



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:09 AM UTC

PDB ID : 8HY0 / pdb_00008hy0
EMDB ID : EMD-35084
Title : Composite cryo-EM structure of the histone deacetylase complex Rpd3S in complex with nucleosome
Authors : Cui, H.; Wang, H.
Deposited on : 2023-01-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

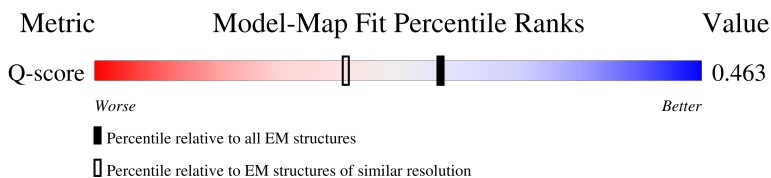
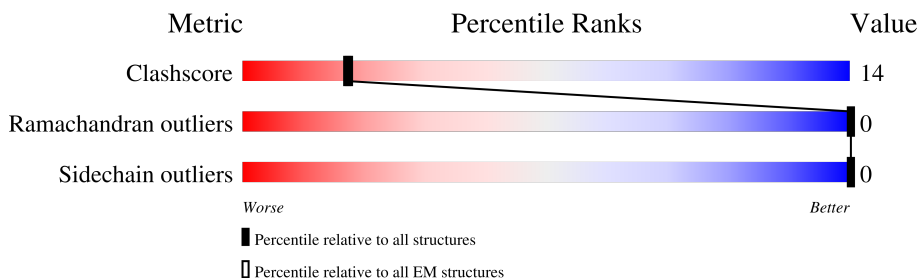
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



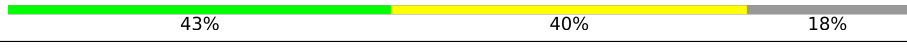
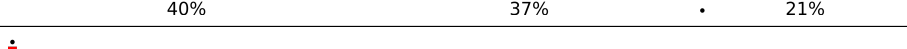
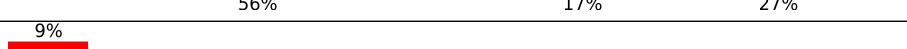
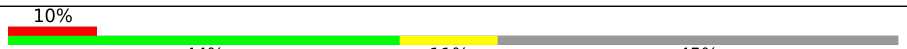
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	
1	E	135	
2	B	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	122	
4	H	122	
5	I	352	
6	J	352	
7	K	1536	
8	L	433	
9	M	401	
9	O	401	
10	N	684	
10	P	684	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28821 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	102	Total	C	N	O	S	0	0
			837	529	162	143	3		
1	E	116	Total	C	N	O	S	0	0
			945	591	189	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	80	Total	C	N	O	S	0	0
			641	405	125	110	1		
2	F	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			843	531	167	145		
3	G	106	Total	C	N	O	0	0
			818	516	160	142		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			757	475	140	140	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	94	Total	C	N	O	S	0	0
			736	463	132	139	2		

- Molecule 5 is a DNA chain called DNA (352-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	170	Total	C	N	O	P	0	0
			3466	1648	623	1025	170		

- Molecule 6 is a DNA chain called DNA (352-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	170	Total	C	N	O	P	0	0
			3504	1659	660	1015	170		

- Molecule 7 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	549	Total	C	N	O	S	0	0
			4597	2954	774	854	15		

- Molecule 8 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	384	Total	C	N	O	S	0	0
			3048	1941	512	569	26		

- Molecule 9 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	294	Total	C	N	O	S	0	0
			2398	1541	394	449	14		
9	O	156	Total	C	N	O	S	0	0
			1275	823	204	240	8		

- Molecule 10 is a protein called RCO1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	375	Total	C	N	O	S	0	0
			3073	1953	529	573	18		

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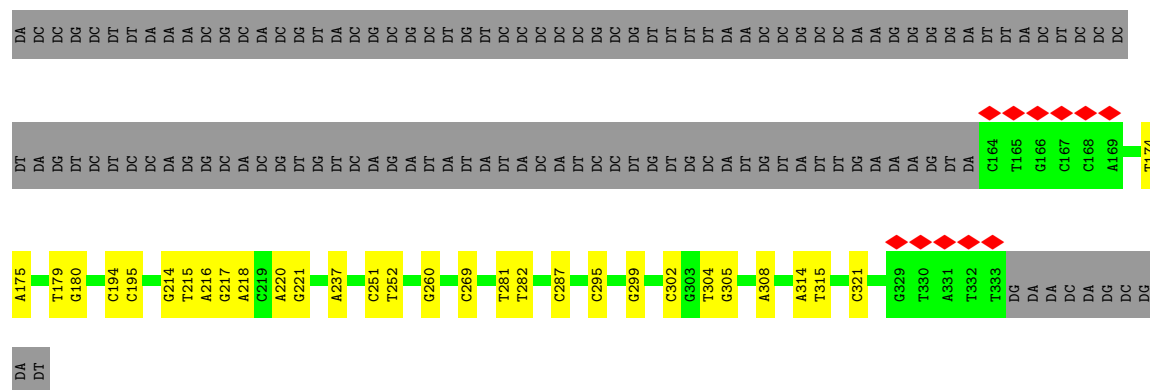
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Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	151	Total	C	N	O	S	0	0
			1249	802	206	231	10		

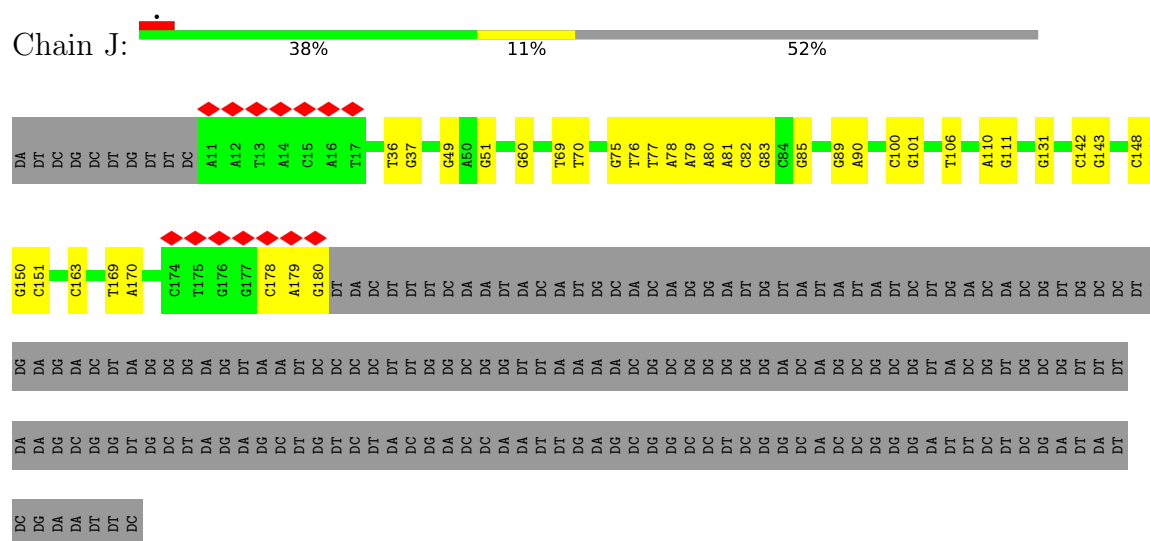
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	L	1	Total	Zn	0
			1	1	
11	N	4	Total	Zn	0
			4	4	
11	P	2	Total	Zn	0
			2	2	

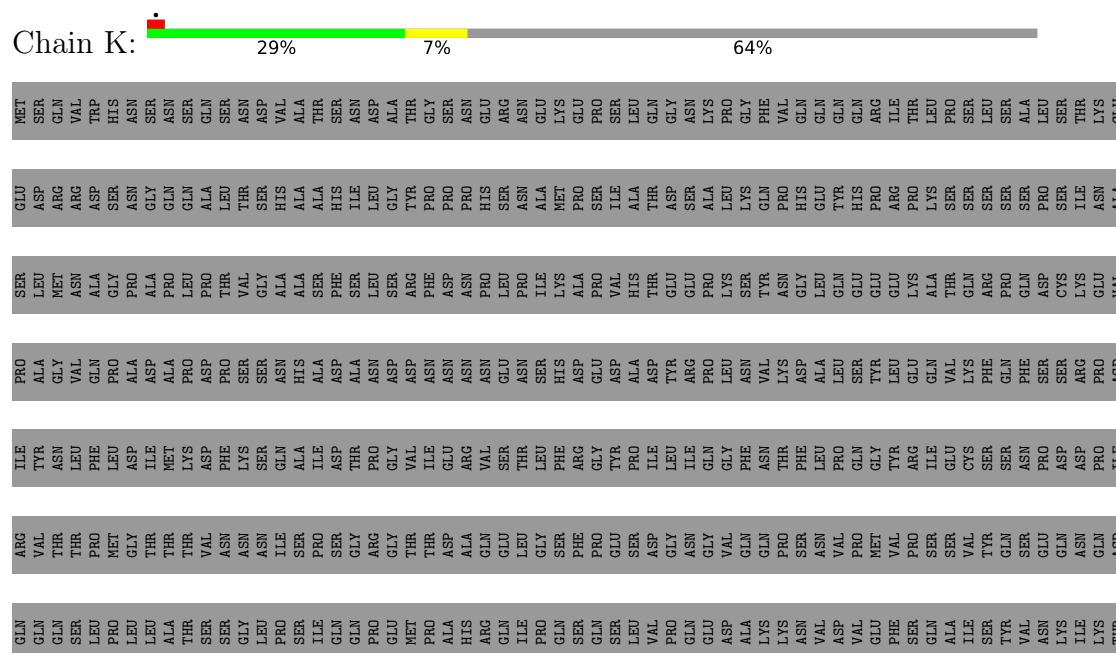


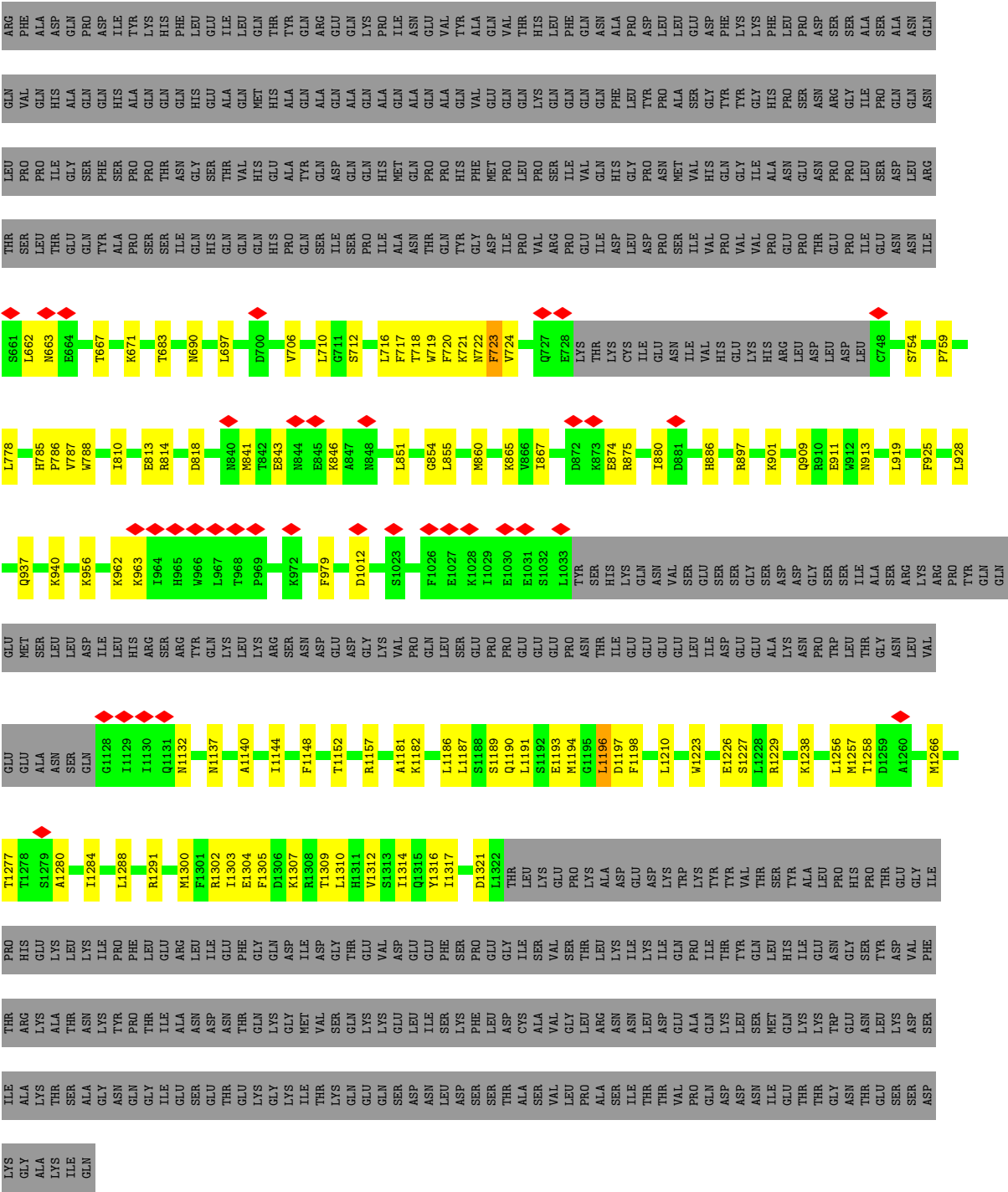


• Molecule 6: DNA (352-MER)



• Molecule 7: Transcriptional regulatory protein SIN3

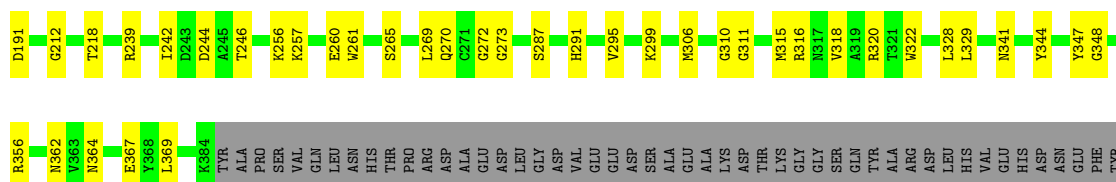




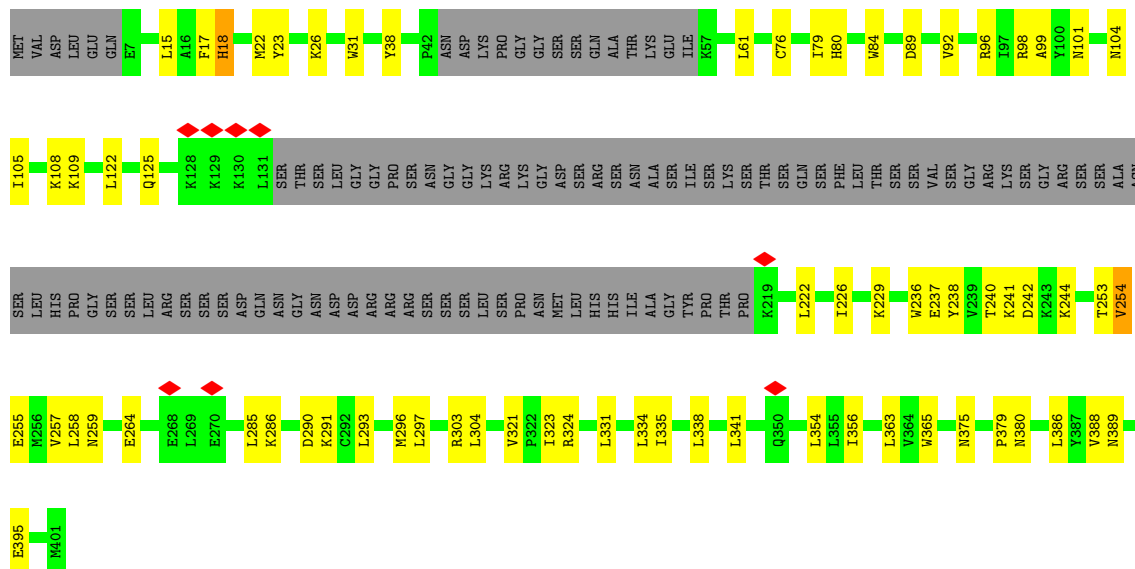
● Molecule 8: Histone deacetylase RPD3

Chain L: 72% 16% 11%

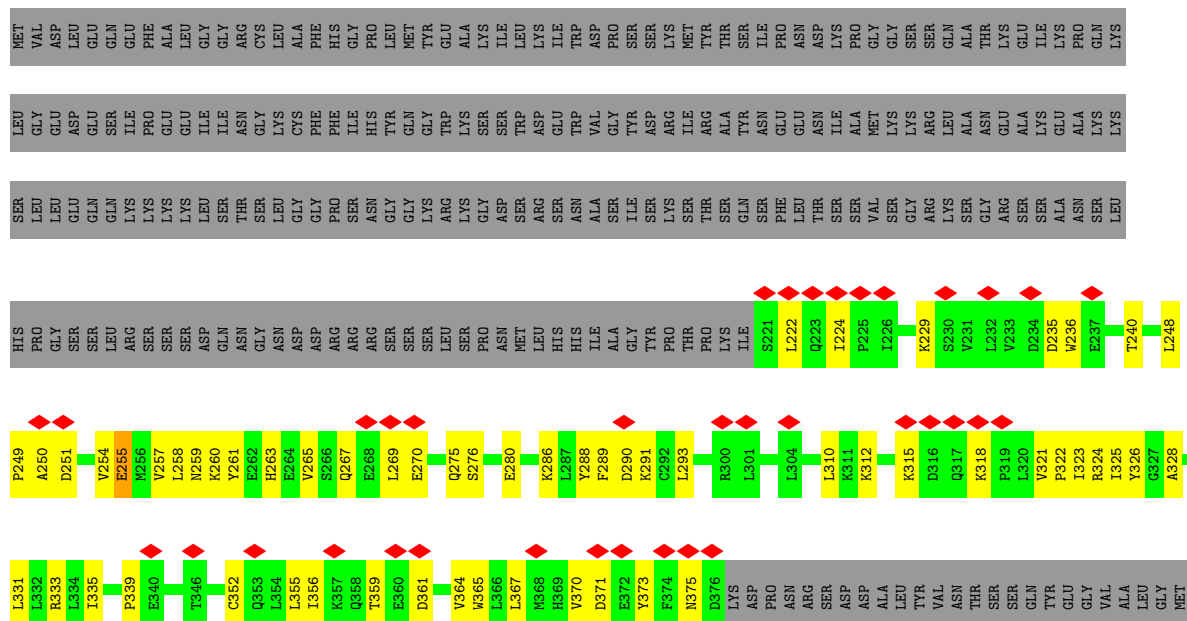




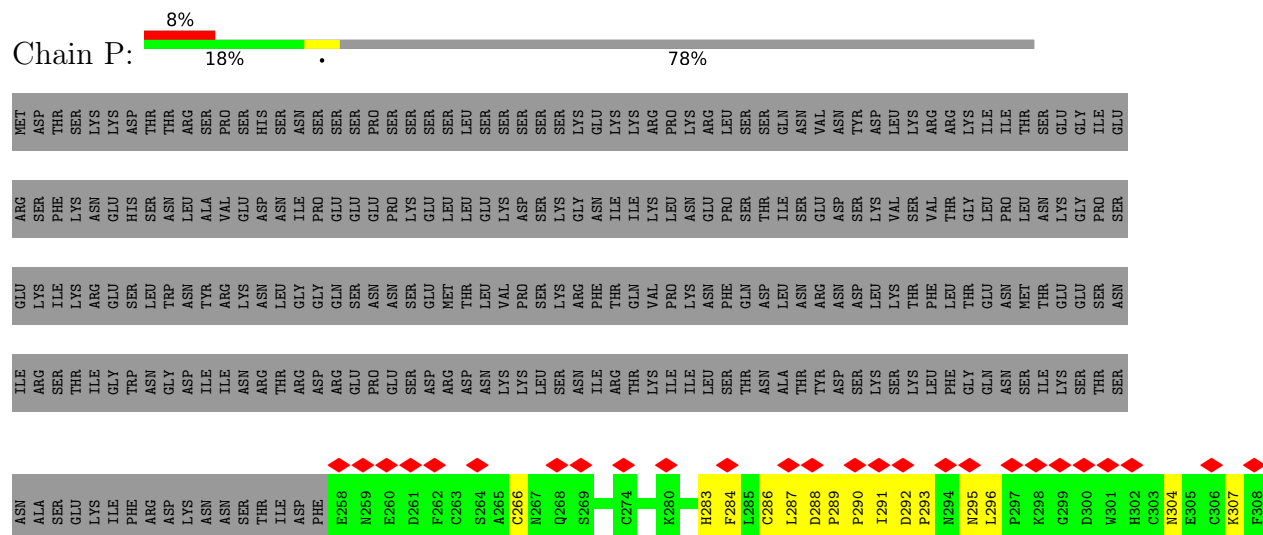
• Molecule 9: Chromatin modification-related protein EAF3



• Molecule 9: Chromatin modification-related protein EAF3



• Molecule 10: RCO1 isoform 1



PHE SER SER ASP GLU ILE LYS HIS LEU LEU TYR SER LEU LYS LYS PHE ASN GLN SER ASP GLU	SER GLU ASN MET VAL LYS ASP ILE ALA LEU LEU TYR PHE GLN VAL SER ASN ASP LEU LEU TYR ASN GLN PHE SER GLU ASN GLN ASP	PRO LEU GLN LYS ILE GLY TYR GLN ASN GLY ILE GLN ILE PRO THR THR SER HIS HIS ASP SER ASP F533 F537 F552 K557 S558 K559 M560 V561 Q562 K563 R564 K565 L566 F569 Q570 E571 VAL VAL PRO ASN GLU ASP SER TLE GLN PHE ASN ASP	ASN THR ASP TYR GLY GLN SER ILE LYS ASP ASN THR GLY LEU ASN GLY SER TRP LYS CYS PRO HIS LEU HIS THR ASP TYR THR ASP F533 F537 F552 K557 S558 K559 M560 V561 Q562 K563 R564 K565 L566 F569 Q570 E571 VAL VAL PRO ASN GLU ASP SER TLE GLN PHE ASN ASP	HIS LEU CYS VAL PRO ARG ALA PHE ASN GLY LEU SER LYS TRP CYS PRO HIS HIS THR PRO THR LYS VAL TYR LYS ILE HIS CYS GLN GLU ASP ASN SER VAL ASN TYR LYS VAL TRP GLU LYS LYS THR GLU TRP LYS GLN ARG LEU ILE ILE ASN LYS LYS ASN GLN TYR TRP GLU	K309 I310 F311 I312 N313 N314 S315 N316 A317 K328 Q329 N330 V333 K334 L339 L340 F341 N342 I343 H346 Q350 F351 Q352 I357 K358 E359 T360 PHE PRO ALA VAL LYS LYS THR GLY SER ARG GLY GLN TYR SER ASP GLU ASN ASP LYS ILE PRO LEU THR ASP ARG LEU PHE	ASN THR ASP TYR GLY GLN SER ILE LYS ASP ASN THR GLY LEU ASN GLY SER TRP LYS CYS PRO HIS LEU HIS CYS GLN GLU ASP ASN SER VAL ASN TYR LYS VAL TRP GLU LYS LYS THR GLU TRP LYS GLN ARG LEU ILE ILE ASN LYS LYS ASN GLN TYR TRP GLU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81856	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.320	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ML3

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	0.76	0/836	0.97	1/1120 (0.1%)
1	E	0.74	0/957	0.97	3/1279 (0.2%)
2	B	0.96	0/648	1.14	3/868 (0.3%)
2	F	0.88	0/634	1.15	6/848 (0.7%)
3	C	0.73	0/853	0.88	2/1149 (0.2%)
3	G	0.80	0/828	0.96	3/1117 (0.3%)
4	D	0.87	0/768	0.99	3/1032 (0.3%)
4	H	0.72	0/747	0.76	1/1004 (0.1%)
5	I	0.21	0/3882	0.46	0/5985
6	J	0.18	0/3936	0.38	0/6077
7	K	0.37	0/4699	0.52	3/6334 (0.0%)
8	L	0.31	1/3127 (0.0%)	0.43	0/4231
9	M	0.29	0/2446	0.50	2/3292 (0.1%)
9	O	0.31	0/1298	0.65	2/1755 (0.1%)
10	N	0.26	0/3144	0.56	5/4234 (0.1%)
10	P	0.25	0/1278	0.68	0/1716
All	All	0.44	1/30081 (0.0%)	0.62	34/42041 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	44	ARG	CA-C	-5.32	1.45	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	259	ASN	CA-C-N	-9.99	101.96	122.03
10	N	259	ASN	C-N-CA	-9.99	101.96	122.03
2	B	50	ILE	N-CA-C	-9.65	104.02	112.12
1	A	133	GLU	N-CA-C	-9.58	101.71	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	259	ASN	O-C-N	8.96	134.15	122.23
2	F	75	HIS	N-CA-C	-7.56	104.30	113.97
2	B	48	GLY	N-CA-C	-7.56	100.95	112.51
9	M	18	HIS	N-CA-C	-6.92	96.06	110.80
2	B	39	ARG	N-CA-C	-6.80	103.80	111.07
1	E	105	GLU	N-CA-C	-6.63	104.13	111.36
4	D	92	GLN	N-CA-C	-6.59	104.13	111.71
7	K	723	PHE	N-CA-C	-6.54	103.84	112.34
2	F	79	LYS	N-CA-C	-6.26	105.96	113.97
10	N	508	PRO	CA-N-CD	-6.22	103.30	112.00
9	O	255	GLU	N-CA-C	-6.14	103.52	111.02
3	C	39	TYR	N-CA-C	-6.12	104.72	111.82
2	F	25	ASN	N-CA-C	-5.98	105.08	112.38
10	N	518	GLY	N-CA-C	-5.75	107.73	115.21
9	O	251	ASP	CB-CA-C	-5.67	110.02	116.54
1	E	64	LYS	N-CA-C	5.61	117.08	110.97
1	E	125	GLN	N-CA-C	-5.54	105.25	112.23
4	H	56	MET	N-CA-C	-5.40	105.08	110.97
2	F	53	GLU	N-CA-C	-5.35	105.90	112.90
3	G	106	GLY	N-CA-C	-5.30	102.61	112.37
3	G	99	ARG	N-CA-C	-5.29	104.41	111.87
2	F	31	LYS	CA-C-N	-5.26	113.37	119.47
2	F	31	LYS	C-N-CA	-5.26	113.37	119.47
7	K	1288	LEU	CA-CB-CG	5.22	134.58	116.30
9	M	254	VAL	CB-CA-C	-5.20	105.39	111.94
7	K	1196	LEU	N-CA-C	-5.18	107.34	113.97
3	C	20	ARG	N-CA-C	-5.14	106.85	113.02
4	D	95	VAL	N-CA-C	-5.11	104.67	111.05
3	G	59	THR	N-CA-C	-5.09	106.58	112.89
4	D	34	TYR	N-CA-C	-5.04	106.38	112.88

There are no chirality outliers.

There are no planarity outliers.

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	837	0	885	91	0
1	E	945	0	1004	97	0
2	B	641	0	684	90	0
2	F	627	0	663	48	0
3	C	843	0	908	60	0
3	G	818	0	877	47	0
4	D	757	0	786	57	0
4	H	736	0	760	36	0
5	I	3466	0	1912	26	0
6	J	3504	0	1907	31	0
7	K	4597	0	4560	94	0
8	L	3048	0	2932	57	0
9	M	2398	0	2429	57	0
9	O	1275	0	1310	55	0
10	N	3073	0	3034	79	0
10	P	1249	0	1215	28	0
11	L	1	0	0	0	0
11	N	4	0	0	0	0
11	P	2	0	0	0	0
All	All	28821	0	25866	743	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 14.

All (743) 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)
3:C:63:LEU:HD22	4:D:59:MET:HE3	1.21	1.14
2:B:91:LYS:HD3	2:B:96:THR:HG22	1.39	1.04
2:B:65:VAL:HG22	2:B:93:GLN:HE22	1.18	1.03
2:B:91:LYS:HD3	2:B:96:THR:CG2	1.90	1.01
7:K:937:GLN:CB	7:K:940:LYS:HE2	1.90	1.00
4:D:51:ILE:HG21	4:D:56:MET:HE2	1.42	0.98
3:C:79:ILE:HG23	3:C:80:PRO:HD2	1.43	0.98
4:D:78:ALA:HB2	4:D:90:GLU:OE1	1.64	0.97
9:M:17:PHE:CD1	9:M:22:MET:HE1	2.00	0.96
7:K:937:GLN:HB2	7:K:940:LYS:HE2	1.49	0.93
3:C:15:LYS:HE2	3:C:20:ARG:HD3	1.51	0.93
9:M:255:GLU:HG3	9:M:286:LYS:HE2	1.50	0.93
3:G:58:LEU:HD21	4:H:99:LEU:HD21	1.51	0.92
9:M:255:GLU:HB2	9:M:323:ILE:CG2	2.01	0.91
9:M:255:GLU:HB2	9:M:323:ILE:HG23	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:102:ILE:HG23	4:H:58:ILE:HD12	1.55	0.87
10:N:304:ASN:HD22	10:N:348:PRO:HD3	1.37	0.87
3:C:79:ILE:CG2	3:C:80:PRO:HD2	2.05	0.87
9:M:17:PHE:HD1	9:M:22:MET:HE1	1.36	0.86
1:A:70:LEU:HD22	2:B:29:ILE:HD11	1.57	0.86
7:K:937:GLN:CA	7:K:940:LYS:HE2	2.06	0.85
3:C:62:ILE:HG23	4:D:59:MET:HE1	1.57	0.85
3:C:115:LEU:HD11	1:E:108:ASN:HD21	1.40	0.85
2:B:26:ILE:HD12	2:B:29:ILE:HD12	1.58	0.84
10:N:466:CYS:SG	10:N:469:HIS:CD2	2.70	0.84
2:B:29:ILE:HD13	2:B:58:LEU:HD23	1.59	0.83
3:C:63:LEU:HD12	4:D:42:LEU:HD13	1.61	0.83
10:P:296:LEU:HD12	10:P:296:LEU:O	1.78	0.81
3:C:111:ILE:CD1	1:E:51:ILE:HG21	2.10	0.81
5:I:217:DG:H2''	5:I:218:DA:C8	2.15	0.81
10:N:304:ASN:ND2	10:N:348:PRO:HD3	1.96	0.81
1:A:46:VAL:HG21	5:I:260:DG:H3'	1.62	0.81
7:K:937:GLN:HA	7:K:940:LYS:HE2	1.62	0.80
3:C:111:ILE:HD11	1:E:51:ILE:HG21	1.63	0.80
1:E:63:ARG:HH21	5:I:237:DA:H5''	1.45	0.79
9:M:18:HIS:HB3	9:M:23:TYR:CE2	2.18	0.78
10:N:122:LYS:HG3	10:N:125:ARG:NH2	1.99	0.78
7:K:937:GLN:O	7:K:940:LYS:HG2	1.84	0.77
4:D:45:VAL:HG23	4:D:46:HIS:H	1.49	0.76
9:O:254:VAL:HA	9:O:257:VAL:HG12	1.67	0.76
10:P:291:ILE:HD11	10:P:296:LEU:HA	1.66	0.76
2:B:65:VAL:HG22	2:B:93:GLN:NE2	1.99	0.75
1:E:7:ALA:HB2	10:N:270:GLY:HA2	1.69	0.75
5:I:215:DT:H2''	5:I:216:DA:N7	2.02	0.75
10:N:443:CYS:SG	10:N:469:HIS:CE1	2.81	0.74
1:E:124:ILE:HD11	2:F:53:GLU:HG2	1.70	0.73
3:C:111:ILE:HD11	1:E:51:ILE:CG2	2.17	0.73
3:C:40:ALA:HB3	4:D:86:ILE:HD13	1.68	0.73
1:E:68:GLN:HE21	1:E:72:ARG:HH21	1.37	0.72
1:A:79:LYS:HB2	2:B:70:VAL:HG21	1.72	0.72
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.22	0.72
1:A:78:PHE:HB3	2:B:70:VAL:HG11	1.70	0.71
3:C:62:ILE:HG23	4:D:59:MET:CE	2.20	0.71
7:K:722:ASN:C	7:K:724:VAL:N	2.46	0.71
2:B:43:VAL:HG21	2:B:46:ILE:HD11	1.73	0.71
3:C:31:HIS:CD2	3:C:35:ARG:HE	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1194:MET:HE1	7:K:1223:TRP:CD1	2.26	0.70
7:K:937:GLN:HA	7:K:940:LYS:HG2	1.72	0.69
1:A:79:LYS:HD3	1:A:82:LEU:HD21	1.72	0.69
2:B:90:LEU:HA	2:B:93:GLN:HE21	1.57	0.69
1:A:103:LEU:HD21	1:A:124:ILE:HG23	1.75	0.69
2:B:84:MET:O	2:B:87:VAL:HG12	1.92	0.69
4:H:36:ILE:HG22	4:H:40:LYS:HE3	1.75	0.69
7:K:925:PHE:HB3	7:K:1229:ARG:HD3	1.75	0.68
1:E:15:ALA:HB3	1:E:16:PRO:HD3	1.75	0.68
10:P:288:ASP:HB2	10:P:289:PRO:HD3	1.73	0.68
10:N:172:THR:HA	10:N:175:MET:HG2	1.75	0.68
2:B:48:GLY:O	2:B:49:LEU:HB2	1.93	0.68
7:K:1148:PHE:CE2	7:K:1312:VAL:HG11	2.29	0.68
1:E:71:VAL:HG13	2:F:66:ILE:HD13	1.75	0.68
3:G:57:TYR:HD2	3:G:58:LEU:HD22	1.60	0.67
1:A:92:LEU:HD21	2:B:66:ILE:CG1	2.24	0.67
9:O:255:GLU:HG2	9:O:259:ASN:ND2	2.10	0.67
1:E:73:GLU:OE1	2:F:25:ASN:HB2	1.95	0.67
1:A:48:LEU:HD21	2:B:44:LYS:HE2	1.77	0.67
1:E:79:LYS:HD3	1:E:82:LEU:HD13	1.77	0.66
3:G:79:ILE:HG22	3:G:81:ARG:H	1.60	0.66
10:N:556:TYR:O	10:N:560:MET:HG2	1.96	0.66
2:B:30:THR:HB	2:B:32:PRO:HD2	1.78	0.66
1:E:17:ARG:HB3	8:L:109:ASP:CG	2.21	0.66
1:A:70:LEU:O	1:A:74:ILE:HG13	1.96	0.65
7:K:722:ASN:C	7:K:724:VAL:H	2.00	0.65
9:O:255:GLU:HG2	9:O:259:ASN:HD21	1.60	0.65
3:C:62:ILE:CG2	4:D:59:MET:HE1	2.27	0.65
10:N:562:GLN:OE1	10:P:560:MET:HE1	1.97	0.65
3:G:49:VAL:HG21	4:H:118:TYR:CD2	2.31	0.64
9:O:290:ASP:OD1	9:O:323:ILE:HG12	1.97	0.64
1:A:125:GLN:HG2	1:A:134:ARG:HH12	1.60	0.64
4:D:36:ILE:HG13	4:D:37:TYR:N	2.10	0.64
1:E:62:ILE:HD13	2:F:33:ALA:HB1	1.79	0.64
9:O:288:TYR:CE1	10:P:343:ILE:HD11	2.33	0.64
7:K:1194:MET:HB2	7:K:1196:LEU:HG	1.78	0.64
7:K:1309:THR:O	7:K:1310:LEU:C	2.38	0.64
9:M:22:MET:SD	9:M:98:ARG:NH2	2.71	0.64
3:G:84:GLN:HA	3:G:87:VAL:HG12	1.80	0.63
1:A:71:VAL:HG13	2:B:66:ILE:HD13	1.79	0.63
7:K:754:SER:HB2	8:L:218:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:GLN:NE2	10:N:271:SER:HB2	2.13	0.63
1:E:65:LEU:HB2	1:E:66:PRO:HD3	1.80	0.63
9:O:222:LEU:HD13	9:O:339:PRO:HG3	1.80	0.63
7:K:1196:LEU:HD22	7:K:1210:LEU:HD11	1.81	0.63
5:I:220:DA:H2''	5:I:221:DG:H5'	1.80	0.63
9:O:286:LYS:HA	9:O:323:ILE:HD11	1.80	0.63
8:L:29:VAL:HG11	8:L:45:ILE:HG21	1.79	0.63
10:N:557:LYS:HB2	9:O:275:GLN:HE22	1.63	0.63
2:B:65:VAL:CG2	2:B:93:GLN:HE22	2.05	0.63
9:M:17:PHE:CE1	9:M:22:MET:HE1	2.34	0.63
10:N:562:GLN:HE22	9:O:270:GLU:HA	1.64	0.63
10:P:339:LEU:HD12	10:P:342:ASN:HD21	1.63	0.63
3:G:57:TYR:CD2	3:G:58:LEU:HD22	2.34	0.62
7:K:937:GLN:C	7:K:940:LYS:HG2	2.23	0.62
2:B:90:LEU:HD23	2:B:93:GLN:NE2	2.14	0.62
1:A:40:ARG:HH22	6:J:85:DG:H21	1.47	0.62
1:A:71:VAL:O	1:A:74:ILE:N	2.31	0.62
3:C:79:ILE:CG2	3:C:80:PRO:CD	2.78	0.62
9:O:260:LYS:HD3	9:O:373:TYR:OH	1.99	0.62
3:G:102:ILE:HG23	4:H:58:ILE:CD1	2.26	0.62
7:K:937:GLN:HA	7:K:940:LYS:CE	2.29	0.62
1:E:124:ILE:HD11	2:F:53:GLU:CG	2.30	0.61
2:B:26:ILE:HG13	2:B:55:ARG:HD3	1.81	0.61
3:C:97:LEU:HD21	4:D:62:PHE:HE1	1.65	0.61
1:E:68:GLN:NE2	1:E:72:ARG:HH21	1.99	0.61
4:H:92:GLN:HA	4:H:95:VAL:HG12	1.82	0.61
1:E:18:LYS:HD2	8:L:188:HIS:CE1	2.36	0.61
1:E:92:LEU:HD12	2:F:62:LEU:CD1	2.30	0.61
1:A:82:LEU:HD11	2:B:70:VAL:CG2	2.29	0.61
3:C:11:ARG:HH21	5:I:295:DC:H1'	1.66	0.61
6:J:79:DA:H2''	6:J:80:DA:H8	1.66	0.61
2:B:32:PRO:HG2	6:J:80:DA:H3'	1.83	0.60
3:C:63:LEU:CD2	4:D:59:MET:HE3	2.13	0.60
1:A:92:LEU:HD21	2:B:66:ILE:HG12	1.82	0.60
1:A:36:ML3:HM2B	9:M:18:HIS:CE1	2.36	0.60
2:B:32:PRO:O	2:B:36:ARG:HG3	2.00	0.60
6:J:142:DC:H2'	6:J:143:DG:C8	2.36	0.60
7:K:788:TRP:NE1	9:M:395:GLU:OE1	2.31	0.60
6:J:80:DA:H2''	6:J:81:DA:H5'	1.82	0.59
7:K:1226:GLU:HA	7:K:1229:ARG:HG2	1.83	0.59
3:C:64:GLU:HA	4:D:46:HIS:CD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:67:ARG:O	2:F:70:VAL:HG12	2.03	0.59
1:A:36:ML3:HM2B	9:M:18:HIS:CD2	2.37	0.59
1:A:70:LEU:CD2	2:B:29:ILE:HD11	2.32	0.59
7:K:937:GLN:CA	7:K:940:LYS:HG2	2.33	0.59
9:M:105:ILE:HG22	9:M:109:LYS:HE3	1.83	0.59
10:N:176:THR:O	10:N:176:THR:HG23	2.02	0.58
9:O:289:PHE:CD2	9:O:323:ILE:HD13	2.38	0.58
1:A:63:ARG:NH2	6:J:79:DA:H5''	2.18	0.58
4:D:45:VAL:HG23	4:D:46:HIS:N	2.19	0.58
9:O:265:VAL:O	9:O:269:LEU:N	2.33	0.58
1:E:2:ARG:HG3	10:N:274:CYS:HB2	1.84	0.58
8:L:73:GLU:OE1	10:N:182:ARG:NH1	2.36	0.58
10:N:414:PHE:HB3	10:N:423:THR:HG21	1.85	0.58
4:D:40:LYS:O	4:D:44:GLN:HG2	2.04	0.58
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.85	0.58
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.86	0.58
5:I:220:DA:H2''	5:I:221:DG:C5'	2.34	0.58
4:D:83:ARG:HH22	6:J:60:DG:P	2.26	0.58
4:D:105:LYS:HD2	4:D:105:LYS:N	2.19	0.57
7:K:911:GLU:HG3	10:N:119:PRO:HD2	1.86	0.57
1:A:60:LEU:HD21	1:A:94:GLU:OE2	2.04	0.57
1:E:7:ALA:HB1	1:E:9:LYS:HE3	1.86	0.57
10:N:173:GLU:O	10:N:176:THR:HG22	2.03	0.57
7:K:706:VAL:HG12	7:K:717:PHE:CD1	2.40	0.57
7:K:937:GLN:O	7:K:940:LYS:CG	2.51	0.57
9:M:18:HIS:HB3	9:M:23:TYR:HE2	1.66	0.57
9:M:335:ILE:HG21	9:M:363:LEU:HD21	1.86	0.57
2:B:91:LYS:HD3	2:B:96:THR:HG21	1.82	0.57
2:F:52:GLU:O	2:F:52:GLU:HG2	2.04	0.57
6:J:77:DT:H2''	6:J:78:DA:C8	2.40	0.57
2:B:61:PHE:O	2:B:65:VAL:HG23	2.04	0.57
3:G:58:LEU:HD21	4:H:99:LEU:CD2	2.30	0.57
7:K:1132:ASN:H	7:K:1277:THR:HG22	1.68	0.57
10:N:559:LYS:O	10:N:563:LYS:HG3	2.05	0.57
9:O:291:LYS:NZ	10:P:343:ILE:HB	2.20	0.57
7:K:818:ASP:OD1	7:K:909:GLN:NE2	2.37	0.57
1:A:120:MET:C	2:B:50:ILE:HD11	2.31	0.56
1:E:109:LEU:HA	1:E:112:ILE:HG22	1.87	0.56
3:G:83:LEU:HD13	4:H:59:MET:HE3	1.86	0.56
8:L:152:ALA:O	8:L:164:ASN:ND2	2.38	0.56
8:L:212:GLY:HA2	10:N:456:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:454:ARG:NH2	10:N:456:SER:OG	2.38	0.56
7:K:1305:PHE:CE1	7:K:1310:LEU:HA	2.40	0.56
8:L:148:GLY:HA3	8:L:310:GLY:HA2	1.86	0.56
10:N:122:LYS:HG3	10:N:125:ARG:HH21	1.70	0.56
10:N:562:GLN:NE2	9:O:270:GLU:O	2.38	0.56
1:E:7:ALA:HB1	1:E:9:LYS:HG2	1.87	0.56
2:B:72:TYR:HE1	4:D:97:LEU:HD13	1.71	0.56
7:K:937:GLN:HA	7:K:940:LYS:CD	2.35	0.56
7:K:1197:ASP:OD1	7:K:1197:ASP:N	2.39	0.56
10:P:266:CYS:HA	10:P:350:GLN:HB2	1.87	0.56
1:A:103:LEU:HD11	1:A:128:ARG:HD2	1.87	0.56
7:K:937:GLN:HA	7:K:940:LYS:CG	2.36	0.56
10:P:339:LEU:HD12	10:P:342:ASN:ND2	2.20	0.56
3:G:25:PHE:CZ	4:H:38:VAL:HG22	2.41	0.56
9:O:291:LYS:HZ3	10:P:343:ILE:HB	1.68	0.56
1:A:79:LYS:HB2	2:B:70:VAL:CG2	2.36	0.56
3:C:51:LEU:O	3:C:54:VAL:HG22	2.06	0.56
1:E:71:VAL:HG13	2:F:66:ILE:CD1	2.37	0.55
1:E:119:ILE:HG23	2:F:43:VAL:HG13	1.88	0.55
3:G:97:LEU:HD21	4:H:62:PHE:CD1	2.41	0.55
8:L:114:ASP:OD1	8:L:114:ASP:N	2.38	0.55
2:B:29:ILE:CD1	2:B:58:LEU:HD23	2.31	0.55
1:E:16:PRO:HG2	7:K:787:VAL:HG22	1.88	0.55
2:B:38:ALA:O	2:B:43:VAL:HG22	2.07	0.55
7:K:851:LEU:HD13	7:K:855:LEU:HD22	1.88	0.55
1:A:99:TYR:CE2	2:B:61:PHE:HB2	2.42	0.55
1:E:84:PHE:CD2	2:F:81:VAL:HG21	2.42	0.55
9:O:260:LYS:HE2	9:O:365:TRP:CZ2	2.42	0.55
8:L:257:LYS:O	8:L:261:TRP:HB2	2.06	0.55
1:E:84:PHE:HA	2:F:81:VAL:HG22	1.88	0.55
7:K:759:PRO:HG3	9:M:388:VAL:HB	1.88	0.55
9:M:297:LEU:HD21	9:M:334:LEU:HB2	1.88	0.55
2:B:38:ALA:HB1	2:B:43:VAL:HG21	1.89	0.55
4:D:38:VAL:O	4:D:41:VAL:HG22	2.07	0.55
1:E:84:PHE:HA	2:F:81:VAL:CG2	2.37	0.55
10:P:292:ASP:CG	10:P:295:ASN:HB3	2.31	0.55
3:G:27:VAL:HG11	3:G:49:VAL:HG22	1.88	0.54
8:L:239:ARG:HE	10:N:455:ALA:HA	1.72	0.54
1:A:82:LEU:HD11	2:B:70:VAL:HG21	1.90	0.54
3:C:58:LEU:HD11	4:D:99:LEU:HD21	1.88	0.54
1:E:5:GLN:HE22	10:N:271:SER:HB2	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:ALA:O	2:B:34:ILE:C	2.46	0.54
3:C:59:THR:HA	3:C:62:ILE:HG22	1.87	0.54
3:C:66:ALA:HB1	3:C:78:ILE:HG23	1.90	0.54
3:G:31:HIS:CE1	3:G:35:ARG:HE	2.25	0.54
2:B:26:ILE:CD1	2:B:29:ILE:HD12	2.33	0.54
3:C:78:ILE:HB	4:D:51:ILE:HG13	1.89	0.54
4:D:105:LYS:HD2	4:D:105:LYS:H	1.72	0.54
8:L:272:GLY:O	8:L:291:HIS:NE2	2.41	0.54
1:E:13:GLY:C	1:E:16:PRO:HD2	2.32	0.54
6:J:79:DA:H2''	6:J:80:DA:C8	2.43	0.54
1:A:51:ILE:HD11	2:B:39:ARG:HD3	1.90	0.54
1:A:61:LEU:N	1:A:97:GLU:OE2	2.36	0.54
2:B:35:ARG:HD3	2:B:46:ILE:HG13	1.89	0.54
4:D:94:ALA:HA	4:D:97:LEU:HD12	1.89	0.54
3:G:39:TYR:O	4:H:75:SER:HB2	2.07	0.54
3:G:56:GLU:HG3	4:H:41:VAL:HG21	1.89	0.54
1:A:106:ASP:HB2	1:E:130:ILE:HG22	1.90	0.54
4:D:76:ARG:O	4:D:77:LEU:C	2.50	0.54
2:F:92:ARG:HE	4:H:98:LEU:HD23	1.72	0.54
2:F:61:PHE:HD2	2:F:62:LEU:HD22	1.73	0.53
1:A:46:VAL:HG21	5:I:260:DG:C3'	2.34	0.53
8:L:149:LEU:HB3	8:L:161:CYS:HB3	1.91	0.53
10:N:498:ILE:HD11	10:P:537:PHE:HD2	1.73	0.53
1:A:40:ARG:HH22	6:J:85:DG:N2	2.06	0.53
9:M:244:LYS:HD3	9:M:379:PRO:HG2	1.90	0.53
4:D:36:ILE:HD11	4:D:37:TYR:CZ	2.43	0.53
1:E:77:ASP:OD1	1:E:78:PHE:N	2.42	0.53
1:E:82:LEU:HG	2:F:81:VAL:HG13	1.91	0.53
8:L:133:ARG:HG2	10:N:181:ILE:HD11	1.91	0.53
9:O:248:LEU:HB2	9:O:249:PRO:HD3	1.91	0.53
3:C:66:ALA:HB2	3:C:83:LEU:HD23	1.91	0.53
4:H:102:GLU:O	4:H:103:LEU:C	2.48	0.53
9:M:18:HIS:HB3	9:M:23:TYR:CD2	2.43	0.53
9:M:303:ARG:HD3	10:N:286:CYS:HA	1.90	0.53
9:O:254:VAL:CA	9:O:257:VAL:HG12	2.38	0.53
2:B:90:LEU:HD23	2:B:93:GLN:HE21	1.72	0.53
3:G:97:LEU:HD21	4:H:62:PHE:HD1	1.74	0.53
1:A:78:PHE:CB	2:B:70:VAL:HG11	2.37	0.53
7:K:723:PHE:CZ	10:P:552:PHE:CE1	2.97	0.53
1:E:11:THR:HA	8:L:102:VAL:HG12	1.91	0.52
4:H:92:GLN:O	4:H:93:THR:C	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1181:ALA:HB1	7:K:1187:LEU:HG	1.90	0.52
3:G:18:SER:O	3:G:22:GLY:N	2.42	0.52
7:K:1256:LEU:HD11	7:K:1266:MET:HE2	1.89	0.52
3:C:66:ALA:HB1	3:C:78:ILE:CG2	2.39	0.52
4:H:38:VAL:HA	4:H:41:VAL:HG12	1.92	0.52
1:E:71:VAL:HA	1:E:74:ILE:HG22	1.92	0.52
8:L:29:VAL:HG21	8:L:45:ILE:HD13	1.90	0.52
1:E:83:ARG:O	2:F:81:VAL:HG22	2.10	0.52
2:F:61:PHE:CD2	2:F:62:LEU:HD22	2.45	0.52
8:L:49:HIS:HE2	10:N:172:THR:HG21	1.74	0.52
1:A:36:ML3:HM2B	9:M:18:HIS:CG	2.44	0.52
1:A:47:ALA:O	1:A:51:ILE:HG12	2.10	0.52
3:G:31:HIS:CD2	3:G:48:PRO:HG3	2.44	0.52
4:H:56:MET:HE3	4:H:56:MET:HA	1.90	0.52
6:J:82:DC:H2"	6:J:83:DG:H8	1.75	0.52
7:K:778:LEU:HD11	8:L:171:ILE:HD11	1.91	0.52
7:K:937:GLN:HB2	7:K:940:LYS:CE	2.32	0.52
1:A:89:VAL:HG23	1:A:90:MET:N	2.24	0.52
1:E:119:ILE:HD11	2:F:46:ILE:HG23	1.90	0.52
9:O:364:VAL:HA	9:O:367:LEU:HD12	1.92	0.52
4:D:102:GLU:O	4:D:103:LEU:C	2.52	0.51
4:H:102:GLU:C	4:H:104:ALA:N	2.66	0.51
7:K:979:PHE:HZ	7:K:1152:THR:HG22	1.75	0.51
1:A:63:ARG:HB2	1:A:66:PRO:HG2	1.92	0.51
2:F:39:ARG:NH1	2:F:46:ILE:HD11	2.25	0.51
4:H:43:LYS:HD2	4:H:47:PRO:HA	1.92	0.51
7:K:1140:ALA:HB1	7:K:1144:ILE:HB	1.91	0.51
7:K:1186:LEU:HD11	8:L:344:TYR:HE2	1.76	0.51
9:O:293:LEU:HD13	9:O:322:PRO:HB3	1.93	0.51
1:A:58:THR:CG2	3:G:81:ARG:HD3	2.41	0.51
1:A:61:LEU:H	1:A:97:GLU:CD	2.19	0.51
1:A:61:LEU:HD23	2:B:37:LEU:HD23	1.93	0.51
4:D:91:ILE:O	4:D:92:GLN:C	2.52	0.51
2:B:71:THR:O	2:B:74:GLU:HG2	2.11	0.51
4:D:58:ILE:HD13	2:F:99:GLY:CA	2.41	0.51
2:F:71:THR:HG22	4:H:93:THR:HG23	1.91	0.51
1:E:92:LEU:HD12	2:F:62:LEU:HD13	1.92	0.51
7:K:683:THR:HG23	10:N:522:ILE:HG13	1.93	0.51
8:L:44:ARG:NH1	8:L:311:GLY:O	2.44	0.51
1:A:79:LYS:HB3	1:A:82:LEU:HG	1.93	0.51
4:H:76:ARG:HB3	4:H:80:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:897:ARG:NH1	10:N:101:THR:OG1	2.43	0.51
7:K:1300:MET:HB3	7:K:1317:ILE:HG13	1.93	0.51
9:M:99:ALA:O	9:M:104:ASN:ND2	2.34	0.51
9:M:254:VAL:O	9:M:257:VAL:HG22	2.11	0.51
10:N:558:SER:O	10:N:562:GLN:HG2	2.11	0.51
1:A:79:LYS:CB	2:B:70:VAL:HG21	2.37	0.51
7:K:690:ASN:ND2	10:N:520:ILE:HD13	2.26	0.51
8:L:76:GLN:OE1	8:L:175:ARG:NH2	2.40	0.51
9:O:289:PHE:HD2	9:O:323:ILE:HD13	1.73	0.51
3:C:85:LEU:O	3:C:89:ASN:HB2	2.11	0.50
1:E:13:GLY:O	1:E:16:PRO:HD2	2.11	0.50
2:B:61:PHE:HE1	2:B:95:ARG:HD2	1.75	0.50
4:D:98:LEU:O	4:D:99:LEU:C	2.54	0.50
2:F:70:VAL:O	2:F:74:GLU:HG2	2.11	0.50
1:A:108:ASN:ND2	2:B:42:GLY:O	2.44	0.50
9:M:101:ASN:OD1	9:M:104:ASN:ND2	2.44	0.50
9:O:293:LEU:HD11	9:O:326:TYR:CG	2.47	0.50
1:A:119:ILE:HD11	2:B:46:ILE:HD13	1.94	0.50
1:A:129:ARG:O	1:A:130:ILE:HD13	2.11	0.50
1:E:61:LEU:N	1:E:97:GLU:OE2	2.45	0.50
6:J:69:DT:H2'	6:J:70:DT:H71	1.93	0.50
8:L:299:LYS:HD2	8:L:329:LEU:HD23	1.92	0.50
9:M:236:TRP:O	9:M:240:THR:OG1	2.29	0.50
1:A:79:LYS:HB3	1:A:82:LEU:CG	2.40	0.50
1:A:117:VAL:HG23	2:B:45:ARG:HD3	1.93	0.50
3:C:40:ALA:HB3	4:D:86:ILE:CD1	2.40	0.50
3:C:93:LEU:HD13	4:D:103:LEU:HD21	1.93	0.50
3:C:58:LEU:HD21	4:D:99:LEU:HD21	1.94	0.50
4:H:36:ILE:O	4:H:40:LYS:HG3	2.12	0.50
2:B:34:ILE:HD11	2:B:55:ARG:HG3	1.94	0.50
3:G:89:ASN:OD1	3:G:108:LEU:HD21	2.12	0.50
7:K:854:GLY:HA3	7:K:860:MET:SD	2.51	0.50
1:E:19:GLN:HB2	8:L:160:PHE:CZ	2.47	0.50
1:E:68:GLN:HE21	1:E:72:ARG:NH2	2.06	0.49
7:K:663:ASN:O	7:K:667:THR:OG1	2.21	0.49
7:K:875:ARG:HE	10:N:99:PRO:HB3	1.77	0.49
8:L:150:HIS:H	8:L:150:HIS:CD2	2.29	0.49
10:N:466:CYS:SG	10:N:469:HIS:HD2	2.23	0.49
10:N:561:VAL:HG11	9:O:269:LEU:O	2.12	0.49
9:O:361:ASP:HA	9:O:364:VAL:HG22	1.93	0.49
3:C:50:TYR:OH	4:D:108:VAL:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:LEU:O	1:E:66:PRO:C	2.53	0.49
1:E:65:LEU:HG	6:J:111:DG:OP2	2.12	0.49
4:D:39:TYR:O	4:D:40:LYS:C	2.55	0.49
4:D:41:VAL:O	4:D:45:VAL:HG22	2.13	0.49
7:K:722:ASN:O	7:K:724:VAL:N	2.45	0.49
9:M:241:LYS:HB2	10:N:372:TYR:HB3	1.94	0.49
10:N:303:CYS:SG	10:N:306:CYS:HB2	2.52	0.49
1:A:38:PRO:HB3	9:M:84:TRP:CZ3	2.47	0.49
4:D:45:VAL:O	4:D:47:PRO:HD3	2.13	0.49
3:G:16:THR:HG23	3:G:19:SER:H	1.76	0.49
1:E:14:LYS:HG2	8:L:108:ASP:OD2	2.13	0.49
5:I:215:DT:H2''	5:I:216:DA:C8	2.47	0.49
8:L:364:ASN:HB3	8:L:369:LEU:HD11	1.95	0.49
8:L:367:GLU:OE1	10:N:435:ARG:NE	2.44	0.49
1:A:71:VAL:HG22	2:B:66:ILE:HD11	1.94	0.49
2:B:91:LYS:CD	2:B:96:THR:HG22	2.26	0.49
3:G:79:ILE:HG23	3:G:80:PRO:HD2	1.94	0.49
6:J:82:DC:H2''	6:J:83:DG:C8	2.48	0.49
3:C:62:ILE:HG12	4:D:59:MET:HE1	1.95	0.49
1:E:11:THR:OG1	8:L:108:ASP:HB3	2.12	0.49
10:N:121:GLU:O	10:N:125:ARG:HG3	2.13	0.49
9:O:257:VAL:HG13	9:O:258:LEU:N	2.27	0.49
3:C:58:LEU:HD21	4:D:99:LEU:CD2	2.43	0.49
3:G:60:ALA:O	3:G:61:GLU:C	2.52	0.49
3:G:110:ASN:O	3:G:111:ILE:HD13	2.13	0.49
9:M:238:TYR:HA	9:M:242:ASP:HB2	1.95	0.49
1:A:54:TYR:OH	2:B:36:ARG:HD2	2.12	0.48
1:A:113:HIS:ND1	1:E:126:LEU:HD22	2.28	0.48
1:E:65:LEU:HD12	6:J:110:DA:H2'	1.95	0.48
7:K:886:HIS:HB3	10:N:93:ILE:HD13	1.95	0.48
1:A:39:HIS:HE1	1:A:41:TYR:CZ	2.30	0.48
1:A:104:PHE:CZ	2:B:54:THR:HG21	2.48	0.48
1:A:129:ARG:O	1:A:129:ARG:HG3	2.13	0.48
2:B:34:ILE:HD13	2:B:54:THR:OG1	2.12	0.48
7:K:865:LYS:NZ	8:L:31:ASN:O	2.42	0.48
3:C:20:ARG:O	4:D:118:TYR:HA	2.13	0.48
1:E:42:ARG:HG3	5:I:321:DC:P	2.53	0.48
1:E:82:LEU:HD12	2:F:79:LYS:O	2.13	0.48
7:K:814:ARG:NH1	7:K:913:ASN:OD1	2.46	0.48
9:M:258:LEU:HD21	9:M:285:LEU:HD23	1.95	0.48
9:M:264:GLU:OE1	9:M:365:TRP:NE1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:LYS:O	2:B:32:PRO:C	2.53	0.48
2:B:80:THR:O	2:B:81:VAL:C	2.56	0.48
4:D:27:ARG:HH22	5:I:302:DC:H5'	1.78	0.48
8:L:63:ILE:O	10:N:176:THR:HA	2.13	0.48
9:O:312:LYS:HA	9:O:315:LYS:HD2	1.94	0.48
9:O:352:CYS:O	9:O:356:ILE:HG12	2.12	0.48
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.96	0.48
2:B:43:VAL:CG2	2:B:46:ILE:HD11	2.42	0.48
4:D:28:LYS:NZ	4:D:28:LYS:H	2.12	0.48
3:G:73:ASN:O	3:G:75:LYS:HG2	2.14	0.48
9:M:253:THR:HG21	9:M:324:ARG:O	2.14	0.48
9:O:222:LEU:HD11	9:O:359:THR:HG21	1.96	0.48
3:C:15:LYS:HG2	6:J:51:DG:OP1	2.14	0.48
1:A:124:ILE:O	1:A:128:ARG:HG3	2.14	0.48
1:E:62:ILE:O	1:E:63:ARG:C	2.54	0.48
3:G:76:THR:H	6:J:151:DC:P	2.36	0.48
3:C:84:GLN:O	3:C:85:LEU:C	2.55	0.48
1:E:74:ILE:HD12	2:F:59:LYS:HG3	1.95	0.48
3:G:102:ILE:CG2	3:G:103:ALA:N	2.77	0.48
5:I:314:DA:H2''	5:I:315:DT:H5''	1.96	0.48
9:M:38:TYR:HE1	9:M:61:LEU:HA	1.79	0.48
9:M:255:GLU:HG2	9:M:259:ASN:ND2	2.28	0.48
1:A:41:TYR:HA	6:J:163:DC:H5''	1.95	0.47
2:F:31:LYS:O	2:F:32:PRO:C	2.51	0.47
2:F:63:GLU:O	2:F:63:GLU:HG2	2.13	0.47
8:L:316:ARG:HH21	8:L:320:ARG:HH22	1.62	0.47
2:B:84:MET:HE1	2:B:101:GLY:HA3	1.95	0.47
1:E:107:THR:CG2	1:E:124:ILE:HG22	2.44	0.47
1:E:126:LEU:O	1:E:127:ALA:C	2.55	0.47
7:K:1305:PHE:HE2	7:K:1307:LYS:HD3	1.79	0.47
10:P:296:LEU:HD12	10:P:296:LEU:C	2.38	0.47
1:A:74:ILE:HG22	1:A:74:ILE:O	2.14	0.47
7:K:1137:ASN:OD1	7:K:1302:ARG:NH1	2.39	0.47
1:A:61:LEU:HB2	1:A:97:GLU:OE2	2.15	0.47
1:E:50:GLU:OE1	2:F:39:ARG:HG3	2.14	0.47
3:G:76:THR:HB	6:J:150:DG:O3'	2.14	0.47
1:E:128:ARG:HB3	1:E:133:GLU:HG3	1.96	0.47
3:G:110:ASN:C	3:G:111:ILE:HD13	2.39	0.47
4:H:92:GLN:C	4:H:94:ALA:N	2.71	0.47
6:J:75:DG:H1'	6:J:76:DT:H5'	1.97	0.47
1:A:61:LEU:HD21	2:B:40:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HG22	1:E:131:ARG:HG2	1.97	0.47
3:C:96:LEU:C	3:C:97:LEU:HD22	2.40	0.47
4:D:54:LYS:O	4:D:58:ILE:HG12	2.14	0.47
1:E:68:GLN:HG3	1:E:89:VAL:HG11	1.96	0.47
1:E:119:ILE:HD13	2:F:43:VAL:HG11	1.97	0.47
7:K:712:SER:OG	10:N:419:LYS:O	2.27	0.47
7:K:1196:LEU:HB3	7:K:1227:SER:HB2	1.97	0.47
10:P:304:ASN:HA	10:P:307:LYS:HG2	1.97	0.47
1:A:61:LEU:O	1:A:62:ILE:C	2.56	0.47
2:B:23:ARG:HA	2:B:23:ARG:NE	2.30	0.47
2:B:82:THR:HG22	2:B:84:MET:H	1.79	0.47
9:M:296:MET:HE3	9:M:341:LEU:HD21	1.97	0.47
10:N:121:GLU:HA	10:N:124:LYS:HB2	1.96	0.47
9:O:250:ALA:HB3	9:O:325:ILE:O	2.14	0.47
9:O:331:LEU:O	9:O:335:ILE:HG12	2.15	0.47
4:H:108:VAL:O	4:H:109:SER:C	2.57	0.47
8:L:169:GLY:HA3	8:L:306:MET:HE1	1.97	0.47
9:O:290:ASP:OD1	9:O:323:ILE:N	2.48	0.47
10:P:287:LEU:O	10:P:288:ASP:C	2.57	0.47
4:D:51:ILE:CG2	4:D:56:MET:HE2	2.30	0.46
1:E:75:ALA:O	1:E:76:GLN:C	2.58	0.46
1:E:120:MET:O	1:E:121:PRO:C	2.57	0.46
3:G:102:ILE:HG22	3:G:103:ALA:N	2.29	0.46
1:E:111:ALA:O	1:E:112:ILE:C	2.56	0.46
5:I:281:DT:H2'	5:I:282:DT:H71	1.97	0.46
10:N:180:ASN:OD1	10:N:180:ASN:N	2.47	0.46
9:M:226:ILE:HA	9:M:229:LYS:HB2	1.98	0.46
10:N:122:LYS:CG	10:N:125:ARG:HH21	2.28	0.46
1:E:6:THR:HG21	10:N:272:PHE:HE2	1.80	0.46
1:A:82:LEU:HD11	2:B:70:VAL:HG23	1.97	0.46
1:A:92:LEU:HD21	2:B:66:ILE:HG13	1.97	0.46
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.51	0.46
3:G:51:LEU:HD12	3:G:51:LEU:HA	1.76	0.46
10:N:296:LEU:N	10:N:296:LEU:HD22	2.31	0.46
9:O:254:VAL:O	9:O:255:GLU:C	2.58	0.46
1:A:51:ILE:CD1	2:B:39:ARG:HD3	2.44	0.46
1:E:57:SER:OG	2:F:40:ARG:NH2	2.45	0.46
7:K:1186:LEU:HD11	8:L:344:TYR:CE2	2.50	0.46
8:L:72:GLN:OE1	10:N:188:ASN:HB2	2.15	0.46
9:O:288:TYR:HD1	10:P:340:LEU:HD23	1.80	0.46
1:A:78:PHE:HZ	2:B:63:GLU:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:178:DC:H2"	6:J:179:DA:C8	2.51	0.46
7:K:1157:ARG:HG2	7:K:1238:LYS:HB3	1.97	0.46
9:M:255:GLU:HB2	9:M:323:ILE:HG22	1.92	0.46
10:N:440:CYS:HB2	10:N:466:CYS:HB3	1.98	0.46
9:O:254:VAL:HG12	9:O:328:ALA:HA	1.98	0.46
9:O:310:LEU:HD21	10:P:290:PRO:CD	2.45	0.46
1:A:54:TYR:HE2	2:B:36:ARG:HB3	1.80	0.46
3:C:81:ARG:HD3	1:E:58:THR:CG2	2.45	0.46
1:E:111:ALA:C	1:E:113:HIS:N	2.74	0.46
1:E:114:ALA:O	1:E:116:ARG:HG3	2.16	0.46
9:O:280:GLU:OE1	10:P:334:LYS:N	2.49	0.46
10:P:562:GLN:HA	10:P:565:LYS:HG2	1.97	0.46
3:C:90:ASP:CG	3:C:91:GLU:H	2.23	0.46
2:F:38:ALA:HB1	2:F:43:VAL:HB	1.98	0.46
3:G:51:LEU:HD12	3:G:54:VAL:CG2	2.46	0.46
1:A:51:ILE:HG21	3:G:111:ILE:HD12	1.98	0.46
3:C:87:VAL:O	3:C:94:ASN:HB2	2.16	0.46
3:G:84:GLN:O	3:G:87:VAL:HG12	2.16	0.46
6:J:89:DG:H2"	6:J:90:DA:C8	2.51	0.46
8:L:44:ARG:HB3	8:L:315:MET:HG2	1.97	0.46
1:A:108:ASN:O	1:A:109:LEU:C	2.57	0.45
3:G:88:ARG:HB2	3:G:108:LEU:HG	1.97	0.45
7:K:1148:PHE:CZ	7:K:1312:VAL:HG11	2.51	0.45
9:O:321:VAL:HG11	9:O:324:ARG:NH1	2.31	0.45
9:O:367:LEU:HA	9:O:370:VAL:HG23	1.99	0.45
1:A:65:LEU:HB2	1:A:66:PRO:HD3	1.96	0.45
1:A:92:LEU:CD2	2:B:66:ILE:HG12	2.45	0.45
4:H:76:ARG:O	4:H:77:LEU:C	2.57	0.45
8:L:316:ARG:NH2	8:L:348:GLY:O	2.49	0.45
9:M:375:ASN:H	9:M:386:LEU:HD11	1.81	0.45
1:A:50:GLU:HA	1:A:53:ARG:HB3	1.99	0.45
3:G:108:LEU:HD23	3:G:108:LEU:HA	1.82	0.45
5:I:304:DT:H2"	5:I:305:DG:C8	2.51	0.45
7:K:956:LYS:HD2	7:K:1316:TYR:HB3	1.98	0.45
9:M:237:GLU:HG3	10:N:372:TYR:CE2	2.51	0.45
10:N:557:LYS:CB	9:O:275:GLN:HE22	2.29	0.45
9:O:248:LEU:HB2	9:O:249:PRO:CD	2.46	0.45
9:O:260:LYS:HE2	9:O:365:TRP:HZ2	1.81	0.45
1:A:75:ALA:C	1:A:77:ASP:N	2.72	0.45
7:K:1012:ASP:OD1	7:K:1012:ASP:N	2.47	0.45
9:M:380:ASN:OD1	9:M:389:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:306:CYS:O	10:N:310:ILE:HG12	2.17	0.45
1:E:80:THR:O	1:E:81:ASP:C	2.59	0.45
3:G:70:ALA:O	3:G:71:ARG:C	2.56	0.45
8:L:244:ASP:OD2	8:L:287:SER:OG	2.28	0.45
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.64	0.45
4:H:102:GLU:O	4:H:104:ALA:N	2.49	0.45
1:A:54:TYR:HE2	2:B:36:ARG:CB	2.29	0.45
1:A:54:TYR:CE2	2:B:36:ARG:HB3	2.52	0.45
4:D:93:THR:O	4:D:96:ARG:HB2	2.16	0.45
1:E:9:LYS:HD2	1:E:14:LYS:CE	2.47	0.45
1:E:47:ALA:O	1:E:51:ILE:HG12	2.17	0.45
7:K:720:PHE:O	7:K:721:LYS:C	2.58	0.45
7:K:843:GLU:HG2	7:K:846:LYS:HE2	1.99	0.45
9:M:254:VAL:HG12	9:M:331:LEU:HB2	1.97	0.45
9:M:291:LYS:HG2	10:N:343:ILE:HD11	1.98	0.45
2:B:43:VAL:HG21	2:B:46:ILE:CD1	2.45	0.45
5:I:214:DG:H2''	5:I:215:DT:OP2	2.17	0.45
1:A:96:SER:O	1:A:97:GLU:C	2.57	0.45
7:K:706:VAL:HG21	7:K:720:PHE:CZ	2.52	0.45
8:L:53:MET:SD	10:N:172:THR:HG22	2.57	0.45
2:B:75:HIS:CD2	4:D:89:ARG:NH1	2.85	0.45
1:E:42:ARG:HG3	5:I:321:DC:OP1	2.16	0.45
1:E:94:GLU:HG3	2:F:100:PHE:CE2	2.51	0.45
8:L:191:ASP:OD1	8:L:191:ASP:N	2.49	0.45
1:A:36:ML3:HM2B	9:M:18:HIS:NE2	2.31	0.44
3:C:17:ARG:HG2	3:C:20:ARG:NH2	2.32	0.44
6:J:142:DC:H2'	6:J:143:DG:H8	1.81	0.44
7:K:1280:ALA:O	7:K:1284:ILE:HD12	2.16	0.44
2:F:46:ILE:HG22	2:F:47:SER:O	2.17	0.44
3:G:27:VAL:HA	3:G:30:VAL:HG22	1.99	0.44
8:L:153:LYS:HB2	8:L:156:GLU:HG2	1.98	0.44
9:M:356:ILE:HD13	9:M:356:ILE:HA	1.88	0.44
2:B:72:TYR:HE1	4:D:97:LEU:CD1	2.28	0.44
1:E:19:GLN:N	8:L:109:ASP:OD1	2.50	0.44
5:I:194:DC:H2''	5:I:195:DC:C5	2.53	0.44
6:J:179:DA:H2''	6:J:180:DG:C8	2.53	0.44
10:N:436:LEU:HD22	10:N:457:PHE:HE2	1.82	0.44
4:D:34:TYR:HA	4:D:37:TYR:HD2	1.83	0.44
10:P:342:ASN:HB2	10:P:346:HIS:CE1	2.53	0.44
4:D:73:GLU:O	4:D:74:ALA:C	2.56	0.44
5:I:251:DC:H2'	5:I:252:DT:H71	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1191:LEU:HD21	7:K:1227:SER:HA	2.00	0.44
8:L:23:TYR:HD2	8:L:63:ILE:HG23	1.82	0.44
10:N:164:ARG:HD2	10:N:164:ARG:HA	1.75	0.44
9:O:235:ASP:OD2	9:O:333:ARG:NH2	2.49	0.44
2:B:59:LYS:HE2	2:B:59:LYS:HB3	1.86	0.44
1:E:127:ALA:O	1:E:130:ILE:HG12	2.18	0.44
9:O:224:ILE:HD11	9:O:229:LYS:HD3	1.99	0.44
1:A:72:ARG:O	1:A:76:GLN:HG2	2.18	0.44
3:G:90:ASP:OD1	3:G:91:GLU:N	2.51	0.44
7:K:813:GLU:HG2	10:N:111:THR:HG22	2.00	0.44
9:M:222:LEU:HD13	9:M:356:ILE:HD12	2.00	0.44
9:O:254:VAL:HG23	9:O:323:ILE:HG23	1.98	0.44
9:O:255:GLU:CG	9:O:259:ASN:HD21	2.27	0.44
1:E:93:GLN:O	1:E:94:GLU:C	2.57	0.44
7:K:841:MET:HE3	7:K:846:LYS:HG3	1.99	0.44
7:K:874:GLU:HG3	7:K:875:ARG:HG2	2.00	0.44
9:M:122:LEU:HD12	9:M:125:GLN:HE21	1.83	0.44
9:M:290:ASP:OD1	9:M:323:ILE:HG12	2.17	0.44
6:J:169:DT:H2"	6:J:170:DA:C8	2.53	0.43
7:K:1198:PHE:HE1	7:K:1227:SER:OG	2.01	0.43
7:K:1321:ASP:OD1	7:K:1321:ASP:N	2.51	0.43
9:M:323:ILE:HD13	9:M:323:ILE:HA	1.90	0.43
1:E:19:GLN:HE22	8:L:38:HIS:CD2	2.36	0.43
1:E:50:GLU:OE2	2:F:39:ARG:NE	2.51	0.43
9:M:304:LEU:HD13	10:N:285:LEU:HD11	1.99	0.43
10:N:372:TYR:OH	10:N:496:ARG:NH1	2.49	0.43
1:A:80:THR:O	1:A:81:ASP:C	2.60	0.43
2:B:78:ARG:NH2	2:B:85:ASP:OD1	2.52	0.43
3:C:90:ASP:CG	3:C:91:GLU:N	2.76	0.43
4:H:104:ALA:O	4:H:105:LYS:C	2.60	0.43
1:A:123:ASP:O	1:A:124:ILE:C	2.61	0.43
2:B:96:THR:OG1	3:G:100:VAL:HG22	2.18	0.43
3:C:18:SER:O	3:C:22:GLY:N	2.52	0.43
1:E:70:LEU:O	1:E:74:ILE:HG22	2.17	0.43
10:N:172:THR:HA	10:N:175:MET:CG	2.47	0.43
9:O:260:LYS:HG3	9:O:261:TYR:N	2.33	0.43
2:F:30:THR:HG23	2:F:33:ALA:H	1.83	0.43
6:J:100:DC:H2"	6:J:101:DG:C8	2.54	0.43
7:K:928:LEU:HD21	8:L:356:ARG:HB2	2.01	0.43
7:K:1189:SER:O	7:K:1193:GLU:HG3	2.18	0.43
9:M:321:VAL:HG22	9:M:323:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:176:THR:O	10:N:176:THR:CG2	2.67	0.43
10:P:330:ASN:HB2	10:P:333:VAL:HG22	2.00	0.43
4:D:51:ILE:HG12	4:D:55:ALA:HB3	2.00	0.43
4:D:81:ASN:O	4:D:82:LYS:C	2.60	0.43
4:H:98:LEU:O	4:H:99:LEU:C	2.58	0.43
7:K:697:LEU:HD12	10:N:474:VAL:HG21	1.99	0.43
7:K:723:PHE:HZ	10:P:552:PHE:CE1	2.37	0.43
7:K:1257:MET:HG3	7:K:1258:THR:HG23	2.01	0.43
10:P:284:PHE:CE2	10:P:293:PRO:HA	2.53	0.43
3:C:18:SER:HB3	3:C:23:LEU:O	2.19	0.43
1:A:67:PHE:CZ	2:B:62:LEU:HD11	2.53	0.43
7:K:706:VAL:HG12	7:K:717:PHE:CE1	2.54	0.43
9:M:354:LEU:HD11	10:N:335:ILE:HG21	2.00	0.43
10:N:562:GLN:O	10:N:563:LYS:C	2.61	0.43
9:O:258:LEU:HD12	9:O:286:LYS:CG	2.49	0.43
1:A:126:LEU:O	1:A:130:ILE:HG12	2.19	0.43
4:D:108:VAL:O	4:D:112:THR:HG23	2.18	0.43
2:F:76:ALA:C	2:F:78:ARG:N	2.75	0.43
7:K:662:LEU:HD13	10:N:559:LYS:NZ	2.33	0.43
8:L:242:ILE:HG13	8:L:246:THR:HB	2.00	0.43
9:M:242:ASP:HB3	9:M:244:LYS:HE2	2.01	0.43
9:M:293:LEU:HA	9:M:297:LEU:HB2	2.00	0.43
3:C:15:LYS:HG3	3:C:20:ARG:NH1	2.33	0.42
10:N:442:TYR:HB2	10:N:469:HIS:CE1	2.53	0.42
1:A:93:GLN:O	1:A:94:GLU:C	2.61	0.42
1:A:104:PHE:HZ	2:B:54:THR:HG21	1.84	0.42
3:C:117:PRO:HD3	1:E:48:LEU:HD22	2.00	0.42
1:E:7:ALA:HB1	1:E:9:LYS:CE	2.49	0.42
1:E:107:THR:OG1	1:E:124:ILE:HG22	2.19	0.42
7:K:1182:LYS:HD2	7:K:1187:LEU:HD12	2.00	0.42
9:O:276:SER:O	9:O:280:GLU:HB2	2.18	0.42
3:C:29:ARG:HG3	3:C:32:ARG:NH2	2.34	0.42
4:H:92:GLN:O	4:H:95:VAL:HG12	2.19	0.42
7:K:722:ASN:O	7:K:723:PHE:C	2.60	0.42
4:D:36:ILE:HG13	4:D:37:TYR:H	1.80	0.42
6:J:148:DC:H2"	6:J:149:DG:C8	2.54	0.42
7:K:718:THR:O	7:K:719:TRP:C	2.61	0.42
7:K:962:LYS:HA	7:K:962:LYS:HD2	1.85	0.42
7:K:1291:ARG:HB2	7:K:1300:MET:HE1	2.01	0.42
2:B:39:ARG:O	2:B:40:ARG:C	2.58	0.42
3:C:92:GLU:O	3:C:93:LEU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:MET:HG2	2:F:47:SER:HB2	2.00	0.42
2:F:92:ARG:HD2	4:H:97:LEU:CD2	2.49	0.42
10:P:266:CYS:HB3	10:P:286:CYS:SG	2.59	0.42
10:P:283:HIS:HB2	10:P:286:CYS:SG	2.59	0.42
1:A:78:PHE:CZ	2:B:63:GLU:HG2	2.55	0.42
2:B:54:THR:O	2:B:55:ARG:C	2.60	0.42
2:B:90:LEU:HB3	2:B:95:ARG:O	2.20	0.42
3:C:63:LEU:HD21	4:D:38:VAL:HG13	2.00	0.42
3:C:76:THR:OG1	5:I:308:DA:O3'	2.37	0.42
4:D:81:ASN:O	4:D:83:ARG:HG3	2.20	0.42
5:I:179:DT:H2''	5:I:180:DG:C8	2.54	0.42
7:K:1303:ILE:HG23	7:K:1314:ILE:HG12	2.01	0.42
7:K:1304:GLU:O	7:K:1312:VAL:HA	2.19	0.42
8:L:269:LEU:HD21	8:L:295:VAL:HG22	2.02	0.42
2:F:70:VAL:O	2:F:71:THR:C	2.60	0.42
10:N:175:MET:HE2	10:N:175:MET:HB3	1.78	0.42
7:K:1194:MET:HE1	7:K:1223:TRP:CG	2.55	0.42
3:G:64:GLU:O	3:G:67:GLY:N	2.53	0.42
4:H:70:ILE:HA	4:H:98:LEU:HD12	2.01	0.42
7:K:1196:LEU:CD2	7:K:1210:LEU:HD11	2.49	0.42
10:N:379:ILE:HD12	10:N:379:ILE:H	1.85	0.42
1:A:108:ASN:O	1:A:111:ALA:N	2.53	0.42
3:C:12:ALA:O	3:C:13:LYS:C	2.62	0.42
4:D:27:ARG:NH2	5:I:302:DC:H5'	2.35	0.42
3:G:32:ARG:O	3:G:33:LEU:C	2.63	0.42
7:K:901:LYS:HB2	7:K:901:LYS:HE2	1.69	0.42
10:N:384:ARG:HA	10:N:388:ASN:HB2	2.01	0.42
1:A:65:LEU:HG	5:I:269:DC:OP2	2.19	0.41
2:B:97:LEU:HD12	3:G:101:THR:O	2.20	0.41
3:C:111:ILE:HD12	1:E:51:ILE:HG21	1.96	0.41
2:F:64:ASN:HA	2:F:67:ARG:NH1	2.34	0.41
8:L:341:ASN:HD21	8:L:347:TYR:HE2	1.68	0.41
9:O:371:ASP:HB3	9:O:375:ASN:HD21	1.85	0.41
4:H:43:LYS:HE2	4:H:49:THR:O	2.20	0.41
7:K:810:ILE:HD11	7:K:919:LEU:HD23	2.02	0.41
3:C:115:LEU:HD11	1:E:108:ASN:ND2	2.20	0.41
4:D:28:LYS:H	4:D:28:LYS:HZ3	1.67	0.41
3:G:84:GLN:CA	3:G:87:VAL:HG12	2.48	0.41
3:G:92:GLU:C	3:G:94:ASN:N	2.77	0.41
7:K:710:LEU:O	7:K:717:PHE:HB2	2.20	0.41
10:N:327:ILE:HD11	10:N:338:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:31:TRP:HB3	9:M:76:CYS:HB2	2.02	0.41
1:A:79:LYS:HB3	1:A:82:LEU:CD1	2.50	0.41
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.86	0.41
3:C:65:LEU:CB	3:C:86:ALA:HB1	2.51	0.41
3:C:119:LYS:HB2	3:C:119:LYS:HE2	1.88	0.41
1:E:64:LYS:O	1:E:65:LEU:C	2.63	0.41
1:E:127:ALA:O	1:E:131:ARG:HG3	2.20	0.41
6:J:106:DT:H6	6:J:106:DT:H2'	1.76	0.41
8:L:270:GLN:NE2	8:L:310:GLY:HA3	2.35	0.41
3:C:67:GLY:HA2	3:C:78:ILE:HD11	2.01	0.41
9:O:260:LYS:O	9:O:263:HIS:N	2.53	0.41
9:O:318:LYS:HA	9:O:318:LYS:HD3	1.81	0.41
1:A:97:GLU:OE2	2:B:37:LEU:HD21	2.21	0.41
1:A:113:HIS:HE1	1:E:123:ASP:HA	1.85	0.41
2:B:63:GLU:O	2:B:64:ASN:C	2.63	0.41
3:G:91:GLU:H	3:G:91:GLU:CD	2.28	0.41
8:L:328:LEU:HD23	8:L:328:LEU:HA	1.91	0.41
10:N:172:THR:O	10:N:173:GLU:C	2.61	0.41
10:N:293:PRO:O	10:N:296:LEU:HD21	2.20	0.41
3:C:79:ILE:HG23	3:C:80:PRO:CD	2.29	0.41
1:E:56:LYS:O	1:E:56:LYS:HG2	2.19	0.41
4:H:73:GLU:OE2	4:H:77:LEU:HG	2.21	0.41
7:K:867:ILE:HG21	7:K:880:ILE:HG13	2.03	0.41
8:L:44:ARG:NH1	8:L:322:TRP:CH2	2.89	0.41
8:L:177:HIS:HB3	8:L:265:SER:HB2	2.03	0.41
9:M:26:LYS:O	9:M:79:ILE:HA	2.21	0.41
3:C:29:ARG:O	3:C:33:LEU:HD23	2.20	0.41
1:E:48:LEU:HD11	2:F:44:LYS:HD2	2.03	0.41
1:E:101:VAL:O	1:E:105:GLU:HG2	2.21	0.41
1:E:105:GLU:O	1:E:109:LEU:HD23	2.20	0.41
2:F:26:ILE:C	2:F:28:GLY:N	2.79	0.41
6:J:36:DT:H2''	6:J:37:DG:C8	2.55	0.41
7:K:785:HIS:CD2	7:K:786:PRO:HD2	2.56	0.41
7:K:1190:GLN:HG3	10:N:129:TRP:CE2	2.56	0.41
8:L:138:LYS:H	8:L:138:LYS:HG2	1.72	0.41
9:M:80:HIS:ND1	9:M:89:ASP:OD1	2.41	0.41
9:M:92:VAL:HB	9:M:96:ARG:HB2	2.02	0.41
1:E:128:ARG:HG2	1:E:133:GLU:OE2	2.21	0.41
5:I:214:DG:N2	6:J:131:DG:C2	2.89	0.41
8:L:256:LYS:O	8:L:260:GLU:HG2	2.21	0.41
10:N:285:LEU:HD23	10:N:285:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:555:ILE:O	10:N:556:TYR:C	2.62	0.41
9:O:236:TRP:O	9:O:240:THR:OG1	2.31	0.41
2:B:33:ALA:C	2:B:35:ARG:N	2.77	0.40
1:E:9:LYS:HD2	1:E:14:LYS:HD3	2.04	0.40
2:F:52:GLU:O	2:F:52:GLU:CG	2.68	0.40
8:L:28:ASP:O	8:L:29:VAL:C	2.62	0.40
8:L:273:GLY:HA3	8:L:318:VAL:HG23	2.04	0.40
10:N:104:GLU:HB3	10:N:107:LYS:HE3	2.03	0.40
10:P:307:LYS:O	10:P:311:PHE:HB2	2.21	0.40
1:A:101:VAL:HG21	2:B:40:ARG:HG2	2.03	0.40
3:C:29:ARG:HA	6:J:49:DG:OP1	2.21	0.40
1:E:9:LYS:HD2	1:E:14:LYS:HE3	2.03	0.40
5:I:287:DC:H6	5:I:287:DC:H2'	1.72	0.40
7:K:671:LYS:HD2	7:K:716:LEU:HD13	2.03	0.40
10:N:296:LEU:HD22	10:N:296:LEU:H	1.85	0.40
9:O:355:LEU:HD23	9:O:355:LEU:HA	1.80	0.40
4:D:36:ILE:HD13	5:I:299:DG:H3'	2.04	0.40
8:L:242:ILE:HA	8:L:362:ASN:ND2	2.36	0.40
9:M:334:LEU:O	9:M:338:LEU:HB2	2.22	0.40
1:A:62:ILE:HD11	2:B:37:LEU:HD11	2.03	0.40
1:A:67:PHE:O	1:A:70:LEU:HB3	2.21	0.40
2:F:71:THR:HG22	4:H:93:THR:CG2	2.51	0.40
2:F:90:LEU:HD12	2:F:97:LEU:CB	2.51	0.40
2:F:39:ARG:HH12	2:F:46:ILE:CD1	2.34	0.40
4:H:56:MET:O	4:H:59:MET:N	2.55	0.40
5:I:174:DT:H2''	5:I:175:DA:C8	2.57	0.40
7:K:963:LYS:HE2	7:K:963:LYS:HB3	1.94	0.40
8:L:299:LYS:HD2	8:L:329:LEU:HA	2.02	0.40
9:M:15:LEU:HD22	9:M:108:LYS:HD2	2.03	0.40
10:N:561:VAL:HG22	9:O:267:GLN:HA	2.04	0.40
9:O:310:LEU:HD21	10:P:290:PRO:CG	2.51	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	99/135 (73%)	90 (91%)	9 (9%)	0	100	100
1	E	112/135 (83%)	108 (96%)	4 (4%)	0	100	100
2	B	78/102 (76%)	72 (92%)	6 (8%)	0	100	100
2	F	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
3	C	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
3	G	104/129 (81%)	98 (94%)	6 (6%)	0	100	100
4	D	94/122 (77%)	86 (92%)	8 (8%)	0	100	100
4	H	92/122 (75%)	81 (88%)	11 (12%)	0	100	100
7	K	543/1536 (35%)	526 (97%)	17 (3%)	0	100	100
8	L	382/433 (88%)	369 (97%)	13 (3%)	0	100	100
9	M	288/401 (72%)	284 (99%)	4 (1%)	0	100	100
9	O	154/401 (38%)	147 (96%)	7 (4%)	0	100	100
10	N	365/684 (53%)	350 (96%)	15 (4%)	0	100	100
10	P	147/684 (22%)	140 (95%)	7 (5%)	0	100	100
All	All	2642/5115 (52%)	2528 (96%)	114 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	E	34/108 (32%)	34 (100%)	0	100	100
2	F	64/78 (82%)	64 (100%)	0	100	100
3	G	84/101 (83%)	84 (100%)	0	100	100
4	H	80/102 (78%)	80 (100%)	0	100	100
7	K	458/1391 (33%)	458 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	286/367 (78%)	286 (100%)	0	100	100
9	M	230/359 (64%)	230 (100%)	0	100	100
10	P	24/653 (4%)	24 (100%)	0	100	100
All	All	1260/3159 (40%)	1260 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	108	ASN
1	E	113	HIS
3	G	68	ASN
4	H	64	ASN
4	H	81	ASN
7	K	886	HIS
7	K	937	GLN
7	K	961	ASN
7	K	1132	ASN
7	K	1190	GLN
8	L	38	HIS
8	L	72	GLN
9	M	82	GLN
9	M	104	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	ML3	A	36	1	10,11,12	0.79	0	11,14,16	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ML3	A	36	1	-	5/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	ML3	SG-CD-CE-NZ
1	A	36	ML3	CD-CE-NZ-CM1
1	A	36	ML3	CD-CE-NZ-CM2
1	A	36	ML3	CD-CE-NZ-CM3
1	A	36	ML3	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	36	ML3	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

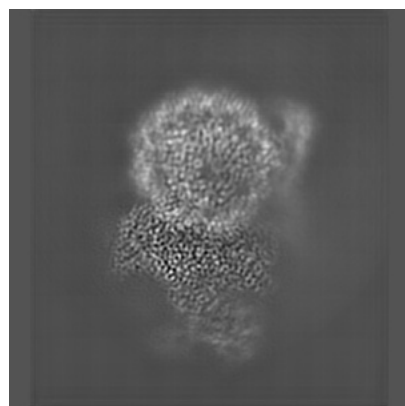
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35084. These allow visual inspection of the internal detail of the map and identification of artifacts.

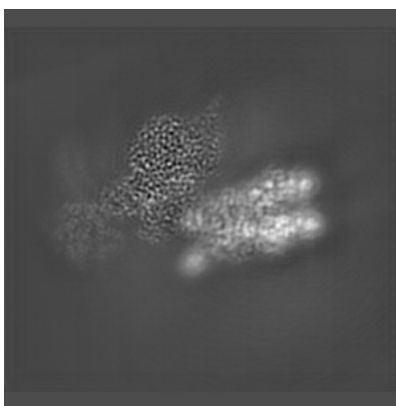
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

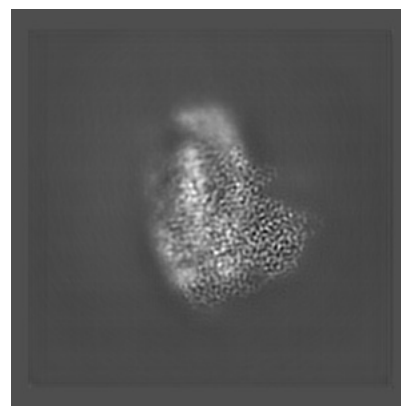
6.1.1 Primary map



X

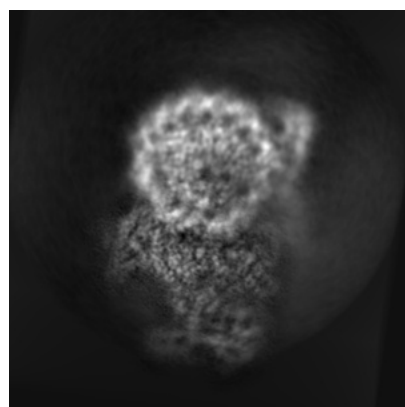


Y

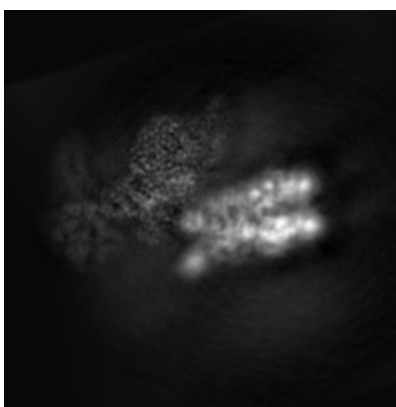


Z

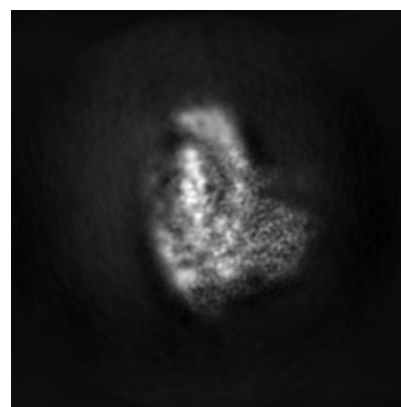
6.1.2 Raw map



X



Y

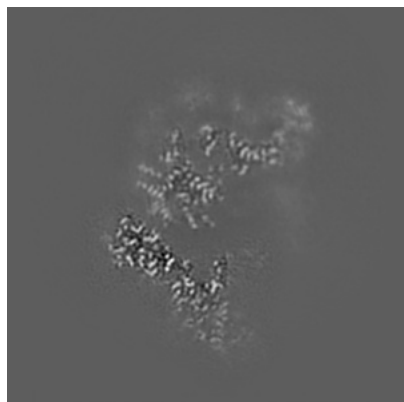


Z

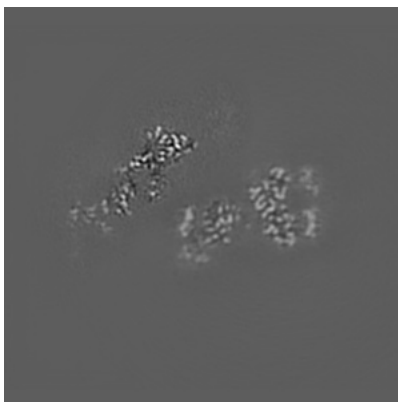
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

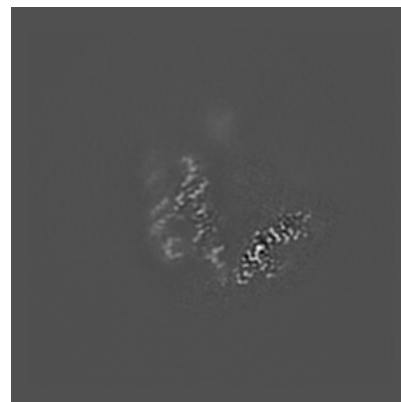
6.2.1 Primary map



X Index: 128

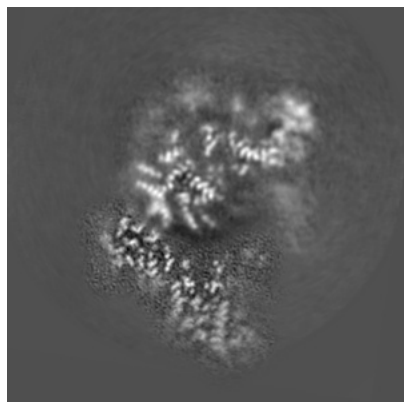


Y Index: 128

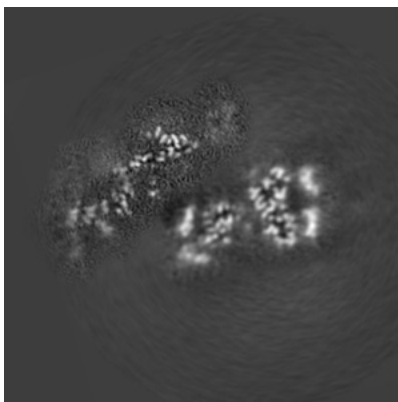


Z Index: 128

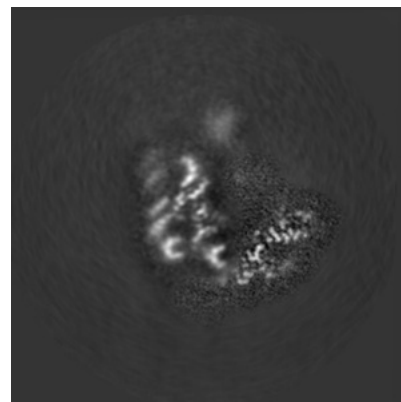
6.2.2 Raw map



X Index: 128



Y Index: 128

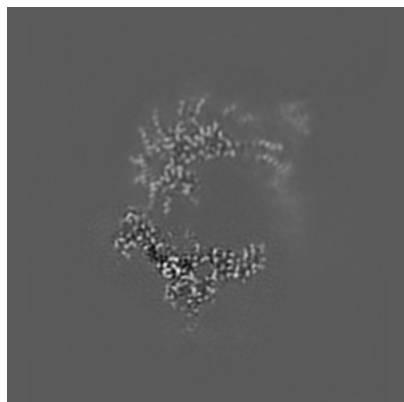


Z Index: 128

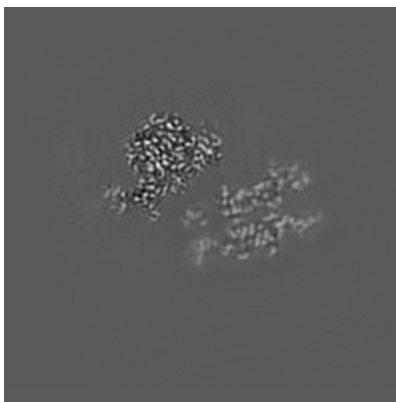
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

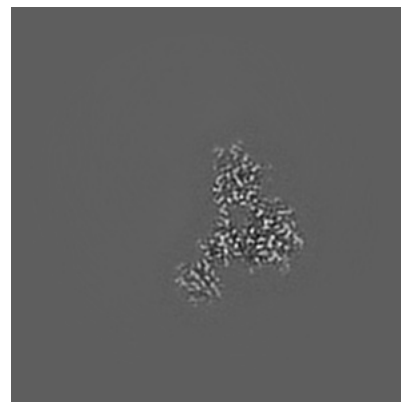
6.3.1 Primary map



X Index: 135

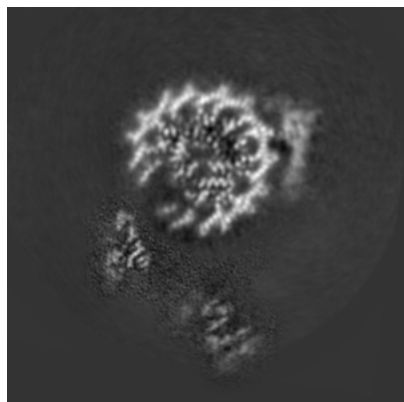


Y Index: 106

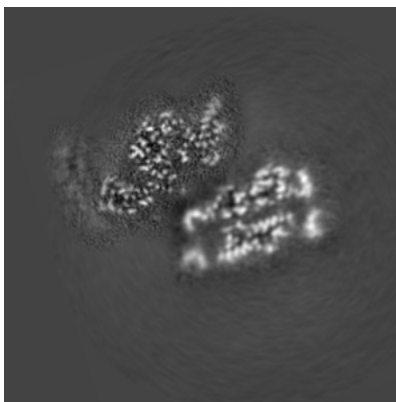


Z Index: 94

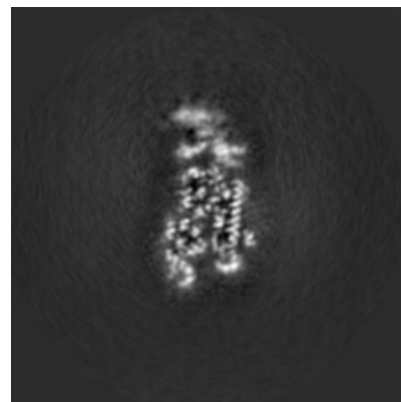
6.3.2 Raw map



X Index: 116



Y Index: 111

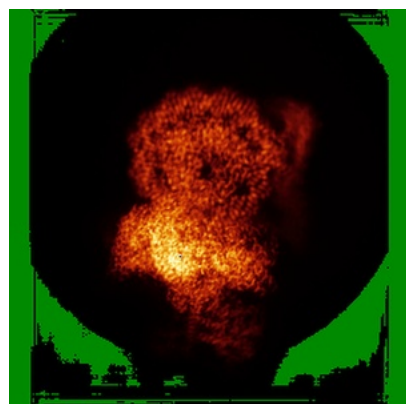


Z Index: 169

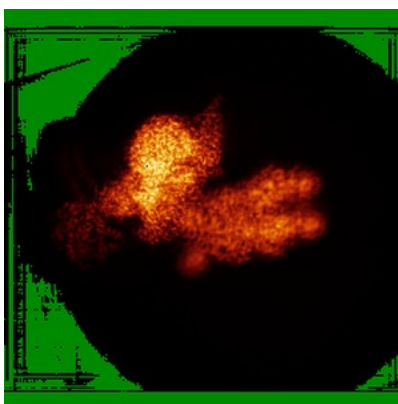
The images above show the largest variance slices of the map in three orthogonal directions.

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

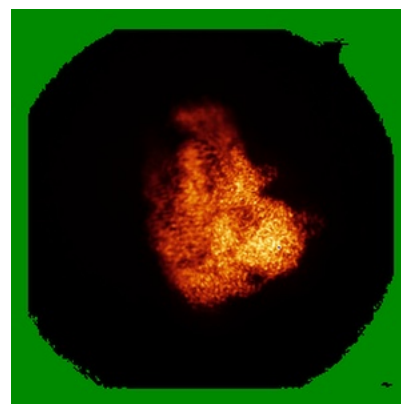
6.4.1 Primary map



X

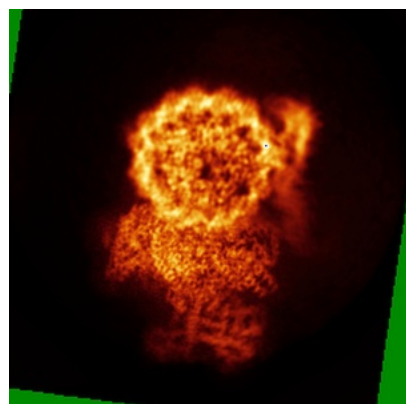


Y

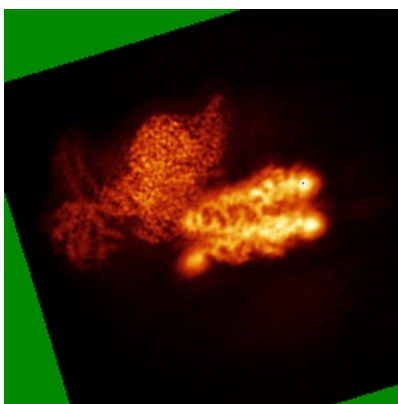


Z

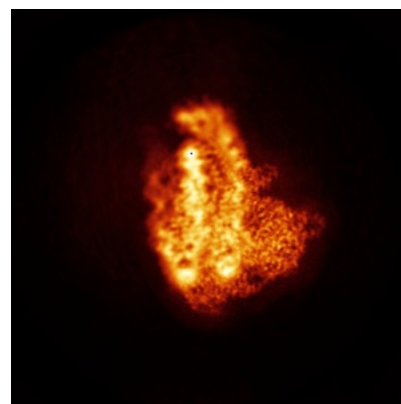
6.4.2 Raw map



X



Y

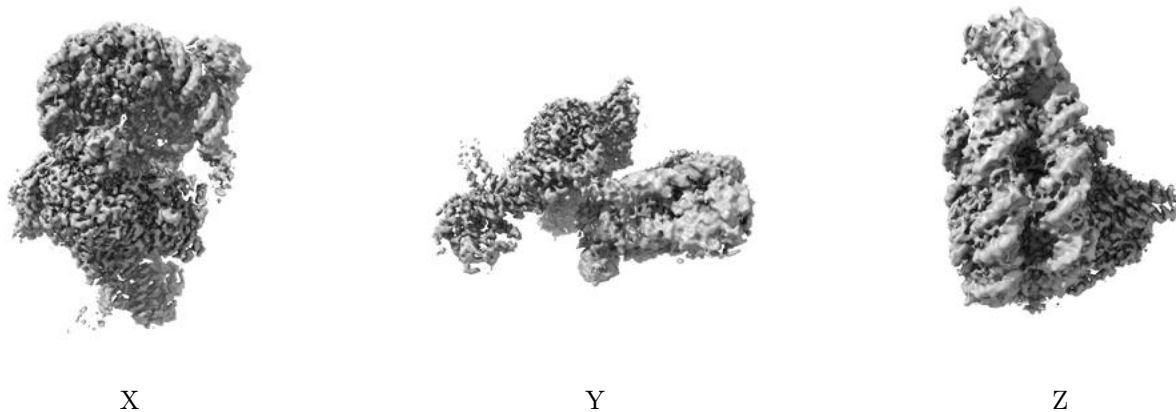


Z

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.

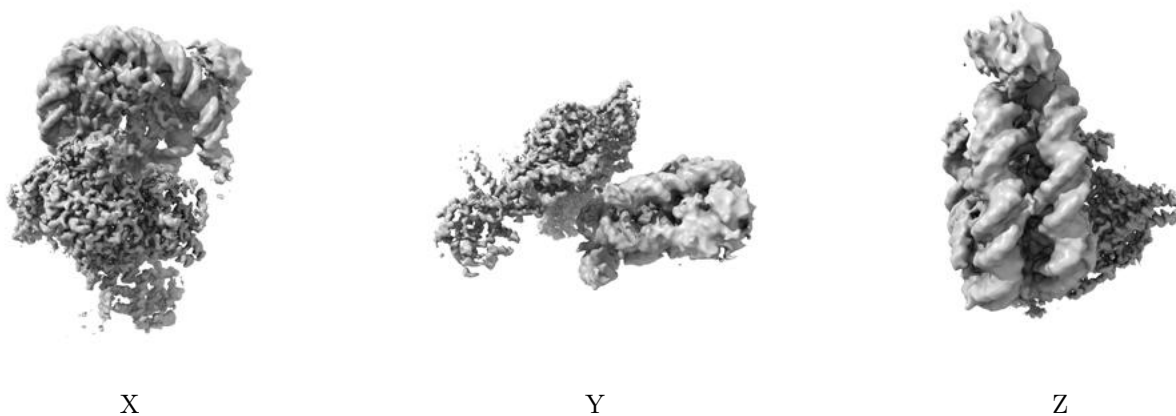
6.5 Orthogonal surface views [i](#)

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.

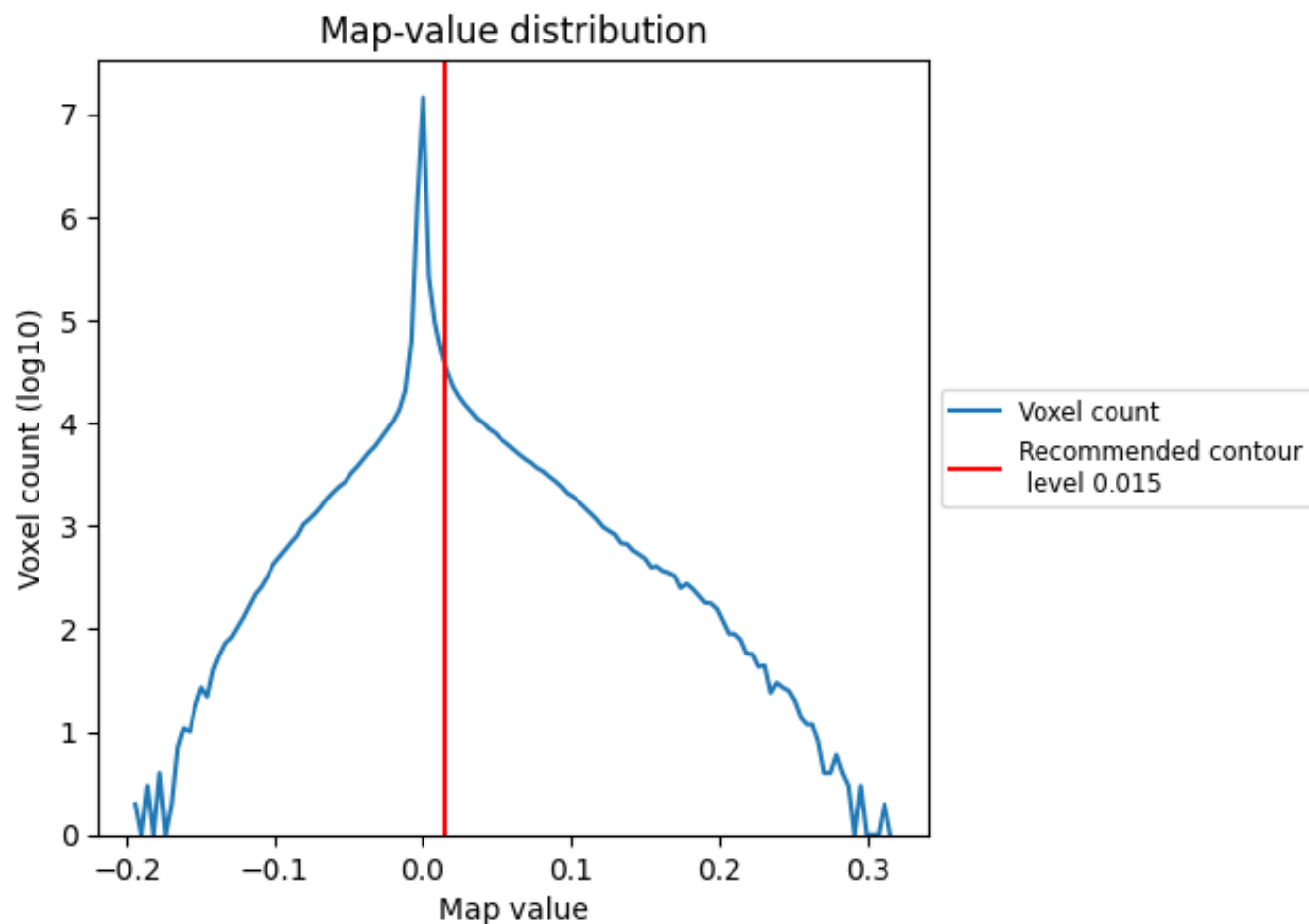
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

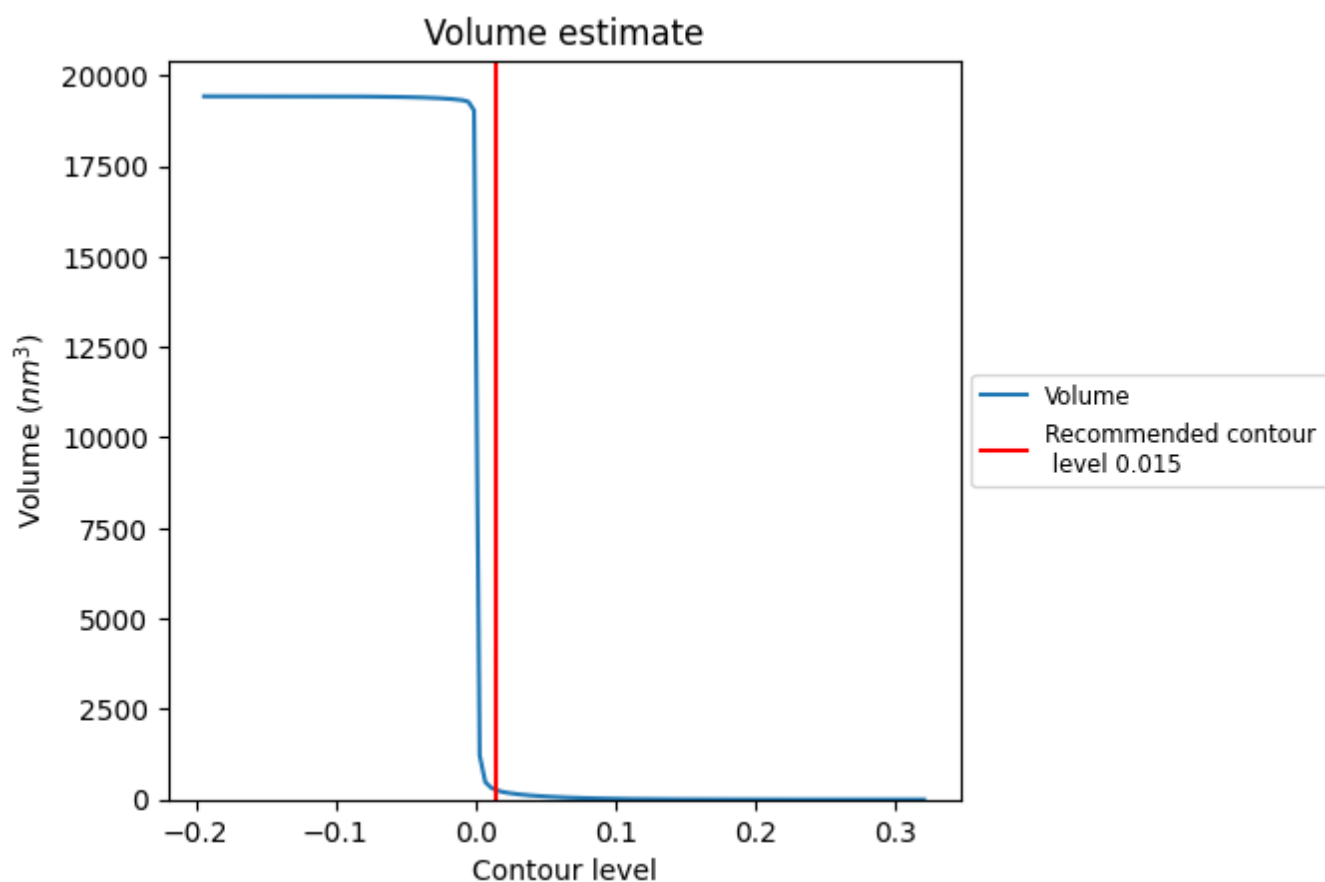
This section contains the results of statistical analysis of the map.

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.

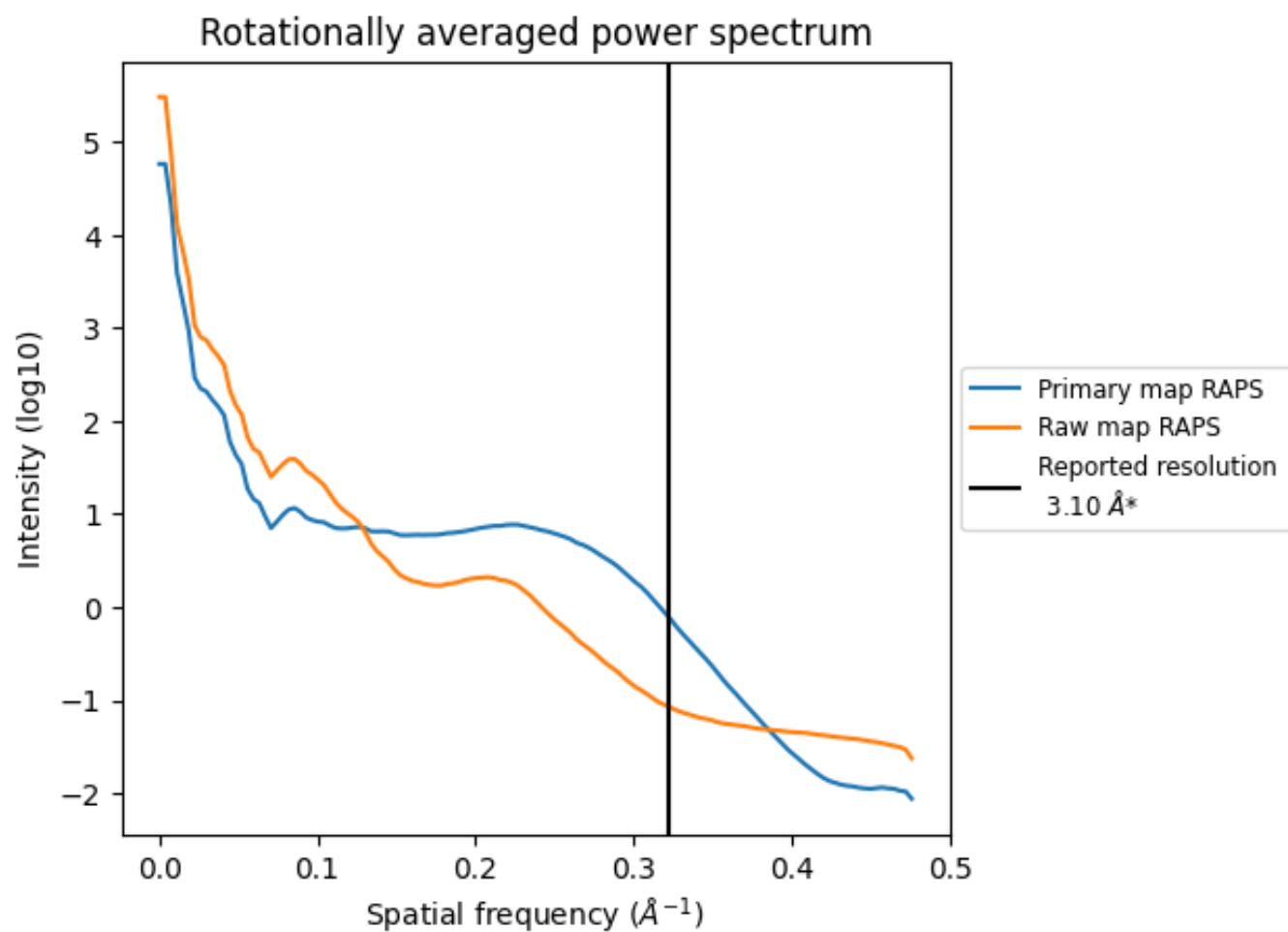
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

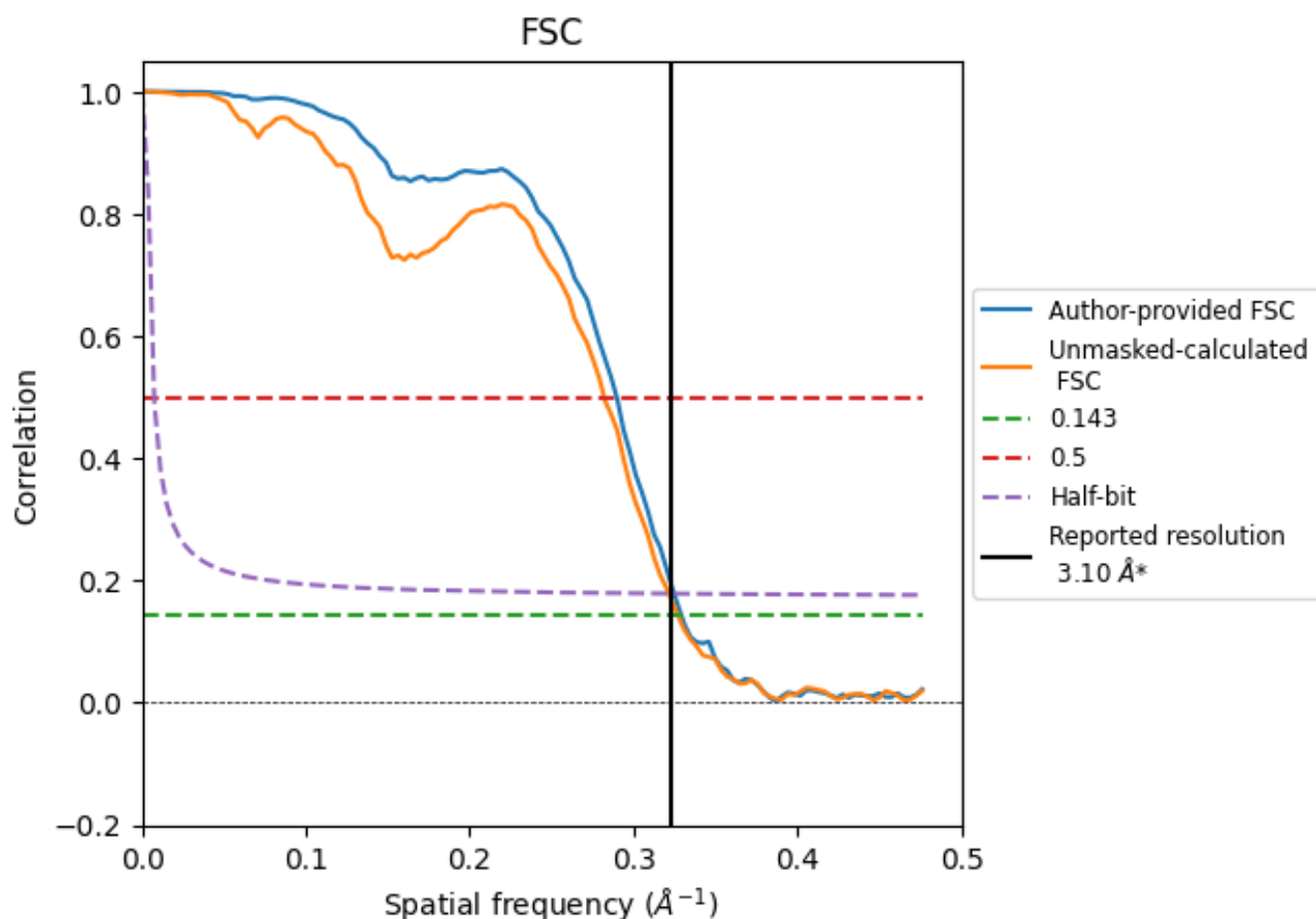


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

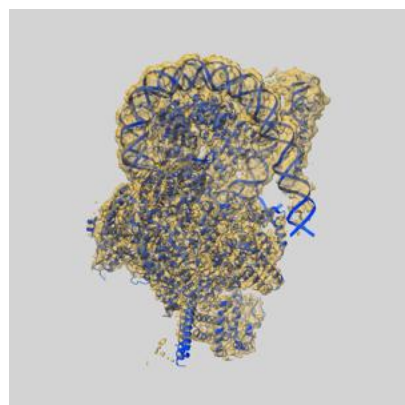
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.45	3.08
Unmasked-calculated*	3.06	3.54	3.11

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

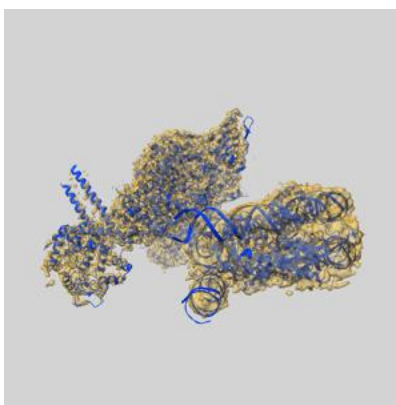
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35084 and PDB model 8HY0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

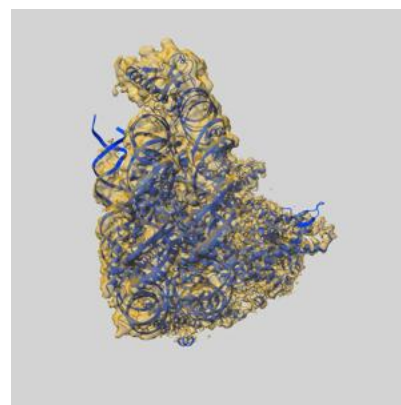
9.1 Map-model overlay [i](#)



X



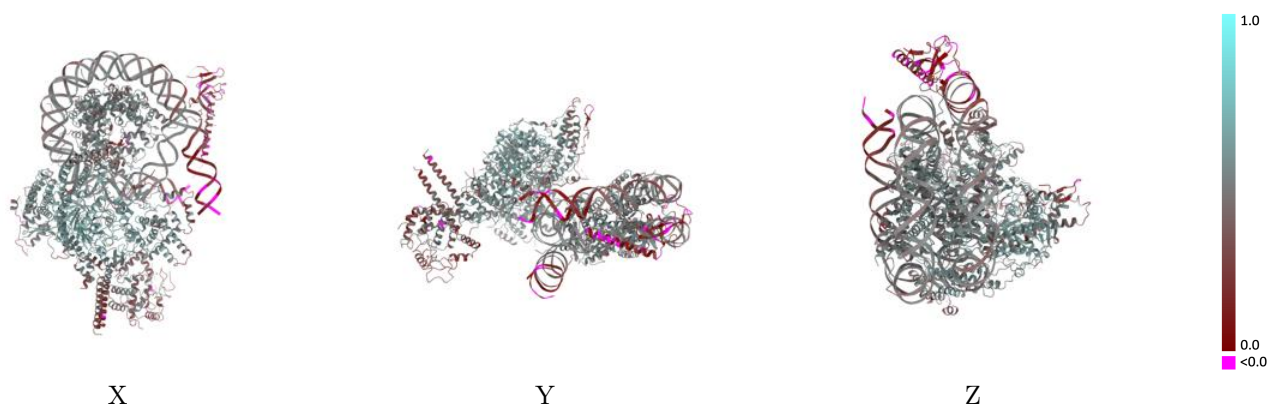
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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](#)

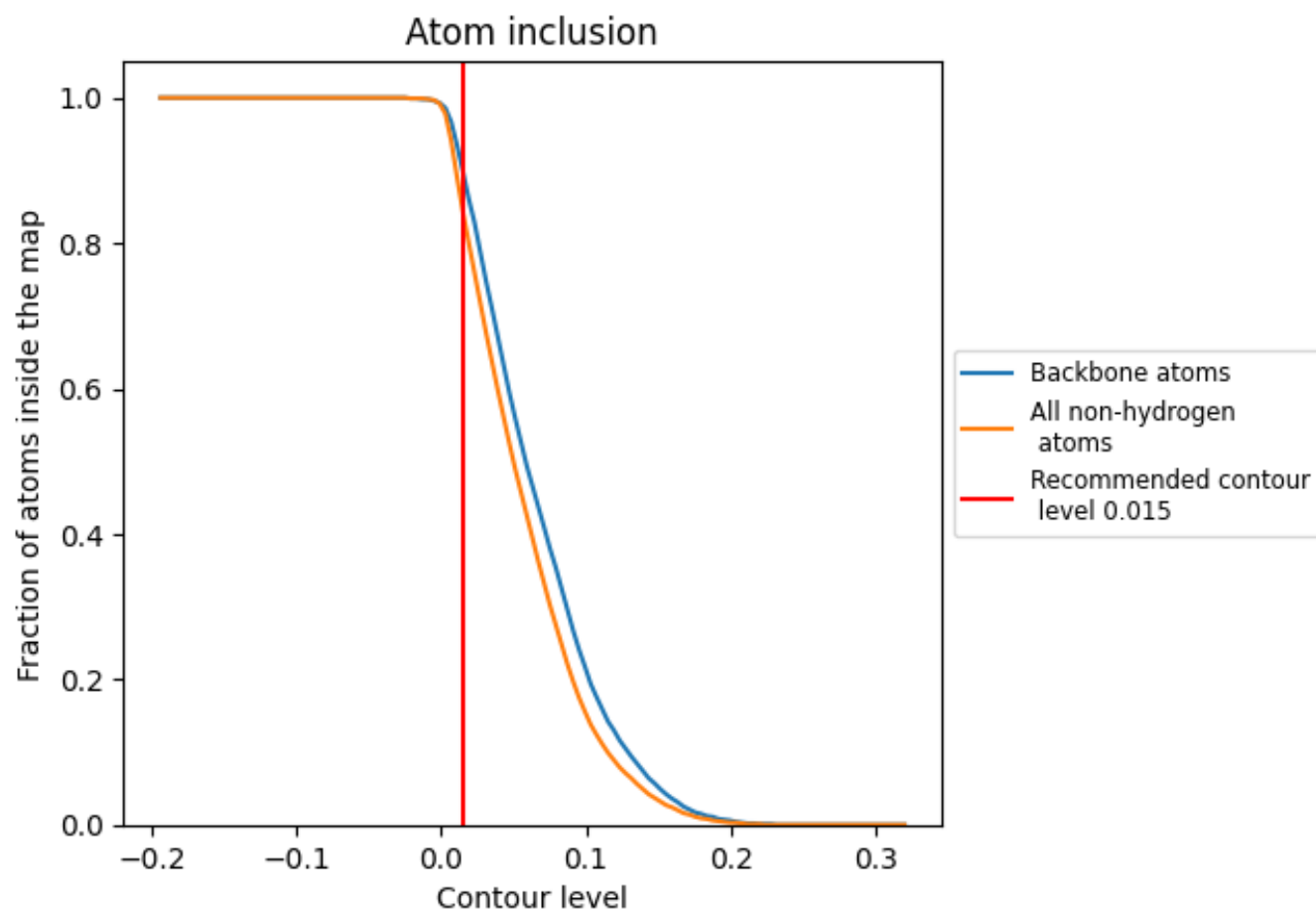


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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	 0.8420	 0.4630
A	 0.9220	 0.4860
B	 0.9480	 0.5250
C	 0.9300	 0.4950
D	 0.9310	 0.4940
E	 0.8130	 0.4670
F	 0.9340	 0.5190
G	 0.9030	 0.5070
H	 0.8980	 0.4740
I	 0.9040	 0.4080
J	 0.8990	 0.4030
K	 0.8340	 0.5190
L	 0.9510	 0.5950
M	 0.8700	 0.3790
N	 0.7160	 0.4770
O	 0.5770	 0.3600
P	 0.4890	 0.3420

