



Full wwPDB EM Validation Report ⓘ

May 6, 2024 – 04:18 AM JST

PDB ID : 8W9D
EMDB ID : EMD-37365
Title : Cryo-EM structure of the Rpd3S-nucleosome complex from budding yeast in State 1
Authors : Wang, C.; Zhan, X.
Deposited on : 2023-09-05
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

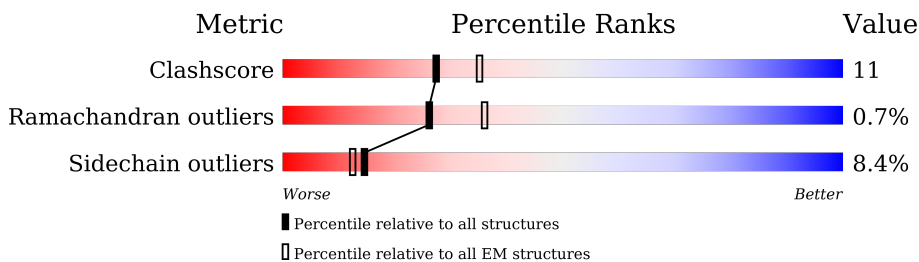
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	E	684	
2	F	684	
3	B	433	
4	C	401	
4	D	401	
4	G	401	
5	a	136	

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Mol	Chain	Length	Quality of chain
5	e	136	<p>7% 74% 9% 24%</p>
6	b	103	<p>71% 9% 20%</p>
6	f	103	<p>71% 9% 20%</p>
7	c	130	<p>78% 9% 18%</p>
7	g	130	<p>80% 9% 17%</p>
8	d	126	<p>6% 69% 6% 25%</p>
8	h	126	<p>74% 9% 25%</p>
9	i	147	<p>99%</p>
10	j	147	<p>100%</p>
11	H	5	<p>60% 40%</p>

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 27990 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
			Total	C	N	O	S		
1	A	606	5066	3253	860	938	15	0	0

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

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

- Molecule 3 is a protein called Histone deacetylase RPD3.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	a	97	801	505	155	137	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	104	Total	C	N	O	S	0	0
			857	538	168	147	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
6	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	c	106	Total	C	N	O	0	0
			812	513	157	142		
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	95	Total	C	N	O	S	0	0
			744	467	136	139	2		
8	h	95	Total	C	N	O	S	0	0
			744	467	136	139	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 a protein called Unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	H	5	29	18	6	5	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

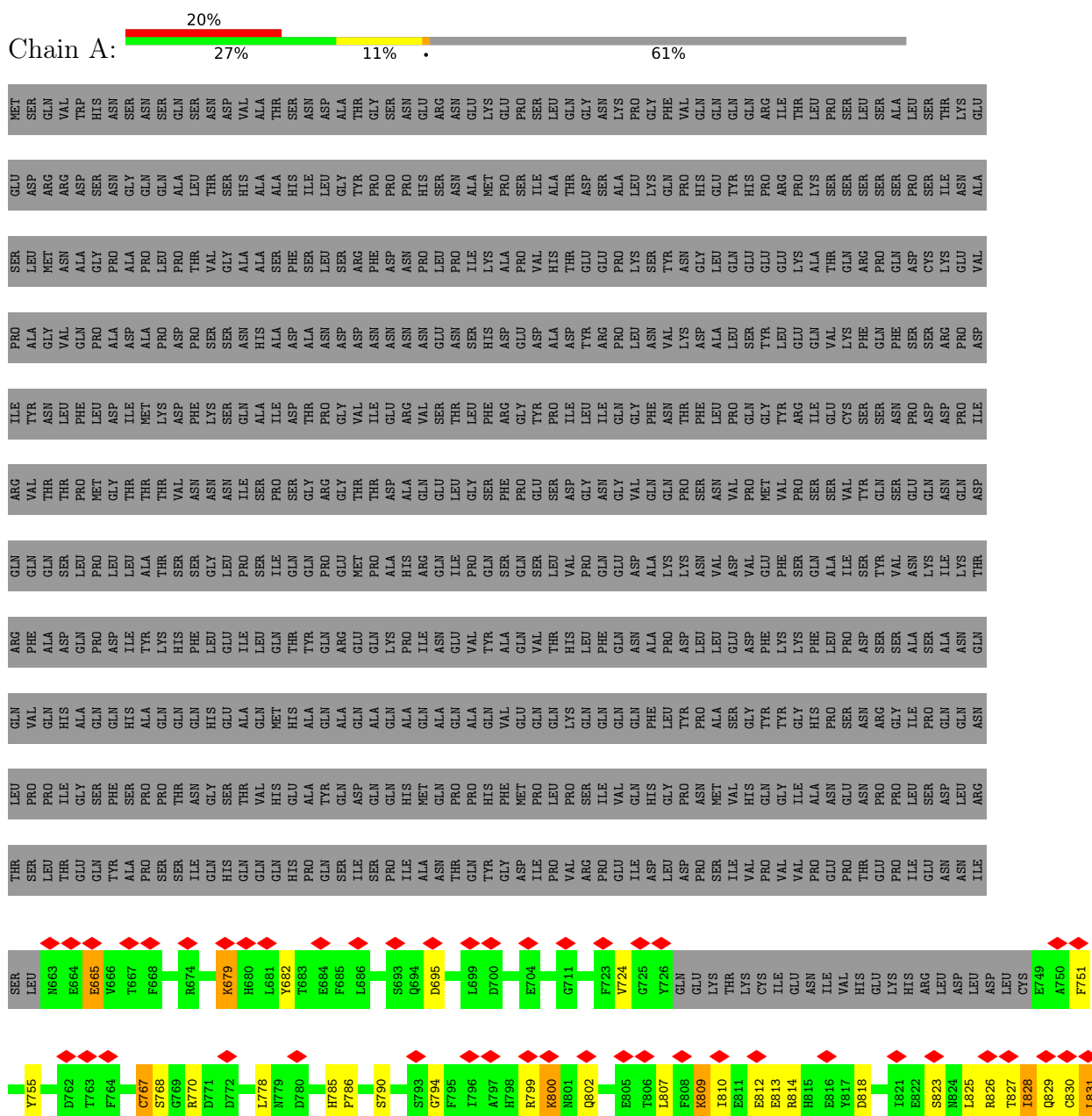
- Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

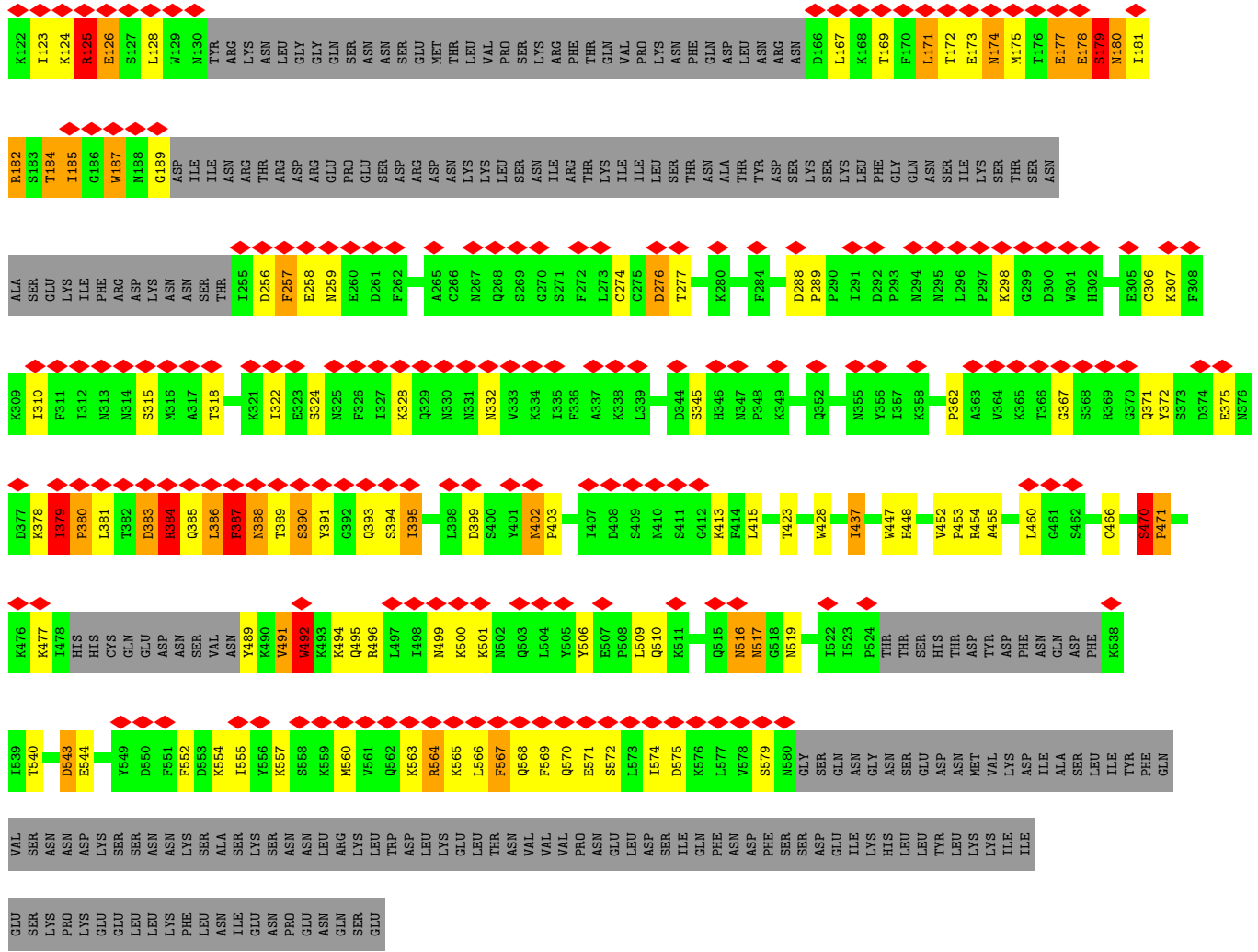
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
13	B	2	2	2	0

3 Residue-property plots

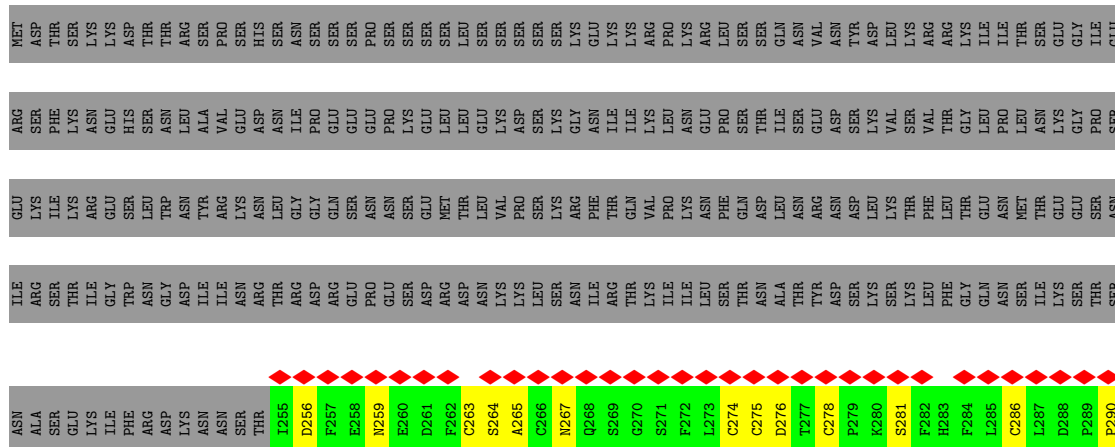
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

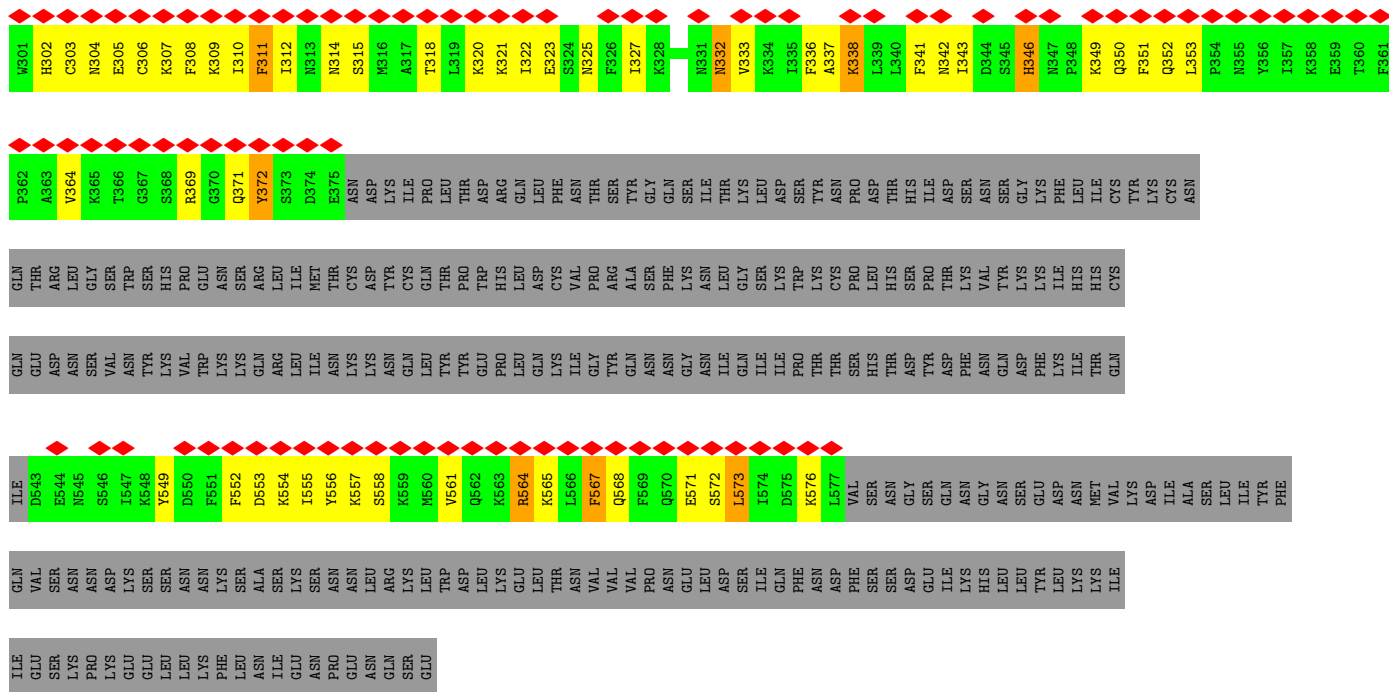
- Molecule 1: Transcriptional regulatory protein SIN3



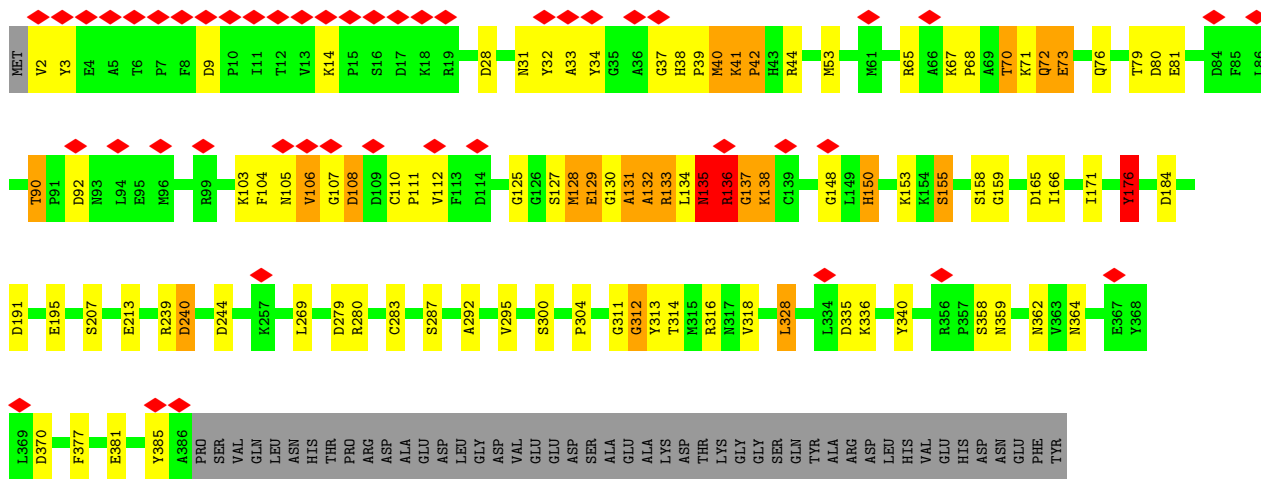


● Molecule 2: Transcriptional regulatory protein RCO1

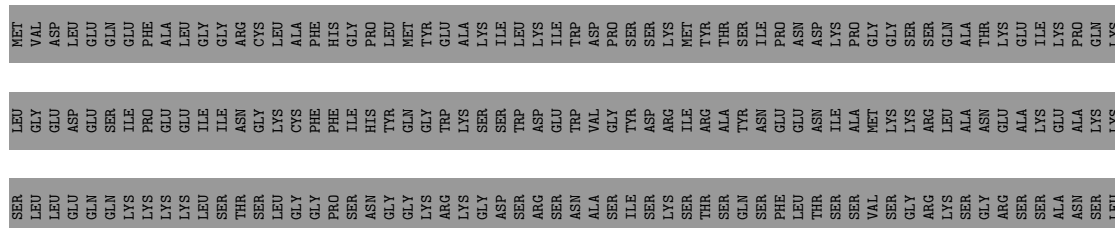
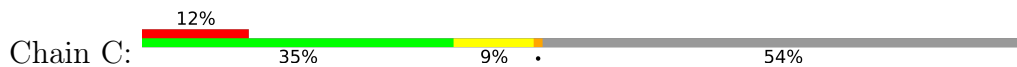


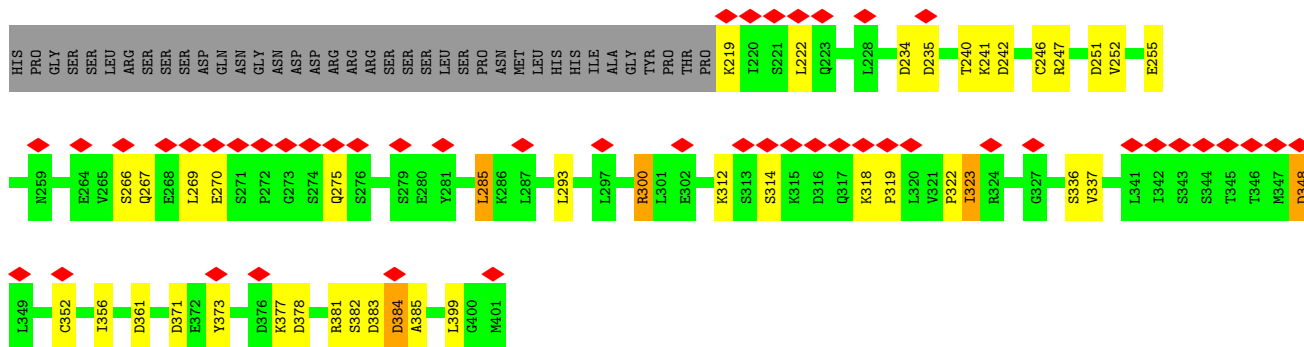


• Molecule 3: Histone deacetylase RPD3

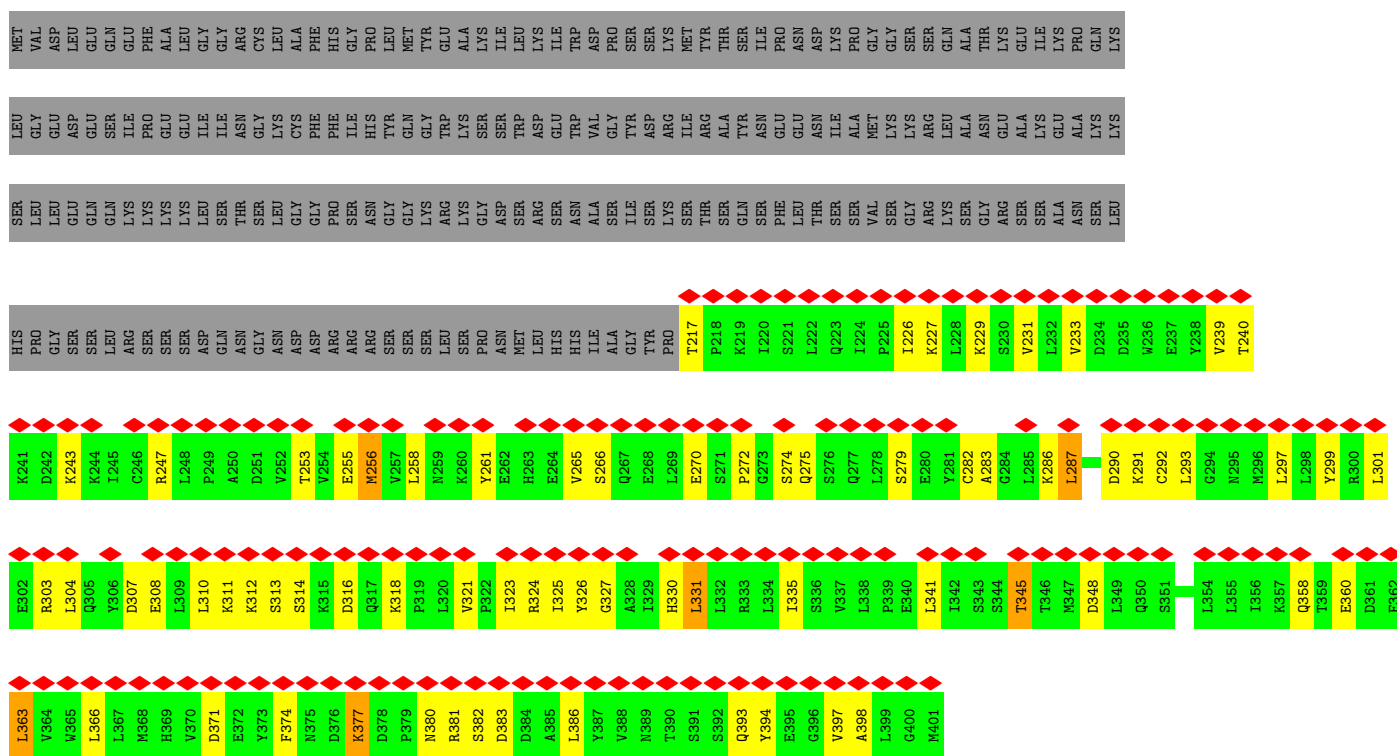
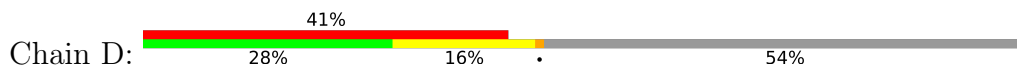


• Molecule 4: Chromatin modification-related protein EAF3

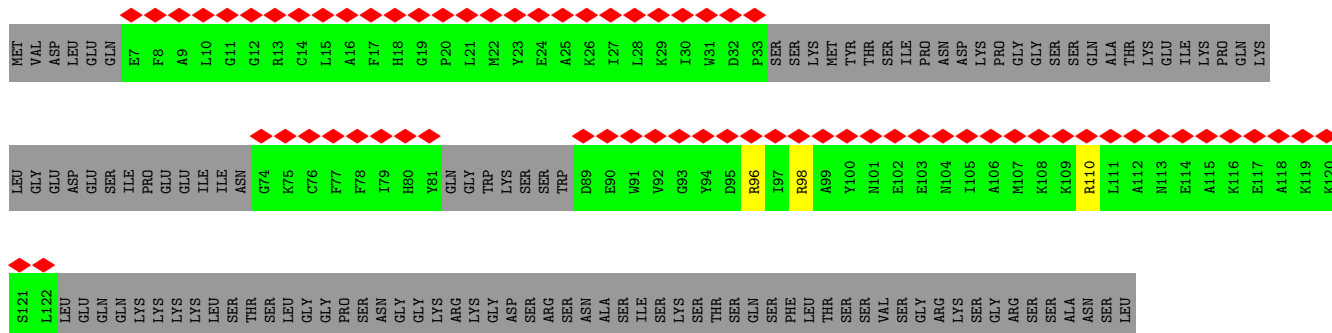


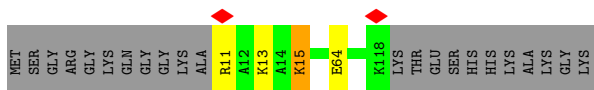


● Molecule 4: Chromatin modification-related protein EAF3

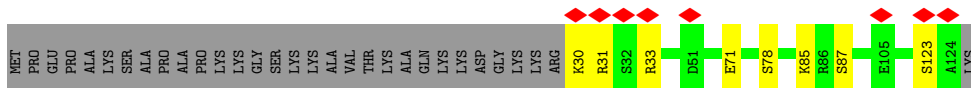


● Molecule 4: Chromatin modification-related protein EAF3

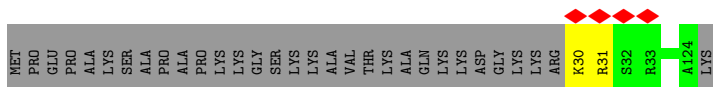




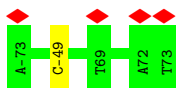
● Molecule 8: Histone H2B type 1-K



● Molecule 8: Histone H2B type 1-K



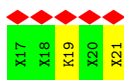
● Molecule 9: 5-DNA



● Molecule 10: 3-DNA



● Molecule 11: Unclear peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	422198	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	0.078	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (\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 (\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: K, 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	0.46	7/5180 (0.1%)	0.54	5/6984 (0.1%)
2	E	0.68	4/2952 (0.1%)	0.97	18/3978 (0.5%)
2	F	0.27	0/1313	0.47	0/1763
3	B	1.07	37/3137 (1.2%)	0.86	19/4246 (0.4%)
4	C	0.30	0/1509	0.48	0/2039
4	D	0.26	0/1524	0.49	0/2061
4	G	0.70	0/583	0.97	3/777 (0.4%)
5	a	0.41	0/813	0.43	0/1090
5	e	0.46	0/868	0.55	0/1160
6	b	0.45	0/660	0.50	0/883
6	f	0.46	0/660	0.64	0/883
7	c	0.46	0/822	0.53	0/1109
7	g	0.40	0/838	0.53	1/1130 (0.1%)
8	d	0.41	0/755	0.49	0/1014
8	h	0.41	0/755	0.51	0/1014
9	i	0.79	0/3378	1.00	1/5212 (0.0%)
10	j	0.80	0/3376	1.00	0/5209
11	H	1.17	0/8	1.69	0/8
All	All	0.65	48/29131 (0.2%)	0.76	47/40560 (0.1%)

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
2	E	0	4
3	B	0	6
All	All	0	10

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	380	PRO	N-CA	13.10	1.69	1.47
1	A	920	GLU	C-O	-11.75	1.01	1.23
3	B	42	PRO	C-O	-10.80	1.01	1.23
3	B	127	SER	CA-CB	-10.55	1.37	1.52
3	B	130	GLY	C-O	-10.10	1.07	1.23
3	B	158	SER	C-O	-10.03	1.04	1.23
3	B	131	ALA	C-O	-9.92	1.04	1.23
1	A	923	VAL	C-O	-9.78	1.04	1.23
3	B	111	PRO	C-O	-9.68	1.03	1.23
3	B	129	GLU	CD-OE1	-9.61	1.15	1.25
3	B	73	GLU	CD-OE2	-9.15	1.15	1.25
3	B	159	GLY	C-O	-9.05	1.09	1.23
3	B	68	PRO	C-O	-9.02	1.05	1.23
3	B	73	GLU	C-O	-8.70	1.06	1.23
3	B	314	THR	C-O	-8.59	1.07	1.23
3	B	71	LYS	C-O	-8.46	1.07	1.23
3	B	176	TYR	C-O	-8.00	1.08	1.23
3	B	72	GLN	C-O	-7.72	1.08	1.23
3	B	105	ASN	C-O	-7.53	1.09	1.23
3	B	128	MET	C-O	-7.42	1.09	1.23
3	B	41	LYS	C-O	-7.14	1.09	1.23
3	B	132	ALA	C-O	-7.00	1.10	1.23
3	B	67	LYS	C-O	-6.97	1.10	1.23
3	B	133	ARG	C-O	-6.83	1.10	1.23
3	B	127	SER	C-O	-6.80	1.10	1.23
3	B	73	GLU	CD-OE1	-6.74	1.18	1.25
3	B	158	SER	CA-CB	-6.73	1.42	1.52
3	B	127	SER	CB-OG	-6.72	1.33	1.42
1	A	915	VAL	C-O	-6.69	1.10	1.23
3	B	312	GLY	C-O	-6.48	1.13	1.23
2	E	179	SER	CA-CB	-6.43	1.43	1.52
1	A	921	GLN	C-O	-6.40	1.11	1.23
1	A	917	ARG	C-O	-6.21	1.11	1.23
3	B	135	ASN	C-O	-6.20	1.11	1.23
3	B	280	ARG	C-O	-6.15	1.11	1.23
3	B	136	ARG	C-O	-5.94	1.12	1.23
3	B	112	VAL	C-O	-5.85	1.12	1.23
3	B	111	PRO	N-CD	-5.82	1.39	1.47
3	B	128	MET	CG-SD	-5.78	1.66	1.81
3	B	106	VAL	C-O	-5.39	1.13	1.23
3	B	129	GLU	CB-CG	-5.39	1.42	1.52
3	B	110	CYS	C-O	-5.37	1.13	1.23
2	E	109	SER	CA-CB	-5.34	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	922	LYS	C-O	-5.33	1.13	1.23
3	B	32	TYR	C-O	-5.29	1.13	1.23
1	A	918	GLU	CD-OE1	-5.25	1.19	1.25
3	B	133	ARG	CD-NE	-5.20	1.37	1.46
2	E	184	THR	C-O	-5.02	1.13	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	384	ARG	CB-CA-C	15.81	142.01	110.40
2	E	379	ILE	O-C-N	-9.56	102.94	121.10
3	B	129	GLU	CB-CA-C	-8.73	92.93	110.40
3	B	133	ARG	CG-CD-NE	-8.46	94.05	111.80
3	B	280	ARG	CB-CG-CD	-8.25	90.15	111.60
3	B	136	ARG	C-N-CA	8.20	139.52	122.30
3	B	314	THR	OG1-CB-CG2	-8.01	91.57	110.00
2	E	383	ASP	CB-CA-C	7.58	125.56	110.40
1	A	922	LYS	CB-CA-C	-7.55	95.29	110.40
1	A	917	ARG	CB-CG-CD	-7.43	92.28	111.60
2	E	182	ARG	CB-CG-CD	-7.40	92.37	111.60
2	E	184	THR	OG1-CB-CG2	-7.29	93.23	110.00
3	B	105	ASN	CB-CA-C	7.16	124.73	110.40
2	E	393	GLN	C-N-CA	7.15	139.58	121.70
3	B	138	LYS	C-N-CA	7.00	139.20	121.70
3	B	135	ASN	O-C-N	-6.92	111.62	122.70
3	B	135	ASN	CB-CA-C	-6.86	96.67	110.40
3	B	34	TYR	CB-CA-C	-6.76	96.87	110.40
2	E	387	PHE	N-CA-CB	6.67	122.60	110.60
2	E	379	ILE	CA-C-N	6.45	135.17	117.10
1	A	917	ARG	CB-CA-C	-6.42	97.57	110.40
3	B	313	TYR	CB-CA-C	6.41	123.22	110.40
2	E	125	ARG	CB-CA-C	-6.39	97.62	110.40
4	G	96	ARG	NE-CZ-NH1	6.35	123.47	120.30
3	B	133	ARG	CB-CA-C	-6.21	97.98	110.40
3	B	137	GLY	C-N-CA	-6.12	106.39	121.70
4	G	98	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	E	257	PHE	CB-CA-C	-5.98	98.44	110.40
2	E	394	SER	C-N-CA	5.86	136.35	121.70
7	g	15	LYS	CB-CA-C	-5.82	98.76	110.40
2	E	172	THR	CA-CB-OG1	5.73	121.03	109.00
3	B	41	LYS	N-CA-CB	-5.61	100.51	110.60
2	E	393	GLN	CB-CA-C	5.52	121.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	176	TYR	CB-CA-C	5.43	121.26	110.40
1	A	921	GLN	CB-CA-C	-5.36	99.67	110.40
2	E	384	ARG	CB-CG-CD	5.36	125.53	111.60
3	B	127	SER	N-CA-CB	-5.33	102.50	110.50
2	E	110	VAL	CG1-CB-CG2	-5.28	102.46	110.90
3	B	176	TYR	N-CA-CB	-5.22	101.20	110.60
4	G	110	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	E	182	ARG	CB-CA-C	-5.13	100.13	110.40
9	i	-49	DC	O4'-C1'-N1	5.10	111.57	108.00
3	B	138	LYS	N-CA-C	5.10	124.76	111.00
1	A	913	ASN	O-C-N	-5.08	114.57	122.70
2	E	174	ASN	CB-CA-C	-5.07	100.26	110.40
2	E	389	THR	CB-CA-C	5.03	125.19	111.60
3	B	328	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	131	ALA	Mainchain
3	B	132	ALA	Mainchain
3	B	135	ASN	Mainchain
3	B	176	TYR	Mainchain
3	B	33	ALA	Mainchain
3	B	70	THR	Mainchain
2	E	379	ILE	Mainchain
2	E	428	TRP	Peptide
2	E	470	SER	Peptide
2	E	492	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5066	0	5024	119	0
2	E	2884	0	2833	119	0
2	F	1282	0	1245	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3057	0	2934	56	0
4	C	1483	0	1510	23	0
4	D	1497	0	1524	50	0
4	G	570	0	563	0	0
5	a	801	0	839	0	0
5	e	857	0	904	0	0
6	b	653	0	696	0	0
6	f	653	0	696	0	0
7	c	812	0	867	0	0
7	g	828	0	885	0	0
8	d	744	0	768	0	0
8	h	744	0	769	0	0
9	i	3011	0	1662	0	0
10	j	3010	0	1663	0	0
11	H	29	0	19	4	0
12	B	1	0	0	0	0
12	E	4	0	0	0	0
12	F	2	0	0	0	0
13	B	2	0	0	1	0
All	All	27990	0	25401	364	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 11.

All (364) 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)
2:E:380:PRO:N	2:E:380:PRO:CA	1.69	1.31
2:E:178:GLU:OE1	3:B:65:ARG:NH1	1.67	1.26
2:E:184:THR:OG1	3:B:73:GLU:OE1	1.68	1.08
2:E:167:LEU:HD21	3:B:340:TYR:CE1	2.03	0.93
1:A:912:TRP:HH2	2:E:113:LEU:HD13	1.36	0.88
3:B:38:HIS:HA	11:H:21:UNK:C	2.05	0.87
4:C:240:THR:O	4:C:242:ASP:N	2.09	0.86
3:B:184:ASP:OD2	13:B:1001:K:K	1.87	0.85
2:E:381:LEU:HB3	2:E:384:ARG:HB2	1.59	0.85
1:A:918:GLU:OE1	2:E:128:LEU:HD12	1.78	0.84
2:E:447:TRP:NE1	2:E:466:CYS:SG	2.51	0.84
3:B:39:PRO:HD2	11:H:21:UNK:C	2.10	0.82
2:E:495:GLN:H	2:E:519:ASN:HD21	1.27	0.80
1:A:794:GLY:HA2	2:E:460:LEU:HD13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:108:ASP:OD2	3:B:108:ASP:N	2.13	0.79
2:E:259:ASN:ND2	2:E:274:CYS:HB3	1.97	0.79
2:E:384:ARG:HA	2:E:387:PHE:HB3	1.65	0.77
3:B:38:HIS:HA	11:H:21:UNK:O	1.84	0.77
2:E:189:GLY:HA2	3:B:72:GLN:HB2	1.68	0.75
1:A:767:CYS:SG	1:A:770:ARG:NH1	2.61	0.74
4:C:318:LYS:HE3	4:C:319:PRO:HD2	1.69	0.74
2:E:257:PHE:HZ	2:E:276:ASP:O	1.72	0.73
1:A:828:ILE:HD11	1:A:899:LYS:HD3	1.69	0.72
2:E:362:PRO:HG3	2:E:499:ASN:HB3	1.72	0.72
2:E:259:ASN:ND2	2:E:274:CYS:CB	2.52	0.72
4:D:240:THR:HG21	2:F:372:TYR:H	1.53	0.71
1:A:831:LEU:HB3	1:A:895:LEU:HD13	1.72	0.71
2:E:259:ASN:ND2	2:E:274:CYS:SG	2.63	0.71
2:E:258:GLU:HA	2:E:258:GLU:OE2	1.88	0.71
4:D:303:ARG:NH1	2:F:286:CYS:SG	2.64	0.70
2:E:113:LEU:HD12	2:E:113:LEU:N	2.07	0.70
2:E:167:LEU:HD21	3:B:340:TYR:CD1	2.26	0.70
1:A:885:GLU:OE1	1:A:886:HIS:ND1	2.24	0.70
4:C:300:ARG:NH2	4:C:399:LEU:O	2.25	0.69
4:D:371:ASP:O	4:D:377:LYS:NZ	2.24	0.69
1:A:919:LEU:HD12	1:A:919:LEU:O	1.92	0.69
2:E:187:TRP:HE3	2:E:187:TRP:N	1.91	0.69
2:E:257:PHE:CZ	2:E:276:ASP:O	2.45	0.69
4:D:243:LYS:HE3	4:D:301:LEU:HD23	1.75	0.69
2:F:275:CYS:SG	2:F:276:ASP:N	2.66	0.68
2:F:320:LYS:HA	2:F:323:GLU:HG2	1.75	0.68
2:E:381:LEU:HD22	2:E:384:ARG:HE	1.58	0.68
3:B:90:THR:HG23	3:B:92:ASP:H	1.59	0.68
4:C:222:LEU:HD12	4:C:356:ILE:HG23	1.77	0.67
1:A:929:ASP:HB3	1:A:1234:ASN:HB3	1.76	0.67
2:E:384:ARG:HG3	2:E:387:PHE:HB3	1.75	0.66
2:E:367:GLY:HA3	2:E:371:GLN:HG3	1.78	0.66
2:E:395:ILE:HD12	2:E:399:ASP:HB2	1.78	0.66
4:D:287:LEU:HB3	4:D:291:LYS:HE3	1.77	0.65
2:F:318:THR:O	2:F:322:ILE:HG13	1.96	0.65
2:E:384:ARG:HB3	2:E:387:PHE:HD2	1.61	0.65
1:A:912:TRP:CH2	2:E:113:LEU:HD13	2.25	0.65
1:A:912:TRP:HH2	2:E:113:LEU:CD1	2.07	0.65
2:E:189:GLY:HA2	3:B:72:GLN:CB	2.27	0.65
2:E:180:ASN:HB2	2:E:185:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:184:THR:HG21	3:B:76:GLN:HE22	1.61	0.64
2:E:380:PRO:N	2:E:380:PRO:C	2.49	0.64
4:D:247:ARG:NH2	4:D:382:SER:O	2.29	0.64
2:E:121:GLU:O	2:E:125:ARG:HG2	1.98	0.64
4:D:226:ILE:HA	4:D:229:LYS:HE2	1.78	0.64
2:E:371:GLN:HA	4:C:240:THR:HG21	1.79	0.64
1:A:695:ASP:OD1	2:E:554:LYS:NZ	2.31	0.64
2:E:259:ASN:HD21	2:E:274:CYS:HB3	1.62	0.64
1:A:1069:LEU:HD11	1:A:1266:MET:HB2	1.80	0.63
1:A:868:ARG:HD2	1:A:873:LYS:HZ3	1.61	0.63
2:E:124:LYS:O	2:E:124:LYS:HG3	1.98	0.63
1:A:1066:LEU:HB2	1:A:1270:VAL:HG11	1.81	0.63
4:C:378:ASP:OD2	4:C:381:ARG:NH2	2.32	0.62
2:E:496:ARG:NH2	4:C:234:ASP:OD1	2.31	0.62
3:B:72:GLN:O	3:B:72:GLN:HG2	1.98	0.62
1:A:851:LEU:HG	1:A:887:PRO:HG3	1.82	0.62
4:D:266:SER:O	4:D:275:GLN:NE2	2.34	0.61
2:E:506:TYR:OH	4:D:348:ASP:OD2	2.18	0.61
2:F:321:LYS:NZ	2:F:321:LYS:O	2.33	0.61
2:E:517:ASN:ND2	2:E:519:ASN:OD1	2.33	0.61
2:E:180:ASN:C	2:E:180:ASN:HD22	2.00	0.61
1:A:1199:VAL:O	1:A:1201:GLU:N	2.34	0.61
1:A:828:ILE:HD12	1:A:898:LEU:HB3	1.81	0.61
1:A:1302:ARG:NH1	1:A:1315:GLN:OE1	2.34	0.61
2:E:543:ASP:OD1	2:E:543:ASP:N	2.34	0.61
2:E:189:GLY:HA3	3:B:70:THR:HB	1.83	0.60
1:A:826:ARG:HG3	3:B:31:ASN:HD21	1.67	0.60
1:A:1066:LEU:HA	1:A:1069:LEU:HB2	1.83	0.60
2:F:565:LYS:HA	2:F:568:GLN:HE21	1.65	0.60
3:B:39:PRO:CD	11:H:21:UNK:C	2.80	0.60
1:A:851:LEU:HD13	1:A:855:LEU:HG	1.84	0.59
3:B:106:VAL:HG12	3:B:106:VAL:O	2.01	0.59
1:A:812:GLU:OE2	3:B:37:GLY:HA2	2.02	0.59
3:B:312:GLY:HA3	3:B:318:VAL:HG21	1.85	0.59
2:E:187:TRP:N	2:E:187:TRP:CE3	2.71	0.59
2:E:171:LEU:O	2:E:173:GLU:N	2.36	0.58
2:E:180:ASN:ND2	2:E:180:ASN:O	2.35	0.58
1:A:921:GLN:HG2	1:A:1188:SER:HB2	1.84	0.58
2:E:167:LEU:CD2	3:B:340:TYR:CD1	2.86	0.58
2:E:184:THR:OG1	2:E:184:THR:O	2.15	0.58
2:F:312:ILE:HG23	2:F:314:ASN:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:573:LEU:HA	2:F:576:LYS:HG3	1.84	0.58
2:E:182:ARG:HD3	3:B:128:MET:HE2	1.85	0.58
1:A:919:LEU:HD12	1:A:919:LEU:C	2.22	0.57
2:E:437:ILE:HG12	2:E:448:HIS:CD2	2.39	0.57
4:D:327:GLY:H	4:D:330:HIS:CE1	2.22	0.57
2:E:107:LYS:HG3	2:E:107:LYS:O	2.05	0.57
4:D:394:TYR:O	4:D:398:ALA:HB2	2.04	0.57
1:A:768:SER:OG	3:B:80:ASP:OD1	2.23	0.57
1:A:826:ARG:NH2	3:B:28:ASP:OD1	2.38	0.57
2:E:372:TYR:OH	2:E:496:ARG:NH1	2.37	0.56
2:E:452:VAL:O	2:E:454:ARG:N	2.38	0.56
4:D:310:LEU:HD13	2:F:290:PRO:HD2	1.86	0.56
2:F:263:CYS:O	2:F:267:ASN:N	2.38	0.56
1:A:1005:PRO:O	1:A:1009:ARG:HG3	2.06	0.56
1:A:1071:ARG:O	1:A:1075:GLN:HG2	2.05	0.56
3:B:292:ALA:HB1	3:B:328:LEU:HD21	1.86	0.56
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.87	0.56
3:B:135:ASN:O	3:B:137:GLY:N	2.38	0.56
3:B:244:ASP:OD2	3:B:287:SER:OG	2.23	0.56
4:D:272:PRO:HB3	2:F:549:TYR:HB3	1.88	0.56
1:A:682:TYR:OH	2:E:544:GLU:OE2	2.20	0.55
3:B:44:ARG:NH1	3:B:311:GLY:O	2.39	0.55
1:A:986:TYR:HE1	1:A:1029:ILE:HD13	1.71	0.55
1:A:1002:TYR:HB3	1:A:1006:ASP:HB2	1.89	0.55
2:F:553:ASP:OD1	2:F:557:LYS:NZ	2.33	0.55
4:C:383:ASP:OD1	4:C:384:ASP:N	2.40	0.55
1:A:1335:LYS:HA	1:A:1338:VAL:HG22	1.87	0.55
3:B:240:ASP:OD1	3:B:240:ASP:N	2.40	0.55
2:F:306:CYS:O	2:F:310:ILE:HG12	2.07	0.55
1:A:965:HIS:NE2	1:A:967:LEU:HB2	2.22	0.54
1:A:814:ARG:NH1	1:A:913:ASN:OD1	2.39	0.54
2:E:460:LEU:HD12	3:B:213:GLU:HG2	1.90	0.54
2:E:517:ASN:HB3	2:E:519:ASN:H	1.72	0.54
1:A:1003:SER:O	1:A:1007:LYS:HG3	2.08	0.54
1:A:1067:ASP:O	1:A:1073:ARG:HB2	2.08	0.54
2:E:560:MET:HG2	2:E:564:ARG:HH12	1.73	0.54
1:A:1064:SER:OG	1:A:1065:LEU:N	2.40	0.54
2:E:126:GLU:O	2:E:126:GLU:HG3	2.08	0.53
4:D:275:GLN:HE22	2:F:552:PHE:HB3	1.74	0.53
2:E:387:PHE:CD1	2:E:387:PHE:C	2.82	0.52
2:E:491:VAL:HG12	2:E:492:TRP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:335:ASP:OD1	3:B:336:LYS:N	2.43	0.52
1:A:1141:ASN:OD1	1:A:1141:ASN:N	2.38	0.52
2:E:402:ASN:N	2:E:403:PRO:HD3	2.24	0.52
4:D:255:GLU:HB2	4:D:323:ILE:HG12	1.91	0.52
1:A:767:CYS:SG	1:A:770:ARG:HD2	2.50	0.52
4:D:256:MET:SD	4:D:256:MET:N	2.83	0.52
1:A:1281:LYS:NZ	1:A:1343:LEU:HB2	2.24	0.51
2:F:259:ASN:HD21	2:F:281:SER:HB3	1.75	0.51
4:D:217:THR:N	4:D:345:THR:O	2.43	0.51
1:A:1169:THR:HA	1:A:1172:ILE:HG22	1.90	0.51
3:B:134:LEU:HD22	3:B:304:PRO:HB3	1.90	0.51
2:E:106:SER:O	2:E:106:SER:OG	2.18	0.51
2:F:554:LYS:HA	2:F:557:LYS:HZ3	1.75	0.51
1:A:976:ASP:OD1	1:A:1313:SER:OG	2.24	0.51
2:F:274:CYS:HB2	2:F:281:SER:HB3	1.92	0.51
2:E:259:ASN:HD21	2:E:274:CYS:CB	2.19	0.50
2:F:312:ILE:HG23	2:F:314:ASN:N	2.27	0.50
2:E:384:ARG:HA	2:E:387:PHE:CB	2.38	0.50
2:E:470:SER:HB2	2:E:471:PRO:CD	2.42	0.50
1:A:918:GLU:OE1	2:E:128:LEU:CD1	2.54	0.50
2:E:318:THR:O	2:E:322:ILE:HD12	2.12	0.50
3:B:3:TYR:HB3	3:B:370:ASP:OD2	2.10	0.50
3:B:148:GLY:HA2	3:B:166:ILE:HD11	1.94	0.50
1:A:1068:ILE:HA	1:A:1074:TYR:HB2	1.94	0.49
1:A:1233:ASN:HD22	1:A:1235:LYS:HD3	1.76	0.49
4:C:348:ASP:N	4:C:348:ASP:OD1	2.45	0.49
2:E:381:LEU:HD22	2:E:384:ARG:NE	2.26	0.49
2:E:182:ARG:HD3	3:B:128:MET:CE	2.42	0.49
4:C:266:SER:O	4:C:275:GLN:NE2	2.44	0.49
2:E:516:ASN:ND2	2:E:540:THR:OG1	2.46	0.49
1:A:1065:LEU:HG	1:A:1069:LEU:HD23	1.94	0.49
2:E:560:MET:SD	2:F:557:LYS:HG2	2.53	0.49
1:A:874:GLU:CD	1:A:874:GLU:H	2.16	0.49
1:A:1343:LEU:HB3	1:A:1345:HIS:ND1	2.28	0.49
2:E:111:THR:HG22	2:E:113:LEU:H	1.77	0.49
2:E:180:ASN:ND2	2:E:180:ASN:N	2.59	0.49
2:E:570:GLN:O	2:E:574:ILE:HG23	2.13	0.49
4:D:321:VAL:HG22	4:D:323:ILE:HG22	1.95	0.49
2:E:181:ILE:HG22	3:B:129:GLU:OE1	2.13	0.49
2:E:385:GLN:OE1	2:E:385:GLN:HA	2.12	0.49
4:C:293:LEU:HD22	4:C:322:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:302:HIS:HB3	2:F:306:CYS:HB2	1.94	0.49
2:F:350:GLN:OE1	2:F:352:GLN:NE2	2.45	0.49
2:F:567:PHE:O	2:F:571:GLU:HG2	2.13	0.49
1:A:1148:PHE:O	1:A:1152:THR:HG23	2.13	0.48
2:E:378:LYS:O	2:E:379:ILE:HG23	2.13	0.48
4:D:394:TYR:O	4:D:398:ALA:CB	2.61	0.48
2:E:509:LEU:HD21	2:F:338:LYS:HB2	1.95	0.48
1:A:828:ILE:CD1	1:A:899:LYS:HD3	2.43	0.48
1:A:665:GLU:HB3	2:E:552:PHE:CZ	2.49	0.48
1:A:953:SER:O	1:A:957:VAL:HG13	2.13	0.48
2:E:179:SER:OG	3:B:133:ARG:NH1	2.47	0.48
4:D:381:ARG:HE	4:D:382:SER:H	1.61	0.47
2:E:560:MET:HG2	2:E:564:ARG:NH1	2.29	0.47
4:C:269:LEU:HD23	4:C:270:GLU:H	1.79	0.47
1:A:956:LYS:O	1:A:960:THR:HG23	2.14	0.47
4:D:360:GLU:HA	4:D:363:LEU:HD23	1.97	0.47
1:A:823:SER:O	1:A:827:THR:HG23	2.14	0.47
1:A:1317:ILE:HG23	1:A:1321:ASP:HB2	1.97	0.47
1:A:919:LEU:C	1:A:919:LEU:CD1	2.83	0.47
2:E:324:SER:O	2:E:328:LYS:HG3	2.14	0.47
2:E:383:ASP:HA	2:E:386:LEU:HB2	1.97	0.47
1:A:1309:THR:HG23	1:A:1311:HIS:HB2	1.96	0.47
3:B:79:THR:HG1	3:B:155:SER:HG	1.62	0.47
2:F:333:VAL:HG22	2:F:336:PHE:HB2	1.97	0.47
1:A:679:LYS:HA	1:A:679:LYS:HD3	1.62	0.47
4:C:247:ARG:NH2	4:C:251:ASP:OD1	2.48	0.47
1:A:825:LEU:O	1:A:828:ILE:HG22	2.15	0.46
1:A:1196:LEU:HB3	1:A:1227:SER:OG	2.14	0.46
2:E:489:TYR:OH	4:C:377:LYS:O	2.31	0.46
2:F:303:CYS:O	2:F:307:LYS:HG3	2.15	0.46
4:D:381:ARG:HE	4:D:382:SER:N	2.12	0.46
1:A:1161:ILE:HG21	1:A:1239:LEU:HD11	1.96	0.46
1:A:1325:LYS:HD2	1:A:1325:LYS:HA	1.51	0.46
3:B:191:ASP:OD1	3:B:191:ASP:N	2.48	0.46
2:E:395:ILE:H	2:E:395:ILE:HG12	1.30	0.46
1:A:921:GLN:HG2	1:A:1188:SER:CB	2.45	0.46
2:F:274:CYS:SG	2:F:275:CYS:N	2.89	0.46
2:E:169:THR:HG22	3:B:53:MET:CE	2.46	0.46
2:E:395:ILE:CD1	2:E:399:ASP:HB2	2.45	0.46
4:D:331:LEU:O	4:D:335:ILE:HG12	2.16	0.46
2:E:175:MET:HE3	2:E:175:MET:HB3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:516:ASN:O	2:E:517:ASN:HB2	2.15	0.46
4:C:247:ARG:NH1	4:C:385:ALA:O	2.46	0.46
4:D:325:ILE:HG13	4:D:326:TYR:CD2	2.51	0.46
1:A:800:LYS:HE2	3:B:279:ASP:O	2.16	0.46
1:A:903:GLU:HG3	1:A:904:GLU:N	2.31	0.46
4:D:290:ASP:OD2	4:D:291:LYS:N	2.50	0.45
1:A:913:ASN:HA	1:A:916:TRP:HE3	1.81	0.45
1:A:983:ASN:HA	1:A:986:TYR:CD2	2.52	0.45
1:A:1119:ASN:OD1	1:A:1119:ASN:N	2.49	0.45
2:E:125:ARG:HD3	2:E:125:ARG:HA	1.31	0.45
4:D:261:TYR:O	4:D:265:VAL:HG22	2.17	0.45
4:D:293:LEU:HA	4:D:297:LEU:HB2	1.98	0.45
3:B:362:ASN:OD1	3:B:364:ASN:ND2	2.43	0.45
2:E:257:PHE:CD2	2:E:257:PHE:C	2.89	0.45
1:A:1005:PRO:HA	1:A:1008:GLU:OE2	2.16	0.45
3:B:269:LEU:HD21	3:B:295:VAL:HG22	1.98	0.45
4:D:299:TYR:O	4:D:303:ARG:HG3	2.17	0.45
2:F:321:LYS:HZ1	2:F:325:ASN:HB3	1.82	0.45
4:D:233:VAL:HG11	2:F:364:VAL:HG21	1.99	0.44
2:F:265:ALA:HA	2:F:349:LYS:HA	1.98	0.44
4:C:252:VAL:HG11	4:C:373:TYR:CE1	2.53	0.44
1:A:1165:ASN:O	1:A:1169:THR:HG22	2.17	0.44
2:E:385:GLN:N	2:E:385:GLN:CD	2.71	0.44
4:D:308:GLU:HA	4:D:311:LYS:HD2	1.99	0.44
2:F:338:LYS:HA	2:F:338:LYS:HD3	1.73	0.44
1:A:755:TYR:HE1	3:B:195:GLU:HG3	1.82	0.44
1:A:960:THR:O	1:A:964:ILE:HG13	2.17	0.44
2:E:288:ASP:HA	2:E:289:PRO:HA	1.86	0.44
3:B:377:PHE:O	3:B:381:GLU:HG2	2.18	0.44
1:A:1235:LYS:HE2	1:A:1235:LYS:HB2	1.55	0.44
1:A:875:ARG:HA	1:A:878:GLU:CG	2.48	0.44
2:E:563:LYS:O	2:E:566:LEU:HG	2.18	0.44
1:A:1338:VAL:O	1:A:1341:TYR:HB2	2.18	0.44
3:B:79:THR:OG1	3:B:155:SER:OG	2.32	0.44
4:D:239:VAL:C	4:D:243:LYS:HA	2.39	0.44
2:F:307:LYS:O	2:F:311:PHE:HB2	2.18	0.44
1:A:921:GLN:CG	1:A:1188:SER:HB2	2.48	0.44
1:A:1168:VAL:HG11	1:A:1232:TYR:CE1	2.53	0.44
2:F:558:SER:HA	2:F:561:VAL:HG22	2.00	0.44
1:A:1241:THR:O	1:A:1245:VAL:HG23	2.18	0.43
4:D:312:LYS:HE2	4:D:313:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:555:ILE:HD12	2:F:556:TYR:N	2.33	0.43
1:A:1261:LYS:O	1:A:1265:ILE:HG13	2.18	0.43
2:F:369:ARG:O	2:F:369:ARG:NH1	2.47	0.43
1:A:1120:LEU:HD21	1:A:1338:VAL:HG23	2.00	0.43
2:F:327:ILE:HG22	2:F:337:ALA:HB1	2.01	0.43
2:E:180:ASN:ND2	2:E:180:ASN:H	2.16	0.43
4:C:382:SER:OG	4:C:383:ASP:N	2.50	0.43
4:D:227:LYS:O	4:D:231:VAL:HG23	2.18	0.43
4:D:270:GLU:HB3	2:F:556:TYR:HD1	1.84	0.43
4:D:282:CYS:SG	4:D:283:ALA:N	2.91	0.43
1:A:835:VAL:O	1:A:838:ILE:HG22	2.19	0.43
4:D:255:GLU:OE2	4:D:324:ARG:NH1	2.52	0.43
1:A:1331:GLU:O	1:A:1335:LYS:HG2	2.18	0.43
2:E:552:PHE:HD1	2:E:555:ILE:HD11	1.83	0.43
4:D:358:GLN:HE21	4:D:358:GLN:HB3	1.65	0.43
1:A:845:GLU:O	1:A:849:PHE:N	2.52	0.43
4:D:304:LEU:HA	4:D:307:ASP:OD2	2.18	0.43
1:A:965:HIS:O	1:A:968:THR:HG22	2.18	0.43
1:A:1007:LYS:O	1:A:1011:LYS:HG3	2.19	0.43
1:A:1178:VAL:HG22	1:A:1180:PHE:H	1.83	0.43
1:A:785:HIS:CD2	1:A:786:PRO:HD2	2.54	0.42
2:E:571:GLU:O	2:E:574:ILE:HG12	2.19	0.42
3:B:80:ASP:OD2	3:B:80:ASP:N	2.52	0.42
4:D:326:TYR:HD1	4:D:330:HIS:NE2	2.17	0.42
4:D:292:CYS:SG	2:F:343:ILE:HG21	2.59	0.42
1:A:842:THR:O	1:A:846:LYS:HD3	2.19	0.42
2:E:388:ASN:HD22	2:E:388:ASN:HA	1.37	0.42
2:E:517:ASN:HB3	2:E:519:ASN:HB2	2.01	0.42
2:F:332:ASN:OD1	2:F:332:ASN:N	2.50	0.42
1:A:1166:GLU:OE1	1:A:1167:ARG:NH1	2.51	0.42
2:E:567:PHE:HD1	2:E:567:PHE:HA	1.77	0.42
1:A:1124:ALA:HB1	1:A:1335:LYS:HE3	2.00	0.42
3:B:153:LYS:NZ	3:B:195:GLU:OE2	2.36	0.42
4:C:352:CYS:O	4:C:356:ILE:HG12	2.19	0.42
1:A:1333:LYS:HD2	1:A:1333:LYS:HA	1.75	0.42
2:F:322:ILE:HD13	2:F:341:PHE:HZ	1.84	0.42
2:E:384:ARG:CG	2:E:387:PHE:HB3	2.44	0.42
4:C:219:LYS:HA	4:C:219:LYS:HD2	1.84	0.42
4:D:377:LYS:HE2	4:D:377:LYS:HB2	1.55	0.42
2:F:333:VAL:HG22	2:F:333:VAL:O	2.19	0.42
1:A:832:GLU:OE2	1:A:895:LEU:HD21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:LYS:HA	1:A:1040:VAL:HG23	2.02	0.42
2:E:177:GLU:H	2:E:177:GLU:HG2	1.52	0.42
2:E:307:LYS:HB3	2:E:307:LYS:HE3	1.85	0.42
2:E:564:ARG:HB3	2:F:564:ARG:NH1	2.34	0.42
4:C:252:VAL:HG11	4:C:373:TYR:HE1	1.85	0.42
4:C:300:ARG:HG2	4:C:399:LEU:HD23	2.01	0.42
2:F:565:LYS:HA	2:F:568:GLN:NE2	2.33	0.42
2:F:275:CYS:HB3	2:F:278:CYS:HB3	2.01	0.42
1:A:995:PHE:CE2	1:A:1247:GLN:HG2	2.55	0.41
1:A:1234:ASN:O	3:B:359:ASN:ND2	2.46	0.41
3:B:150:HIS:CD2	3:B:150:HIS:H	2.38	0.41
4:D:290:ASP:OD2	4:D:291:LYS:HG3	2.20	0.41
1:A:936:LYS:NZ	1:A:1225:GLU:OE2	2.46	0.41
1:A:1006:ASP:OD2	1:A:1006:ASP:N	2.52	0.41
2:E:499:ASN:CG	2:E:500:LYS:H	2.23	0.41
2:E:565:LYS:O	2:E:568:GLN:HG3	2.19	0.41
2:F:564:ARG:HA	2:F:567:PHE:HB2	2.02	0.41
1:A:831:LEU:O	1:A:834:ILE:HG13	2.20	0.41
3:B:38:HIS:CD2	3:B:40:MET:HB2	2.55	0.41
4:D:393:GLN:O	4:D:397:VAL:HG23	2.20	0.41
1:A:1318:ALA:O	1:A:1321:ASP:N	2.53	0.41
1:A:878:GLU:H	1:A:878:GLU:HG2	1.71	0.41
1:A:1281:LYS:HZ1	1:A:1343:LEU:HB2	1.85	0.41
2:E:455:ALA:HA	3:B:239:ARG:HH11	1.85	0.41
1:A:835:VAL:HA	1:A:838:ILE:HG22	2.03	0.41
3:B:125:GLY:O	3:B:129:GLU:HB2	2.19	0.41
1:A:1336:TYR:O	1:A:1339:THR:HG22	2.20	0.41
2:E:277:THR:HG21	2:E:306:CYS:SG	2.61	0.41
1:A:942:LEU:HD21	2:E:403:PRO:HG2	2.02	0.41
1:A:1139:PHE:CE1	1:A:1302:ARG:HG3	2.56	0.41
2:E:381:LEU:O	2:E:385:GLN:NE2	2.54	0.41
4:D:258:LEU:HD22	4:D:286:LYS:HG3	2.03	0.41
4:D:307:ASP:HB2	4:D:311:LYS:NZ	2.36	0.41
1:A:778:LEU:HD11	3:B:171:ILE:HD11	2.03	0.41
1:A:809:LYS:O	1:A:813:GLU:HG3	2.21	0.41
1:A:1016:TYR:HB3	1:A:1065:LEU:HD13	2.03	0.41
1:A:1150:HIS:O	1:A:1154:ILE:HG13	2.21	0.41
1:A:1279:SER:O	1:A:1283:GLN:HG2	2.21	0.41
2:E:307:LYS:HA	2:E:310:ILE:HG22	2.02	0.41
1:A:867:ILE:O	1:A:871:TYR:HB2	2.21	0.41
1:A:877:PHE:O	1:A:880:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:LYS:HB2	1:A:1271:LYS:HE2	1.87	0.41
2:E:277:THR:CG2	2:E:306:CYS:SG	3.09	0.41
2:F:342:ASN:O	2:F:346:HIS:HB2	2.20	0.41
2:E:415:LEU:O	2:E:423:THR:HB	2.21	0.40
4:C:285:LEU:HA	4:C:285:LEU:HD23	1.80	0.40
4:D:299:TYR:CE1	2:F:351:PHE:HD1	2.39	0.40
2:F:305:GLU:O	2:F:309:LYS:HG2	2.21	0.40
1:A:912:TRP:CH2	2:E:111:THR:HG23	2.57	0.40
3:B:128:MET:HE2	3:B:128:MET:HB3	1.68	0.40
4:D:363:LEU:O	4:D:366:LEU:HB3	2.22	0.40
1:A:1286:TYR:O	1:A:1290:VAL:HG12	2.21	0.40
2:E:572:SER:HA	2:E:575:ASP:OD1	2.22	0.40
4:D:253:THR:HG21	4:D:324:ARG:C	2.42	0.40
4:D:283:ALA:O	4:D:287:LEU:HD22	2.21	0.40
1:A:810:ILE:HD11	1:A:919:LEU:HG	2.04	0.40
2:E:107:LYS:HB2	2:E:107:LYS:NZ	2.35	0.40
2:E:177:GLU:CG	2:E:177:GLU:O	2.70	0.40
2:E:501:LYS:HA	2:E:501:LYS:HD2	1.90	0.40
3:B:103:LYS:HD2	3:B:104:PHE:CE1	2.57	0.40
4:C:255:GLU:HB2	4:C:323:ILE:HG12	2.02	0.40
4:D:313:SER:HA	4:D:316:ASP:HB2	2.04	0.40
1:A:876:GLY:O	1:A:879:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	598/1536 (39%)	568 (95%)	27 (4%)	3 (0%)	29 67
2	E	343/684 (50%)	293 (85%)	41 (12%)	9 (3%)	5 35
2	F	152/684 (22%)	146 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	383/433 (88%)	365 (95%)	16 (4%)	2 (0%)	29	67
4	C	181/401 (45%)	168 (93%)	12 (7%)	1 (1%)	25	63
4	D	183/401 (46%)	172 (94%)	11 (6%)	0	100	100
4	G	63/401 (16%)	62 (98%)	1 (2%)	0	100	100
5	a	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
5	e	100/136 (74%)	96 (96%)	4 (4%)	0	100	100
6	b	80/103 (78%)	77 (96%)	1 (1%)	2 (2%)	5	36
6	f	80/103 (78%)	77 (96%)	2 (2%)	1 (1%)	12	48
7	c	104/130 (80%)	101 (97%)	3 (3%)	0	100	100
7	g	106/130 (82%)	104 (98%)	2 (2%)	0	100	100
8	d	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
8	h	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
11	H	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2655/5535 (48%)	2507 (94%)	130 (5%)	18 (1%)	26	60

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	171	LEU
2	E	174	ASN
2	E	470	SER
4	C	241	LYS
6	b	25	ASN
1	A	873	LYS
1	A	1200	GLY
2	E	125	ARG
2	E	390	SER
2	E	517	ASN
6	b	24	ASP
1	A	1233	ASN
2	E	471	PRO
3	B	136	ARG
2	E	492	TRP
6	f	24	ASP
2	E	453	PRO
3	B	107	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/1391 (40%)	508 (91%)	52 (9%)	9	34
2	E	332/653 (51%)	288 (87%)	44 (13%)	4	22
2	F	148/653 (23%)	132 (89%)	16 (11%)	6	29
3	B	326/367 (89%)	304 (93%)	22 (7%)	16	46
4	C	172/359 (48%)	158 (92%)	14 (8%)	11	40
4	D	174/359 (48%)	159 (91%)	15 (9%)	10	38
4	G	56/359 (16%)	56 (100%)	0	100	100
5	a	85/111 (77%)	83 (98%)	2 (2%)	49	69
5	e	90/111 (81%)	87 (97%)	3 (3%)	38	63
6	b	67/79 (85%)	60 (90%)	7 (10%)	7	29
6	f	67/79 (85%)	59 (88%)	8 (12%)	5	25
7	c	83/100 (83%)	79 (95%)	4 (5%)	25	54
7	g	84/100 (84%)	80 (95%)	4 (5%)	25	54
8	d	81/105 (77%)	73 (90%)	8 (10%)	8	31
8	h	81/105 (77%)	79 (98%)	2 (2%)	47	69
11	H	1/1 (100%)	0	1 (100%)	0	0
All	All	2407/4932 (49%)	2205 (92%)	202 (8%)	14	39

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	665	GLU
1	A	679	LYS
1	A	724	VAL
1	A	751	PHE
1	A	767	CYS
1	A	790	SER
1	A	799	ARG
1	A	800	LYS

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Mol	Chain	Res	Type
1	A	802	GLN
1	A	807	LEU
1	A	809	LYS
1	A	818	ASP
1	A	828	ILE
1	A	829	GLN
1	A	830	CYS
1	A	831	LEU
1	A	837	LYS
1	A	839	GLU
1	A	850	LYS
1	A	860	MET
1	A	871	TYR
1	A	872	ASP
1	A	879	ILE
1	A	911	GLU
1	A	912	TRP
1	A	919	LEU
1	A	920	GLU
1	A	921	GLN
1	A	961	ASN
1	A	962	LYS
1	A	963	LYS
1	A	1006	ASP
1	A	1008	GLU
1	A	1012	ASP
1	A	1016	TYR
1	A	1023	SER
1	A	1025	SER
1	A	1036	HIS
1	A	1063	MET
1	A	1069	LEU
1	A	1076	LYS
1	A	1079	ARG
1	A	1141	ASN
1	A	1182	LYS
1	A	1233	ASN
1	A	1243	ASP
1	A	1287	ARG
1	A	1313	SER
1	A	1320	ASP
1	A	1335	LYS

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Mol	Chain	Res	Type
1	A	1337	TYR
1	A	1339	THR
2	E	105	ASP
2	E	107	LYS
2	E	110	VAL
2	E	111	THR
2	E	113	LEU
2	E	114	PRO
2	E	123	ILE
2	E	125	ARG
2	E	126	GLU
2	E	177	GLU
2	E	178	GLU
2	E	179	SER
2	E	180	ASN
2	E	185	ILE
2	E	187	TRP
2	E	256	ASP
2	E	276	ASP
2	E	298	LYS
2	E	315	SER
2	E	332	ASN
2	E	345	SER
2	E	375	GLU
2	E	384	ARG
2	E	386	LEU
2	E	387	PHE
2	E	388	ASN
2	E	390	SER
2	E	391	TYR
2	E	395	ILE
2	E	402	ASN
2	E	413	LYS
2	E	437	ILE
2	E	477	LYS
2	E	491	VAL
2	E	492	TRP
2	E	494	LYS
2	E	510	GLN
2	E	516	ASN
2	E	543	ASP
2	E	557	LYS

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Mol	Chain	Res	Type
2	E	564	ARG
2	E	567	PHE
2	E	569	PHE
2	E	579	SER
3	B	2	VAL
3	B	9	ASP
3	B	14	LYS
3	B	40	MET
3	B	41	LYS
3	B	42	PRO
3	B	81	GLU
3	B	90	THR
3	B	108	ASP
3	B	136	ARG
3	B	138	LYS
3	B	150	HIS
3	B	155	SER
3	B	165	ASP
3	B	176	TYR
3	B	207	SER
3	B	240	ASP
3	B	283	CYS
3	B	300	SER
3	B	316	ARG
3	B	358	SER
3	B	385	TYR
4	C	235	ASP
4	C	246	CYS
4	C	267	GLN
4	C	285	LEU
4	C	300	ARG
4	C	312	LYS
4	C	314	SER
4	C	323	ILE
4	C	336	SER
4	C	337	VAL
4	C	348	ASP
4	C	361	ASP
4	C	371	ASP
4	C	384	ASP
4	D	256	MET
4	D	274	SER

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Mol	Chain	Res	Type
4	D	279	SER
4	D	287	LEU
4	D	314	SER
4	D	318	LYS
4	D	331	LEU
4	D	341	LEU
4	D	345	THR
4	D	363	LEU
4	D	374	PHE
4	D	377	LYS
4	D	380	ASN
4	D	383	ASP
4	D	386	LEU
2	F	256	ASP
2	F	264	SER
2	F	304	ASN
2	F	308	PHE
2	F	311	PHE
2	F	315	SER
2	F	332	ASN
2	F	338	LYS
2	F	346	HIS
2	F	353	LEU
2	F	371	GLN
2	F	372	TYR
2	F	564	ARG
2	F	567	PHE
2	F	572	SER
2	F	573	LEU
5	a	86	SER
5	a	123	ASP
6	b	21	VAL
6	b	50	ILE
6	b	52	GLU
6	b	54	THR
6	b	74	GLU
6	b	79	LYS
6	b	92	ARG
7	c	13	LYS
7	c	19	SER
7	c	36	LYS
7	c	90	ASP

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Mol	Chain	Res	Type
8	d	30	LYS
8	d	31	ARG
8	d	33	ARG
8	d	71	GLU
8	d	78	SER
8	d	85	LYS
8	d	87	SER
8	d	123	SER
5	e	2	ARG
5	e	37	LYS
5	e	63	ARG
6	f	22	LEU
6	f	23	ARG
6	f	50	ILE
6	f	52	GLU
6	f	54	THR
6	f	74	GLU
6	f	79	LYS
6	f	92	ARG
7	g	11	ARG
7	g	13	LYS
7	g	15	LYS
7	g	64	GLU
8	h	30	LYS
8	h	31	ARG
11	H	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	690	ASN
1	A	722	ASN
1	A	798	HIS
1	A	802	GLN
1	A	1038	GLN
1	A	1233	ASN
1	A	1234	ASN
1	A	1254	HIS
2	E	180	ASN
2	E	259	ASN
2	E	376	ASN
2	E	388	ASN

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Continued from previous page...

Mol	Chain	Res	Type
2	E	448	HIS
2	E	495	GLN
2	E	516	ASN
2	E	517	ASN
2	E	519	ASN
2	E	541	GLN
3	B	76	GLN
3	B	105	ASN
3	B	375	ASN
4	C	267	GLN
4	C	353	GLN
4	D	277	GLN
4	D	350	GLN
4	D	358	GLN
4	D	389	ASN
2	F	259	ASN
2	F	294	ASN
2	F	568	GLN
5	a	39	HIS
6	b	75	HIS
7	c	38	ASN
7	c	112	GLN
5	e	5	GLN
5	e	39	HIS
5	e	76	GLN
5	e	125	GLN
7	g	31	HIS
7	g	38	ASN
8	h	47	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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.

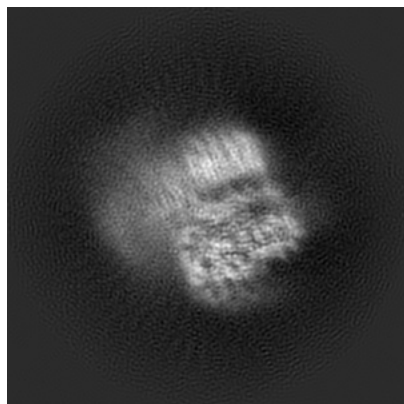
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37365. These allow visual inspection of the internal detail of the map and identification of artifacts.

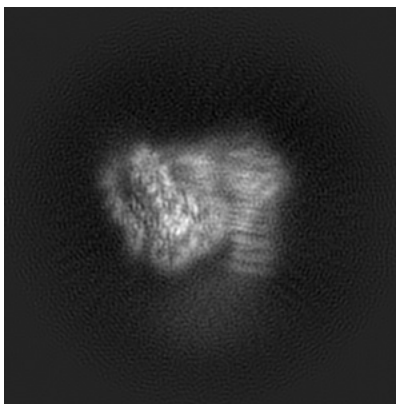
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

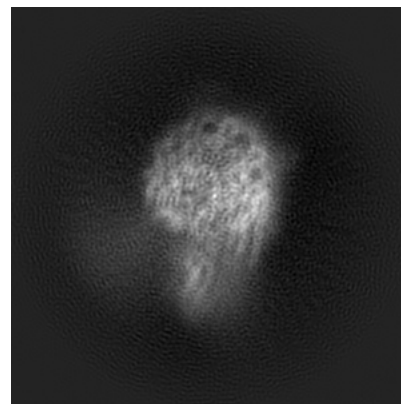
6.1.1 Primary map



X

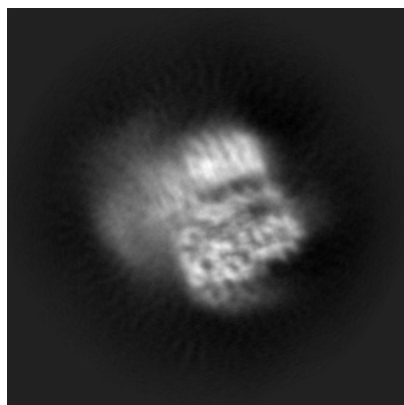


Y

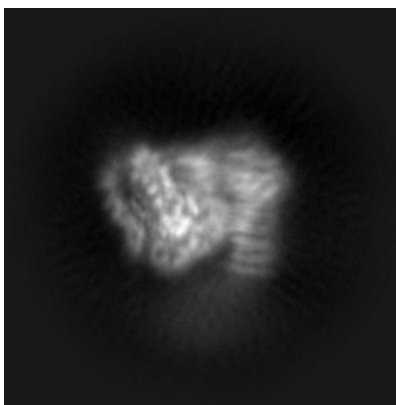


Z

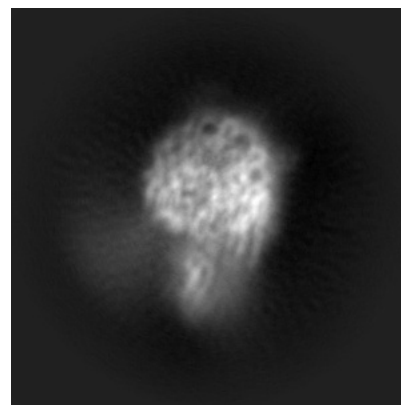
6.1.2 Raw map



X



Y

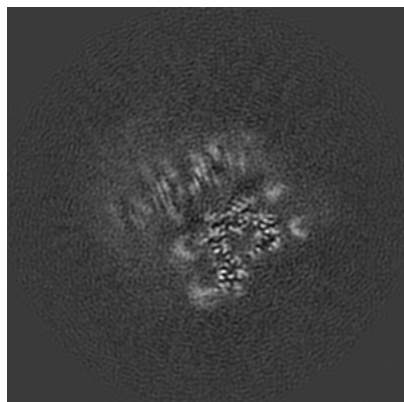


Z

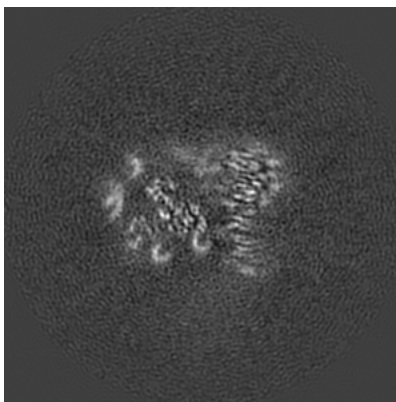
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

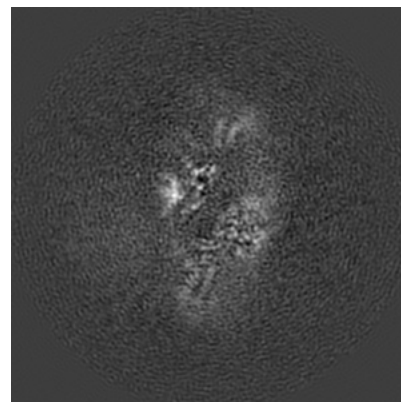
6.2.1 Primary map



X Index: 140

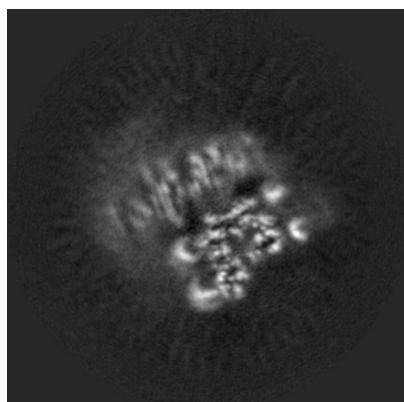


Y Index: 140

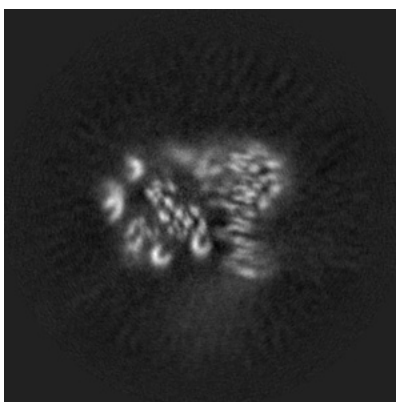


Z Index: 140

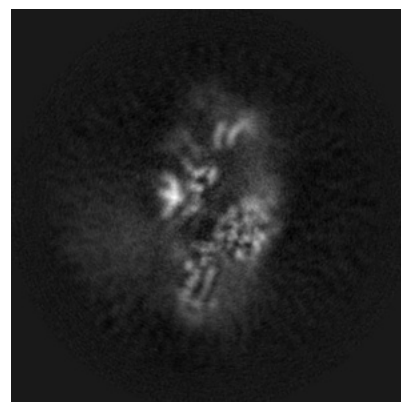
6.2.2 Raw map



X Index: 140



Y Index: 140

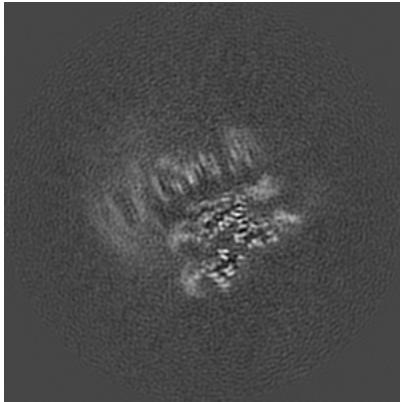


Z Index: 140

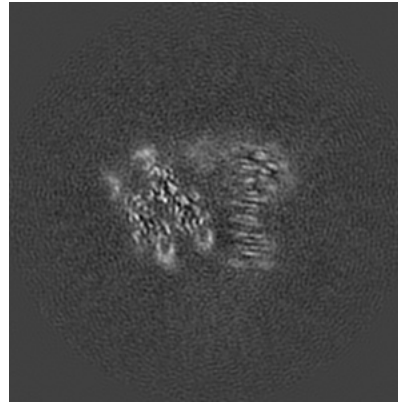
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

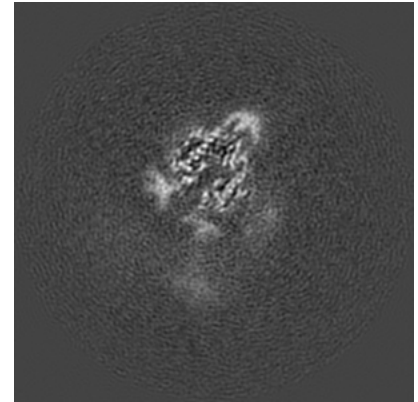
6.3.1 Primary map



X Index: 130

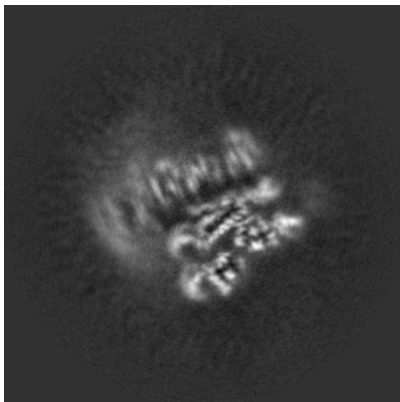


Y Index: 147

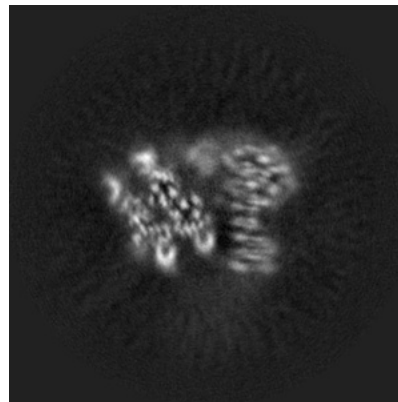


Z Index: 113

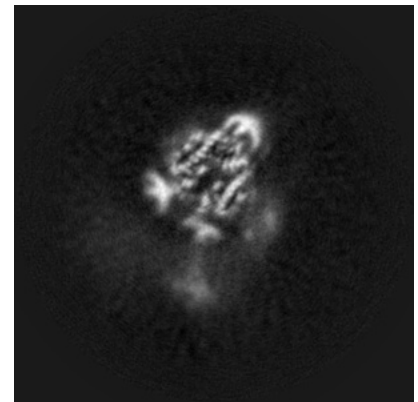
6.3.2 Raw map



X Index: 131



Y Index: 146

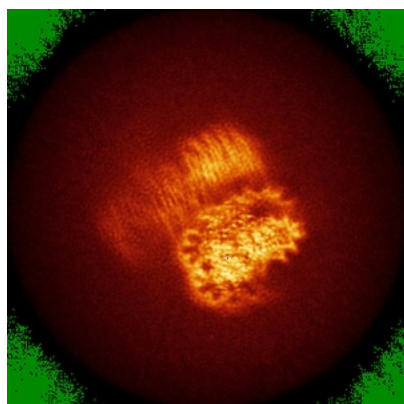


Z Index: 113

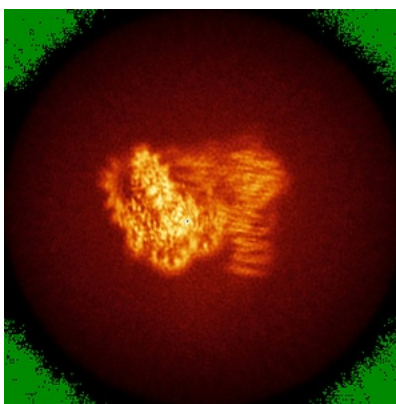
The images above show the largest variance slices of the map in three orthogonal directions.

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

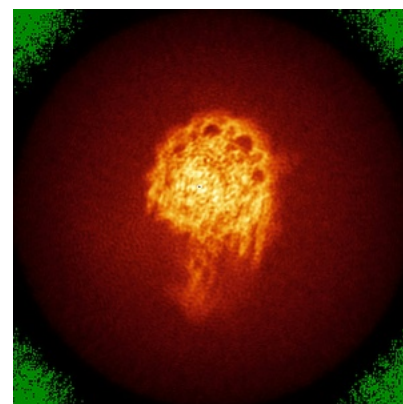
6.4.1 Primary map



X

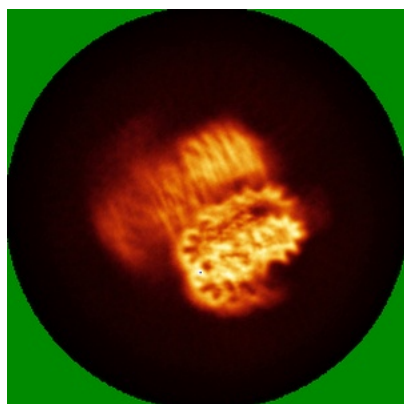


Y

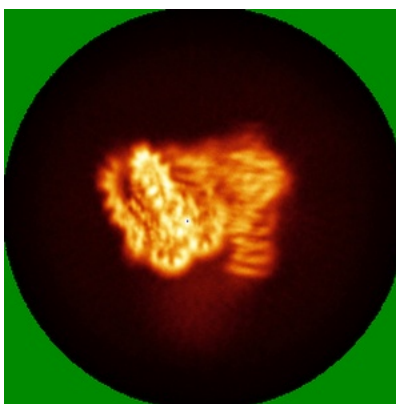


Z

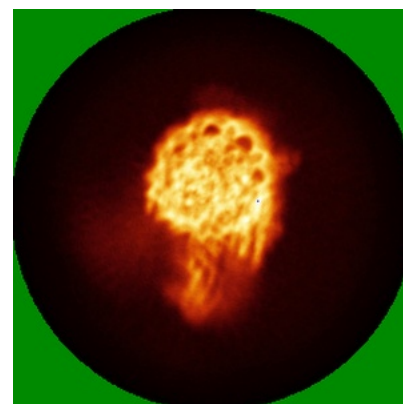
6.4.2 Raw map



X



Y

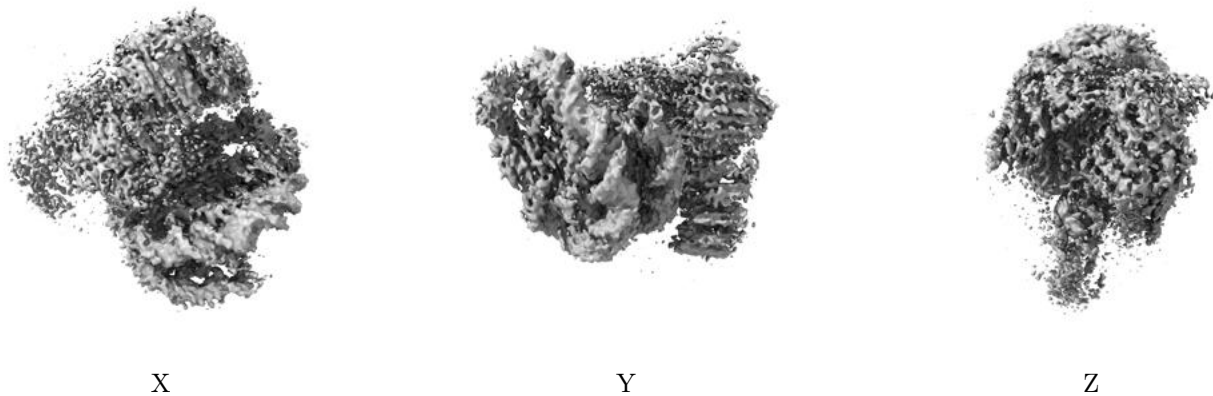


Z

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.

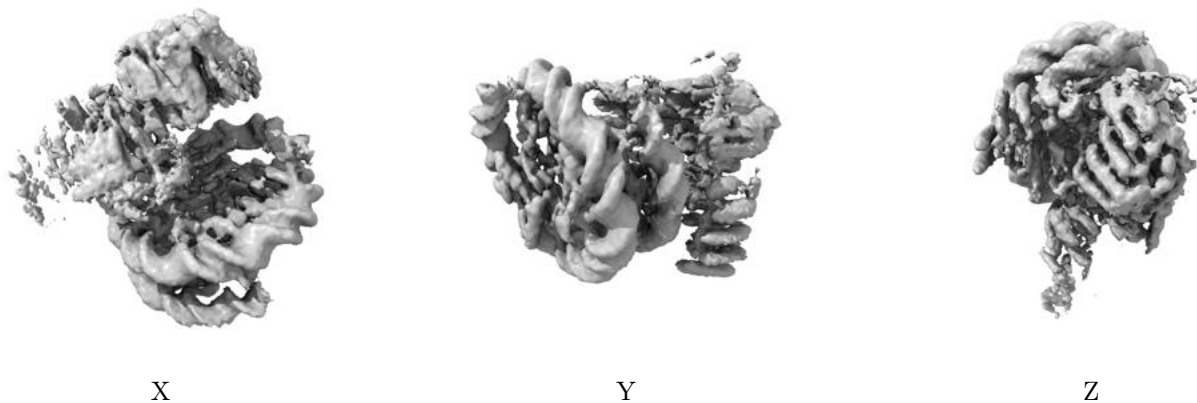
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

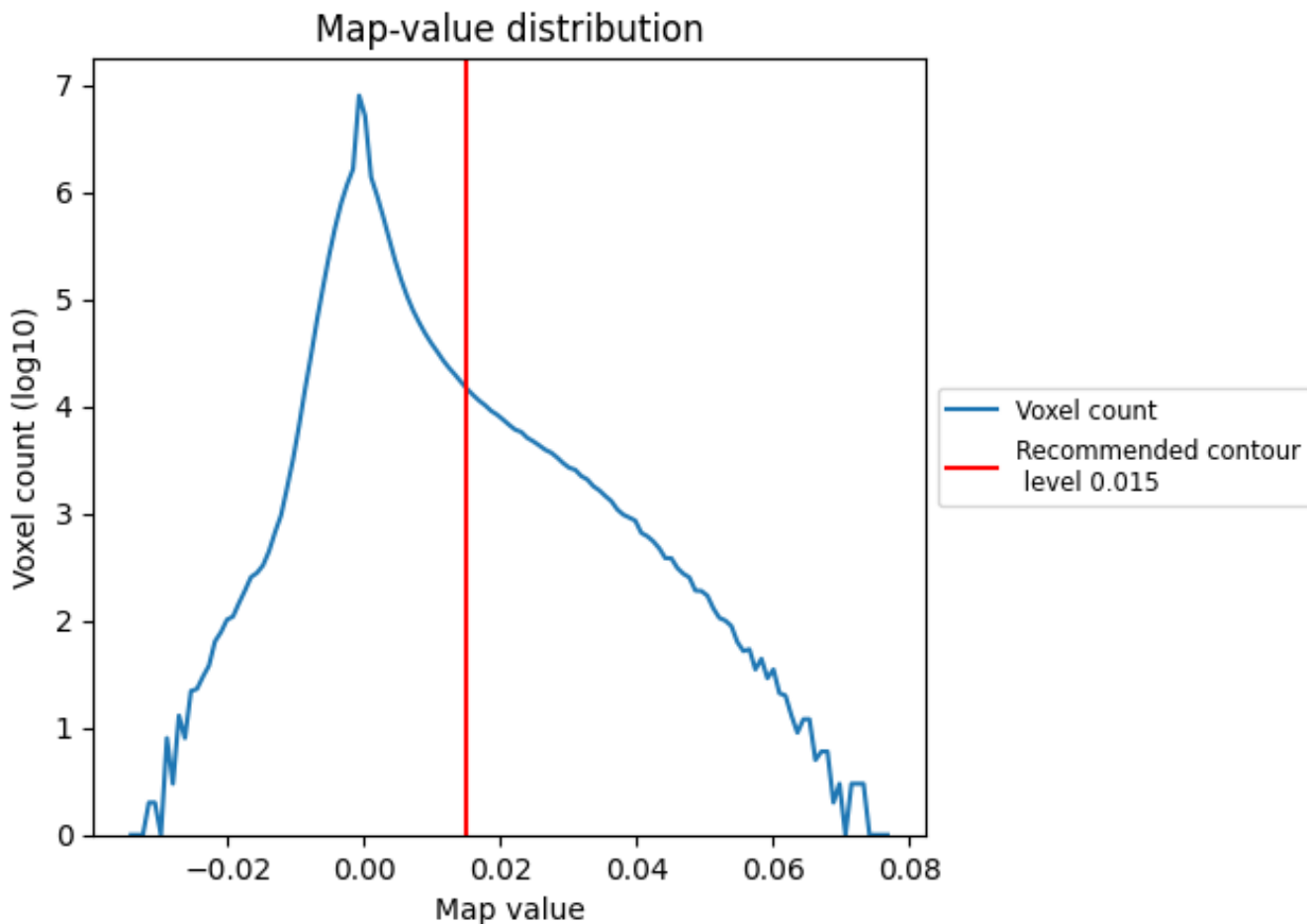
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

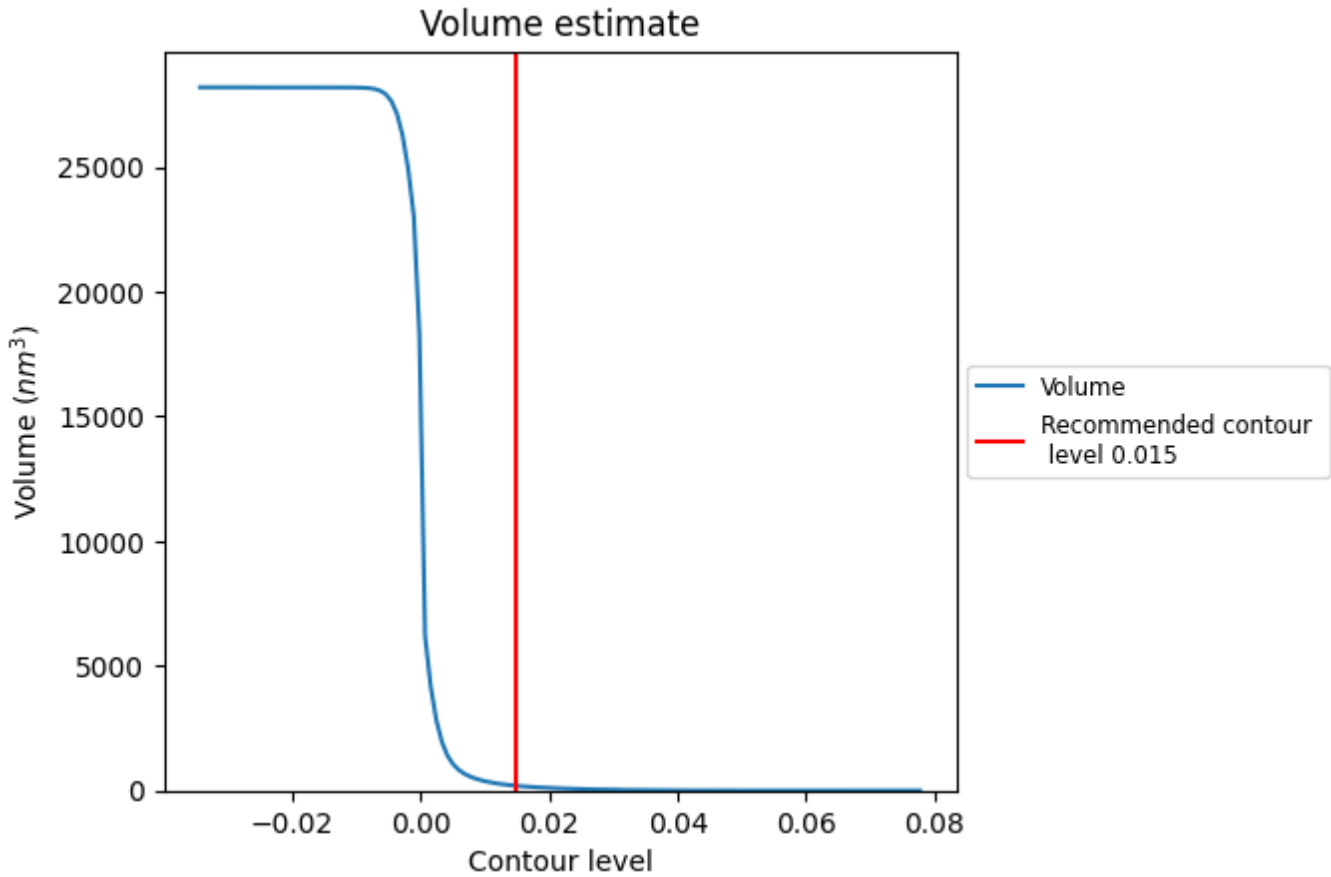
This section contains the results of statistical analysis of the map.

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.

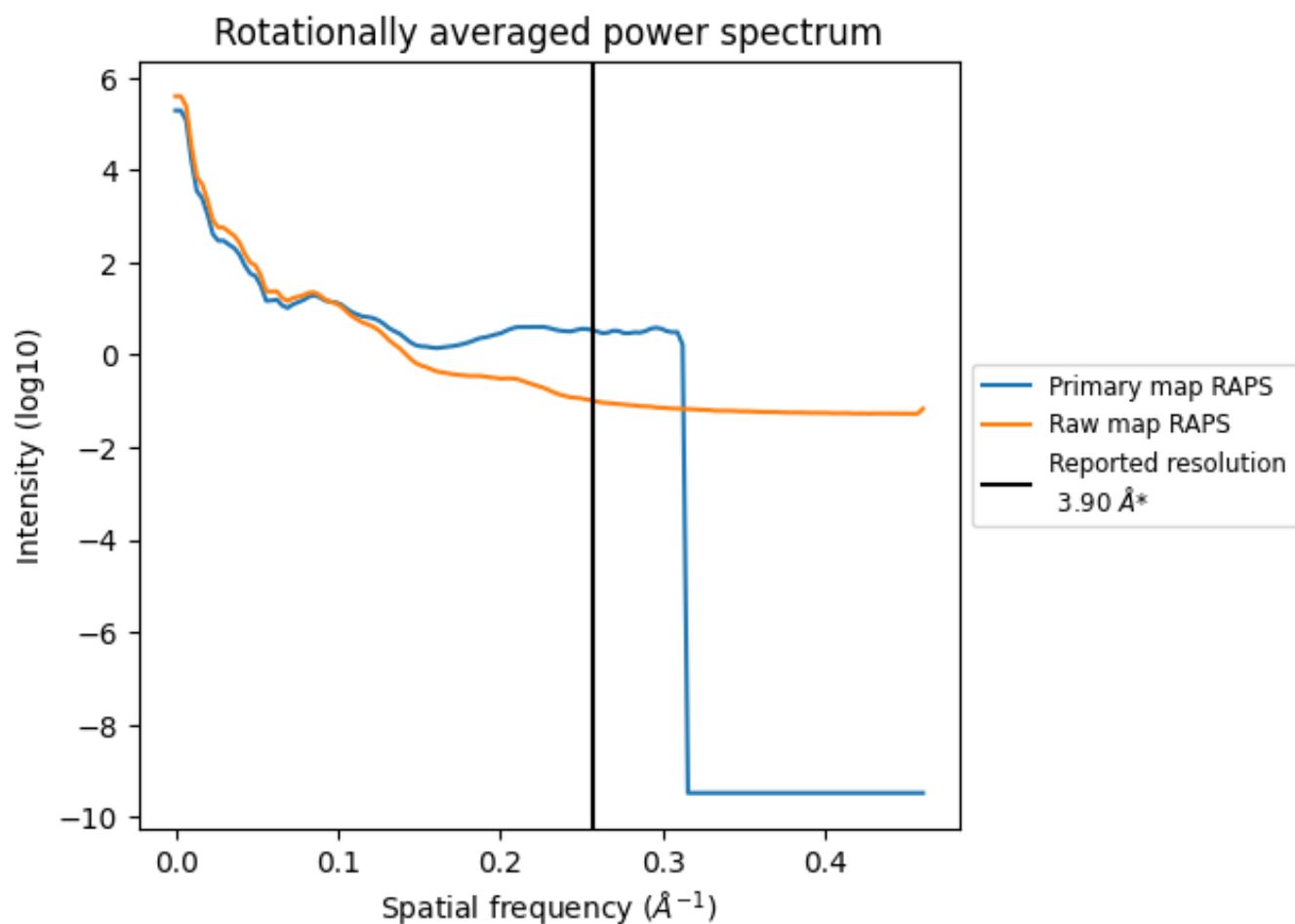
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 189 nm^3 ; this corresponds to an approximate mass of 171 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

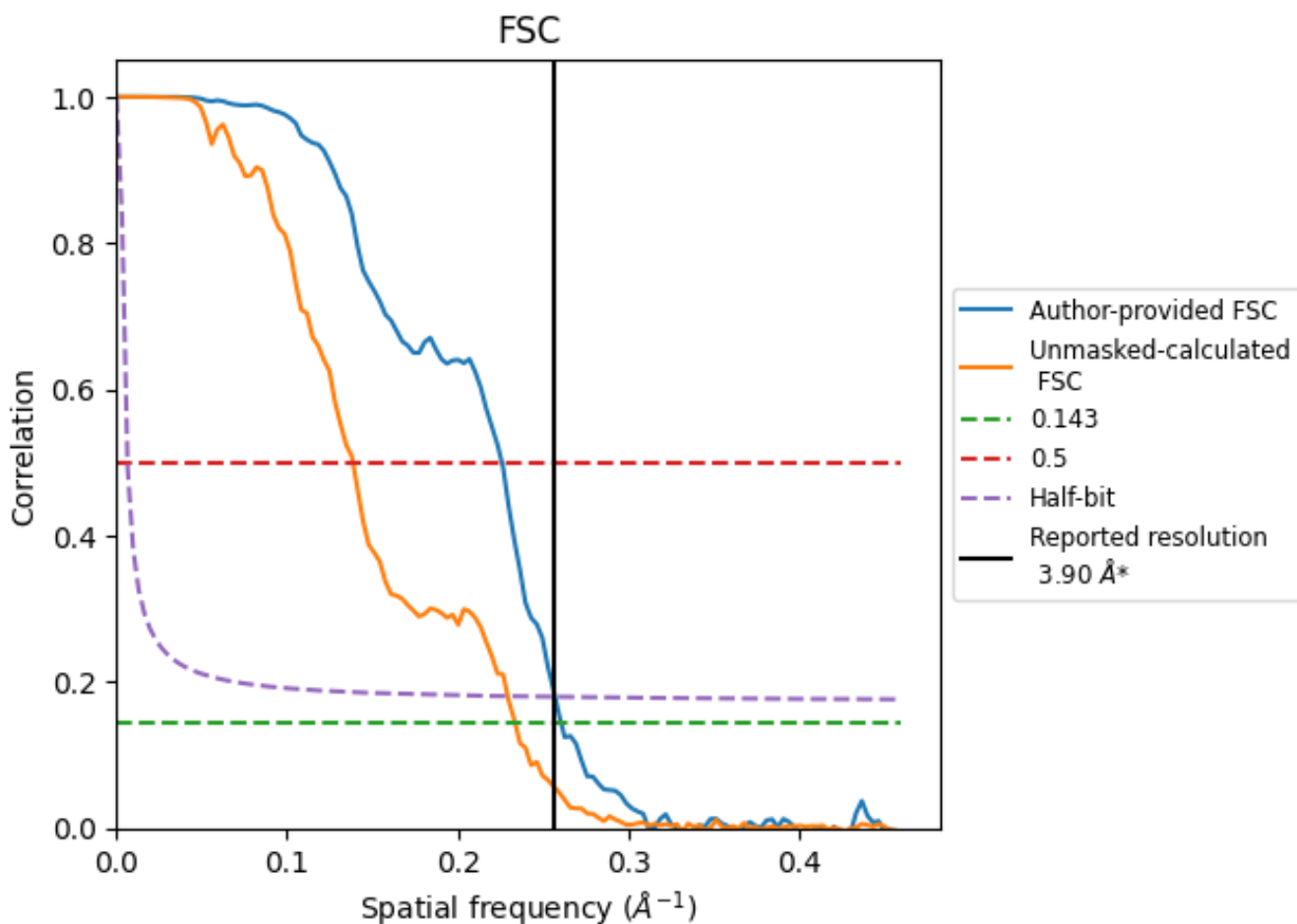


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

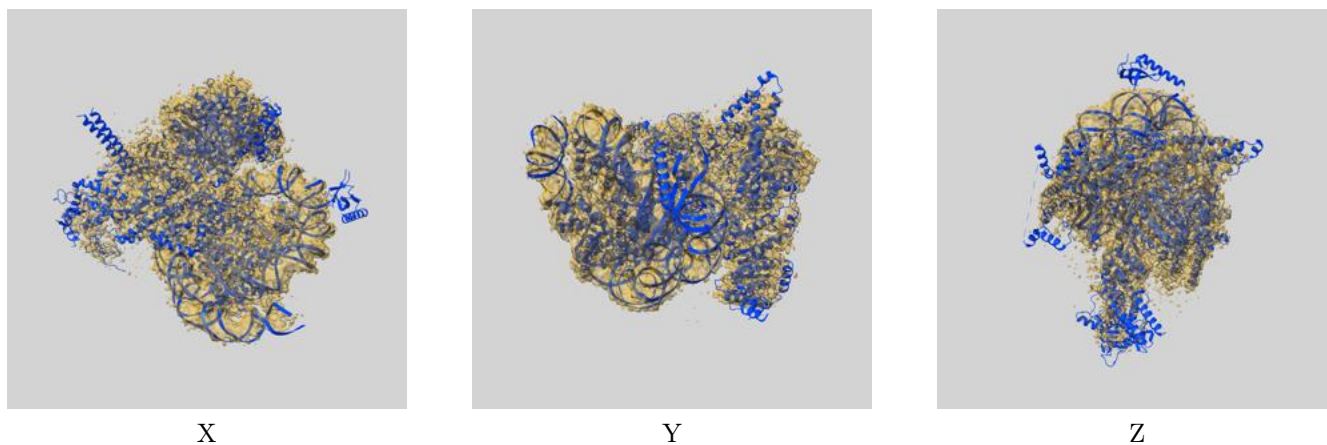
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.42	3.89
Unmasked-calculated*	4.28	7.22	4.36

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

9 Map-model fit [i](#)

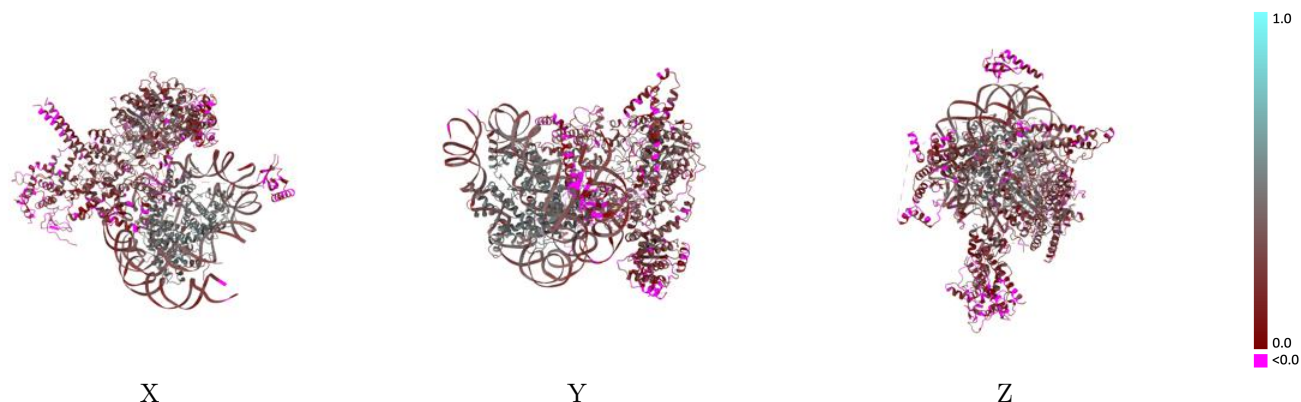
This section contains information regarding the fit between EMDB map EMD-37365 and PDB model 8W9D. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



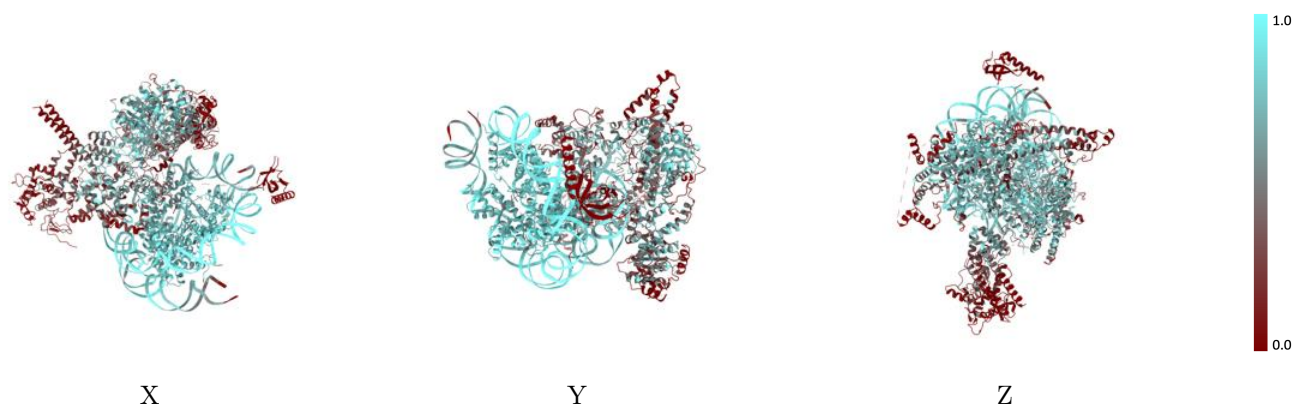
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



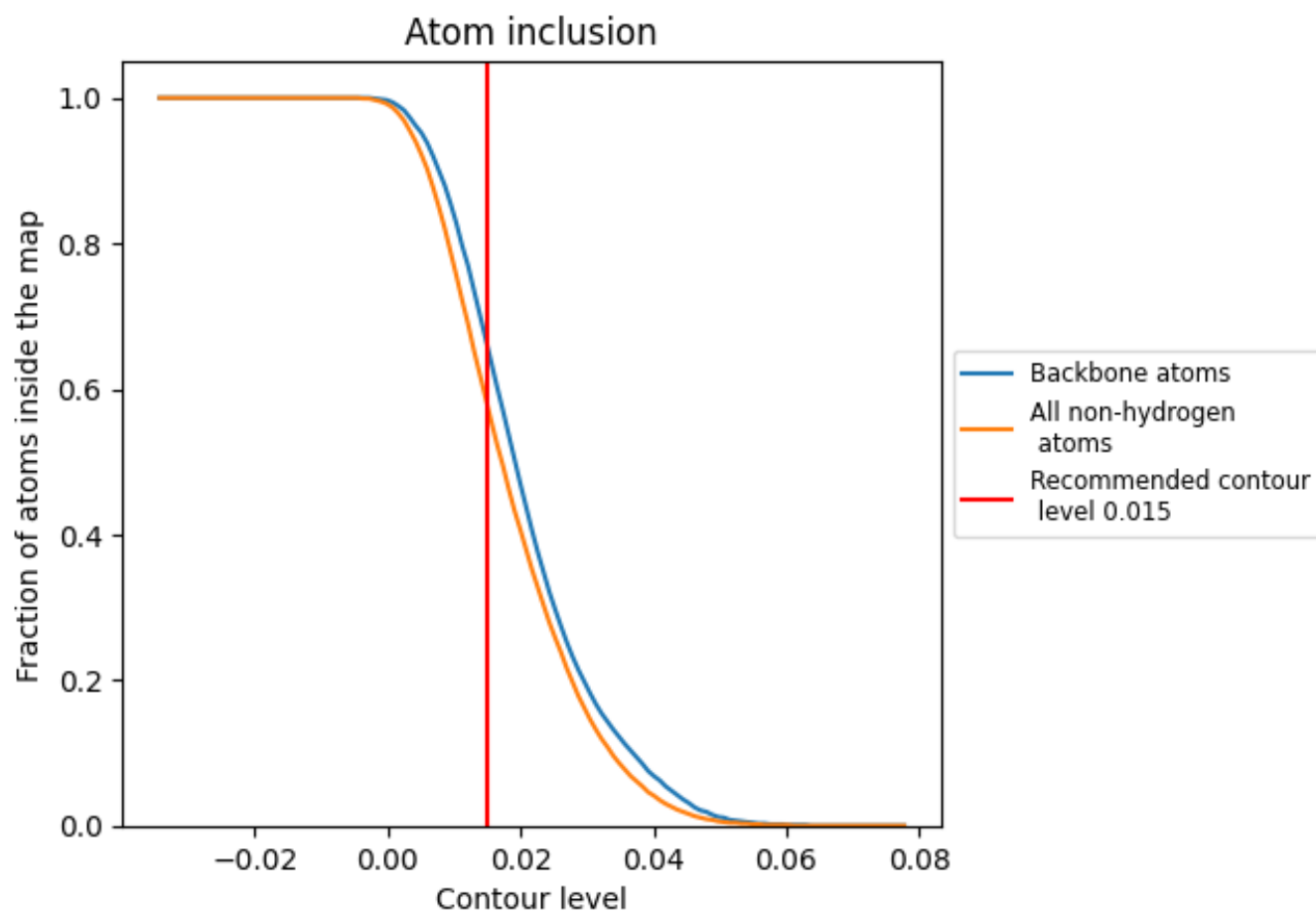
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.2630
A	 0.3950	 0.1890
B	 0.6660	 0.2830
C	 0.5420	 0.2350
D	 0.1440	 0.1220
E	 0.3520	 0.1680
F	 0.1270	 0.0710
G	 0.0000	 -0.0020
H	 0.1380	 0.1700
a	 0.8130	 0.4420
b	 0.8260	 0.4720
c	 0.7540	 0.4290
d	 0.7310	 0.4020
e	 0.7920	 0.4370
f	 0.8690	 0.4680
g	 0.8090	 0.4530
h	 0.8180	 0.4470
i	 0.8300	 0.2880
j	 0.8530	 0.2860

