



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:23 AM UTC

PDB ID : 8JH3 / pdb_00008jh3
EMDB ID : EMD-36252
Title : RNA polymerase II elongation complex containing 40 bp upstream DNA loop, stalled at SHL(-1) of the nucleosome
Authors : Akatsu, M.; Fujita, R.; Ogasawara, M.; Ehara, H.; Kujirai, T.; Takizawa, Y.; Sekine, S.; Kurumizaka, H.
Deposited on : 2023-05-22
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

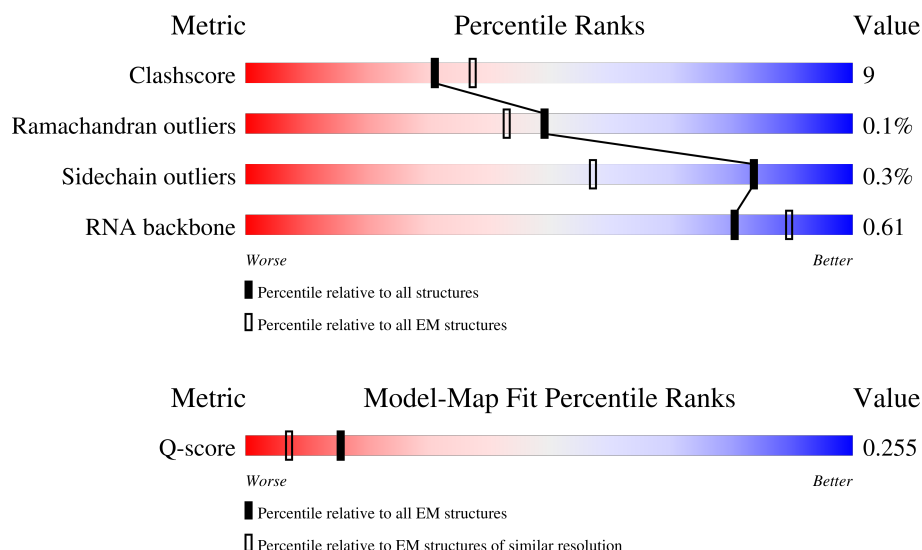
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1743	
2	B	1227	
3	C	304	

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Mol	Chain	Length	Quality of chain
4	D	186	78% 65% 25% 10%
5	E	214	10% 85% 15%
6	F	155	47% 7% 46%
7	G	171	59% 65% 35%
8	H	145	75% 17% 8%
9	I	115	34% 70% 26%
10	J	72	79% 12% 8%
11	K	118	82% 14%
12	L	72	51% 11% 38%
13	N	198	9% 43% 28% 29%
14	P	13	46% 46% 8%
15	T	198	10% 48% 32% 20%
16	a	136	11% 60% 8% 30%
16	e	136	58% 8% 32%
17	b	103	6% 68% 7% 25%
17	f	103	70% 6% 24%
18	c	130	6% 66% 12% 18%
18	g	130	11% 62% 10% 28%
19	d	126	68% 5% 27%
19	h	126	6% 57% 12% 30%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 43416 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1412	Total	C	N	O	S	0	0
			11120	7015	1936	2099	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1155	Total	C	N	O	S	0	0
			9210	5806	1626	1720	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	141	Total	C	N	O	P	0	0
			2897	1376	514	866	141		

- Molecule 14 is a RNA chain called RNA (5'-R(P*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*GP)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	13	Total	C	N	O	P	0	0
			281	124	48	96	13		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	159	Total	C	N	O	P	0	0
			3243	1536	624	925	158		

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	95	Total	C	N	O	S	0	0
			779	492	150	135	2		
16	e	92	Total	C	N	O	S	0	0
			746	471	142	131	2		

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	106	Total	C	N	O	0	0
			815	514	159	142		
18	g	93	Total	C	N	O	0	0
			720	452	142	126		

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	92	Total	C	N	O	S	0	0
			720	453	129	136	2		
19	h	88	Total	C	N	O	S	0	0
			685	433	121	129	2		

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	

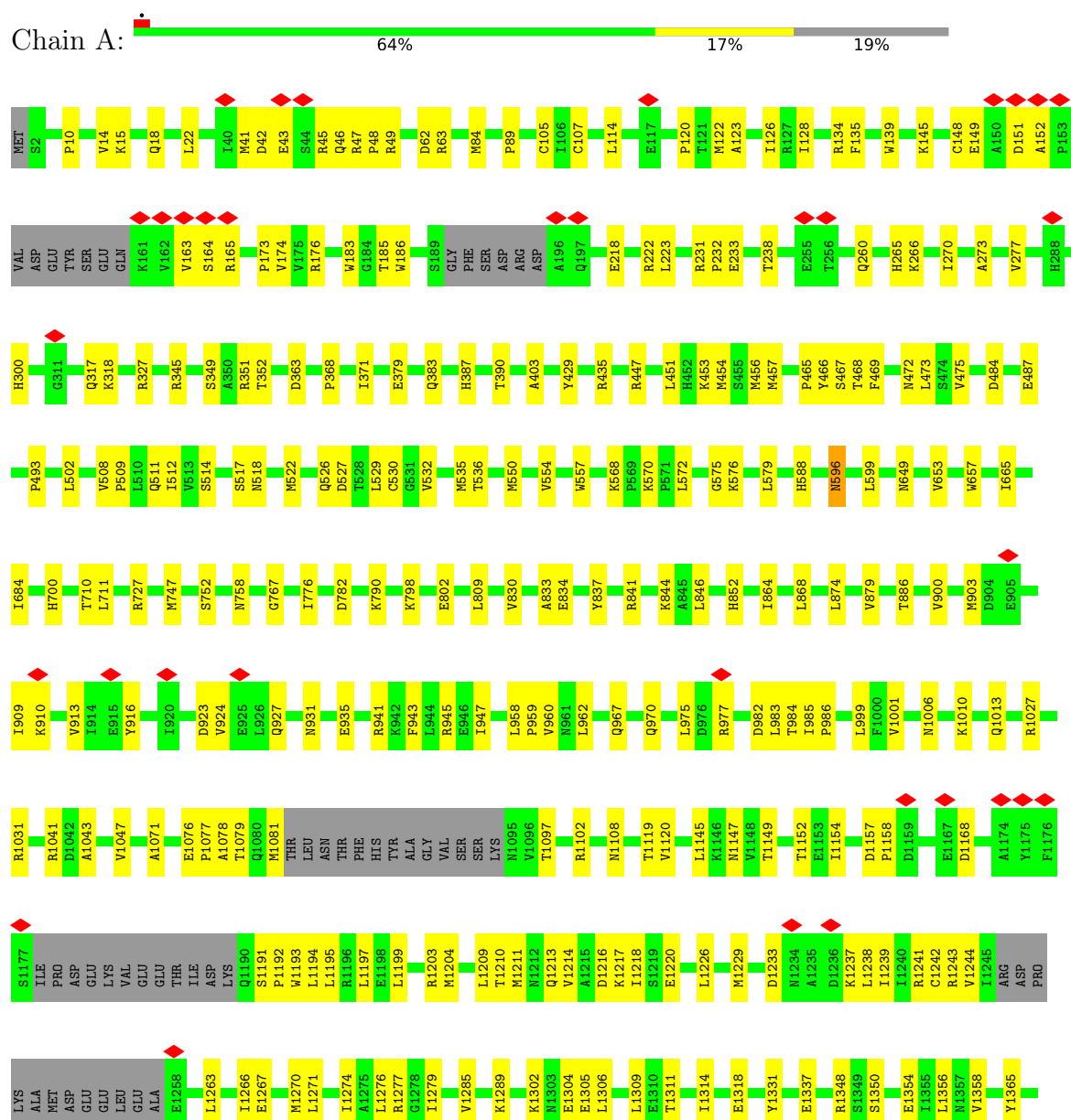
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

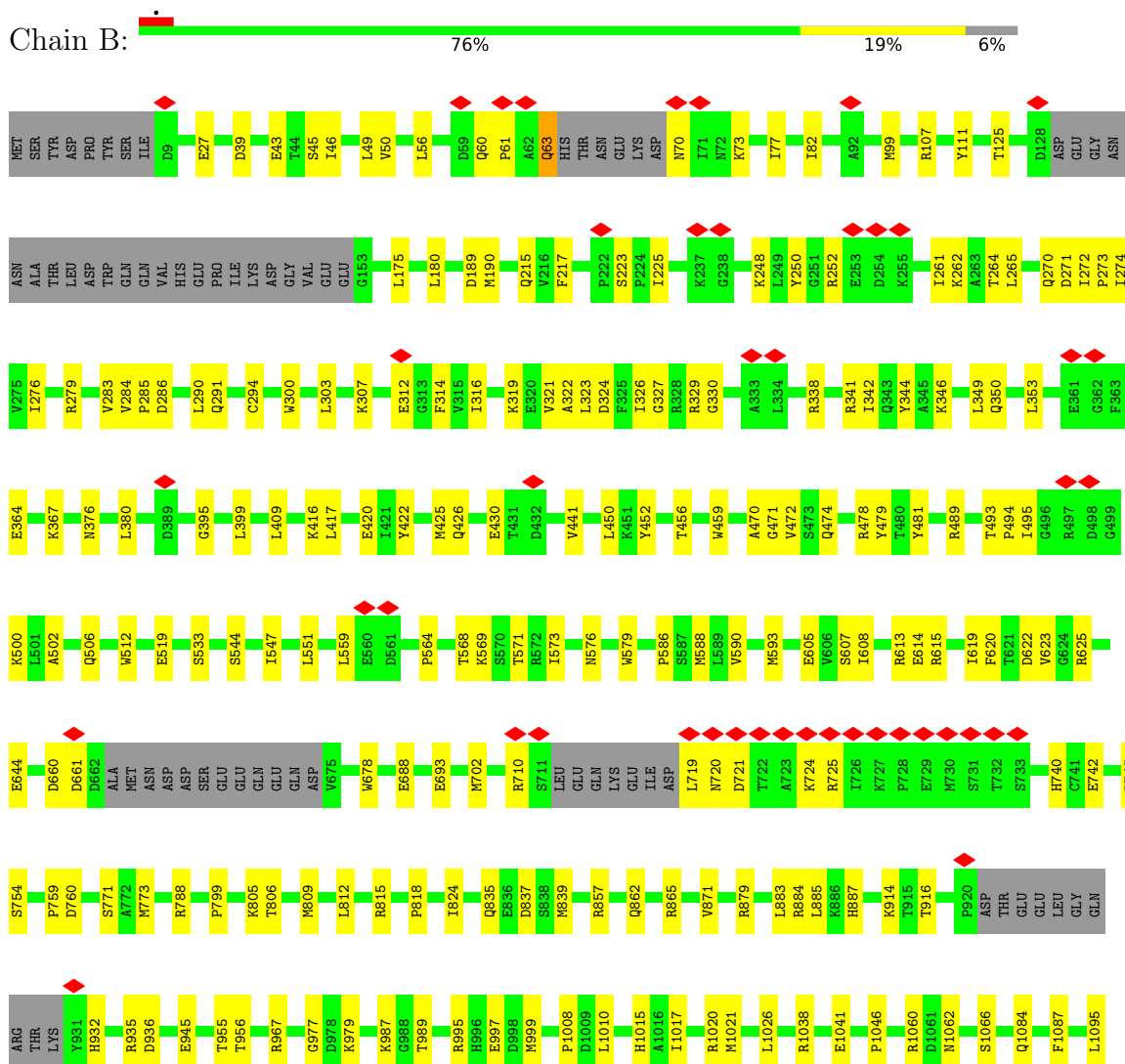
3 Residue-property plots

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: DNA-directed RNA polymerase subunit

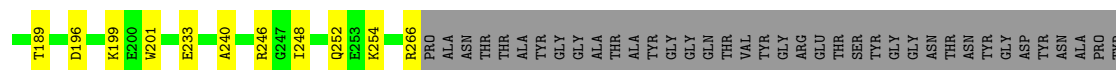
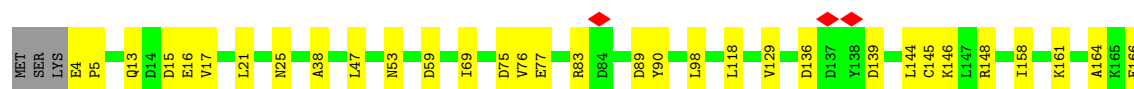


- Molecule 2: DNA-directed RNA polymerase subunit beta

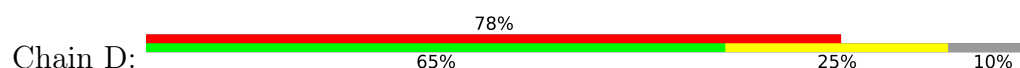




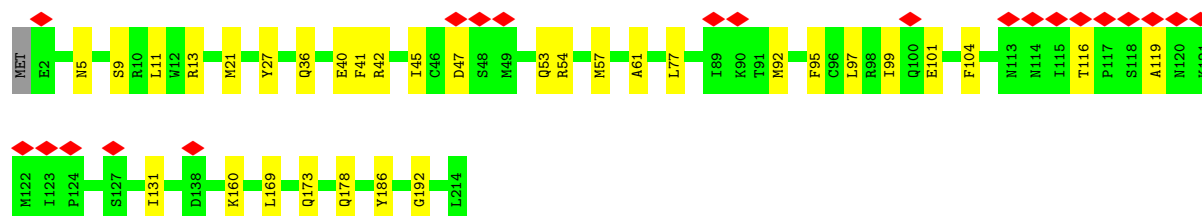
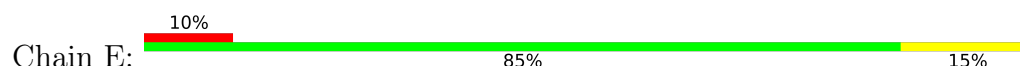
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



- Molecule 4: RNA polymerase II subunit B32



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

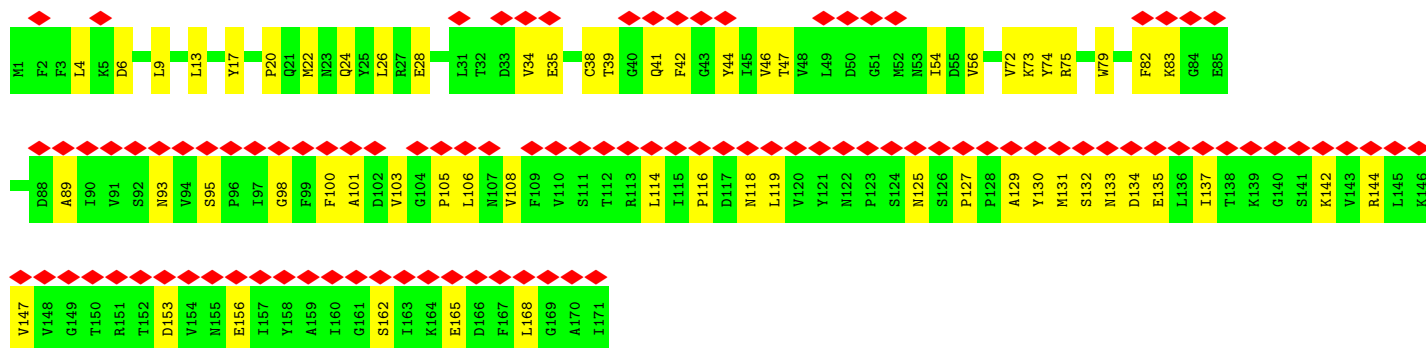


- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

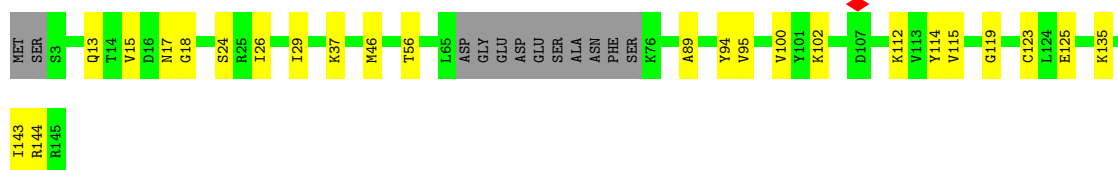
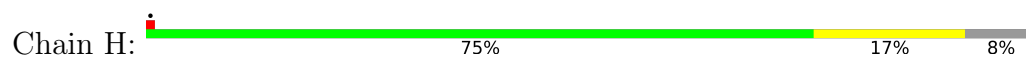




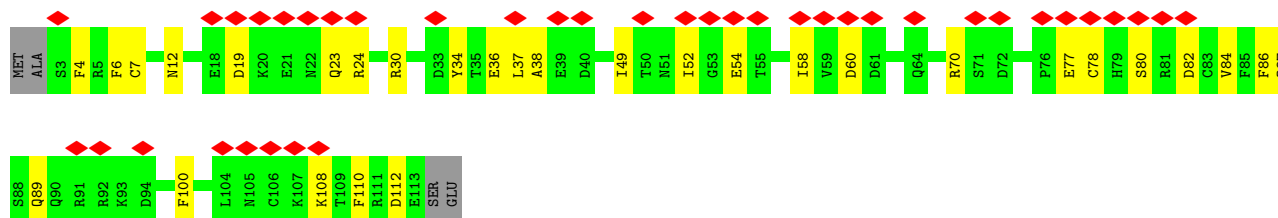
• Molecule 7: RNA polymerase II subunit



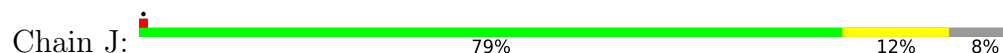
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase subunit



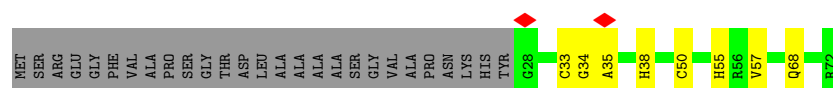
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

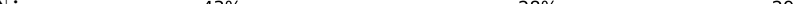


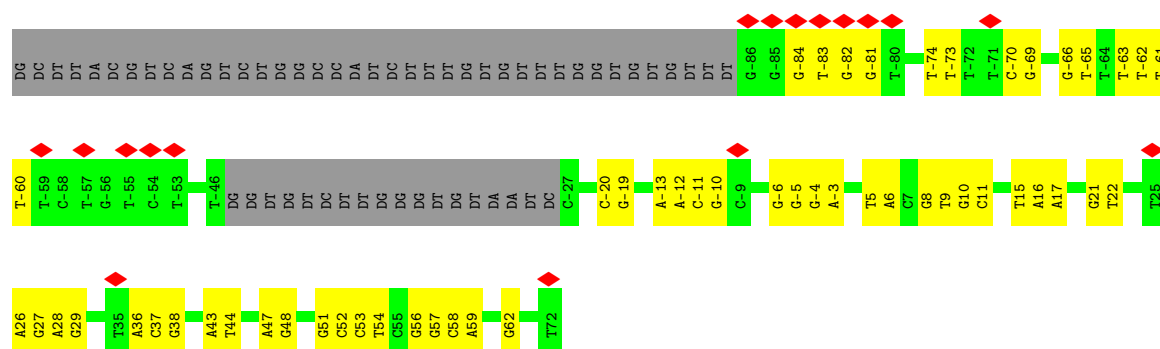
• Molecule 11: RNA polymerase II subunit B12.5

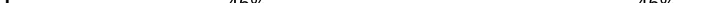


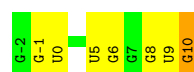
- Chain L: 51% 11% 38%

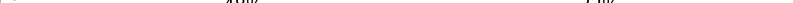


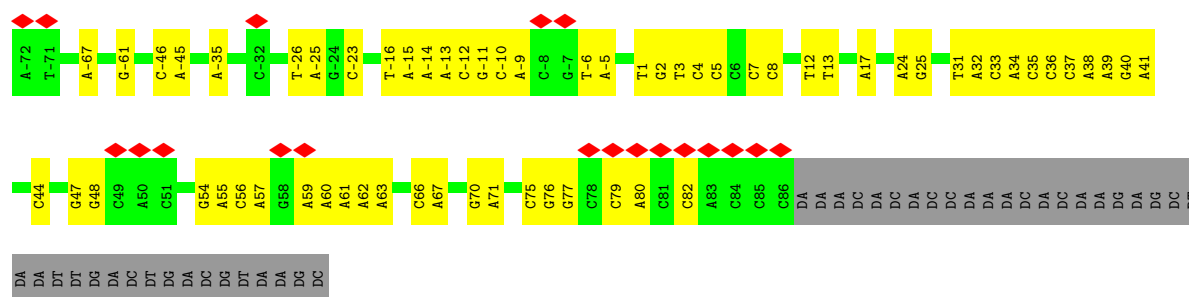
- Chain N: 



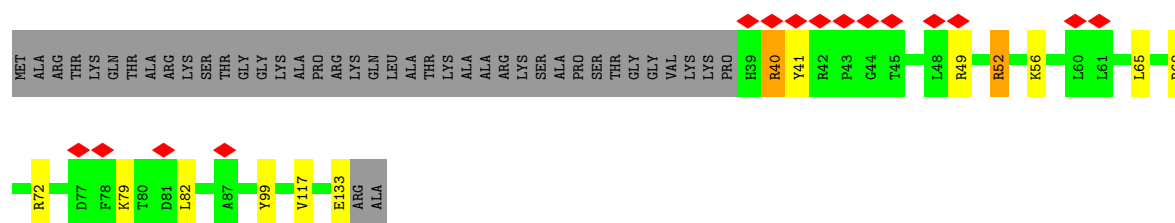
- Chain P:  46% 46% 8%



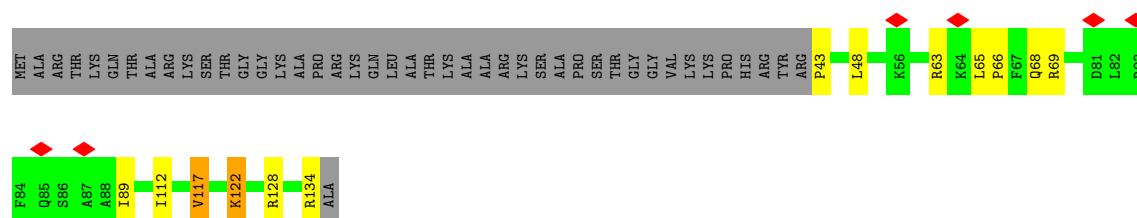
- Chain T: 



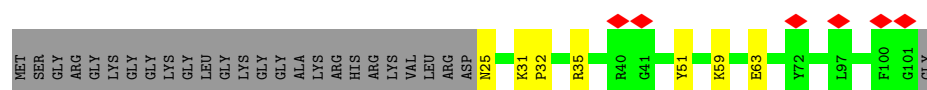
- WORLDWIDE
PDB
PROTEIN DATA BANK



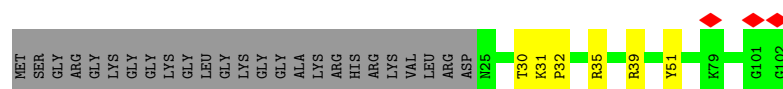
- Molecule 16: Histone H3.3



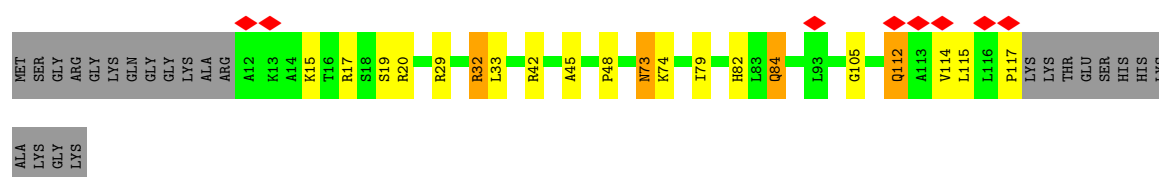
- Molecule 17: Histone H4



- Molecule 17: Histone H4

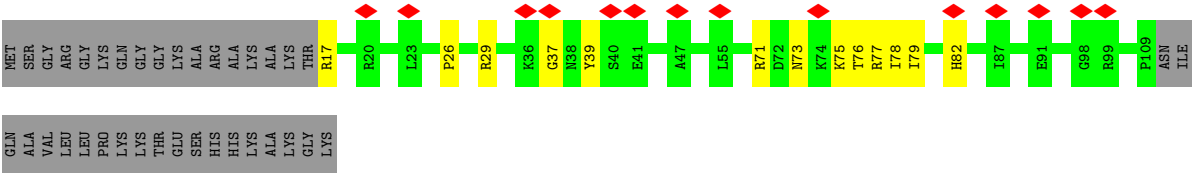


- Molecule 18: Histone H2A type 1-B/E

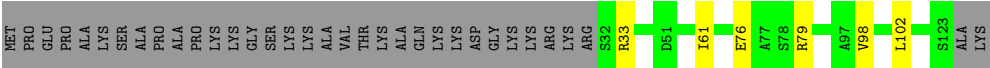


- Molecule 18: Histone H2A type 1-B/E

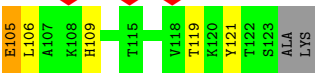
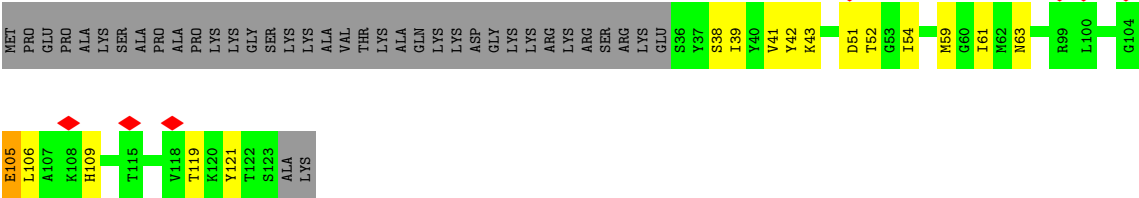




● Molecule 19: Histone H2B type 1-J



● Molecule 19: Histone H2B type 1-J



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51652	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 ($e^-/\text{\AA}^2$)	59.84	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0121	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: MG, 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	0.23	0/11326	0.43	0/15306
2	B	0.23	0/9388	0.43	0/12659
3	C	0.26	0/2139	0.41	0/2895
4	D	0.15	0/1326	0.41	0/1788
5	E	0.21	0/1772	0.43	0/2385
6	F	0.20	0/687	0.39	0/931
7	G	0.20	0/1353	0.43	0/1837
8	H	0.21	0/1069	0.42	0/1444
9	I	0.16	0/934	0.44	0/1257
10	J	0.23	0/554	0.39	0/742
11	K	0.21	0/953	0.40	0/1291
12	L	0.18	0/365	0.47	0/484
13	N	0.15	0/3243	0.31	0/5005
14	P	0.13	0/313	0.27	0/487
15	T	0.15	0/3644	0.27	0/5614
16	a	0.41	1/790 (0.1%)	0.77	1/1060 (0.1%)
16	e	0.35	0/755	0.75	1/1012 (0.1%)
17	b	0.36	0/621	0.86	0/832
17	f	0.35	0/626	0.81	0/837
18	c	0.44	1/825 (0.1%)	0.81	0/1114
18	g	0.32	0/729	0.75	0/983
19	d	0.37	0/731	0.78	0/983
19	h	0.32	0/696	0.76	0/938
All	All	0.24	2/44839 (0.0%)	0.47	2/61884 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	52	ARG	C-O	-6.17	1.17	1.24
18	c	112	GLN	C-O	5.04	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	117	VAL	N-CA-C	-7.13	106.27	113.47
16	e	117	VAL	N-CA-C	-5.83	107.58	113.47

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	11120	0	11150	229	0
2	B	9210	0	9221	179	0
3	C	2098	0	2057	27	0
4	D	1314	0	1314	38	0
5	E	1740	0	1754	22	0
6	F	677	0	693	9	0
7	G	1324	0	1342	52	0
8	H	1052	0	1050	18	0
9	I	917	0	865	23	0
10	J	545	0	560	6	0
11	K	932	0	944	11	0
12	L	359	0	358	7	0
13	N	2897	0	1594	53	0
14	P	281	0	138	24	0
15	T	3243	0	1772	80	0
16	a	779	0	814	26	0
16	e	746	0	786	11	0
17	b	614	0	656	14	0
17	f	619	0	659	8	0
18	c	815	0	869	26	0
18	g	720	0	760	24	0
19	d	720	0	740	6	0
19	h	685	0	703	21	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
All	All	43416	0	40799	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 9.

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)
18:g:73:ASN:ND2	18:g:75:LYS:HE3	1.64	1.13
13:N:9:DT:H4'	16:a:40:ARG:HB2	1.34	1.09
13:N:9:DT:H4'	16:a:40:ARG:CB	1.84	1.07
19:h:38:SER:O	19:h:42:TYR:CD2	2.19	0.96
2:B:63:GLN:NE2	19:h:119:THR:HG21	1.83	0.93
15:T:76:DG:OP1	18:g:75:LYS:HB3	1.70	0.91
2:B:1129:ARG:NE	15:T:34:DA:OP1	2.05	0.89
13:N:48:DG:C4'	19:d:33:ARG:HH12	1.86	0.88
14:P:6:G:C2	15:T:38:DA:C2	2.63	0.87
2:B:316:ILE:HG21	2:B:322:ALA:HB2	1.56	0.87
18:c:17:ARG:HG2	18:c:20:ARG:HH22	1.40	0.85
2:B:63:GLN:NE2	2:B:63:GLN:O	2.09	0.85
16:a:69:ARG:HD2	17:b:25:ASN:ND2	1.92	0.85
15:T:76:DG:OP1	18:g:75:LYS:CB	2.24	0.85
13:N:48:DG:H4'	19:d:33:ARG:HH12	1.43	0.84
16:a:69:ARG:CD	17:b:25:ASN:ND2	2.41	0.83
15:T:-45:DA:H3'	18:c:32:ARG:NH2	1.93	0.83
1:A:962:LEU:CD1	1:A:1027:ARG:HG3	2.08	0.83
1:A:318:LYS:HD3	1:A:318:LYS:N	1.94	0.83
15:T:76:DG:OP1	18:g:75:LYS:CA	2.28	0.81
1:A:526:GLN:HG2	2:B:835:GLN:HB3	1.64	0.80
13:N:9:DT:H4'	16:a:40:ARG:HB3	1.64	0.79
13:N:9:DT:C4'	16:a:40:ARG:HB2	2.11	0.79
14:P:8:G:C2	15:T:36:DC:O2	2.36	0.78
14:P:8:G:N2	15:T:36:DC:O2	2.17	0.78
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.17	0.77
2:B:262:LYS:NZ	2:B:312:GLU:OE1	2.19	0.75
15:T:-13:DA:P	17:b:32:PRO:HG3	2.27	0.74
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HA	1:A:164:SER:HA	1.68	0.74
1:A:962:LEU:HD12	1:A:1027:ARG:HG3	1.68	0.74
2:B:702:MET:HE2	2:B:745:PRO:HB3	1.69	0.74
7:G:56:VAL:HA	7:G:72:VAL:HG12	1.70	0.73
1:A:1393:ASN:HD22	1:A:1402:ARG:HG2	1.52	0.73
4:D:137:LEU:HB3	4:D:142:ILE:HD11	1.68	0.73
18:g:76:THR:O	19:h:52:THR:HG23	1.90	0.72
18:c:29:ARG:HA	18:c:32:ARG:NE	2.03	0.72
2:B:470:ALA:HB1	14:P:5:U:H4'	1.70	0.72
16:e:128:ARG:HH12	16:e:134:ARG:HE	1.38	0.72
1:A:874:LEU:HD11	1:A:959:PRO:HG3	1.72	0.71
1:A:1229:MET:HE1	1:A:1243:ARG:HG3	1.72	0.71
2:B:470:ALA:CB	14:P:5:U:H4'	2.20	0.71
18:g:73:ASN:HD21	18:g:75:LYS:HE3	1.53	0.71
13:N:-83:DT:H5'	16:a:49:ARG:NH1	2.06	0.71
1:A:1456:LEU:HB2	7:G:20:PRO:HB3	1.73	0.71
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.17	0.71
13:N:17:DA:P	16:a:65:LEU:HD23	2.31	0.70
1:A:152:ALA:HB3	1:A:163:VAL:HG12	1.74	0.70
1:A:318:LYS:HA	15:T:44:DC:C5	2.27	0.70
1:A:1266:ILE:HG22	1:A:1270:MET:HE2	1.71	0.70
1:A:345:ARG:NH2	15:T:35:DC:OP1	2.22	0.70
3:C:21:LEU:HD11	11:K:101:LEU:HD11	1.74	0.70
1:A:1402:ARG:HB3	1:A:1411:ILE:HD13	1.72	0.69
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.72	0.69
4:D:149:GLY:O	7:G:144:ARG:NH1	2.24	0.69
11:K:7:PHE:HB2	11:K:11:ILE:HD12	1.72	0.69
16:a:69:ARG:HD3	17:b:25:ASN:HD21	1.56	0.69
1:A:1289:LYS:HD2	1:A:1305:GLU:HG2	1.75	0.69
1:A:41:MET:HA	1:A:48:PRO:HB3	1.75	0.69
4:D:86:ASP:HB3	4:D:106:LEU:HB3	1.74	0.69
7:G:119:LEU:HA	7:G:132:SER:HG	1.56	0.69
2:B:721:ASP:HB3	2:B:724:LYS:HG2	1.75	0.69
6:F:128:ARG:NH1	6:F:151:LEU:O	2.26	0.69
7:G:119:LEU:HD22	7:G:130:TYR:HB3	1.74	0.69
5:E:36:GLN:HE22	5:E:40:GLU:HG2	1.58	0.69
1:A:900:VAL:HA	1:A:1031:ARG:HH11	1.57	0.68
1:A:962:LEU:HD13	1:A:1027:ARG:HG3	1.76	0.68
1:A:1415:ALA:HA	1:A:1420:GLU:HG3	1.74	0.68
13:N:-81:DG:C2	15:T:82:DC:C2	2.81	0.68
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:31:DT:H5''	15:T:32:DA:H5'	1.76	0.68
2:B:63:GLN:NE2	19:h:119:THR:CG2	2.57	0.68
13:N:10:DG:H2''	13:N:11:DC:H5''	1.74	0.68
1:A:43:GLU:HB2	1:A:45:ARG:HE	1.59	0.67
1:A:1400:LEU:HB2	1:A:1429:GLU:HG2	1.76	0.67
18:c:112:GLN:HG3	16:e:112:ILE:CD1	2.24	0.67
18:c:17:ARG:HG2	18:c:20:ARG:NH2	2.09	0.67
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.58	0.67
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.76	0.67
13:N:48:DG:H4'	19:d:33:ARG:NH1	2.09	0.67
4:D:90:ALA:HB2	4:D:106:LEU:HD12	1.77	0.67
7:G:119:LEU:HA	7:G:132:SER:OG	1.95	0.67
2:B:279:ARG:NH1	2:B:286:ASP:OD1	2.28	0.67
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.76	0.66
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.77	0.66
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.78	0.65
17:f:31:LYS:N	17:f:32:PRO:HD2	2.12	0.65
1:A:42:ASP:HA	1:A:49:ARG:HB2	1.77	0.65
1:A:1226:LEU:HD11	1:A:1242:CYS:HB3	1.78	0.65
2:B:1129:ARG:HD3	15:T:34:DA:H5''	1.79	0.64
1:A:1423:ASP:O	2:B:1220:ARG:NH2	2.27	0.64
2:B:1084:GLN:NE2	3:C:189:THR:OG1	2.30	0.64
18:c:32:ARG:HG2	18:c:33:LEU:N	2.11	0.64
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.37	0.64
19:h:38:SER:HB3	19:h:42:TYR:HE2	1.62	0.64
1:A:529:LEU:O	1:A:532:VAL:HG12	1.98	0.64
11:K:50:LEU:HD13	11:K:75:LEU:HD13	1.80	0.64
13:N:-84:DG:H2''	16:a:49:ARG:HH12	1.61	0.64
13:N:-81:DG:N2	15:T:82:DC:C2	2.65	0.64
7:G:133:ASN:O	7:G:134:ASP:HB2	1.97	0.64
1:A:1210:THR:OG1	1:A:1233:ASP:OD2	2.15	0.63
16:a:69:ARG:CD	17:b:25:ASN:HD21	2.09	0.63
2:B:327:GLY:O	2:B:341:ARG:NH2	2.32	0.63
2:B:350:GLN:O	2:B:367:LYS:NZ	2.31	0.63
1:A:833:ALA:HB1	15:T:31:DT:O3'	1.99	0.63
17:b:31:LYS:N	17:b:32:PRO:HD2	2.14	0.63
19:h:38:SER:O	19:h:42:TYR:HD2	1.80	0.63
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.80	0.63
18:g:73:ASN:CG	18:g:75:LYS:HE3	2.22	0.63
2:B:987:LYS:NZ	14:P:10:G:OP1	2.31	0.63
13:N:9:DT:C5'	16:a:40:ARG:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:ALA:HA	15:T:32:DA:C8	2.33	0.62
2:B:474:GLN:HE21	14:P:6:G:H4'	1.63	0.62
13:N:-84:DG:H2''	16:a:49:ARG:NH1	2.13	0.62
13:N:9:DT:OP1	16:a:41:TYR:HB2	1.99	0.62
17:f:30:THR:HB	17:f:32:PRO:HD2	1.80	0.62
2:B:569:LYS:NZ	9:I:60:ASP:OD2	2.29	0.62
2:B:995:ARG:NH2	2:B:997:GLU:OE2	2.33	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.35	0.62
1:A:916:TYR:OH	1:A:983:LEU:O	2.17	0.61
1:A:1448:ILE:HG12	7:G:22:MET:HE1	1.82	0.61
4:D:37:LYS:HE3	4:D:45:GLU:HG2	1.80	0.61
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.81	0.61
14:P:6:G:N1	15:T:38:DA:C2	2.69	0.61
17:b:31:LYS:HE3	17:b:51:TYR:CZ	2.35	0.61
18:c:15:LYS:NZ	18:c:19:SER:HB2	2.15	0.61
1:A:1229:MET:N	1:A:1241:ARG:O	2.31	0.61
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.81	0.61
16:a:40:ARG:O	16:a:40:ARG:HD3	2.01	0.61
1:A:700:HIS:NE2	9:I:112:ASP:OD2	2.33	0.61
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.25	0.61
1:A:1350:SER:O	1:A:1354:GLU:HG2	2.01	0.61
1:A:231:ARG:HH21	1:A:232:PRO:HD2	1.66	0.61
1:A:352:THR:HG22	1:A:469:PHE:CE2	2.36	0.60
18:c:45:ALA:O	18:c:48:PRO:HD2	2.01	0.60
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.33	0.60
4:D:128:LEU:HD13	4:D:142:ILE:HG23	1.82	0.60
5:E:97:LEU:O	5:E:101:GLU:HB2	2.01	0.60
2:B:613:ARG:NH2	9:I:89:GLN:OE1	2.26	0.60
1:A:568:LYS:NZ	8:H:89:ALA:O	2.27	0.60
19:h:38:SER:HA	19:h:59:MET:HE2	1.84	0.60
5:E:92:MET:HG3	5:E:119:ALA:HB1	1.83	0.59
1:A:318:LYS:HD3	1:A:318:LYS:H	1.67	0.59
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.27	0.59
15:T:60:DA:OP2	15:T:60:DA:H2'	2.02	0.59
15:T:76:DG:P	18:g:75:LYS:HA	2.42	0.59
2:B:290:LEU:O	2:B:294:CYS:N	2.32	0.59
18:g:78:ILE:H	19:h:54:ILE:HA	1.66	0.59
1:A:456:MET:HE3	2:B:1138:MET:HE3	1.84	0.59
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.84	0.59
3:C:148:ARG:HG2	10:J:60:LEU:HD22	1.84	0.59
1:A:456:MET:HE2	2:B:1137:CYS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:HIS:NE2	14:P:-1:G:N2	2.50	0.59
15:T:17:DA:OP1	16:e:69:ARG:NH1	2.35	0.59
3:C:83:ARG:NH1	3:C:166:GLU:OE2	2.36	0.59
15:T:76:DG:OP1	18:g:75:LYS:HA	2.01	0.59
15:T:-23:DC:OP1	16:a:72:ARG:NH1	2.34	0.59
2:B:607:SER:HB2	2:B:620:PHE:HB2	1.85	0.58
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.84	0.58
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.85	0.58
2:B:788:ARG:O	2:B:967:ARG:NH2	2.36	0.58
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.85	0.58
4:D:67:ARG:NH2	7:G:35:GLU:OE2	2.31	0.58
5:E:160:LYS:NZ	5:E:192:GLY:O	2.24	0.58
17:b:31:LYS:HG3	17:b:51:TYR:CE1	2.38	0.58
2:B:887:HIS:CE1	14:P:-1:G:H1	2.21	0.58
13:N:47:DA:H2''	13:N:48:DG:N7	2.19	0.58
1:A:120:PRO:HA	1:A:123:ALA:HB3	1.86	0.57
1:A:173:PRO:HB3	1:A:186:TRP:CD2	2.39	0.57
2:B:883:LEU:HB3	2:B:932:HIS:CE1	2.38	0.57
2:B:987:LYS:CE	14:P:10:G:OP1	2.53	0.57
11:K:36:GLU:OE1	11:K:37:ARG:NH2	2.37	0.57
2:B:474:GLN:CD	14:P:6:G:O2'	2.48	0.57
15:T:41:DA:O5'	15:T:41:DA:H8	1.87	0.57
1:A:923:ASP:OD1	1:A:924:VAL:N	2.37	0.57
1:A:1304:GLU:HG2	1:A:1306:LEU:HD11	1.86	0.57
8:H:17:ASN:CG	8:H:24:SER:HG	2.09	0.57
15:T:-23:DC:P	16:a:72:ARG:HH12	2.27	0.57
2:B:225:ILE:O	2:B:252:ARG:NH1	2.38	0.57
7:G:13:LEU:HD22	7:G:26:LEU:HD11	1.84	0.57
1:A:874:LEU:HD13	1:A:959:PRO:HB3	1.86	0.57
9:I:70:ARG:NH1	9:I:82:ASP:OD2	2.38	0.57
15:T:-45:DA:C3'	18:c:32:ARG:NH2	2.63	0.57
4:D:33:GLU:HG3	7:G:41:GLN:HG2	1.87	0.57
1:A:1229:MET:HB2	1:A:1241:ARG:HB2	1.86	0.57
4:D:38:GLN:N	4:D:46:HIS:O	2.38	0.57
7:G:153:ASP:HB3	7:G:156:GLU:O	2.05	0.57
18:g:76:THR:HG23	19:h:51:ASP:O	2.04	0.57
1:A:572:LEU:HD11	8:H:46:MET:HE3	1.86	0.56
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.87	0.56
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.86	0.56
13:N:-81:DG:N1	15:T:82:DC:N3	2.54	0.56
13:N:-13:DA:H5'	17:f:32:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:d:76:GLU:OE1	19:d:79:ARG:NH2	2.38	0.56
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.87	0.56
3:C:233:GLU:OE2	10:J:41:LYS:NZ	2.31	0.56
1:A:1403:CYS:HB2	1:A:1408:THR:HG23	1.88	0.56
7:G:95:SER:OG	7:G:98:GLY:O	2.16	0.56
7:G:116:PRO:HG2	7:G:119:LEU:HD12	1.88	0.56
2:B:63:GLN:HA	2:B:70:ASN:HB3	1.88	0.56
1:A:1449:ASP:HB2	6:F:133:VAL:HG23	1.87	0.56
1:A:909:ILE:HD11	1:A:985:ILE:HD11	1.86	0.56
2:B:613:ARG:HG3	2:B:614:GLU:HG2	1.88	0.56
2:B:865:ARG:HA	2:B:871:VAL:HG12	1.88	0.56
1:A:830:VAL:O	2:B:500:LYS:NZ	2.39	0.55
2:B:250:TYR:HE2	2:B:262:LYS:HB2	1.70	0.55
2:B:533:SER:OG	2:B:747:MET:O	2.25	0.55
15:T:-16:DT:H2''	15:T:-15:DA:N7	2.20	0.55
2:B:887:HIS:CE1	14:P:-1:G:N1	2.74	0.55
4:D:175:LEU:O	4:D:179:ASN:ND2	2.39	0.55
2:B:326:ILE:HD13	2:B:349:LEU:HD21	1.88	0.55
13:N:17:DA:OP2	16:a:65:LEU:HD23	2.06	0.55
2:B:660:ASP:OD1	2:B:661:ASP:N	2.39	0.55
2:B:883:LEU:HB3	2:B:932:HIS:HE1	1.70	0.55
5:E:27:TYR:HB3	5:E:61:ALA:HB1	1.88	0.55
18:c:117:PRO:HD3	16:e:48:LEU:HD11	1.89	0.55
1:A:512:ILE:HA	1:A:522:MET:HE3	1.88	0.55
2:B:568:THR:O	2:B:615:ARG:NH1	2.40	0.55
1:A:874:LEU:CD1	1:A:959:PRO:HG3	2.36	0.55
7:G:44:TYR:CZ	7:G:106:LEU:HD21	2.41	0.55
2:B:916:THR:N	2:B:935:ARG:O	2.27	0.54
5:E:11:LEU:HD11	5:E:57:MET:HE1	1.88	0.54
5:E:27:TYR:CZ	5:E:77:LEU:HB2	2.41	0.54
13:N:8:DG:H2'	13:N:9:DT:H71	1.88	0.54
1:A:43:GLU:HB2	1:A:45:ARG:NE	2.23	0.54
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.07	0.54
18:g:73:ASN:ND2	18:g:75:LYS:CE	2.56	0.54
6:F:108:LEU:HB3	6:F:129:LYS:HE2	1.89	0.54
9:I:7:CYS:N	9:I:12:ASN:O	2.35	0.54
18:g:37:GLY:HA3	18:g:39:TYR:CE2	2.43	0.54
1:A:467:SER:HB3	2:B:1103:ILE:HD12	1.90	0.54
1:A:550:MET:HE3	1:A:657:TRP:HB2	1.90	0.54
7:G:24:GLN:O	7:G:28:GLU:HG2	2.07	0.54
17:f:30:THR:OG1	17:f:32:PRO:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:LEU:HB3	1:A:959:PRO:HD2	1.90	0.54
2:B:493:THR:HG22	2:B:495:ILE:HG12	1.90	0.54
1:A:270:ILE:HG12	1:A:300:HIS:HB3	1.91	0.53
1:A:557:TRP:O	11:K:26:ARG:NH2	2.40	0.53
2:B:223:SER:O	2:B:252:ARG:NH1	2.32	0.53
2:B:512:TRP:HZ2	2:B:702:MET:HE1	1.73	0.53
5:E:36:GLN:NE2	5:E:40:GLU:HG2	2.23	0.53
1:A:841:ARG:NH1	1:A:1108:ASN:OD1	2.40	0.53
4:D:25:ALA:HB1	4:D:140:PHE:HZ	1.73	0.53
1:A:176:ARG:N	1:A:183:TRP:O	2.39	0.53
5:E:61:ALA:HB3	5:E:77:LEU:HB3	1.90	0.53
13:N:62:DG:N1	15:T:-61:DG:O6	2.41	0.53
1:A:457:MET:HE2	1:A:508:VAL:HA	1.89	0.53
4:D:53:LEU:HD21	4:D:108:TYR:HE1	1.74	0.53
1:A:727:ARG:HD3	1:A:767:GLY:HA3	1.89	0.53
2:B:291:GLN:HG2	2:B:564:PRO:HG2	1.90	0.53
2:B:319:LYS:HE2	2:B:346:LYS:HE3	1.90	0.53
2:B:586:PRO:O	2:B:590:VAL:HG23	2.09	0.53
1:A:529:LEU:HD23	1:A:752:SER:HB3	1.90	0.53
19:h:38:SER:HB3	19:h:42:TYR:CE2	2.44	0.53
2:B:702:MET:HE3	2:B:742:GLU:HG3	1.89	0.53
7:G:93:ASN:HB2	7:G:100:PHE:HB2	1.89	0.53
1:A:174:VAL:HB	1:A:185:THR:HB	1.91	0.53
1:A:846:LEU:HD12	1:A:1071:ALA:HB2	1.91	0.52
1:A:977:ARG:HA	8:H:135:LYS:NZ	2.24	0.52
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.90	0.52
2:B:56:LEU:HD12	2:B:77:ILE:HD11	1.90	0.52
9:I:54:GLU:HG2	9:I:100:PHE:HZ	1.75	0.52
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.52
9:I:24:ARG:HH21	9:I:37:LEU:HD13	1.74	0.52
13:N:26:DA:H2"	13:N:27:DG:N7	2.24	0.52
1:A:758:ASN:ND2	2:B:1021:MET:HE2	2.25	0.52
5:E:21:MET:HE2	5:E:186:TYR:CD2	2.45	0.52
2:B:459:TRP:HB2	2:B:472:VAL:HG21	1.91	0.52
1:A:318:LYS:N	1:A:318:LYS:CD	2.65	0.52
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.45	0.52
13:N:51:DG:H2"	13:N:52:DC:H5"	1.91	0.52
1:A:536:THR:HG21	1:A:579:LEU:HD22	1.92	0.52
1:A:368:PRO:HB3	1:A:466:TYR:O	2.10	0.52
1:A:596:ASN:C	1:A:596:ASN:HD22	2.18	0.52
1:A:809:LEU:O	2:B:725:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:33:CYS:HB2	12:L:50:CYS:SG	2.50	0.52
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.74	0.52
13:N:-84:DG:H2'	13:N:-83:DT:C6	2.45	0.52
13:N:-62:DT:O4	15:T:61:DA:N6	2.43	0.52
1:A:1450:GLU:O	1:A:1454:THR:HG23	2.10	0.51
6:F:107:VAL:HG11	6:F:111:ILE:HD11	1.92	0.51
13:N:36:DA:H2''	13:N:37:DC:C5	2.45	0.51
8:H:37:LYS:HE3	8:H:125:GLU:HG3	1.91	0.51
17:b:31:LYS:HE3	17:b:51:TYR:OH	2.10	0.51
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.10	0.51
1:A:318:LYS:HA	15:T:44:DC:C4	2.46	0.51
1:A:1285:VAL:HG13	1:A:1311:THR:HG22	1.93	0.51
1:A:1302:LYS:NZ	1:A:1304:GLU:OE2	2.39	0.51
2:B:644:GLU:N	2:B:644:GLU:OE1	2.42	0.51
13:N:-74:DT:H4'	13:N:-73:DT:OP1	2.10	0.51
1:A:782:ASP:HB2	1:A:790:LYS:HG2	1.93	0.51
1:A:970:GLN:HA	1:A:975:LEU:HG	1.91	0.51
2:B:862:GLN:O	2:B:914:LYS:NZ	2.36	0.51
18:c:45:ALA:C	18:c:48:PRO:HD2	2.35	0.51
1:A:588:HIS:HB2	1:A:967:GLN:NE2	2.26	0.51
2:B:857:ARG:NE	2:B:945:GLU:OE2	2.43	0.51
13:N:-61:DT:H2''	13:N:-60:DT:C4	2.44	0.51
15:T:35:DC:H2'	15:T:36:DC:C6	2.45	0.51
1:A:468:THR:HG21	2:B:977:GLY:HA3	1.92	0.51
2:B:1038:ARG:NE	2:B:1062:ASN:OD1	2.43	0.51
18:c:73:ASN:O	18:c:73:ASN:ND2	2.38	0.51
2:B:1017:ILE:HG21	2:B:1026:LEU:HD11	1.91	0.51
1:A:1289:LYS:HD3	1:A:1306:LEU:O	2.11	0.51
2:B:307:LYS:HZ1	9:I:4:PHE:HD2	1.58	0.51
2:B:544:SER:OG	2:B:576:ASN:ND2	2.44	0.51
1:A:84:MET:HE1	1:A:270:ILE:HG22	1.93	0.51
1:A:484:ASP:HB2	2:B:987:LYS:HG3	1.93	0.51
1:A:852:HIS:ND1	6:F:139:PRO:HG3	2.25	0.51
13:N:56:DG:H2''	13:N:57:DG:N7	2.26	0.51
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.94	0.50
12:L:33:CYS:SG	12:L:34:GLY:N	2.84	0.50
1:A:152:ALA:HB2	1:A:165:ARG:HB3	1.91	0.50
1:A:758:ASN:HD22	2:B:1021:MET:HE2	1.76	0.50
15:T:-46:DC:H2''	15:T:-45:DA:C8	2.46	0.50
15:T:39:DA:H2'	15:T:40:DG:C8	2.46	0.50
15:T:47:DG:N2	15:T:48:DG:O6	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:31:LYS:HG3	17:b:51:TYR:CZ	2.46	0.50
19:h:38:SER:HA	19:h:59:MET:CE	2.41	0.50
2:B:883:LEU:HD12	2:B:884:ARG:HB2	1.93	0.50
4:D:139:PRO:HA	4:D:142:ILE:HB	1.93	0.50
13:N:-83:DT:H5'	16:a:49:ARG:CZ	2.40	0.50
1:A:943:PHE:HD1	1:A:947:ILE:HD12	1.75	0.50
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.76	0.50
9:I:78:CYS:SG	9:I:80:SER:OG	2.61	0.50
15:T:-10:DC:H2''	15:T:-9:DA:H8	1.77	0.50
1:A:903:MET:HE1	1:A:927:GLN:HG2	1.94	0.50
15:T:-35:DA:H4'	18:c:42:ARG:HD2	1.94	0.50
1:A:371:ILE:HD11	2:B:1103:ILE:HG13	1.94	0.50
1:A:1097:THR:HG22	1:A:1102:ARG:HB2	1.94	0.50
1:A:1354:GLU:O	1:A:1358:VAL:HG23	2.12	0.50
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	1.94	0.50
3:C:266:ARG:HH22	11:K:85:GLN:HE22	1.60	0.50
9:I:58:ILE:HG12	9:I:86:PHE:HZ	1.76	0.50
2:B:323:LEU:HD22	2:B:342:ILE:HG23	1.93	0.49
18:c:79:ILE:HG12	18:c:82:HIS:CE1	2.46	0.49
1:A:345:ARG:HH22	15:T:35:DC:P	2.33	0.49
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.46	0.49
10:J:24:LEU:HD22	10:J:29:LYS:HD2	1.93	0.49
1:A:1270:MET:HA	1:A:1274:ILE:HG12	1.94	0.49
16:e:68:GLN:HG3	16:e:89:ILE:HD13	1.93	0.49
2:B:815:ARG:NH1	2:B:1041:GLU:HG3	2.26	0.49
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.95	0.49
18:g:17:ARG:N	19:h:121:TYR:HE1	2.11	0.49
13:N:15:DT:H2''	13:N:16:DA:C8	2.47	0.49
15:T:75:DC:O4'	18:g:77:ARG:NH1	2.46	0.49
17:f:30:THR:CB	17:f:32:PRO:HD2	2.41	0.49
1:A:105:CYS:SG	1:A:139:TRP:HD1	2.36	0.49
1:A:472:ASN:O	1:A:475:VAL:HG22	2.13	0.49
7:G:38:CYS:HB2	7:G:44:TYR:CE2	2.47	0.49
1:A:834:GLU:HG2	2:B:500:LYS:NZ	2.28	0.49
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.94	0.49
14:P:9:U:C2'	14:P:10:G:H5'	2.43	0.49
9:I:70:ARG:HG2	9:I:84:VAL:HG12	1.94	0.49
15:T:-6:DT:H2''	15:T:-5:DA:N7	2.27	0.49
15:T:76:DG:OP1	18:g:75:LYS:C	2.55	0.49
19:h:38:SER:C	19:h:42:TYR:CD2	2.91	0.49
1:A:1214:VAL:O	1:A:1218:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:GLN:OE1	1:A:1277:ARG:NH1	2.46	0.48
2:B:547:ILE:HG21	2:B:619:ILE:HG21	1.94	0.48
3:C:15:ASP:OD1	3:C:16:GLU:N	2.46	0.48
2:B:39:ASP:O	2:B:43:GLU:HG2	2.13	0.48
2:B:839:MET:HG2	2:B:989:THR:O	2.14	0.48
7:G:83:LYS:HA	7:G:147:VAL:HG12	1.95	0.48
13:N:5:DT:H2''	13:N:6:DA:N7	2.28	0.48
17:b:59:LYS:HE2	17:b:63:GLU:OE2	2.13	0.48
1:A:684:ILE:HG21	1:A:802:GLU:HG3	1.96	0.48
1:A:1145:LEU:O	1:A:1149:THR:OG1	2.16	0.48
2:B:107:ARG:NH1	2:B:956:THR:O	2.36	0.48
12:L:33:CYS:SG	12:L:35:ALA:N	2.82	0.48
18:c:29:ARG:HA	18:c:32:ARG:CD	2.43	0.48
19:d:76:GLU:HA	19:d:79:ARG:NH2	2.29	0.48
1:A:1006:ASN:O	1:A:1010:LYS:HG2	2.13	0.48
4:D:85:ASP:O	4:D:89:LEU:N	2.44	0.48
15:T:33:DC:H2'	15:T:34:DA:C8	2.49	0.48
19:h:105:GLU:HG3	19:h:109:HIS:CE1	2.48	0.48
1:A:403:ALA:HA	1:A:435:ARG:HA	1.96	0.48
1:A:1452:LEU:HD23	6:F:131:PRO:HA	1.96	0.48
15:T:-14:DA:H2''	15:T:-13:DA:N7	2.28	0.48
1:A:379:GLU:OE1	1:A:435:ARG:NE	2.34	0.48
1:A:1447:MET:HB2	6:F:133:VAL:HB	1.95	0.48
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.78	0.48
3:C:136:ASP:H	3:C:139:ASP:HB2	1.79	0.48
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.96	0.48
1:A:526:GLN:HG3	1:A:527:ASP:N	2.29	0.48
3:C:47:LEU:HD11	12:L:68:GLN:HB3	1.95	0.48
16:a:79:LYS:HD3	16:a:82:LEU:HD21	1.94	0.48
1:A:62:ASP:OD1	1:A:63:ARG:N	2.47	0.48
1:A:1195:LEU:HD11	1:A:1267:GLU:HB2	1.95	0.48
2:B:471:GLY:HA3	14:P:6:G:H5'	1.96	0.48
7:G:125:ASN:ND2	7:G:127:PRO:O	2.41	0.48
1:A:931:ASN:O	1:A:935:GLU:HG3	2.14	0.47
2:B:605:GLU:O	2:B:625:ARG:NH1	2.42	0.47
5:E:169:LEU:HD22	5:E:173:GLN:HB2	1.95	0.47
1:A:14:VAL:N	1:A:1435:GLN:OE1	2.46	0.47
1:A:886:THR:O	1:A:941:ARG:HD3	2.14	0.47
1:A:1152:THR:HG21	1:A:1271:LEU:HD11	1.96	0.47
2:B:593:MET:HB3	2:B:608:ILE:HD13	1.96	0.47
13:N:9:DT:H5''	16:a:40:ARG:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.97	0.47
2:B:824:ILE:HD11	10:J:47:ARG:HE	1.79	0.47
4:D:41:HIS:ND1	7:G:73:LYS:HB3	2.29	0.47
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.96	0.47
9:I:19:ASP:O	9:I:23:GLN:N	2.41	0.47
18:c:112:GLN:HG3	16:e:112:ILE:HD11	1.96	0.47
1:A:457:MET:HE3	1:A:511:GLN:HB2	1.97	0.47
1:A:1216:ASP:O	1:A:1220:GLU:HG2	2.14	0.47
13:N:-11:DC:H2''	13:N:-10:DG:C8	2.50	0.47
18:c:29:ARG:HA	18:c:32:ARG:HE	1.78	0.47
1:A:1403:CYS:O	1:A:1408:THR:OG1	2.23	0.47
2:B:46:ILE:HG22	2:B:82:ILE:HG13	1.95	0.47
14:P:10:G:O6	15:T:34:DA:N6	2.48	0.47
1:A:451:LEU:HD13	1:A:1079:THR:HG21	1.97	0.47
1:A:149:GLU:O	1:A:165:ARG:NH2	2.45	0.47
1:A:453:LYS:O	2:B:1141:HIS:NE2	2.48	0.47
1:A:864:ILE:HD12	5:E:169:LEU:HD11	1.95	0.47
1:A:1193:TRP:HB3	1:A:1263:LEU:HD22	1.97	0.47
1:A:1203:ARG:NH1	9:I:49:ILE:HD11	2.30	0.47
2:B:290:LEU:HD23	2:B:303:LEU:HD22	1.97	0.47
2:B:806:THR:H	2:B:809:MET:HE2	1.79	0.47
2:B:839:MET:HE2	2:B:1010:LEU:HD11	1.96	0.47
3:C:77:GLU:OE1	3:C:246:ARG:NH2	2.48	0.47
4:D:60:ILE:HG23	7:G:47:THR:HG21	1.97	0.47
12:L:55:HIS:NE2	12:L:57:VAL:HG12	2.30	0.47
15:T:62:DA:H2''	15:T:63:DA:C8	2.50	0.47
1:A:349:SER:HB2	2:B:1128:LEU:HD12	1.96	0.47
7:G:6:ASP:OD1	7:G:75:ARG:HB2	2.15	0.47
7:G:54:ILE:HG23	7:G:74:TYR:HB3	1.97	0.47
1:A:1154:ILE:HG23	1:A:1263:LEU:HD23	1.97	0.47
1:A:977:ARG:HA	8:H:135:LYS:HZ1	1.78	0.47
13:N:53:DC:H2''	13:N:54:DT:H5''	1.97	0.47
4:D:49:ILE:HG21	7:G:4:LEU:HB2	1.97	0.46
1:A:526:GLN:HG3	1:A:527:ASP:H	1.78	0.46
2:B:760:ASP:OD1	2:B:760:ASP:N	2.44	0.46
3:C:254:LYS:HD3	11:K:42:LEU:HB2	1.97	0.46
5:E:92:MET:CG	5:E:119:ALA:HB1	2.45	0.46
15:T:66:DC:H2''	15:T:67:DA:C8	2.50	0.46
15:T:75:DC:C1'	18:g:77:ARG:HH11	2.28	0.46
19:h:42:TYR:OH	19:h:59:MET:HG2	2.16	0.46
1:A:554:VAL:HB	1:A:557:TRP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:ARG:NE	1:A:1376:ASP:OD1	2.46	0.46
15:T:3:DT:H2''	15:T:4:DC:OP2	2.15	0.46
2:B:376:ASN:O	2:B:380:LEU:HD23	2.15	0.46
4:D:33:GLU:HG3	7:G:41:GLN:O	2.15	0.46
4:D:39:TYR:HD1	4:D:45:GLU:HA	1.80	0.46
1:A:1145:LEU:HG	1:A:1271:LEU:HD23	1.98	0.46
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.80	0.46
5:E:99:ILE:HG23	5:E:104:PHE:HB2	1.97	0.46
15:T:62:DA:H2''	15:T:63:DA:N7	2.31	0.46
1:A:1195:LEU:O	1:A:1241:ARG:HA	2.15	0.46
1:A:1462:PRO:HB3	7:G:17:TYR:HD1	1.81	0.46
1:A:517:SER:OG	1:A:1365:TYR:O	2.33	0.46
1:A:900:VAL:HA	1:A:1031:ARG:NH1	2.26	0.46
2:B:284:VAL:HG23	2:B:285:PRO:HD3	1.98	0.46
2:B:324:ASP:OD2	2:B:338:ARG:HG3	2.15	0.46
3:C:76:VAL:HG22	3:C:161:LYS:HG3	1.98	0.46
9:I:77:GLU:HB2	9:I:108:LYS:HD3	1.97	0.46
19:h:105:GLU:HG3	19:h:109:HIS:HE1	1.80	0.46
1:A:1289:LYS:HD2	1:A:1305:GLU:CG	2.44	0.46
5:E:116:THR:HG23	5:E:119:ALA:H	1.81	0.46
13:N:-63:DT:H2''	13:N:-62:DT:H72	1.97	0.46
15:T:4:DC:H4'	15:T:5:DC:OP1	2.15	0.46
19:d:98:VAL:HG13	19:d:102:LEU:HD22	1.97	0.46
2:B:190:MET:HE3	2:B:481:TYR:OH	2.15	0.46
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.97	0.46
15:T:1:DT:H2''	15:T:2:DG:C8	2.50	0.46
1:A:570:LYS:HD3	8:H:46:MET:HE1	1.98	0.46
1:A:962:LEU:HB2	1:A:1027:ARG:NH2	2.31	0.46
2:B:571:THR:HG21	2:B:586:PRO:HB3	1.97	0.46
4:D:10:ALA:HB1	4:D:12:ARG:HG3	1.98	0.46
2:B:63:GLN:NE2	2:B:63:GLN:C	2.73	0.45
3:C:248:ILE:O	3:C:252:GLN:HG3	2.15	0.45
4:D:106:LEU:HD23	4:D:106:LEU:HA	1.83	0.45
8:H:89:ALA:HB1	8:H:95:VAL:HG21	1.98	0.45
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.50	0.45
2:B:364:GLU:OE1	2:B:364:GLU:N	2.43	0.45
13:N:17:DA:O5'	16:a:65:LEU:HD23	2.16	0.45
2:B:286:ASP:H	9:I:12:ASN:ND2	2.15	0.45
3:C:89:ASP:O	3:C:90:TYR:C	2.60	0.45
17:b:31:LYS:HE3	17:b:51:TYR:CE2	2.51	0.45
1:A:266:LYS:HA	1:A:266:LYS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:HB3	1:A:429:TYR:CE2	2.51	0.45
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.45
2:B:987:LYS:HE3	14:P:10:G:OP1	2.16	0.45
4:D:93:THR:HG21	4:D:102:VAL:HG21	1.97	0.45
15:T:75:DC:H1'	18:g:77:ARG:HH11	1.81	0.45
18:c:29:ARG:HG3	18:c:32:ARG:HD2	1.98	0.45
18:c:112:GLN:HB2	18:c:115:LEU:HG	1.97	0.45
1:A:962:LEU:HB2	1:A:1027:ARG:HH21	1.82	0.45
1:A:1157:ASP:CG	1:A:1243:ARG:HH12	2.24	0.45
2:B:215:GLN:HB3	2:B:217:PHE:CE1	2.52	0.45
2:B:805:LYS:HE3	2:B:1041:GLU:HB2	1.98	0.45
7:G:34:VAL:HG11	7:G:74:TYR:OH	2.17	0.45
15:T:67:DA:OP2	19:h:39:ILE:HG21	2.17	0.45
4:D:105:THR:OG1	7:G:105:PRO:HG3	2.17	0.45
1:A:454:MET:HE1	1:A:514:SER:HA	1.99	0.45
1:A:493:PRO:HG3	1:A:502:LEU:HD12	1.98	0.45
1:A:1043:ALA:O	1:A:1047:VAL:HG23	2.16	0.45
2:B:270:GLN:HB3	2:B:329:ARG:HG2	1.99	0.45
2:B:409:LEU:HD23	2:B:450:LEU:HD23	1.99	0.45
8:H:56:THR:HG21	8:H:144:ARG:HH11	1.81	0.45
15:T:60:DA:H1'	15:T:61:DA:C4	2.51	0.45
1:A:535:MET:O	1:A:575:GLY:HA3	2.17	0.45
1:A:1199:LEU:HD12	1:A:1211:MET:HE1	1.98	0.45
3:C:75:ASP:HB2	3:C:129:VAL:HG13	1.98	0.45
1:A:260:GLN:HB2	1:A:265:HIS:CD2	2.52	0.45
1:A:941:ARG:HE	1:A:945:ARG:HD2	1.82	0.45
1:A:1078:ALA:HA	1:A:1081:MET:HG2	1.99	0.45
1:A:1279:ILE:HD12	1:A:1318:GLU:HB3	1.99	0.45
1:A:114:LEU:HD13	1:A:145:LYS:O	2.17	0.44
2:B:276:ILE:HG23	2:B:322:ALA:HB1	1.98	0.44
9:I:87:GLN:O	9:I:89:GLN:NE2	2.45	0.44
13:N:43:DA:H2'	13:N:44:DT:H71	1.98	0.44
18:g:71:ARG:HB2	18:g:71:ARG:NH2	2.32	0.44
19:h:59:MET:HE3	19:h:59:MET:O	2.17	0.44
1:A:526:GLN:OE1	2:B:1015:HIS:HB2	2.17	0.44
1:A:576:LYS:HD2	8:H:119:GLY:HA3	1.98	0.44
2:B:416:LYS:O	2:B:420:GLU:HG2	2.16	0.44
2:B:422:TYR:HA	2:B:425:MET:HG2	1.99	0.44
2:B:559:LEU:HD21	2:B:579:TRP:CE2	2.52	0.44
4:D:30:LEU:HD21	4:D:140:PHE:HE2	1.83	0.44
15:T:7:DC:H2''	15:T:8:DC:H5'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:32:DA:O5'	15:T:32:DA:H8	2.00	0.44
1:A:273:ALA:O	1:A:277:VAL:HG23	2.17	0.44
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.82	0.44
4:D:3:VAL:HG12	7:G:9:LEU:HD11	1.98	0.44
7:G:114:LEU:HD13	7:G:162:SER:HB2	2.00	0.44
13:N:-83:DT:H2''	13:N:-82:DG:H8	1.82	0.44
1:A:1194:LEU:HD12	1:A:1242:CYS:O	2.17	0.44
2:B:474:GLN:NE2	14:P:6:G:O2'	2.51	0.44
2:B:519:GLU:HG3	2:B:771:SER:HB3	1.99	0.44
15:T:56:DC:H2''	15:T:57:DA:C8	2.52	0.44
16:a:99:TYR:OH	16:a:133:GLU:OE1	2.31	0.44
17:f:31:LYS:N	17:f:32:PRO:CD	2.79	0.44
1:A:122:MET:O	1:A:126:ILE:HG12	2.17	0.44
2:B:885:LEU:HA	2:B:936:ASP:OD2	2.18	0.44
2:B:1171:VAL:HG11	2:B:1191:ILE:HG21	2.00	0.44
16:a:65:LEU:HG	16:a:69:ARG:HH12	1.83	0.44
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.83	0.44
1:A:41:MET:HA	1:A:48:PRO:CB	2.46	0.44
1:A:844:LYS:HA	1:A:844:LYS:HD2	1.75	0.44
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.74	0.44
18:c:32:ARG:HE	18:c:32:ARG:HB3	1.70	0.44
1:A:473:LEU:CD2	2:B:835:GLN:HB2	2.48	0.44
5:E:41:PHE:CE1	5:E:45:ILE:HG13	2.53	0.44
15:T:76:DG:OP1	18:g:76:THR:N	2.50	0.44
1:A:135:PHE:HB2	1:A:223:LEU:O	2.18	0.44
1:A:868:LEU:HD21	1:A:1001:VAL:HG11	2.00	0.44
1:A:1120:VAL:HB	1:A:1309:LEU:HB2	1.98	0.44
1:A:1194:LEU:HD11	1:A:1241:ARG:HB3	1.98	0.44
13:N:-66:DG:H2'	13:N:-65:DT:H71	2.00	0.44
13:N:38:DG:OP1	18:c:45:ALA:HB2	2.17	0.44
15:T:59:DA:H2''	15:T:60:DA:C8	2.52	0.44
1:A:665:ILE:HD12	1:A:747:MET:HE1	2.00	0.44
1:A:1381:ARG:NH1	1:A:1385:MET:SD	2.91	0.44
1:A:1461:ALA:HA	7:G:20:PRO:HD2	1.99	0.44
13:N:-70:DC:H2''	13:N:-69:DG:C8	2.53	0.44
17:f:35:ARG:O	17:f:39:ARG:HG2	2.18	0.44
1:A:317:GLN:OE1	1:A:318:LYS:HE2	2.18	0.43
5:E:5:ASN:OD1	5:E:42:ARG:NH1	2.51	0.43
16:a:40:ARG:HD3	16:a:40:ARG:C	2.43	0.43
16:a:52:ARG:O	16:a:56:LYS:HG3	2.18	0.43
18:c:15:LYS:HZ2	18:c:19:SER:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:TYR:OH	2:B:271:ASP:OD2	2.35	0.43
13:N:-70:DC:H2''	13:N:-69:DG:H8	1.83	0.43
1:A:456:MET:SD	2:B:1134:GLU:HG3	2.58	0.43
1:A:1191:SER:HB3	1:A:1244:VAL:HB	1.99	0.43
1:A:1204:MET:HB3	1:A:1209:LEU:O	2.17	0.43
2:B:364:GLU:H	2:B:364:GLU:CD	2.25	0.43
7:G:44:TYR:N	7:G:79:TRP:O	2.51	0.43
15:T:32:DA:C8	15:T:32:DA:O5'	2.71	0.43
3:C:47:LEU:HB3	3:C:158:ILE:HB	2.01	0.43
13:N:28:DA:H2''	13:N:29:DG:C8	2.53	0.43
1:A:1158:PRO:HA	1:A:1192:PRO:CB	2.48	0.43
3:C:98:LEU:HB3	3:C:118:LEU:HD22	2.01	0.43
17:f:31:LYS:HG3	17:f:51:TYR:CE1	2.54	0.43
1:A:43:GLU:CD	1:A:45:ARG:HH11	2.26	0.43
1:A:910:LYS:O	1:A:913:VAL:HG22	2.17	0.43
1:A:983:LEU:HD13	1:A:1041:ARG:HA	1.99	0.43
2:B:719:LEU:HB3	2:B:720:ASN:H	1.47	0.43
1:A:15:LYS:O	1:A:1424:CYS:HB2	2.18	0.43
1:A:1425:ARG:HE	2:B:1220:ARG:CZ	2.31	0.43
2:B:300:TRP:CD1	9:I:52:ILE:HD12	2.54	0.43
9:I:108:LYS:HE3	9:I:110:PHE:HB3	2.01	0.43
15:T:24:DA:H2''	15:T:25:DG:C8	2.54	0.43
1:A:710:THR:HG22	1:A:711:LEU:N	2.34	0.43
1:A:1383:TYR:HB3	5:E:178:GLN:NE2	2.34	0.43
4:D:51:LEU:HD11	7:G:4:LEU:HG	2.00	0.43
7:G:24:GLN:NE2	7:G:28:GLU:OE2	2.43	0.43
13:N:-5:DG:H5'	16:e:43:PRO:HG2	2.00	0.43
1:A:984:THR:HB	1:A:986:PRO:HD2	2.01	0.43
1:A:1214:VAL:HG22	1:A:1276:LEU:HD22	2.00	0.43
2:B:1060:ARG:HB2	2:B:1066:SER:HB3	2.01	0.43
3:C:196:ASP:OD2	3:C:199:LYS:HG2	2.19	0.43
14:P:6:G:C2	15:T:38:DA:N3	2.87	0.43
18:c:17:ARG:HA	18:c:20:ARG:NH2	2.33	0.43
2:B:452:TYR:CE1	2:B:456:THR:HG21	2.54	0.43
5:E:47:ASP:CG	5:E:53:GLN:HE22	2.26	0.43
13:N:-4:DG:H2''	13:N:-3:DA:C8	2.54	0.43
17:b:31:LYS:HB3	17:b:32:PRO:CD	2.49	0.43
2:B:489:ARG:NH1	2:B:533:SER:O	2.52	0.42
15:T:76:DG:H2''	15:T:77:DG:C8	2.54	0.42
16:e:122:LYS:HB2	16:e:122:LYS:NZ	2.33	0.42
19:h:41:VAL:HG21	19:h:59:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:HG2	2:B:1192:TYR:CD1	2.54	0.42
1:A:447:ARG:NH1	14:P:10:G:O2'	2.46	0.42
1:A:465:PRO:HB2	11:K:4:PRO:HD3	2.00	0.42
1:A:833:ALA:HA	15:T:32:DA:H8	1.79	0.42
1:A:837:TYR:O	1:A:841:ARG:HG3	2.18	0.42
1:A:1314:ILE:HB	1:A:1337:GLU:OE1	2.18	0.42
2:B:815:ARG:HG2	2:B:815:ARG:HH21	1.85	0.42
1:A:1217:LYS:HE3	1:A:1276:LEU:O	2.19	0.42
4:D:172:GLN:NE2	4:D:176:ASP:OD2	2.41	0.42
18:c:112:GLN:HB2	18:c:115:LEU:HD12	2.01	0.42
1:A:46:GLN:HB2	1:A:47:ARG:NH2	2.33	0.42
2:B:314:PHE:HZ	9:I:30:ARG:HB3	1.84	0.42
7:G:129:ALA:HB1	7:G:137:ILE:O	2.19	0.42
11:K:84:LYS:O	11:K:88:GLU:OE1	2.37	0.42
15:T:37:DC:H2''	15:T:38:DA:C8	2.53	0.42
1:A:1237:LYS:HB3	1:A:1239:ILE:HD11	2.00	0.42
2:B:955:THR:HB	12:L:57:VAL:HG23	2.01	0.42
15:T:54:DG:H2''	15:T:55:DA:H8	1.85	0.42
16:e:65:LEU:HB3	16:e:66:PRO:HD3	2.00	0.42
18:g:73:ASN:CG	18:g:75:LYS:CE	2.91	0.42
1:A:173:PRO:HB3	1:A:186:TRP:CE2	2.55	0.42
1:A:231:ARG:HG3	1:A:233:GLU:OE1	2.20	0.42
1:A:1076:GLU:O	1:A:1079:THR:OG1	2.35	0.42
1:A:1147:ASN:O	1:A:1203:ARG:HD3	2.20	0.42
2:B:417:LEU:HD11	2:B:441:VAL:HG13	2.01	0.42
2:B:815:ARG:HG2	2:B:815:ARG:NH2	2.34	0.42
7:G:46:VAL:HG13	7:G:47:THR:N	2.34	0.42
2:B:99:MET:HE3	2:B:111:TYR:HA	2.01	0.42
2:B:189:ASP:OD1	2:B:478:ARG:NH1	2.42	0.42
5:E:9:SER:O	5:E:13:ARG:HG3	2.19	0.42
15:T:-26:DT:H2''	15:T:-25:DA:C8	2.55	0.42
2:B:283:VAL:HG23	2:B:283:VAL:O	2.20	0.42
2:B:710:ARG:NE	2:B:719:LEU:HD11	2.35	0.42
7:G:101:ALA:N	7:G:108:VAL:O	2.39	0.42
14:P:6:G:N2	15:T:38:DA:N3	2.67	0.42
19:h:39:ILE:O	19:h:43:LYS:HG3	2.20	0.42
1:A:776:ILE:HD13	1:A:776:ILE:HA	1.94	0.42
1:A:1168:ASP:OD2	1:A:1241:ARG:NH2	2.51	0.42
2:B:307:LYS:HE2	2:B:307:LYS:HB2	1.80	0.42
13:N:-13:DA:H2''	13:N:-12:DA:N7	2.35	0.42
15:T:12:DT:H2''	15:T:13:DT:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:67:DA:OP2	19:h:39:ILE:CG2	2.68	0.42
1:A:41:MET:HE3	1:A:45:ARG:O	2.20	0.42
4:D:39:TYR:CD1	4:D:45:GLU:HA	2.55	0.42
4:D:59:LEU:HD23	4:D:59:LEU:HA	1.90	0.42
15:T:56:DC:H2''	15:T:57:DA:H8	1.85	0.42
1:A:363:ASP:HB3	1:A:509:PRO:HD3	2.02	0.41
2:B:45:SER:O	2:B:49:LEU:HG	2.20	0.41
15:T:-12:DC:H2''	15:T:-11:DG:H8	1.85	0.41
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	2.01	0.41
1:A:327:ARG:HD2	1:A:1409:VAL:HG11	2.02	0.41
5:E:95:PHE:CE2	5:E:131:ILE:HD12	2.55	0.41
7:G:4:LEU:HD23	7:G:4:LEU:HA	1.85	0.41
8:H:100:VAL:HG22	8:H:115:VAL:HG22	2.02	0.41
9:I:34:TYR:CZ	9:I:36:GLU:HB3	2.56	0.41
13:N:21:DG:H2'	13:N:22:DT:H71	2.01	0.41
18:g:79:ILE:HG12	18:g:82:HIS:CE1	2.55	0.41
1:A:1410:GLU:O	1:A:1414:GLU:HG3	2.20	0.41
2:B:773:MET:SD	2:B:987:LYS:HB3	2.60	0.41
2:B:879:ARG:HD3	2:B:885:LEU:HD12	2.03	0.41
4:D:25:ALA:HB2	7:G:82:PHE:HB2	2.03	0.41
7:G:116:PRO:HB2	7:G:118:ASN:ND2	2.35	0.41
10:J:35:LEU:HD11	10:J:50:LEU:HD13	2.01	0.41
13:N:-6:DG:H2''	13:N:-5:DG:C8	2.56	0.41
1:A:218:GLU:OE1	1:A:222:ARG:NE	2.46	0.41
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.52	0.41
1:A:1199:LEU:O	1:A:1238:LEU:HB2	2.20	0.41
1:A:1457:PRO:O	7:G:20:PRO:HG3	2.19	0.41
10:J:54:ASP:OD2	10:J:57:GLU:HG2	2.20	0.41
13:N:-81:DG:C2	15:T:82:DC:O2	2.73	0.41
1:A:231:ARG:HD2	1:A:231:ARG:HA	1.97	0.41
1:A:649:ASN:O	1:A:653:VAL:HG23	2.21	0.41
2:B:622:ASP:OD1	2:B:623:VAL:N	2.54	0.41
7:G:39:THR:OG1	7:G:42:PHE:HB2	2.20	0.41
1:A:776:ILE:O	1:A:798:LYS:NZ	2.47	0.41
4:D:98:ALA:O	4:D:102:VAL:HG23	2.20	0.41
13:N:-20:DC:H2''	13:N:-19:DG:H5'	2.02	0.41
1:A:518:ASN:HD22	1:A:879:VAL:HG23	1.86	0.41
2:B:175:LEU:O	2:B:180:LEU:HG	2.21	0.41
2:B:395:GLY:HA3	2:B:693:GLU:HG2	2.02	0.41
4:D:141:GLU:O	4:D:145:LEU:HG	2.20	0.41
14:P:9:U:H2'	14:P:10:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:32:DA:H2'	15:T:33:DC:C6	2.56	0.41
16:e:63:ARG:HD3	16:e:63:ARG:HA	1.66	0.41
1:A:1412:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.41
4:D:112:PHE:CE1	7:G:142:LYS:HD3	2.56	0.41
7:G:89:ALA:CB	7:G:103:VAL:HG22	2.47	0.41
9:I:54:GLU:HG2	9:I:100:PHE:CZ	2.55	0.41
12:L:33:CYS:HB3	12:L:38:HIS:H	1.86	0.41
1:A:387:HIS:O	1:A:390:THR:HG22	2.20	0.41
1:A:487:GLU:OE2	2:B:1102:LYS:HD3	2.20	0.41
1:A:943:PHE:CD1	1:A:947:ILE:HD12	2.54	0.41
2:B:60:GLN:HG2	2:B:60:GLN:O	2.21	0.41
2:B:316:ILE:HD12	2:B:321:VAL:HG23	2.03	0.41
2:B:426:GLN:O	2:B:430:GLU:HG3	2.21	0.41
2:B:551:LEU:HD13	2:B:573:ILE:HG21	2.03	0.41
4:D:54:SER:O	4:D:58:LEU:HG	2.21	0.41
4:D:120:THR:O	4:D:124:VAL:HG23	2.21	0.41
14:P:6:G:C2	15:T:38:DA:H2	2.32	0.41
17:b:35:ARG:HD3	17:b:51:TYR:OH	2.20	0.41
18:c:115:LEU:CD2	16:e:117:VAL:HG22	2.51	0.41
1:A:318:LYS:H	1:A:318:LYS:CD	2.22	0.41
2:B:502:ALA:O	2:B:506:GLN:HG3	2.21	0.41
2:B:1149:GLU:HA	2:B:1153:GLU:OE1	2.21	0.41
3:C:25:ASN:HB3	11:K:48:GLU:OE1	2.21	0.41
18:c:84:GLN:HG3	18:c:105:GLY:HA3	2.03	0.41
2:B:493:THR:HA	2:B:494:PRO:HD3	1.94	0.40
2:B:588:MET:HE3	2:B:588:MET:HB3	1.89	0.40
2:B:884:ARG:NE	14:P:-1:G:C8	2.70	0.40
7:G:119:LEU:HD23	7:G:131:MET:O	2.20	0.40
9:I:37:LEU:HD12	9:I:38:ALA:H	1.86	0.40
13:N:58:DC:H2''	13:N:59:DA:N7	2.36	0.40
1:A:833:ALA:HB3	2:B:500:LYS:HZ1	1.84	0.40
1:A:1076:GLU:HB3	1:A:1077:PRO:HD3	2.02	0.40
1:A:1119:THR:CG2	1:A:1331:TYR:HB3	2.51	0.40
1:A:1195:LEU:HD22	1:A:1197:LEU:HD23	2.04	0.40
2:B:272:ILE:HG22	2:B:273:PRO:O	2.21	0.40
5:E:54:ARG:HA	5:E:57:MET:HE2	2.03	0.40
7:G:22:MET:HG2	7:G:26:LEU:HD13	2.04	0.40
8:H:102:LYS:HB3	8:H:114:TYR:HB2	2.03	0.40
1:A:985:ILE:N	1:A:986:PRO:HD2	2.36	0.40
2:B:837:ASP:CG	2:B:1020:ARG:HH12	2.29	0.40
8:H:56:THR:HG21	8:H:144:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:-67:DA:H8	15:T:-67:DA:OP2	2.05	0.40
15:T:-10:DC:H2''	15:T:-9:DA:C8	2.57	0.40
15:T:59:DA:H2''	15:T:60:DA:N7	2.36	0.40
15:T:70:DG:H2''	15:T:71:DA:C8	2.56	0.40
18:g:26:PRO:HB2	18:g:29:ARG:HB3	2.03	0.40
2:B:272:ILE:HG12	2:B:326:ILE:HG12	2.03	0.40
4:D:6:SER:HB3	7:G:42:PHE:CZ	2.56	0.40
7:G:46:VAL:HG13	7:G:47:THR:H	1.86	0.40
8:H:13:GLN:HG3	8:H:29:ILE:HD12	2.04	0.40
18:g:71:ARG:HB2	18:g:71:ARG:CZ	2.52	0.40
1:A:128:ILE:O	1:A:134:ARG:NH2	2.53	0.40
1:A:529:LEU:O	1:A:530:CYS:C	2.64	0.40
2:B:261:ILE:O	2:B:274:ILE:HG12	2.21	0.40
2:B:805:LYS:HD3	2:B:815:ARG:CZ	2.52	0.40
2:B:1219:GLU:O	4:D:12:ARG:NH1	2.54	0.40
4:D:54:SER:OG	4:D:115:PHE:HD2	2.04	0.40
15:T:79:DC:H2''	15:T:80:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1400/1743 (80%)	1342 (96%)	57 (4%)	1 (0%)	48	78
2	B	1143/1227 (93%)	1101 (96%)	41 (4%)	1 (0%)	48	78
3	C	261/304 (86%)	256 (98%)	5 (2%)	0	100	100
4	D	162/186 (87%)	153 (94%)	9 (6%)	0	100	100
5	E	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	129/145 (89%)	124 (96%)	4 (3%)	1 (1%)	16	48
9	I	109/115 (95%)	106 (97%)	3 (3%)	0	100	100
10	J	64/72 (89%)	63 (98%)	1 (2%)	0	100	100
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	a	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
16	e	90/136 (66%)	90 (100%)	0	0	100	100
17	b	75/103 (73%)	73 (97%)	2 (3%)	0	100	100
17	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
18	c	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
18	g	91/130 (70%)	91 (100%)	0	0	100	100
19	d	90/126 (71%)	90 (100%)	0	0	100	100
19	h	86/126 (68%)	86 (100%)	0	0	100	100
All	All	4589/5512 (83%)	4439 (97%)	147 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	18	GLY
2	B	61	PRO
1	A	960	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1528 (80%)	1224 (100%)	1 (0%)	88	88
2	B	1010/1077 (94%)	1009 (100%)	1 (0%)	88	88
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	38 (100%)	0	100	100
16	a	81/110 (74%)	80 (99%)	1 (1%)	63	72
16	e	78/110 (71%)	77 (99%)	1 (1%)	61	71
17	b	63/79 (80%)	63 (100%)	0	100	100
17	f	63/79 (80%)	63 (100%)	0	100	100
18	c	83/100 (83%)	78 (94%)	5 (6%)	17	44
18	g	73/100 (73%)	73 (100%)	0	100	100
19	d	79/105 (75%)	78 (99%)	1 (1%)	61	71
19	h	75/105 (71%)	71 (95%)	4 (5%)	20	46
All	All	4056/4769 (85%)	4042 (100%)	14 (0%)	84	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	ASN
2	B	63	GLN
16	a	40	ARG
18	c	32	ARG
18	c	73	ASN
18	c	74	LYS
18	c	84	GLN
18	c	114	VAL
19	d	61	ILE
16	e	122	LYS
19	h	61	ILE
19	h	63	ASN
19	h	105	GLU
19	h	106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	291	ASN
1	A	314	GLN
1	A	359	ASN
1	A	588	HIS
1	A	596	ASN
1	A	761	GLN
1	A	769	GLN
1	A	955	ASN
1	A	971	GLN
1	A	1014	GLN
1	A	1021	GLN
1	A	1072	GLN
1	A	1212	ASN
1	A	1303	ASN
1	A	1357	ASN
1	A	1393	ASN
2	B	63	GLN
2	B	206	GLN
2	B	359	GLN
2	B	438	ASN
2	B	474	GLN
2	B	477	ASN
2	B	932	HIS
2	B	1084	GLN
2	B	1193	GLN
4	D	179	ASN
5	E	31	GLN
5	E	51	ASN
5	E	165	GLN
5	E	173	GLN
7	G	41	GLN
9	I	105	ASN
11	K	85	GLN
16	a	68	GLN
17	b	25	ASN
18	c	24	GLN
18	c	38	ASN
18	c	104	GLN
18	c	112	GLN
19	d	95	GLN

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Mol	Chain	Res	Type
19	d	109	HIS
16	e	113	HIS
18	g	24	GLN
19	h	82	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	12/13 (92%)	2 (16%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	0	U
14	P	10	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

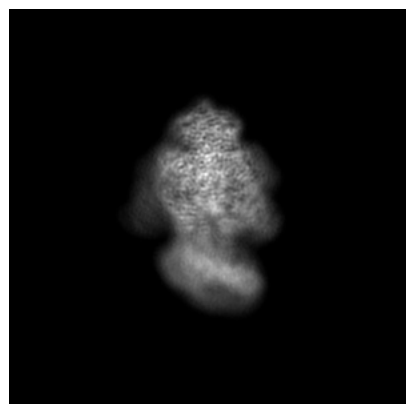
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36252. These allow visual inspection of the internal detail of the map and identification of artifacts.

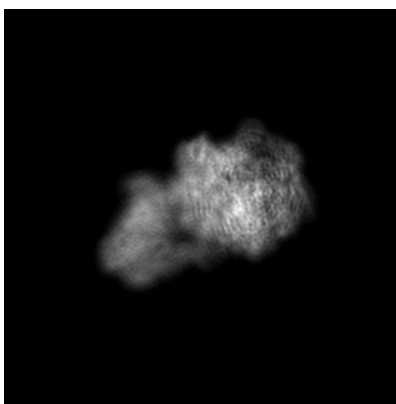
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

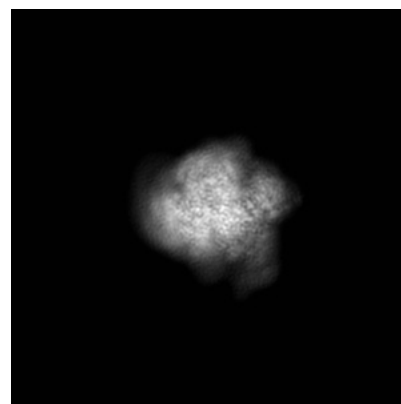
6.1.1 Primary map



X

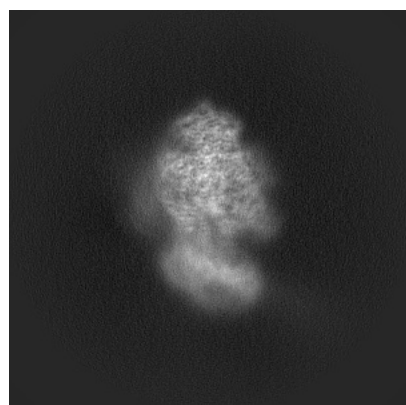


Y

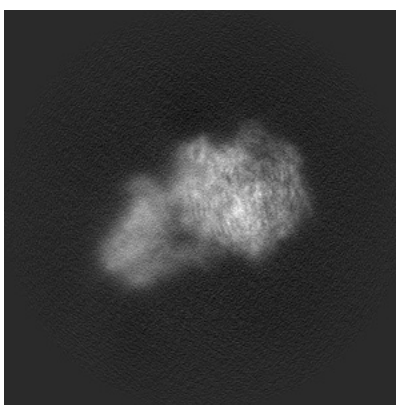


Z

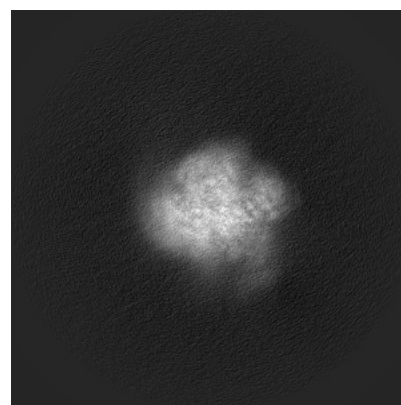
6.1.2 Raw map



X



Y

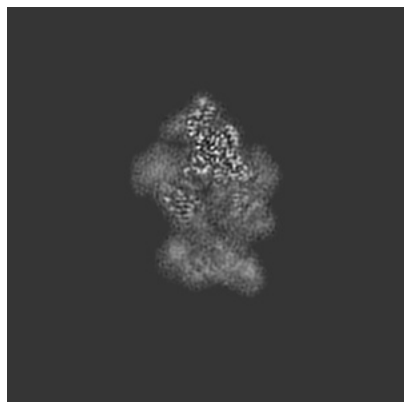


Z

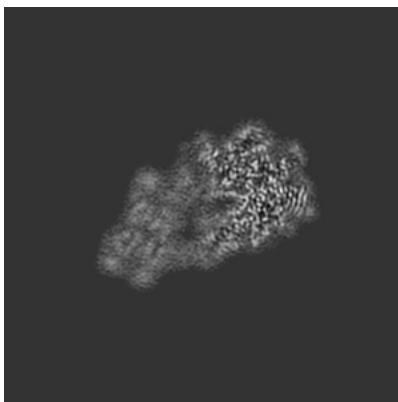
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

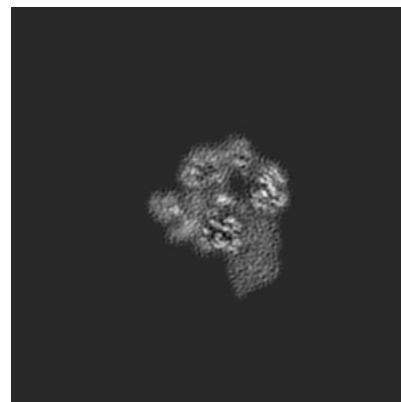
6.2.1 Primary map



X Index: 180

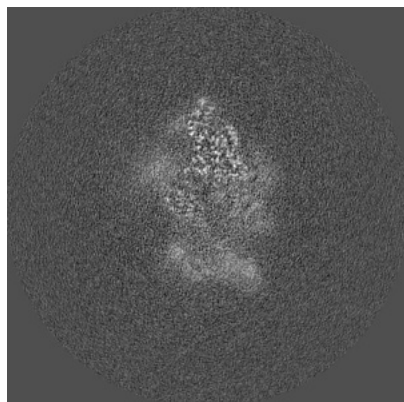


Y Index: 180

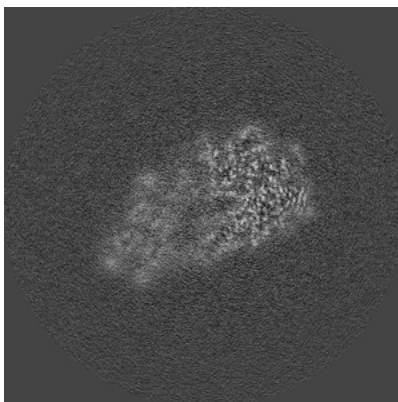


Z Index: 180

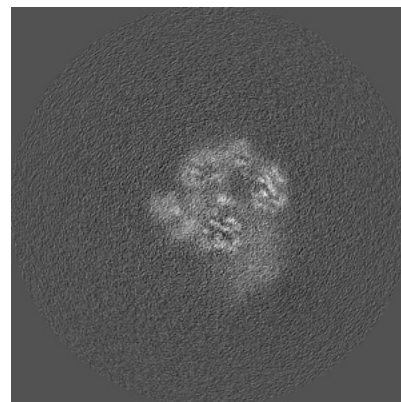
6.2.2 Raw map



X Index: 180



Y Index: 180

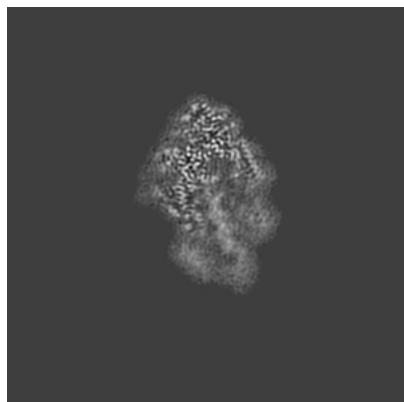


Z Index: 180

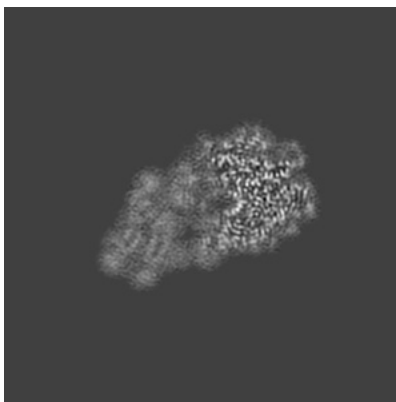
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

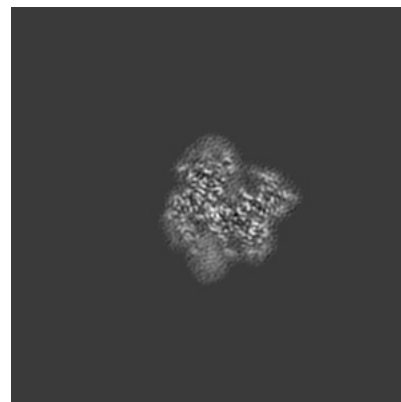
6.3.1 Primary map



X Index: 193

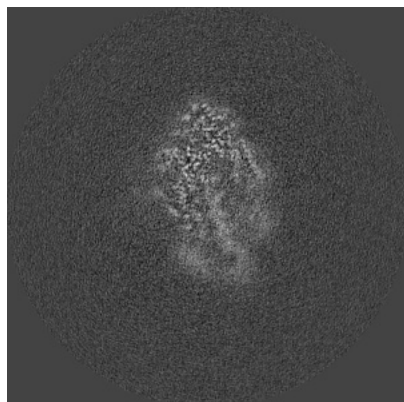


Y Index: 177

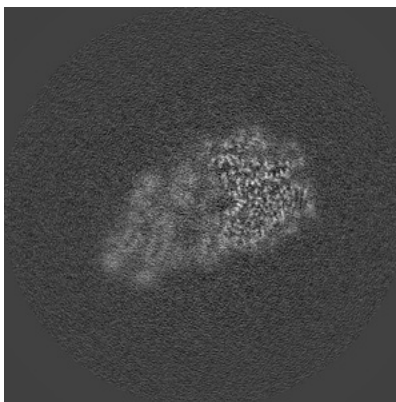


Z Index: 212

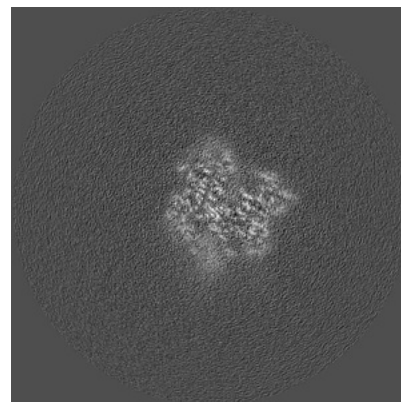
6.3.2 Raw map



X Index: 193



Y Index: 177

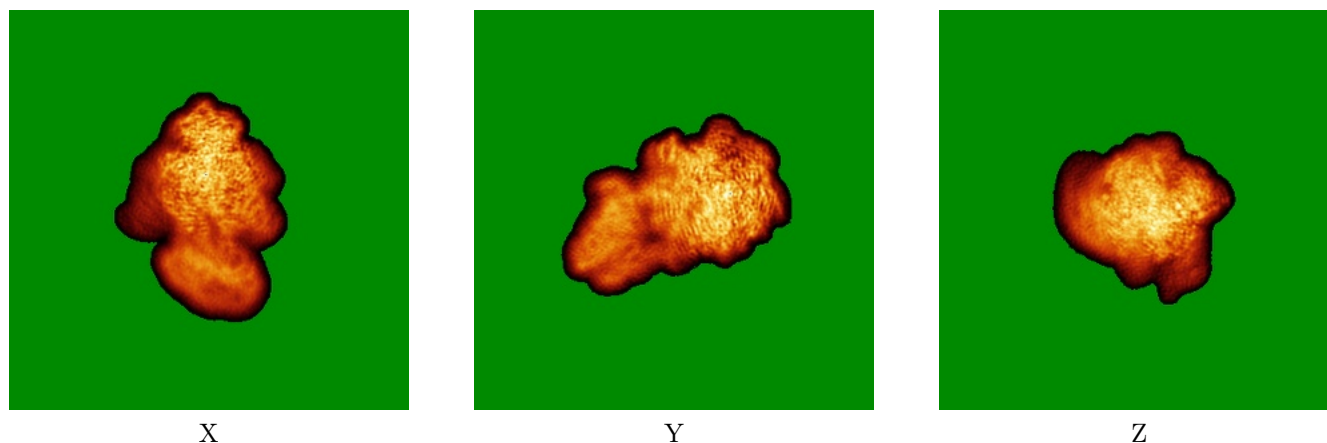


Z Index: 212

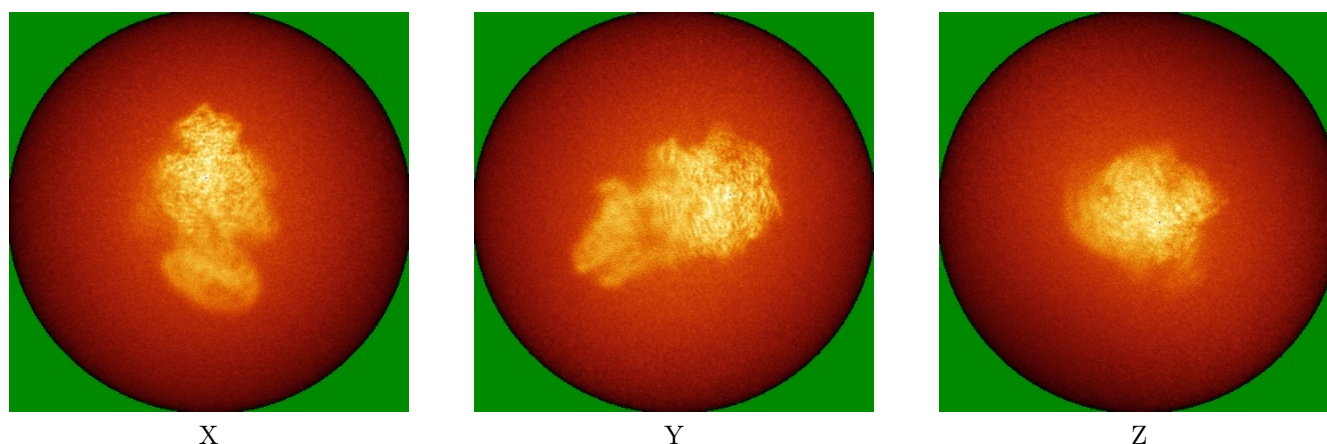
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

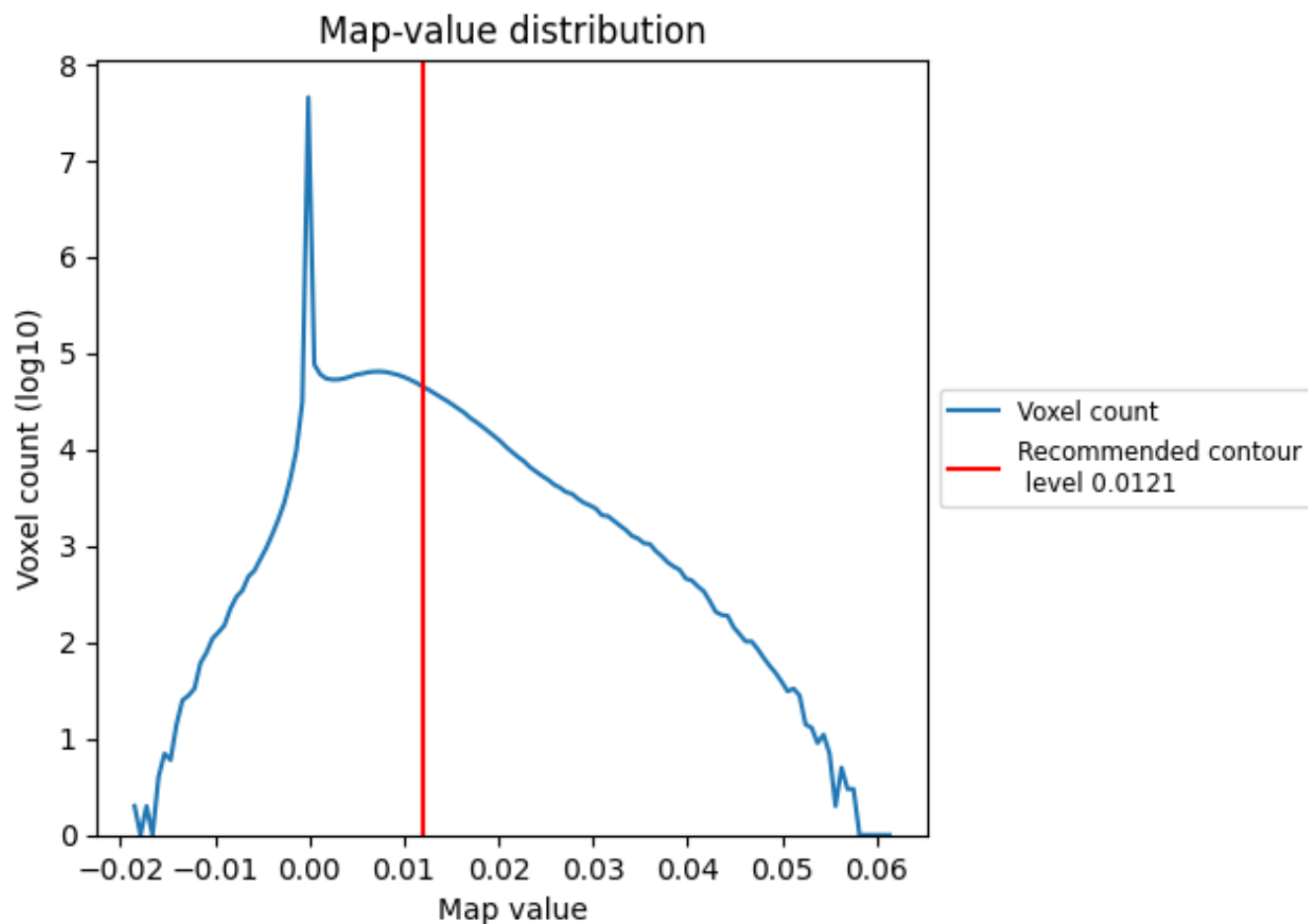
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

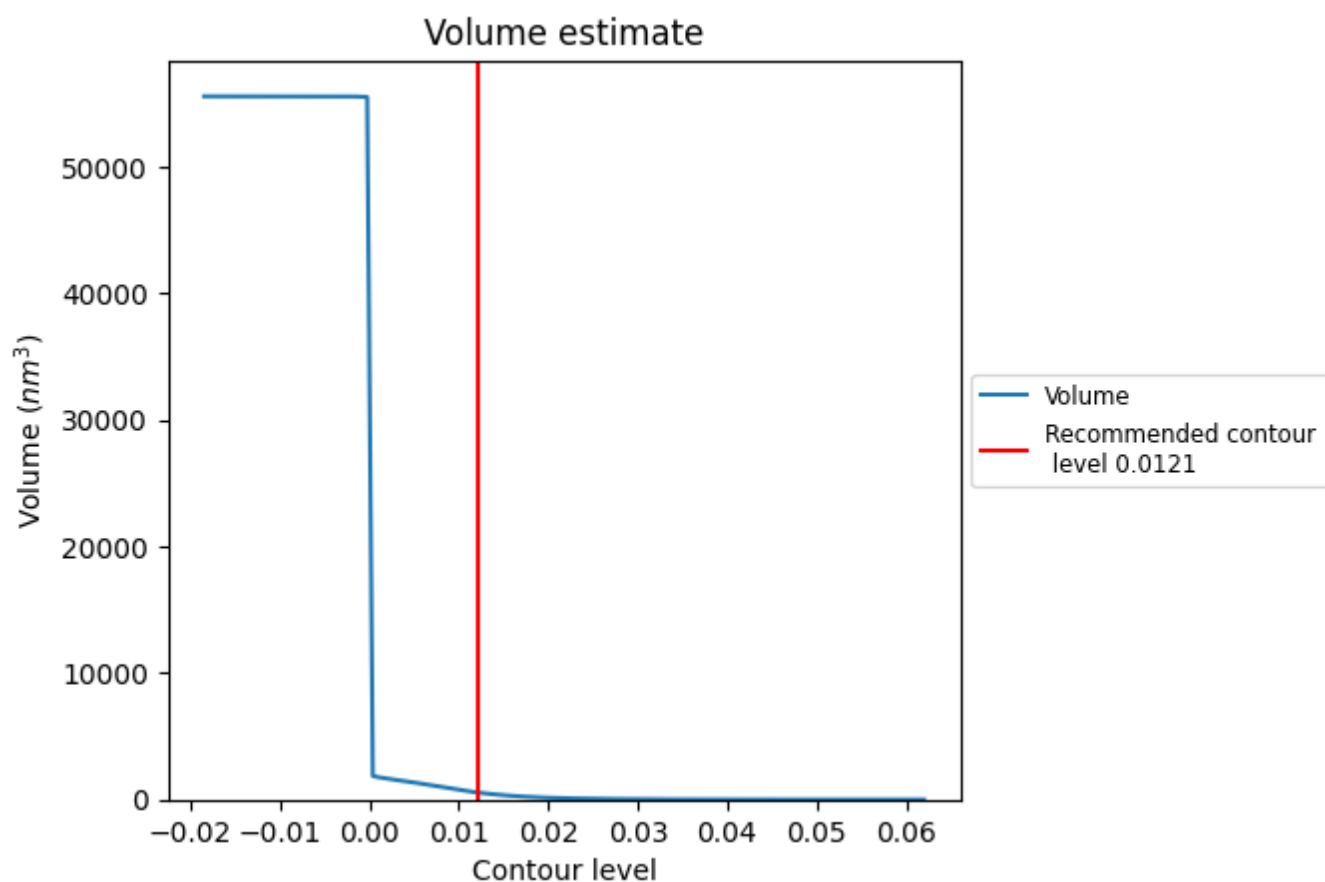
This section contains the results of statistical analysis of the map.

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.

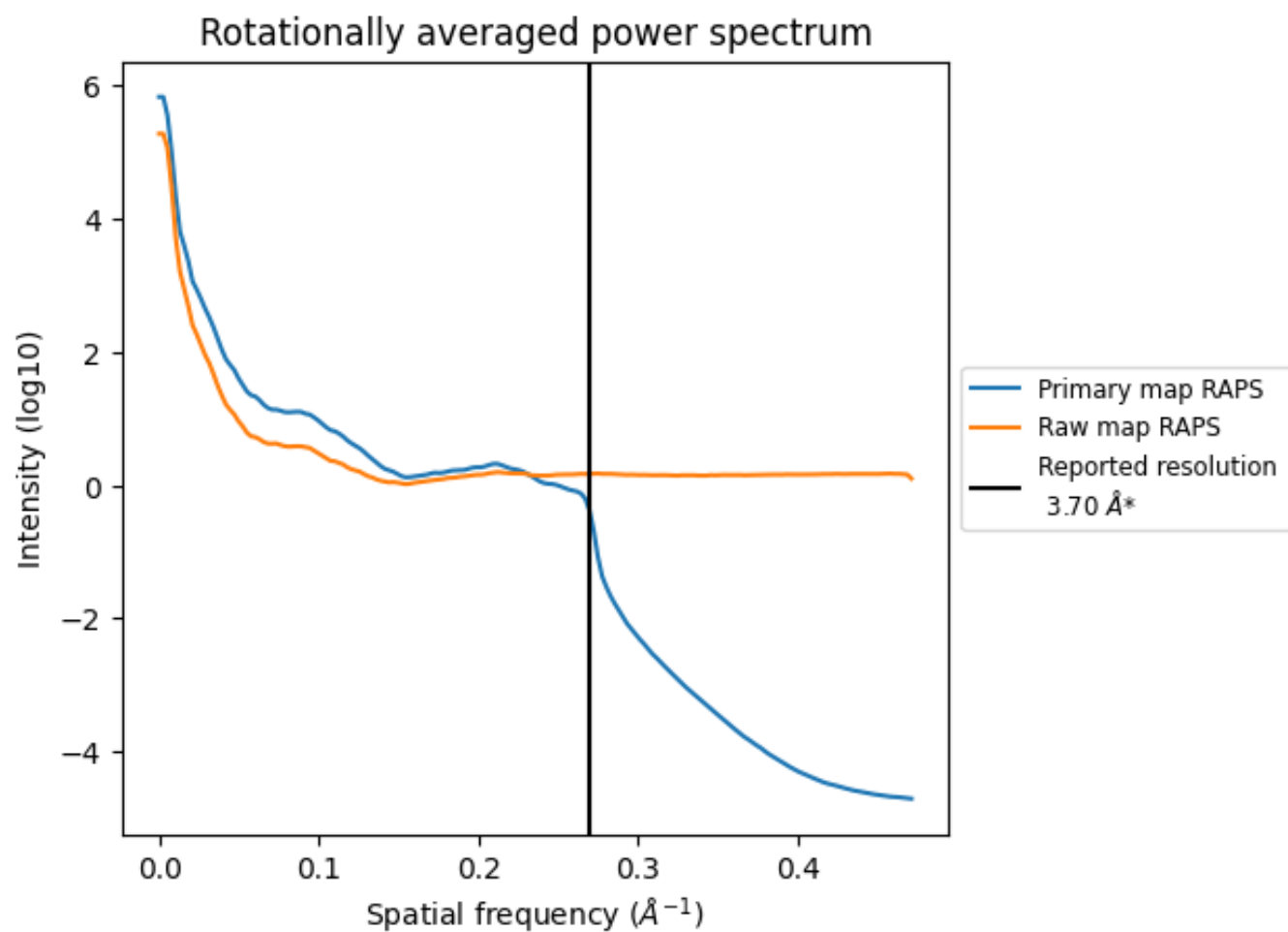
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm³; this corresponds to an approximate mass of 501 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 ⓘ

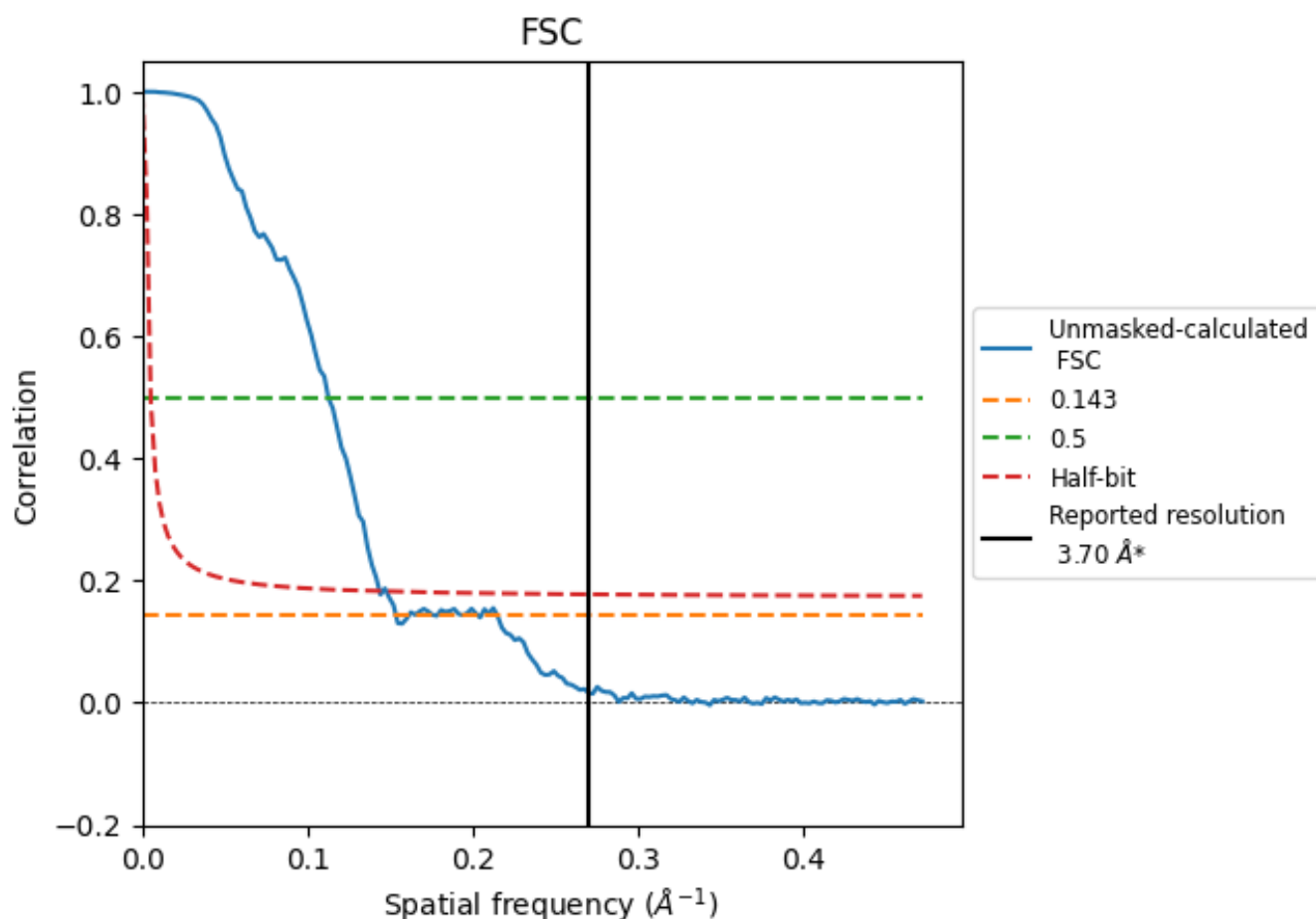


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.51	8.89	6.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.51 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36252 and PDB model 8JH3. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

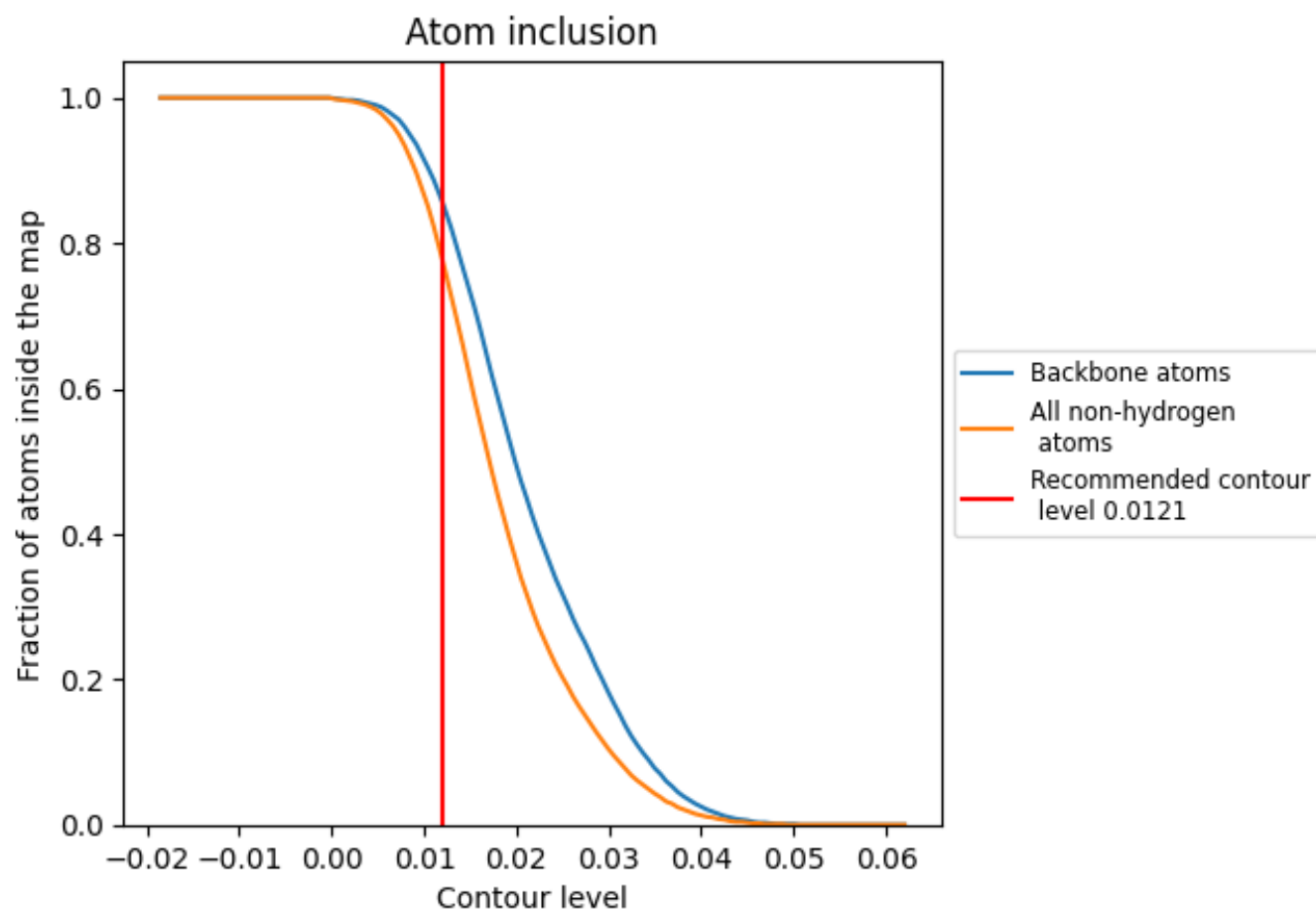


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 77% 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 (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.2550
A	 0.8550	 0.3530
B	 0.8490	 0.3480
C	 0.8610	 0.3810
D	 0.1560	 0.0710
E	 0.7730	 0.2790
F	 0.9040	 0.3930
G	 0.3370	 0.1140
H	 0.8510	 0.3550
I	 0.5250	 0.1120
J	 0.8910	 0.4030
K	 0.8870	 0.3770
L	 0.8650	 0.2910
N	 0.6670	 0.0460
P	 0.9070	 0.2530
T	 0.7010	 0.0780
a	 0.7040	 0.0770
b	 0.7690	 0.0750
c	 0.7950	 0.0970
d	 0.8150	 0.1150
e	 0.7760	 0.1170
f	 0.7810	 0.1380
g	 0.7070	 0.0830
h	 0.7280	 0.0730

