9:i:-28:DG:OP2	9:i:-28:DG:H8	2.04	0.41
9:i:-19:DA:H1'	9:i:-18:DA:C8	2.55	0.41
9:i:14:DG:H2''	9:i:15:DC:C5	2.56	0.41
1:A:759:PRO:C	1:A:761:SER:H	2.30	0.40
1:A:785:HIS:CE1	1:A:787:VAL:HG13	2.56	0.40
2:E:555:ILE:HD13	2:E:555:ILE:HA	1.98	0.40
2:E:557:LYS:O	2:E:561:VAL:HG22	2.22	0.40
3:B:39:PRO:CB	3:B:281:LEU:HD21	2.51	0.40
3:B:41:LYS:HA	3:B:42:PRO:HD3	1.84	0.40
3:B:173:LEU:HD23	3:B:173:LEU:HA	1.86	0.40
2:F:358:LYS:HG2	2:F:372:TYR:CE1	2.56	0.40
7:g:16:THR:OG1	7:g:17:ARG:N	2.54	0.40
1:A:698:ASP:OD1	1:A:699:LEU:N	2.54	0.40
1:A:835:VAL:HG12	1:A:839:GLU:OE1	2.21	0.40
2:E:362:PRO:CG	2:E:499:ASN:HB2	2.52	0.40
2:E:556:TYR:HB3	4:D:270:GLU:OE2	2.21	0.40
2:F:556:TYR:O	2:F:560:MET:HG2	2.21	0.40
1:A:836:ASN:HA	1:A:839:GLU:OE2	2.21	0.40
1:A:933:LEU:C	1:A:935:PHE:H	2.29	0.40
1:A:1027:GLU:N	1:A:1027:GLU:OE2	2.55	0.40
1:A:1251:LYS:HE2	1:A:1251:LYS:HB3	1.84	0.40
2:E:126:GLU:O	2:E:126:GLU:CG	2.69	0.40
2:E:563:LYS:HD3	2:E:563:LYS:HA	1.77	0.40
4:D:262:GLU:HB3	4:D:282:CYS:SG	2.61	0.40
4:D:301:LEU:HD12	4:D:302:GLU:N	2.37	0.40
1:A:675:TYR:OH	1:A:712:SER:HB3	2.21	0.40
1:A:805:GLU:HA	1:A:808:PHE:CD2	2.56	0.40
4:D:363:LEU:HD23	4:D:363:LEU:HA	1.81	0.40
2:F:324:SER:HA	2:F:327:ILE:HG12	2.04	0.40
2:F:557:LYS:O	2:F:561:VAL:HG13	2.21	0.40
7:c:88:ARG:HD3	7:c:88:ARG:HA	1.85	0.40
9:i:46:DT:H5''	9:i:46:DT:H6	1.87	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	598/1536 (39%)	564 (94%)	32 (5%)	2 (0%)	36	65
2	E	343/684 (50%)	286 (83%)	49 (14%)	8 (2%)	5	30
2	F	152/684 (22%)	148 (97%)	4 (3%)	0	100	100
3	B	383/433 (88%)	348 (91%)	32 (8%)	3 (1%)	16	49
4	C	181/401 (45%)	167 (92%)	13 (7%)	1 (1%)	21	54
4	D	183/401 (46%)	176 (96%)	7 (4%)	0	100	100
4	G	63/401 (16%)	62 (98%)	1 (2%)	0	100	100
5	a	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
5	e	96/136 (71%)	96 (100%)	0	0	100	100
6	b	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
6	f	79/103 (77%)	78 (99%)	1 (1%)	0	100	100
7	c	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
7	g	106/130 (82%)	101 (95%)	3 (3%)	2 (2%)	6	33
8	d	92/126 (73%)	88 (96%)	3 (3%)	1 (1%)	11	43
8	h	92/126 (73%)	89 (97%)	3 (3%)	0	100	100
All	All	2647/5530 (48%)	2476 (94%)	154 (6%)	17 (1%)	23	54

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	171	LEU
2	E	174	ASN
3	B	32	TYR
3	B	34	TYR
2	E	125	ARG
2	E	393	GLN
2	E	500	LYS
4	C	241	LYS

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Mol	Chain	Res	Type
8	d	32	SER
7	g	12	ALA
1	A	873	LYS
1	A	1233	ASN
2	E	470	SER
7	g	16	THR
2	E	471	PRO
2	E	492	TRP
3	B	107	GLY

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	560/1391 (40%)	558 (100%)	2 (0%)	84	81
2	E	332/653 (51%)	305 (92%)	27 (8%)	11	36
2	F	148/653 (23%)	148 (100%)	0	100	100
3	B	326/367 (89%)	321 (98%)	5 (2%)	57	70
4	C	172/359 (48%)	171 (99%)	1 (1%)	78	79
4	D	174/359 (48%)	174 (100%)	0	100	100
4	G	56/359 (16%)	56 (100%)	0	100	100
5	a	85/111 (77%)	83 (98%)	2 (2%)	43	63
5	e	86/111 (78%)	85 (99%)	1 (1%)	63	73
6	b	65/79 (82%)	62 (95%)	3 (5%)	24	51
6	f	67/79 (85%)	63 (94%)	4 (6%)	17	45
7	c	83/100 (83%)	74 (89%)	9 (11%)	6	28
7	g	84/100 (84%)	73 (87%)	11 (13%)	4	21
8	d	80/105 (76%)	70 (88%)	10 (12%)	4	22
8	h	80/105 (76%)	69 (86%)	11 (14%)	3	20
All	All	2398/4931 (49%)	2312 (96%)	86 (4%)	32	56

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	922	LYS
1	A	1190	GLN
2	E	105	ASP
2	E	107	LYS
2	E	108	VAL
2	E	110	VAL
2	E	111	THR
2	E	113	LEU
2	E	114	PRO
2	E	115	LEU
2	E	123	ILE
2	E	125	ARG
2	E	126	GLU
2	E	175	MET
2	E	177	GLU
2	E	178	GLU
2	E	179	SER
2	E	180	ASN
2	E	181	ILE
2	E	185	ILE
2	E	187	TRP
2	E	381	LEU
2	E	382	THR
2	E	386	LEU
2	E	389	THR
2	E	500	LYS
2	E	501	LYS
2	E	504	LEU
2	E	505	TYR
3	B	20	ARG
3	B	41	LYS
3	B	136	ARG
3	B	138	LYS
3	B	281	LEU
4	C	395	GLU
5	a	57	SER
5	a	87	SER
6	b	50	ILE
6	b	82	THR
6	b	93	GLN
7	c	18	SER
7	c	19	SER

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Mol	Chain	Res	Type
7	c	59	THR
7	c	72	ASP
7	c	74	LYS
7	c	76	THR
7	c	91	GLU
7	c	95	LYS
7	c	100	VAL
8	d	34	LYS
8	d	52	THR
8	d	55	SER
8	d	78	SER
8	d	91	SER
8	d	105	GLU
8	d	112	SER
8	d	113	GLU
8	d	115	THR
8	d	123	SER
5	e	59	GLU
6	f	21	VAL
6	f	22	LEU
6	f	50	ILE
6	f	92	ARG
7	g	11	ARG
7	g	13	LYS
7	g	18	SER
7	g	19	SER
7	g	59	THR
7	g	72	ASP
7	g	74	LYS
7	g	76	THR
7	g	91	GLU
7	g	95	LYS
7	g	100	VAL
8	h	33	ARG
8	h	34	LYS
8	h	52	THR
8	h	55	SER
8	h	78	SER
8	h	91	SER
8	h	105	GLU
8	h	112	SER
8	h	113	GLU

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Mol	Chain	Res	Type
8	h	115	THR
8	h	123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	663	ASN
1	A	785	HIS
1	A	798	HIS
1	A	801	ASN
1	A	857	HIS
1	A	974	GLN
1	A	1039	ASN
1	A	1070	HIS
1	A	1081	ASN
1	A	1127	GLN
1	A	1163	GLN
1	A	1190	GLN
1	A	1221	HIS
1	A	1234	ASN
1	A	1283	GLN
1	A	1293	HIS
1	A	1315	GLN
1	A	1345	HIS
2	E	130	ASN
2	E	180	ASN
2	E	259	ASN
2	E	283	HIS
2	E	314	ASN
2	E	346	HIS
2	E	355	ASN
2	E	376	ASN
2	E	385	GLN
2	E	388	ASN
2	E	421	ASN
2	E	422	GLN
2	E	430	HIS
2	E	433	ASN
2	E	499	ASN
2	E	503	GLN
2	E	510	GLN
2	E	521	GLN

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Mol	Chain	Res	Type
3	B	43	HIS
3	B	54	ASN
3	B	72	GLN
3	B	150	HIS
3	B	177	HIS
3	B	188	HIS
3	B	231	ASN
4	C	275	GLN
4	C	305	GLN
4	D	375	ASN
2	F	259	ASN
2	F	268	GLN
2	F	302	HIS
2	F	325	ASN
2	F	331	ASN
2	F	355	ASN
5	a	39	HIS
5	a	113	HIS
6	b	93	GLN
7	c	24	GLN
7	c	31	HIS
8	d	63	ASN
5	e	113	HIS
5	e	125	GLN
7	g	31	HIS
8	h	63	ASN

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

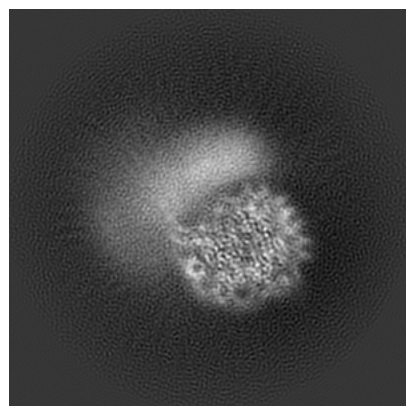
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37366. These allow visual inspection of the internal detail of the map and identification of artifacts.

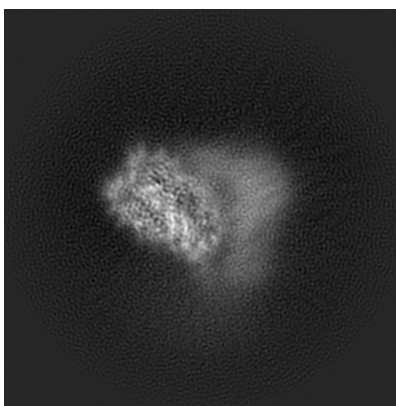
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

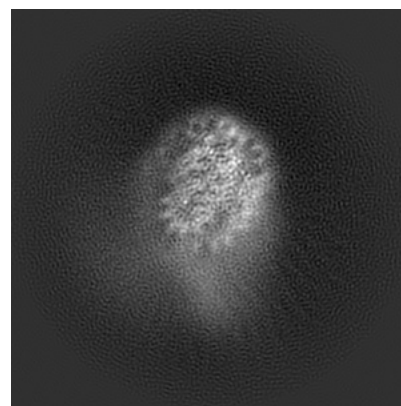
6.1.1 Primary map



X

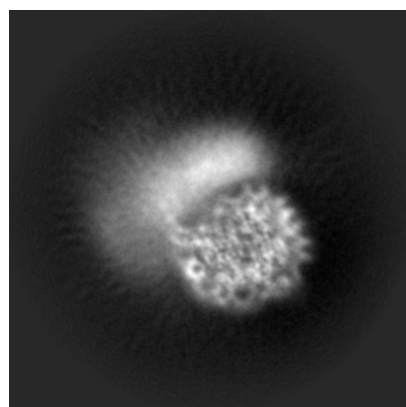


Y

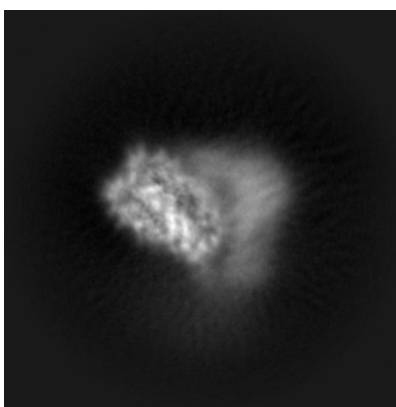


Z

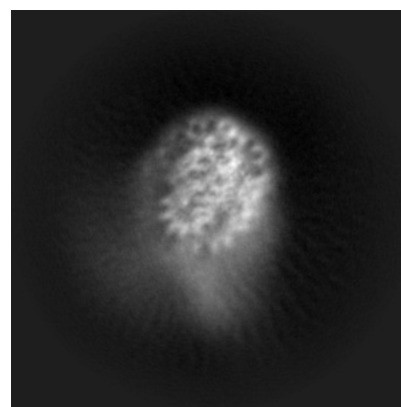
6.1.2 Raw map



X



Y

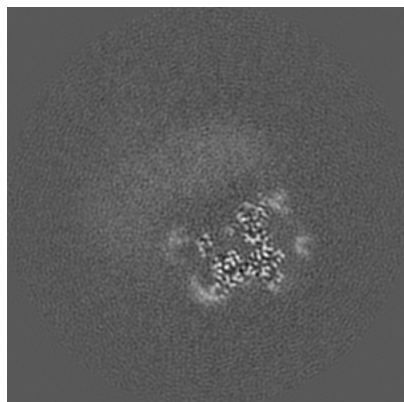


Z

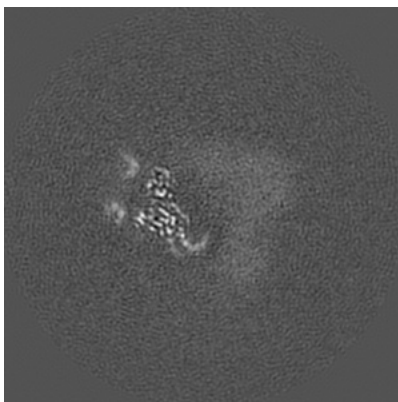
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

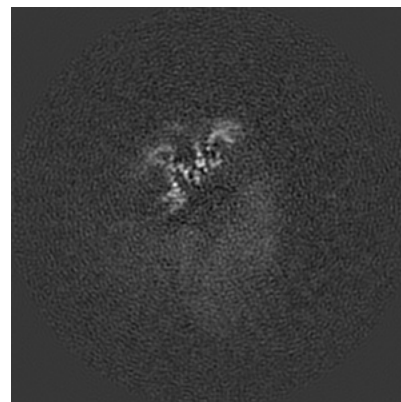
6.2.1 Primary map



X Index: 140

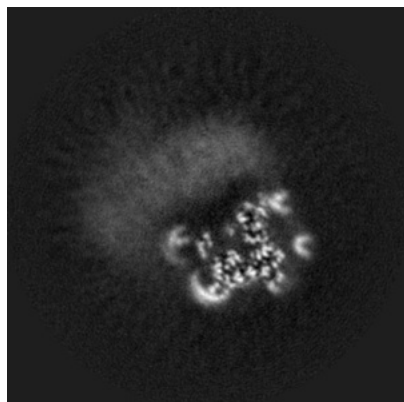


Y Index: 140

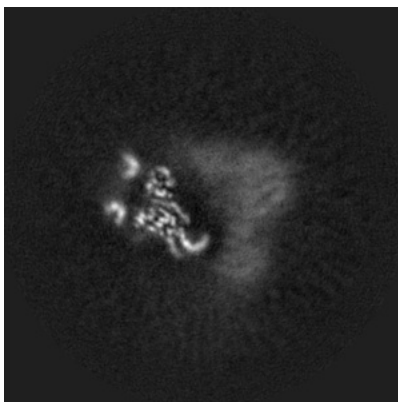


Z Index: 140

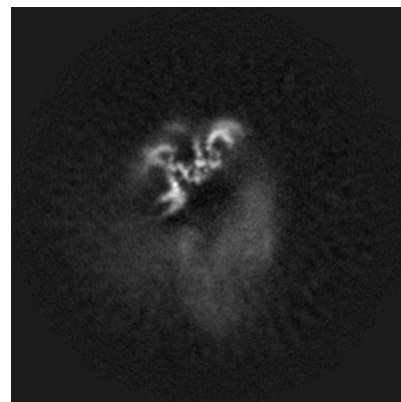
6.2.2 Raw map



X Index: 140



Y Index: 140

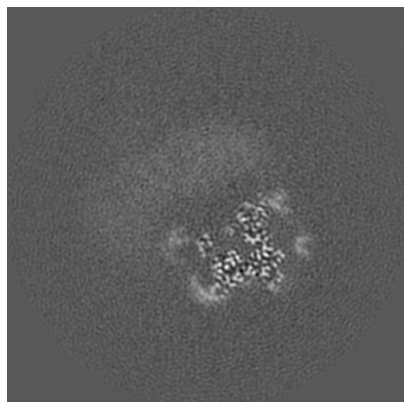


Z Index: 140

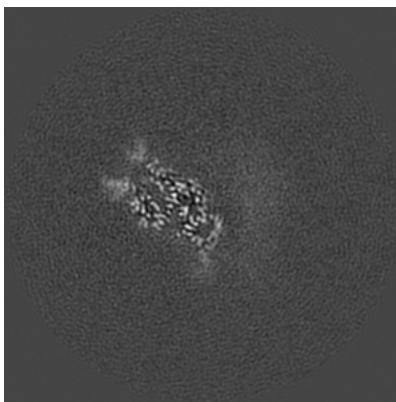
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

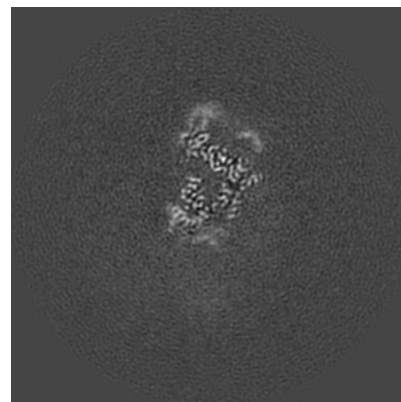
6.3.1 Primary map



X Index: 140

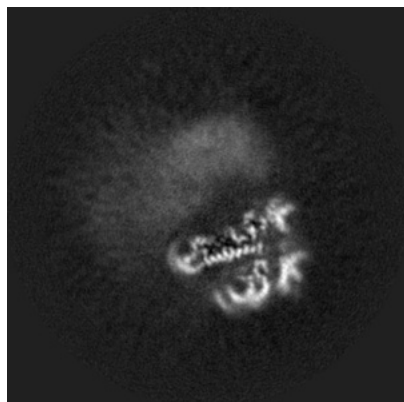


Y Index: 171

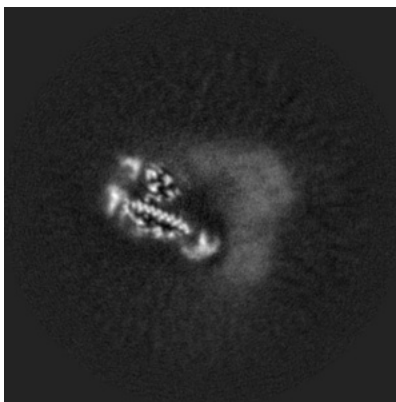


Z Index: 117

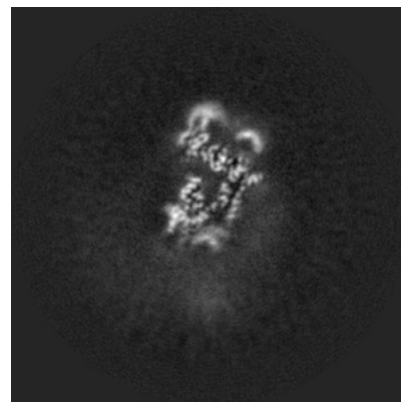
6.3.2 Raw map



X Index: 154



Y Index: 147

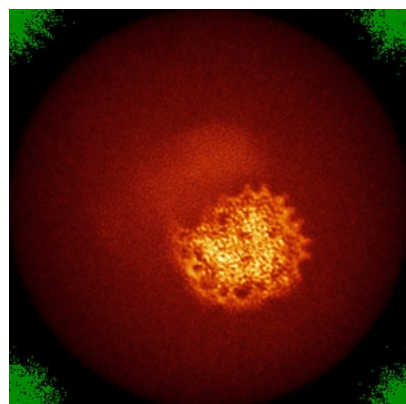


Z Index: 117

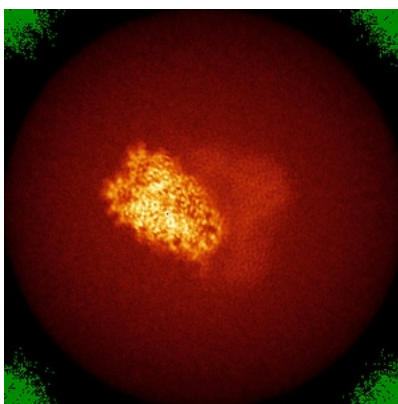
The images above show the largest variance slices of the map in three orthogonal directions.

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

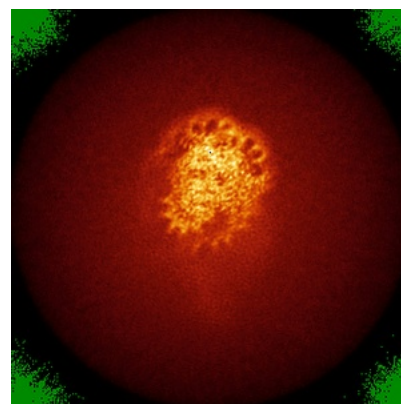
6.4.1 Primary map



X

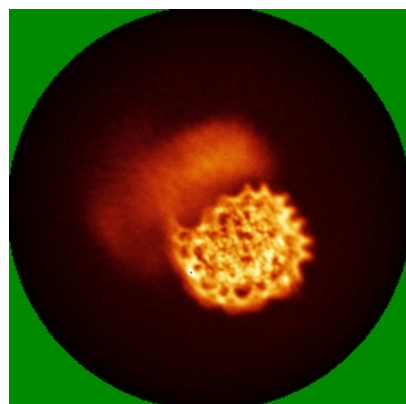


Y

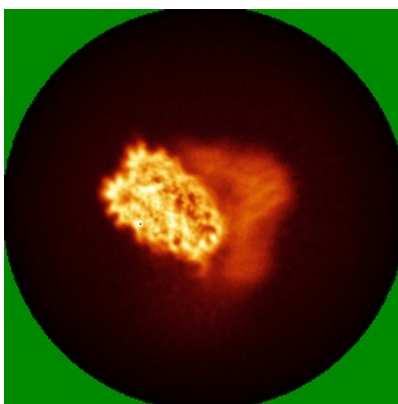


Z

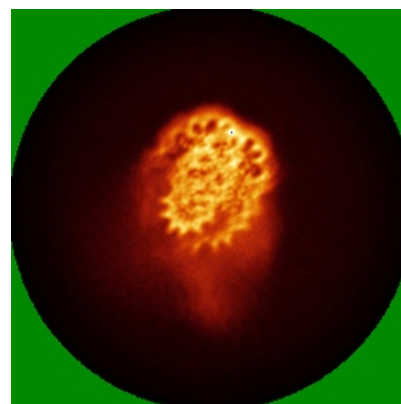
6.4.2 Raw map



X



Y

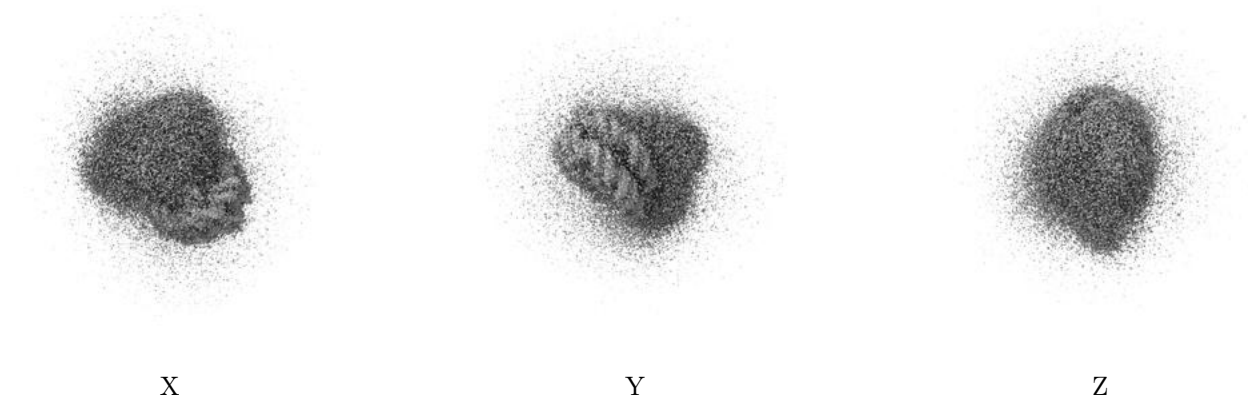


Z

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.

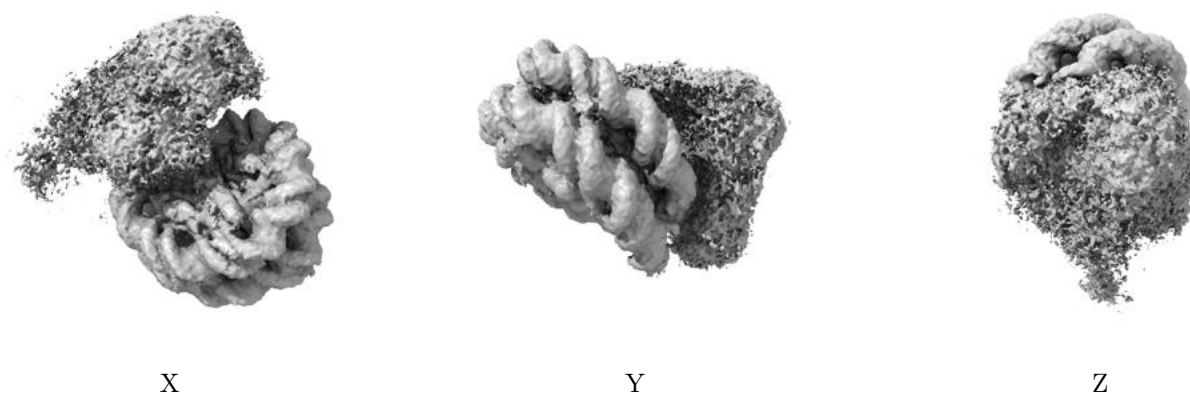
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

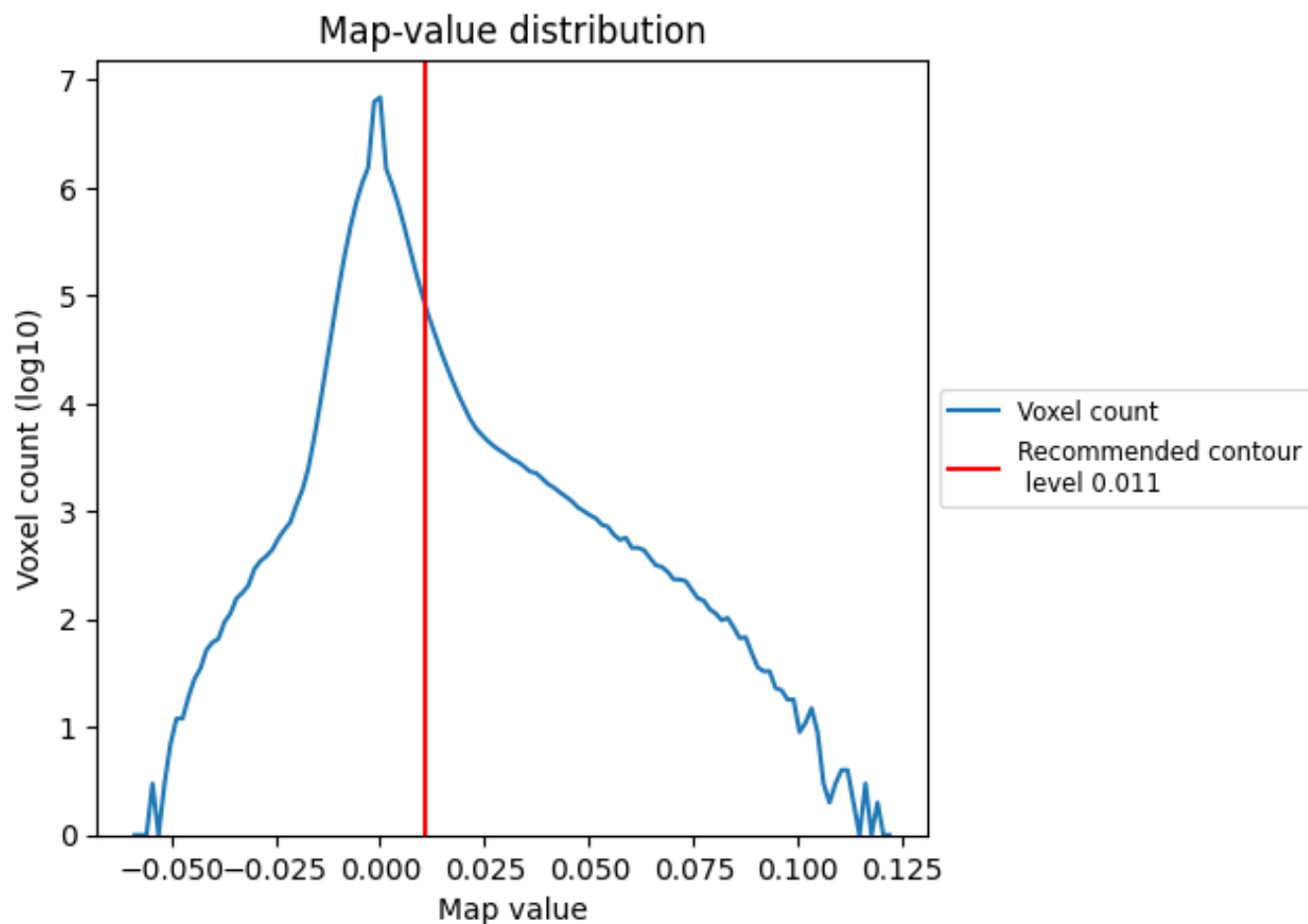
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

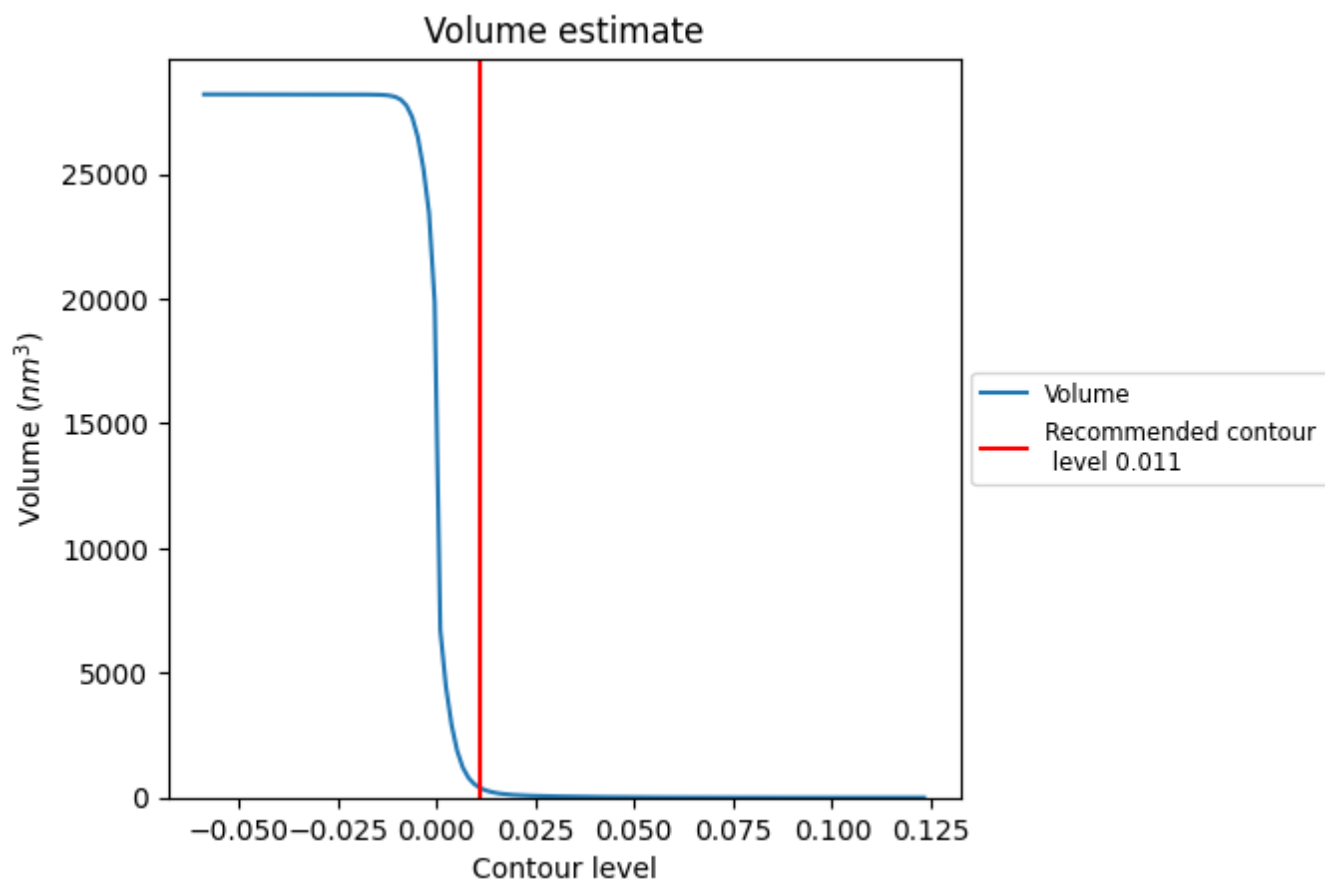
This section contains the results of statistical analysis of the map.

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.

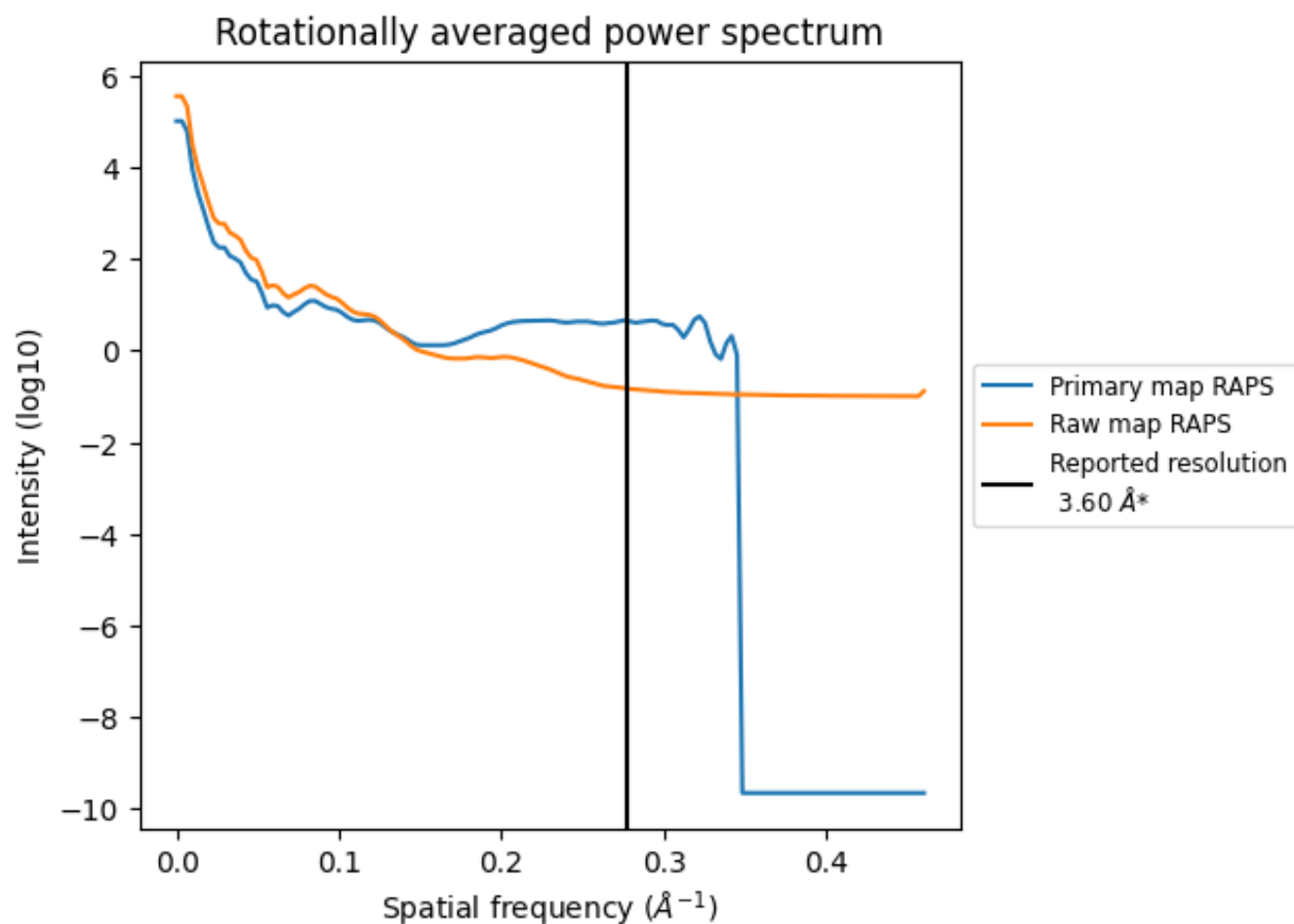
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 393 nm^3 ; this corresponds to an approximate mass of 355 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 ⓘ

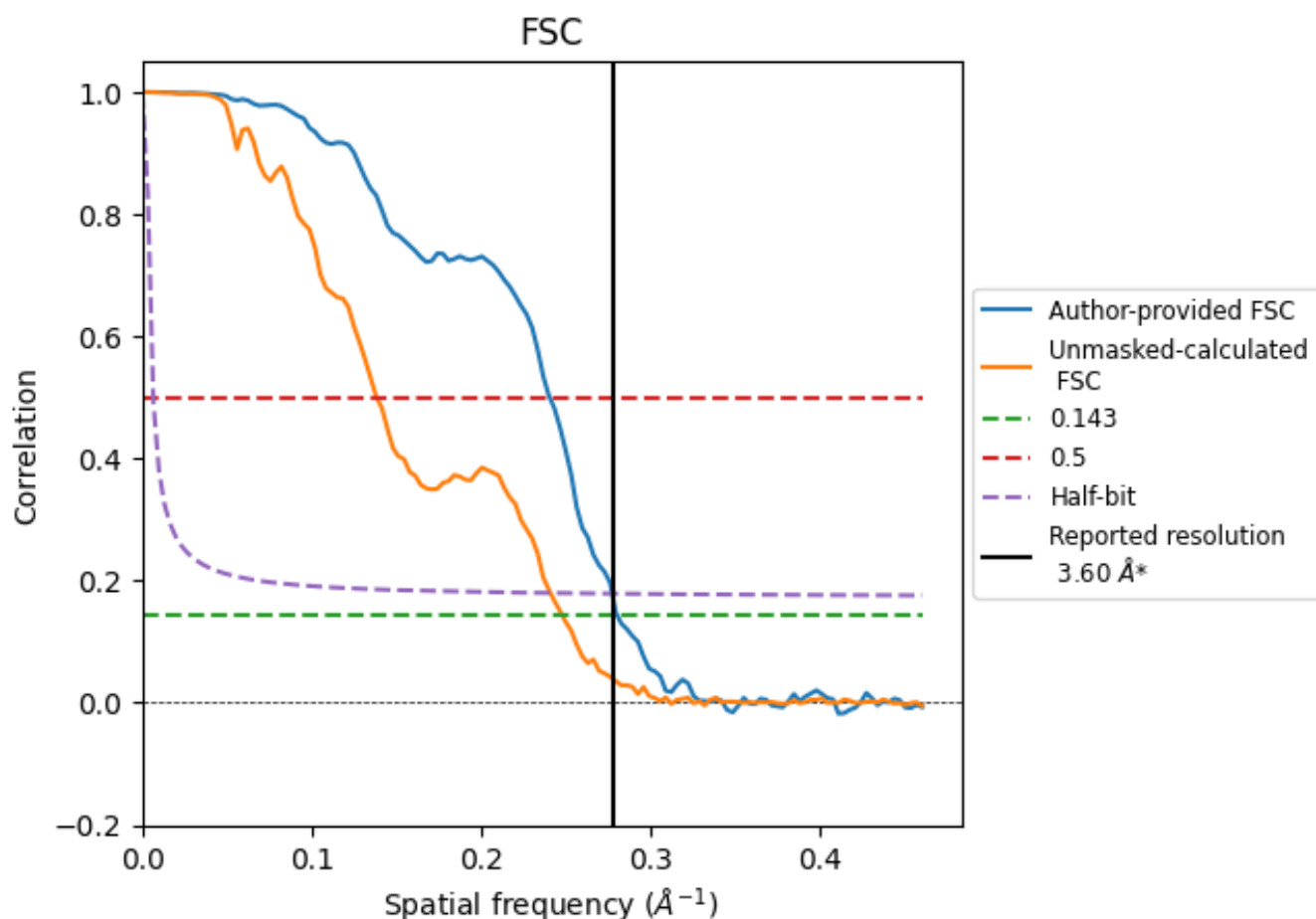


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

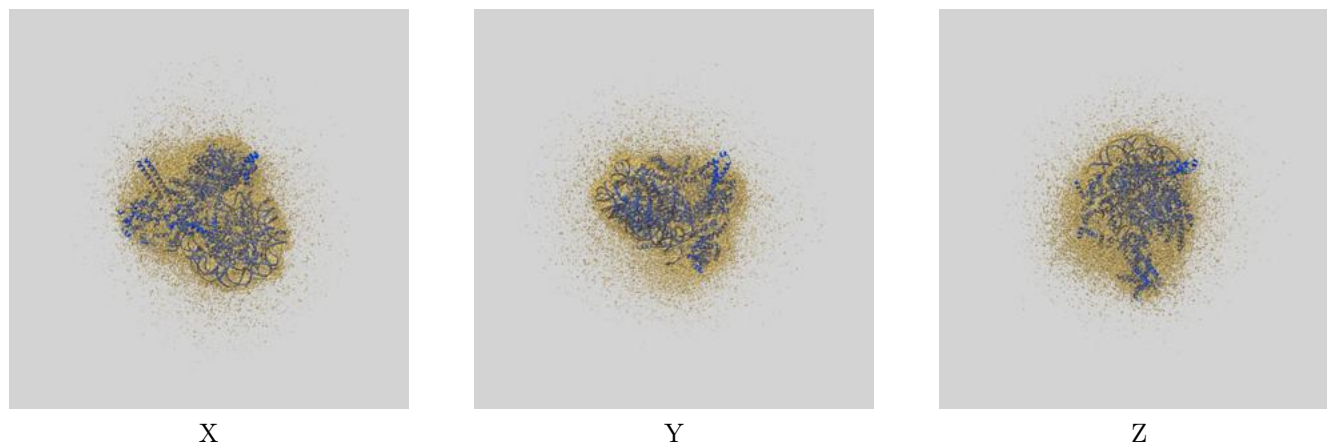
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.16	3.61
Unmasked-calculated*	4.04	7.24	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

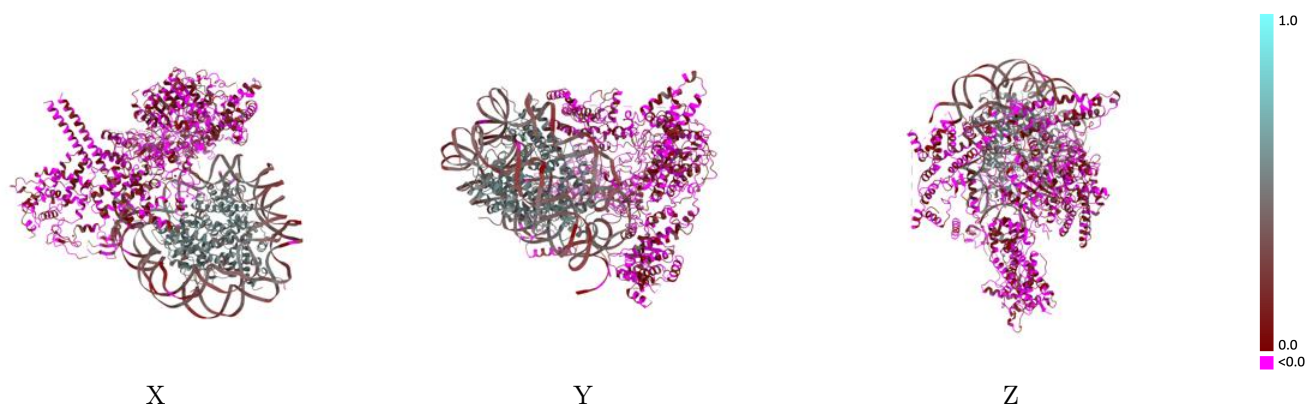
This section contains information regarding the fit between EMDB map EMD-37366 and PDB model 8W9E. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



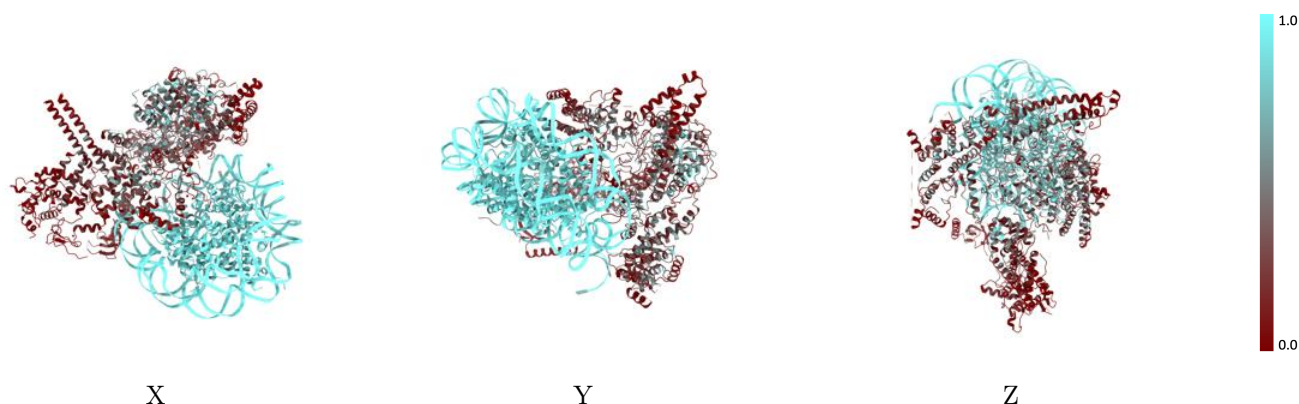
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



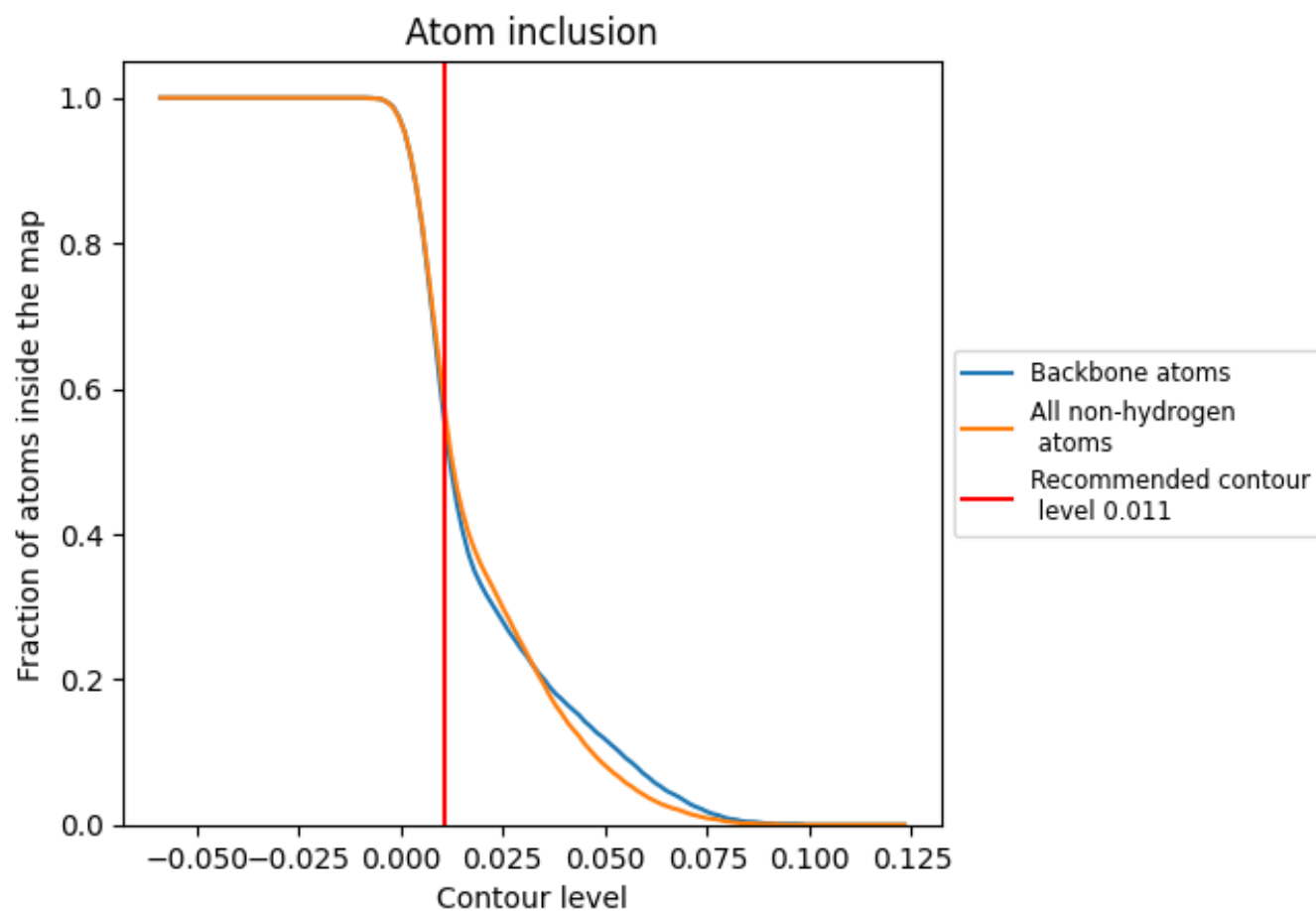
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion ⓘ



At the recommended contour level, 54% of all backbone atoms, 56% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5620	 0.1880
A	 0.2630	 0.0180
B	 0.4840	 0.0350
C	 0.3460	 0.0440
D	 0.1130	 -0.0030
E	 0.1990	 -0.0060
F	 0.0970	 -0.0260
G	 0.0720	 0.0050
a	 0.9510	 0.5200
b	 0.9640	 0.5420
c	 0.9220	 0.5050
d	 0.9330	 0.4960
e	 0.9410	 0.5090
f	 0.9490	 0.5300
g	 0.9470	 0.5060
h	 0.9400	 0.5060
i	 0.9520	 0.3210
j	 0.9600	 0.3240

