



Full wwPDB EM Validation Report ⓘ

Jul 18, 2026 – 07:48 am BST

PDB ID : 9TAX / pdb_00009tax
EMDB ID : EMD-55758
Title : Structure of the human inner kinetochore CCAN bound to a mono-CENP-A nucleosome
Authors : Yu, C.; Barford, D.
Deposited on : 2025-11-18
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

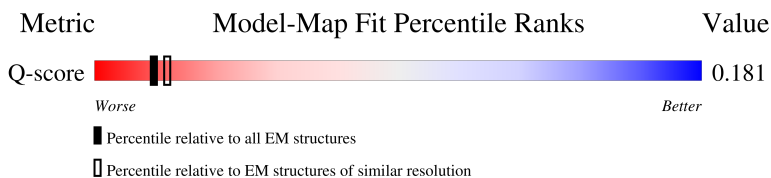
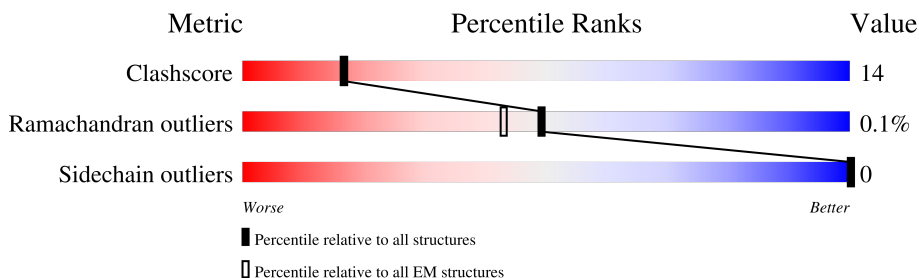
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	H	247	 49% 34% 17%
2	I	762	 53% 28% 18%
3	K	269	 60% 26% 13%
4	M	180	 69% 27% .

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Mol	Chain	Length	Quality of chain
5	L	348	
6	N	347	
7	O	300	
8	P	288	
9	Q	215	
10	U	211	
11	R	177	
12	T	777	
13	W	88	
14	S	138	
15	X	81	
16	V	212	
17	Y	212	
18	a	775	
18	b	775	
19	c	140	
19	g	140	
20	d	103	
20	h	103	
21	e	153	
21	i	153	
22	f	126	
22	j	126	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 40202 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 Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	204	Total	C	N	O	S	0	0
			1678	1052	292	323	11		

- Molecule 2 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	622	Total	C	N	O	S	0	0
			5051	3306	818	896	31		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	699	GLU	-	insertion	UNP A0A8C8KX99
I	700	SER	-	insertion	UNP A0A8C8KX99
I	701	PRO	-	insertion	UNP A0A8C8KX99
I	702	GLU	-	insertion	UNP A0A8C8KX99
I	703	GLU	-	insertion	UNP A0A8C8KX99
I	704	ARG	-	insertion	UNP A0A8C8KX99
I	705	THR	-	insertion	UNP A0A8C8KX99
I	706	VAL	-	insertion	UNP A0A8C8KX99
I	707	ASN	-	insertion	UNP A0A8C8KX99
I	708	VAL	-	insertion	UNP A0A8C8KX99
I	709	SER	-	insertion	UNP A0A8C8KX99
I	710	SER	-	insertion	UNP A0A8C8KX99
I	711	ILE	-	insertion	UNP A0A8C8KX99
I	712	ARG	-	insertion	UNP A0A8C8KX99
I	757	GLU	-	expression tag	UNP A0A8C8KX99
I	758	ASN	-	expression tag	UNP A0A8C8KX99
I	759	LEU	-	expression tag	UNP A0A8C8KX99
I	760	TYR	-	expression tag	UNP A0A8C8KX99
I	761	PHE	-	expression tag	UNP A0A8C8KX99
I	762	GLN	-	expression tag	UNP A0A8C8KX99

- Molecule 3 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	233	Total	C	N	O	S	0	0
			1936	1227	321	378	10		

- Molecule 4 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	172	Total	C	N	O	S	0	0
			1325	839	236	243	7		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	312	Total	C	N	O	S	0	0
			2506	1630	409	453	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q8N0S6
L	-2	PRO	-	expression tag	UNP Q8N0S6
L	-1	LEU	-	expression tag	UNP Q8N0S6
L	0	GLY	-	expression tag	UNP Q8N0S6

- Molecule 6 is a protein called Isoform 3 of Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	318	Total	C	N	O	S	0	0
			2631	1688	456	476	11		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	288	LYS	GLU	conflict	UNP Q96H22
N	313	GLY	ALA	conflict	UNP Q96H22
N	314	ILE	LEU	conflict	UNP Q96H22
N	315	ALA	VAL	conflict	UNP Q96H22
N	316	ASP	-	expression tag	UNP Q96H22
N	317	ALA	-	expression tag	UNP Q96H22
N	318	PRO	-	expression tag	UNP Q96H22
N	319	LEU	-	expression tag	UNP Q96H22
N	320	SER	-	expression tag	UNP Q96H22

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Chain	Residue	Modelled	Actual	Comment	Reference
N	321	PRO	-	expression tag	UNP Q96H22
N	322	LEU	-	expression tag	UNP Q96H22
N	323	LEU	-	expression tag	UNP Q96H22
N	324	THR	-	expression tag	UNP Q96H22
N	325	CYS	-	expression tag	UNP Q96H22
N	326	ILE	-	expression tag	UNP Q96H22
N	327	PRO	-	expression tag	UNP Q96H22
N	328	ASN	-	expression tag	UNP Q96H22
N	329	LYS	-	expression tag	UNP Q96H22
N	330	ARG	-	expression tag	UNP Q96H22
N	331	MET	-	expression tag	UNP Q96H22
N	332	ASN	-	expression tag	UNP Q96H22
N	333	TYR	-	expression tag	UNP Q96H22
N	334	PHE	-	expression tag	UNP Q96H22
N	335	LYS	-	expression tag	UNP Q96H22
N	336	ILE	-	expression tag	UNP Q96H22
N	337	ARG	-	expression tag	UNP Q96H22
N	338	ASP	-	expression tag	UNP Q96H22
N	339	LYS	-	expression tag	UNP Q96H22
N	340	SER	-	expression tag	UNP Q96H22
N	341	ASP	-	expression tag	UNP Q96H22
N	342	LEU	-	expression tag	UNP Q96H22
N	343	GLU	-	expression tag	UNP Q96H22
N	344	VAL	-	expression tag	UNP Q96H22
N	345	LEU	-	expression tag	UNP Q96H22
N	346	PHE	-	expression tag	UNP Q96H22
N	347	GLN	-	expression tag	UNP Q96H22

- Molecule 7 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	210	Total	C	N	O	S	0	0
			1681	1079	283	312	7		

- Molecule 8 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	224	Total	C	N	O	S	0	0
			1819	1158	316	337	8		

- Molecule 9 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	191	Total	C	N	O	S	0	0
			1530	955	259	305	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	54	MET	-	initiating methionine	UNP Q7L2Z9

- Molecule 10 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	166	Total	C	N	O	S	0	0
			1377	869	244	259	5		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	419	GLU	-	expression tag	UNP Q71F23
U	420	ASN	-	expression tag	UNP Q71F23
U	421	LEU	-	expression tag	UNP Q71F23
U	422	TYR	-	expression tag	UNP Q71F23
U	423	PHE	-	expression tag	UNP Q71F23
U	424	GLN	-	expression tag	UNP Q71F23
U	425	SER	-	expression tag	UNP Q71F23
U	426	TRP	-	expression tag	UNP Q71F23
U	427	SER	-	expression tag	UNP Q71F23
U	428	HIS	-	expression tag	UNP Q71F23
U	429	PRO	-	expression tag	UNP Q71F23
U	430	GLN	-	expression tag	UNP Q71F23
U	431	PHE	-	expression tag	UNP Q71F23
U	432	GLU	-	expression tag	UNP Q71F23
U	433	LYS	-	expression tag	UNP Q71F23
U	434	GLY	-	expression tag	UNP Q71F23
U	435	GLY	-	expression tag	UNP Q71F23
U	436	GLY	-	expression tag	UNP Q71F23
U	437	SER	-	expression tag	UNP Q71F23
U	438	GLY	-	expression tag	UNP Q71F23
U	439	GLY	-	expression tag	UNP Q71F23
U	440	GLY	-	expression tag	UNP Q71F23
U	441	SER	-	expression tag	UNP Q71F23
U	442	GLY	-	expression tag	UNP Q71F23
U	443	GLY	-	expression tag	UNP Q71F23
U	444	GLY	-	expression tag	UNP Q71F23

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Chain	Residue	Modelled	Actual	Comment	Reference
U	445	SER	-	expression tag	UNP Q71F23
U	446	TRP	-	expression tag	UNP Q71F23
U	447	SER	-	expression tag	UNP Q71F23
U	448	HIS	-	expression tag	UNP Q71F23
U	449	PRO	-	expression tag	UNP Q71F23
U	450	GLN	-	expression tag	UNP Q71F23
U	451	PHE	-	expression tag	UNP Q71F23
U	452	GLU	-	expression tag	UNP Q71F23
U	453	LYS	-	expression tag	UNP Q71F23

- Molecule 11 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	80	Total	C	N	O	S	0	0
			649	412	105	125	7		

- Molecule 12 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	112	Total	C	N	O	S	0	0
			915	586	163	159	7		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-215	MET	-	initiating methionine	UNP Q96BT3
T	-214	SER	-	expression tag	UNP Q96BT3
T	-213	TYR	-	expression tag	UNP Q96BT3
T	-212	TYR	-	expression tag	UNP Q96BT3
T	-211	HIS	-	expression tag	UNP Q96BT3
T	-210	HIS	-	expression tag	UNP Q96BT3
T	-209	HIS	-	expression tag	UNP Q96BT3
T	-208	HIS	-	expression tag	UNP Q96BT3
T	-207	HIS	-	expression tag	UNP Q96BT3
T	-206	HIS	-	expression tag	UNP Q96BT3
T	-205	ASP	-	expression tag	UNP Q96BT3
T	-204	TYR	-	expression tag	UNP Q96BT3
T	-203	ASP	-	expression tag	UNP Q96BT3
T	-202	ILE	-	expression tag	UNP Q96BT3
T	-201	PRO	-	expression tag	UNP Q96BT3
T	-200	THR	-	expression tag	UNP Q96BT3
T	-199	THR	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-198	GLU	-	expression tag	UNP Q96BT3
T	-197	ASN	-	expression tag	UNP Q96BT3
T	-196	LEU	-	expression tag	UNP Q96BT3
T	-195	TYR	-	expression tag	UNP Q96BT3
T	-194	PHE	-	expression tag	UNP Q96BT3
T	-193	GLN	-	expression tag	UNP Q96BT3
T	-192	GLY	-	expression tag	UNP Q96BT3
T	-191	MET	-	expression tag	UNP Q96BT3
T	-190	ASP	-	expression tag	UNP Q96BT3
T	-189	LYS	-	expression tag	UNP Q96BT3
T	-188	ASP	-	expression tag	UNP Q96BT3
T	-187	CYS	-	expression tag	UNP Q96BT3
T	-186	GLU	-	expression tag	UNP Q96BT3
T	-185	MET	-	expression tag	UNP Q96BT3
T	-184	LYS	-	expression tag	UNP Q96BT3
T	-183	ARG	-	expression tag	UNP Q96BT3
T	-182	THR	-	expression tag	UNP Q96BT3
T	-181	THR	-	expression tag	UNP Q96BT3
T	-180	LEU	-	expression tag	UNP Q96BT3
T	-179	ASP	-	expression tag	UNP Q96BT3
T	-178	SER	-	expression tag	UNP Q96BT3
T	-177	PRO	-	expression tag	UNP Q96BT3
T	-176	LEU	-	expression tag	UNP Q96BT3
T	-175	GLY	-	expression tag	UNP Q96BT3
T	-174	LYS	-	expression tag	UNP Q96BT3
T	-173	LEU	-	expression tag	UNP Q96BT3
T	-172	GLU	-	expression tag	UNP Q96BT3
T	-171	LEU	-	expression tag	UNP Q96BT3
T	-170	SER	-	expression tag	UNP Q96BT3
T	-169	GLY	-	expression tag	UNP Q96BT3
T	-168	CYS	-	expression tag	UNP Q96BT3
T	-167	GLU	-	expression tag	UNP Q96BT3
T	-166	GLN	-	expression tag	UNP Q96BT3
T	-165	GLY	-	expression tag	UNP Q96BT3
T	-164	LEU	-	expression tag	UNP Q96BT3
T	-163	HIS	-	expression tag	UNP Q96BT3
T	-162	ARG	-	expression tag	UNP Q96BT3
T	-161	ILE	-	expression tag	UNP Q96BT3
T	-160	ILE	-	expression tag	UNP Q96BT3
T	-159	PHE	-	expression tag	UNP Q96BT3
T	-158	LEU	-	expression tag	UNP Q96BT3
T	-157	GLY	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-156	LYS	-	expression tag	UNP Q96BT3
T	-155	GLY	-	expression tag	UNP Q96BT3
T	-154	THR	-	expression tag	UNP Q96BT3
T	-153	SER	-	expression tag	UNP Q96BT3
T	-152	ALA	-	expression tag	UNP Q96BT3
T	-151	ALA	-	expression tag	UNP Q96BT3
T	-150	ASP	-	expression tag	UNP Q96BT3
T	-149	ALA	-	expression tag	UNP Q96BT3
T	-148	VAL	-	expression tag	UNP Q96BT3
T	-147	GLU	-	expression tag	UNP Q96BT3
T	-146	VAL	-	expression tag	UNP Q96BT3
T	-145	PRO	-	expression tag	UNP Q96BT3
T	-144	ALA	-	expression tag	UNP Q96BT3
T	-143	PRO	-	expression tag	UNP Q96BT3
T	-142	ALA	-	expression tag	UNP Q96BT3
T	-141	ALA	-	expression tag	UNP Q96BT3
T	-140	VAL	-	expression tag	UNP Q96BT3
T	-139	LEU	-	expression tag	UNP Q96BT3
T	-138	GLY	-	expression tag	UNP Q96BT3
T	-137	GLY	-	expression tag	UNP Q96BT3
T	-136	PRO	-	expression tag	UNP Q96BT3
T	-135	GLU	-	expression tag	UNP Q96BT3
T	-134	PRO	-	expression tag	UNP Q96BT3
T	-133	LEU	-	expression tag	UNP Q96BT3
T	-132	MET	-	expression tag	UNP Q96BT3
T	-131	GLN	-	expression tag	UNP Q96BT3
T	-130	ALA	-	expression tag	UNP Q96BT3
T	-129	THR	-	expression tag	UNP Q96BT3
T	-128	ALA	-	expression tag	UNP Q96BT3
T	-127	TRP	-	expression tag	UNP Q96BT3
T	-126	LEU	-	expression tag	UNP Q96BT3
T	-125	ASN	-	expression tag	UNP Q96BT3
T	-124	ALA	-	expression tag	UNP Q96BT3
T	-123	TYR	-	expression tag	UNP Q96BT3
T	-122	PHE	-	expression tag	UNP Q96BT3
T	-121	HIS	-	expression tag	UNP Q96BT3
T	-120	GLN	-	expression tag	UNP Q96BT3
T	-119	PRO	-	expression tag	UNP Q96BT3
T	-118	GLU	-	expression tag	UNP Q96BT3
T	-117	ALA	-	expression tag	UNP Q96BT3
T	-116	ILE	-	expression tag	UNP Q96BT3
T	-115	GLU	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-114	GLU	-	expression tag	UNP Q96BT3
T	-113	PHE	-	expression tag	UNP Q96BT3
T	-112	PRO	-	expression tag	UNP Q96BT3
T	-111	VAL	-	expression tag	UNP Q96BT3
T	-110	PRO	-	expression tag	UNP Q96BT3
T	-109	ALA	-	expression tag	UNP Q96BT3
T	-108	LEU	-	expression tag	UNP Q96BT3
T	-107	HIS	-	expression tag	UNP Q96BT3
T	-106	HIS	-	expression tag	UNP Q96BT3
T	-105	PRO	-	expression tag	UNP Q96BT3
T	-104	VAL	-	expression tag	UNP Q96BT3
T	-103	PHE	-	expression tag	UNP Q96BT3
T	-102	GLN	-	expression tag	UNP Q96BT3
T	-101	GLN	-	expression tag	UNP Q96BT3
T	-100	GLU	-	expression tag	UNP Q96BT3
T	-99	SER	-	expression tag	UNP Q96BT3
T	-98	PHE	-	expression tag	UNP Q96BT3
T	-97	THR	-	expression tag	UNP Q96BT3
T	-96	ARG	-	expression tag	UNP Q96BT3
T	-95	GLN	-	expression tag	UNP Q96BT3
T	-94	VAL	-	expression tag	UNP Q96BT3
T	-93	LEU	-	expression tag	UNP Q96BT3
T	-92	TRP	-	expression tag	UNP Q96BT3
T	-91	LYS	-	expression tag	UNP Q96BT3
T	-90	LEU	-	expression tag	UNP Q96BT3
T	-89	LEU	-	expression tag	UNP Q96BT3
T	-88	LYS	-	expression tag	UNP Q96BT3
T	-87	VAL	-	expression tag	UNP Q96BT3
T	-86	VAL	-	expression tag	UNP Q96BT3
T	-85	LYS	-	expression tag	UNP Q96BT3
T	-84	PHE	-	expression tag	UNP Q96BT3
T	-83	GLY	-	expression tag	UNP Q96BT3
T	-82	GLU	-	expression tag	UNP Q96BT3
T	-81	VAL	-	expression tag	UNP Q96BT3
T	-80	ILE	-	expression tag	UNP Q96BT3
T	-79	SER	-	expression tag	UNP Q96BT3
T	-78	TYR	-	expression tag	UNP Q96BT3
T	-77	SER	-	expression tag	UNP Q96BT3
T	-76	HIS	-	expression tag	UNP Q96BT3
T	-75	LEU	-	expression tag	UNP Q96BT3
T	-74	ALA	-	expression tag	UNP Q96BT3
T	-73	ALA	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-72	LEU	-	expression tag	UNP Q96BT3
T	-71	ALA	-	expression tag	UNP Q96BT3
T	-70	GLY	-	expression tag	UNP Q96BT3
T	-69	ASN	-	expression tag	UNP Q96BT3
T	-68	PRO	-	expression tag	UNP Q96BT3
T	-67	ALA	-	expression tag	UNP Q96BT3
T	-66	ALA	-	expression tag	UNP Q96BT3
T	-65	THR	-	expression tag	UNP Q96BT3
T	-64	ALA	-	expression tag	UNP Q96BT3
T	-63	ALA	-	expression tag	UNP Q96BT3
T	-62	VAL	-	expression tag	UNP Q96BT3
T	-61	LYS	-	expression tag	UNP Q96BT3
T	-60	THR	-	expression tag	UNP Q96BT3
T	-59	ALA	-	expression tag	UNP Q96BT3
T	-58	LEU	-	expression tag	UNP Q96BT3
T	-57	SER	-	expression tag	UNP Q96BT3
T	-56	GLY	-	expression tag	UNP Q96BT3
T	-55	ASN	-	expression tag	UNP Q96BT3
T	-54	PRO	-	expression tag	UNP Q96BT3
T	-53	VAL	-	expression tag	UNP Q96BT3
T	-52	PRO	-	expression tag	UNP Q96BT3
T	-51	ILE	-	expression tag	UNP Q96BT3
T	-50	LEU	-	expression tag	UNP Q96BT3
T	-49	ILE	-	expression tag	UNP Q96BT3
T	-48	PRO	-	expression tag	UNP Q96BT3
T	-47	CYS	-	expression tag	UNP Q96BT3
T	-46	HIS	-	expression tag	UNP Q96BT3
T	-45	ARG	-	expression tag	UNP Q96BT3
T	-44	VAL	-	expression tag	UNP Q96BT3
T	-43	VAL	-	expression tag	UNP Q96BT3
T	-42	GLN	-	expression tag	UNP Q96BT3
T	-41	GLY	-	expression tag	UNP Q96BT3
T	-40	ASP	-	expression tag	UNP Q96BT3
T	-39	LEU	-	expression tag	UNP Q96BT3
T	-38	ASP	-	expression tag	UNP Q96BT3
T	-37	VAL	-	expression tag	UNP Q96BT3
T	-36	GLY	-	expression tag	UNP Q96BT3
T	-35	GLY	-	expression tag	UNP Q96BT3
T	-34	TYR	-	expression tag	UNP Q96BT3
T	-33	GLU	-	expression tag	UNP Q96BT3
T	-32	GLY	-	expression tag	UNP Q96BT3
T	-31	GLY	-	expression tag	UNP Q96BT3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-30	LEU	-	expression tag	UNP Q96BT3
T	-29	ALA	-	expression tag	UNP Q96BT3
T	-28	VAL	-	expression tag	UNP Q96BT3
T	-27	LYS	-	expression tag	UNP Q96BT3
T	-26	GLU	-	expression tag	UNP Q96BT3
T	-25	TRP	-	expression tag	UNP Q96BT3
T	-24	LEU	-	expression tag	UNP Q96BT3
T	-23	LEU	-	expression tag	UNP Q96BT3
T	-22	ALA	-	expression tag	UNP Q96BT3
T	-21	HIS	-	expression tag	UNP Q96BT3
T	-20	GLU	-	expression tag	UNP Q96BT3
T	-19	GLY	-	expression tag	UNP Q96BT3
T	-18	HIS	-	expression tag	UNP Q96BT3
T	-17	ARG	-	expression tag	UNP Q96BT3
T	-16	LEU	-	expression tag	UNP Q96BT3
T	-15	GLY	-	expression tag	UNP Q96BT3
T	-14	LYS	-	expression tag	UNP Q96BT3
T	-13	PRO	-	expression tag	UNP Q96BT3
T	-12	GLY	-	expression tag	UNP Q96BT3
T	-11	LEU	-	expression tag	UNP Q96BT3
T	-10	GLY	-	expression tag	UNP Q96BT3
T	-9	SER	-	expression tag	UNP Q96BT3
T	-8	ASP	-	expression tag	UNP Q96BT3
T	-7	LEU	-	expression tag	UNP Q96BT3
T	-6	GLU	-	expression tag	UNP Q96BT3
T	-5	VAL	-	expression tag	UNP Q96BT3
T	-4	LEU	-	expression tag	UNP Q96BT3
T	-3	PHE	-	expression tag	UNP Q96BT3
T	-2	GLN	-	expression tag	UNP Q96BT3
T	-1	GLY	-	expression tag	UNP Q96BT3
T	0	PRO	-	expression tag	UNP Q96BT3

- Molecule 13 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	86	Total	C	N	O	S	0	0
			691	437	141	110	3		

- Molecule 14 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	120	Total	C	N	O	S	0	0
			982	607	174	195	6		

- Molecule 15 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 16 is a DNA chain called DNA (199-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	199	Total	C	N	O	P	0	0
			4078	1943	736	1200	199		

- Molecule 17 is a DNA chain called DNA (199-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	199	Total	C	N	O	P	0	0
			4081	1942	752	1188	199		

- Molecule 18 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	a	21	Total	C	N	O	0	0
			178	111	37	30		
18	b	57	Total	C	N	O	0	0
			476	298	85	93		

There are 460 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	546	ASP	-	expression tag	UNP Q03188
a	547	LEU	-	expression tag	UNP Q03188
a	548	GLU	-	expression tag	UNP Q03188
a	549	VAL	-	expression tag	UNP Q03188
a	550	LEU	-	expression tag	UNP Q03188
a	551	PHE	-	expression tag	UNP Q03188
a	552	GLN	-	expression tag	UNP Q03188
a	553	GLY	-	expression tag	UNP Q03188
a	554	PRO	-	expression tag	UNP Q03188
a	555	LEU	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	556	GLY	-	expression tag	UNP Q03188
a	557	MET	-	expression tag	UNP Q03188
a	558	ASP	-	expression tag	UNP Q03188
a	559	LYS	-	expression tag	UNP Q03188
a	560	ASP	-	expression tag	UNP Q03188
a	561	CYS	-	expression tag	UNP Q03188
a	562	GLU	-	expression tag	UNP Q03188
a	563	MET	-	expression tag	UNP Q03188
a	564	LYS	-	expression tag	UNP Q03188
a	565	ARG	-	expression tag	UNP Q03188
a	566	THR	-	expression tag	UNP Q03188
a	567	THR	-	expression tag	UNP Q03188
a	568	LEU	-	expression tag	UNP Q03188
a	569	ASP	-	expression tag	UNP Q03188
a	570	SER	-	expression tag	UNP Q03188
a	571	PRO	-	expression tag	UNP Q03188
a	572	LEU	-	expression tag	UNP Q03188
a	573	GLY	-	expression tag	UNP Q03188
a	574	LYS	-	expression tag	UNP Q03188
a	575	LEU	-	expression tag	UNP Q03188
a	576	GLU	-	expression tag	UNP Q03188
a	577	LEU	-	expression tag	UNP Q03188
a	578	SER	-	expression tag	UNP Q03188
a	579	GLY	-	expression tag	UNP Q03188
a	580	CYS	-	expression tag	UNP Q03188
a	581	GLU	-	expression tag	UNP Q03188
a	582	GLN	-	expression tag	UNP Q03188
a	583	GLY	-	expression tag	UNP Q03188
a	584	LEU	-	expression tag	UNP Q03188
a	585	HIS	-	expression tag	UNP Q03188
a	586	ARG	-	expression tag	UNP Q03188
a	587	ILE	-	expression tag	UNP Q03188
a	588	ILE	-	expression tag	UNP Q03188
a	589	PHE	-	expression tag	UNP Q03188
a	590	LEU	-	expression tag	UNP Q03188
a	591	GLY	-	expression tag	UNP Q03188
a	592	LYS	-	expression tag	UNP Q03188
a	593	GLY	-	expression tag	UNP Q03188
a	594	THR	-	expression tag	UNP Q03188
a	595	SER	-	expression tag	UNP Q03188
a	596	ALA	-	expression tag	UNP Q03188
a	597	ALA	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	598	ASP	-	expression tag	UNP Q03188
a	599	ALA	-	expression tag	UNP Q03188
a	600	VAL	-	expression tag	UNP Q03188
a	601	GLU	-	expression tag	UNP Q03188
a	602	VAL	-	expression tag	UNP Q03188
a	603	PRO	-	expression tag	UNP Q03188
a	604	ALA	-	expression tag	UNP Q03188
a	605	PRO	-	expression tag	UNP Q03188
a	606	ALA	-	expression tag	UNP Q03188
a	607	ALA	-	expression tag	UNP Q03188
a	608	VAL	-	expression tag	UNP Q03188
a	609	LEU	-	expression tag	UNP Q03188
a	610	GLY	-	expression tag	UNP Q03188
a	611	GLY	-	expression tag	UNP Q03188
a	612	PRO	-	expression tag	UNP Q03188
a	613	GLU	-	expression tag	UNP Q03188
a	614	PRO	-	expression tag	UNP Q03188
a	615	LEU	-	expression tag	UNP Q03188
a	616	MET	-	expression tag	UNP Q03188
a	617	GLN	-	expression tag	UNP Q03188
a	618	ALA	-	expression tag	UNP Q03188
a	619	THR	-	expression tag	UNP Q03188
a	620	ALA	-	expression tag	UNP Q03188
a	621	TRP	-	expression tag	UNP Q03188
a	622	LEU	-	expression tag	UNP Q03188
a	623	ASN	-	expression tag	UNP Q03188
a	624	ALA	-	expression tag	UNP Q03188
a	625	TYR	-	expression tag	UNP Q03188
a	626	PHE	-	expression tag	UNP Q03188
a	627	HIS	-	expression tag	UNP Q03188
a	628	GLN	-	expression tag	UNP Q03188
a	629	PRO	-	expression tag	UNP Q03188
a	630	GLU	-	expression tag	UNP Q03188
a	631	ALA	-	expression tag	UNP Q03188
a	632	ILE	-	expression tag	UNP Q03188
a	633	GLU	-	expression tag	UNP Q03188
a	634	GLU	-	expression tag	UNP Q03188
a	635	PHE	-	expression tag	UNP Q03188
a	636	PRO	-	expression tag	UNP Q03188
a	637	VAL	-	expression tag	UNP Q03188
a	638	PRO	-	expression tag	UNP Q03188
a	639	ALA	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	640	LEU	-	expression tag	UNP Q03188
a	641	HIS	-	expression tag	UNP Q03188
a	642	HIS	-	expression tag	UNP Q03188
a	643	PRO	-	expression tag	UNP Q03188
a	644	VAL	-	expression tag	UNP Q03188
a	645	PHE	-	expression tag	UNP Q03188
a	646	GLN	-	expression tag	UNP Q03188
a	647	GLN	-	expression tag	UNP Q03188
a	648	GLU	-	expression tag	UNP Q03188
a	649	SER	-	expression tag	UNP Q03188
a	650	PHE	-	expression tag	UNP Q03188
a	651	THR	-	expression tag	UNP Q03188
a	652	ARG	-	expression tag	UNP Q03188
a	653	GLN	-	expression tag	UNP Q03188
a	654	VAL	-	expression tag	UNP Q03188
a	655	LEU	-	expression tag	UNP Q03188
a	656	TRP	-	expression tag	UNP Q03188
a	657	LYS	-	expression tag	UNP Q03188
a	658	LEU	-	expression tag	UNP Q03188
a	659	LEU	-	expression tag	UNP Q03188
a	660	LYS	-	expression tag	UNP Q03188
a	661	VAL	-	expression tag	UNP Q03188
a	662	VAL	-	expression tag	UNP Q03188
a	663	LYS	-	expression tag	UNP Q03188
a	664	PHE	-	expression tag	UNP Q03188
a	665	GLY	-	expression tag	UNP Q03188
a	666	GLU	-	expression tag	UNP Q03188
a	667	VAL	-	expression tag	UNP Q03188
a	668	ILE	-	expression tag	UNP Q03188
a	669	SER	-	expression tag	UNP Q03188
a	670	TYR	-	expression tag	UNP Q03188
a	671	SER	-	expression tag	UNP Q03188
a	672	HIS	-	expression tag	UNP Q03188
a	673	LEU	-	expression tag	UNP Q03188
a	674	ALA	-	expression tag	UNP Q03188
a	675	ALA	-	expression tag	UNP Q03188
a	676	LEU	-	expression tag	UNP Q03188
a	677	ALA	-	expression tag	UNP Q03188
a	678	GLY	-	expression tag	UNP Q03188
a	679	ASN	-	expression tag	UNP Q03188
a	680	PRO	-	expression tag	UNP Q03188
a	681	ALA	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	682	ALA	-	expression tag	UNP Q03188
a	683	THR	-	expression tag	UNP Q03188
a	684	ALA	-	expression tag	UNP Q03188
a	685	ALA	-	expression tag	UNP Q03188
a	686	VAL	-	expression tag	UNP Q03188
a	687	LYS	-	expression tag	UNP Q03188
a	688	THR	-	expression tag	UNP Q03188
a	689	ALA	-	expression tag	UNP Q03188
a	690	LEU	-	expression tag	UNP Q03188
a	691	SER	-	expression tag	UNP Q03188
a	692	GLY	-	expression tag	UNP Q03188
a	693	ASN	-	expression tag	UNP Q03188
a	694	PRO	-	expression tag	UNP Q03188
a	695	VAL	-	expression tag	UNP Q03188
a	696	PRO	-	expression tag	UNP Q03188
a	697	ILE	-	expression tag	UNP Q03188
a	698	LEU	-	expression tag	UNP Q03188
a	699	ILE	-	expression tag	UNP Q03188
a	700	PRO	-	expression tag	UNP Q03188
a	701	CYS	-	expression tag	UNP Q03188
a	702	HIS	-	expression tag	UNP Q03188
a	703	ARG	-	expression tag	UNP Q03188
a	704	VAL	-	expression tag	UNP Q03188
a	705	VAL	-	expression tag	UNP Q03188
a	706	GLN	-	expression tag	UNP Q03188
a	707	GLY	-	expression tag	UNP Q03188
a	708	ASP	-	expression tag	UNP Q03188
a	709	LEU	-	expression tag	UNP Q03188
a	710	ASP	-	expression tag	UNP Q03188
a	711	VAL	-	expression tag	UNP Q03188
a	712	GLY	-	expression tag	UNP Q03188
a	713	GLY	-	expression tag	UNP Q03188
a	714	TYR	-	expression tag	UNP Q03188
a	715	GLU	-	expression tag	UNP Q03188
a	716	GLY	-	expression tag	UNP Q03188
a	717	GLY	-	expression tag	UNP Q03188
a	718	LEU	-	expression tag	UNP Q03188
a	719	ALA	-	expression tag	UNP Q03188
a	720	VAL	-	expression tag	UNP Q03188
a	721	LYS	-	expression tag	UNP Q03188
a	722	GLU	-	expression tag	UNP Q03188
a	723	TRP	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	724	LEU	-	expression tag	UNP Q03188
a	725	LEU	-	expression tag	UNP Q03188
a	726	ALA	-	expression tag	UNP Q03188
a	727	HIS	-	expression tag	UNP Q03188
a	728	GLU	-	expression tag	UNP Q03188
a	729	GLY	-	expression tag	UNP Q03188
a	730	HIS	-	expression tag	UNP Q03188
a	731	ARG	-	expression tag	UNP Q03188
a	732	LEU	-	expression tag	UNP Q03188
a	733	GLY	-	expression tag	UNP Q03188
a	734	LYS	-	expression tag	UNP Q03188
a	735	PRO	-	expression tag	UNP Q03188
a	736	GLY	-	expression tag	UNP Q03188
a	737	LEU	-	expression tag	UNP Q03188
a	738	GLY	-	expression tag	UNP Q03188
a	739	GLU	-	expression tag	UNP Q03188
a	740	ASN	-	expression tag	UNP Q03188
a	741	LEU	-	expression tag	UNP Q03188
a	742	TYR	-	expression tag	UNP Q03188
a	743	PHE	-	expression tag	UNP Q03188
a	744	GLN	-	expression tag	UNP Q03188
a	745	SER	-	expression tag	UNP Q03188
a	746	SER	-	expression tag	UNP Q03188
a	747	ALA	-	expression tag	UNP Q03188
a	748	TRP	-	expression tag	UNP Q03188
a	749	SER	-	expression tag	UNP Q03188
a	750	HIS	-	expression tag	UNP Q03188
a	751	PRO	-	expression tag	UNP Q03188
a	752	GLN	-	expression tag	UNP Q03188
a	753	PHE	-	expression tag	UNP Q03188
a	754	GLU	-	expression tag	UNP Q03188
a	755	LYS	-	expression tag	UNP Q03188
a	756	GLY	-	expression tag	UNP Q03188
a	757	GLY	-	expression tag	UNP Q03188
a	758	GLY	-	expression tag	UNP Q03188
a	759	SER	-	expression tag	UNP Q03188
a	760	GLY	-	expression tag	UNP Q03188
a	761	GLY	-	expression tag	UNP Q03188
a	762	GLY	-	expression tag	UNP Q03188
a	763	SER	-	expression tag	UNP Q03188
a	764	GLY	-	expression tag	UNP Q03188
a	765	GLY	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
a	766	SER	-	expression tag	UNP Q03188
a	767	ALA	-	expression tag	UNP Q03188
a	768	TRP	-	expression tag	UNP Q03188
a	769	SER	-	expression tag	UNP Q03188
a	770	HIS	-	expression tag	UNP Q03188
a	771	PRO	-	expression tag	UNP Q03188
a	772	GLN	-	expression tag	UNP Q03188
a	773	PHE	-	expression tag	UNP Q03188
a	774	GLU	-	expression tag	UNP Q03188
a	775	LYS	-	expression tag	UNP Q03188
b	546	ASP	-	expression tag	UNP Q03188
b	547	LEU	-	expression tag	UNP Q03188
b	548	GLU	-	expression tag	UNP Q03188
b	549	VAL	-	expression tag	UNP Q03188
b	550	LEU	-	expression tag	UNP Q03188
b	551	PHE	-	expression tag	UNP Q03188
b	552	GLN	-	expression tag	UNP Q03188
b	553	GLY	-	expression tag	UNP Q03188
b	554	PRO	-	expression tag	UNP Q03188
b	555	LEU	-	expression tag	UNP Q03188
b	556	GLY	-	expression tag	UNP Q03188
b	557	MET	-	expression tag	UNP Q03188
b	558	ASP	-	expression tag	UNP Q03188
b	559	LYS	-	expression tag	UNP Q03188
b	560	ASP	-	expression tag	UNP Q03188
b	561	CYS	-	expression tag	UNP Q03188
b	562	GLU	-	expression tag	UNP Q03188
b	563	MET	-	expression tag	UNP Q03188
b	564	LYS	-	expression tag	UNP Q03188
b	565	ARG	-	expression tag	UNP Q03188
b	566	THR	-	expression tag	UNP Q03188
b	567	THR	-	expression tag	UNP Q03188
b	568	LEU	-	expression tag	UNP Q03188
b	569	ASP	-	expression tag	UNP Q03188
b	570	SER	-	expression tag	UNP Q03188
b	571	PRO	-	expression tag	UNP Q03188
b	572	LEU	-	expression tag	UNP Q03188
b	573	GLY	-	expression tag	UNP Q03188
b	574	LYS	-	expression tag	UNP Q03188
b	575	LEU	-	expression tag	UNP Q03188
b	576	GLU	-	expression tag	UNP Q03188
b	577	LEU	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
b	578	SER	-	expression tag	UNP Q03188
b	579	GLY	-	expression tag	UNP Q03188
b	580	CYS	-	expression tag	UNP Q03188
b	581	GLU	-	expression tag	UNP Q03188
b	582	GLN	-	expression tag	UNP Q03188
b	583	GLY	-	expression tag	UNP Q03188
b	584	LEU	-	expression tag	UNP Q03188
b	585	HIS	-	expression tag	UNP Q03188
b	586	ARG	-	expression tag	UNP Q03188
b	587	ILE	-	expression tag	UNP Q03188
b	588	ILE	-	expression tag	UNP Q03188
b	589	PHE	-	expression tag	UNP Q03188
b	590	LEU	-	expression tag	UNP Q03188
b	591	GLY	-	expression tag	UNP Q03188
b	592	LYS	-	expression tag	UNP Q03188
b	593	GLY	-	expression tag	UNP Q03188
b	594	THR	-	expression tag	UNP Q03188
b	595	SER	-	expression tag	UNP Q03188
b	596	ALA	-	expression tag	UNP Q03188
b	597	ALA	-	expression tag	UNP Q03188
b	598	ASP	-	expression tag	UNP Q03188
b	599	ALA	-	expression tag	UNP Q03188
b	600	VAL	-	expression tag	UNP Q03188
b	601	GLU	-	expression tag	UNP Q03188
b	602	VAL	-	expression tag	UNP Q03188
b	603	PRO	-	expression tag	UNP Q03188
b	604	ALA	-	expression tag	UNP Q03188
b	605	PRO	-	expression tag	UNP Q03188
b	606	ALA	-	expression tag	UNP Q03188
b	607	ALA	-	expression tag	UNP Q03188
b	608	VAL	-	expression tag	UNP Q03188
b	609	LEU	-	expression tag	UNP Q03188
b	610	GLY	-	expression tag	UNP Q03188
b	611	GLY	-	expression tag	UNP Q03188
b	612	PRO	-	expression tag	UNP Q03188
b	613	GLU	-	expression tag	UNP Q03188
b	614	PRO	-	expression tag	UNP Q03188
b	615	LEU	-	expression tag	UNP Q03188
b	616	MET	-	expression tag	UNP Q03188
b	617	GLN	-	expression tag	UNP Q03188
b	618	ALA	-	expression tag	UNP Q03188
b	619	THR	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
b	620	ALA	-	expression tag	UNP Q03188
b	621	TRP	-	expression tag	UNP Q03188
b	622	LEU	-	expression tag	UNP Q03188
b	623	ASN	-	expression tag	UNP Q03188
b	624	ALA	-	expression tag	UNP Q03188
b	625	TYR	-	expression tag	UNP Q03188
b	626	PHE	-	expression tag	UNP Q03188
b	627	HIS	-	expression tag	UNP Q03188
b	628	GLN	-	expression tag	UNP Q03188
b	629	PRO	-	expression tag	UNP Q03188
b	630	GLU	-	expression tag	UNP Q03188
b	631	ALA	-	expression tag	UNP Q03188
b	632	ILE	-	expression tag	UNP Q03188
b	633	GLU	-	expression tag	UNP Q03188
b	634	GLU	-	expression tag	UNP Q03188
b	635	PHE	-	expression tag	UNP Q03188
b	636	PRO	-	expression tag	UNP Q03188
b	637	VAL	-	expression tag	UNP Q03188
b	638	PRO	-	expression tag	UNP Q03188
b	639	ALA	-	expression tag	UNP Q03188
b	640	LEU	-	expression tag	UNP Q03188
b	641	HIS	-	expression tag	UNP Q03188
b	642	HIS	-	expression tag	UNP Q03188
b	643	PRO	-	expression tag	UNP Q03188
b	644	VAL	-	expression tag	UNP Q03188
b	645	PHE	-	expression tag	UNP Q03188
b	646	GLN	-	expression tag	UNP Q03188
b	647	GLN	-	expression tag	UNP Q03188
b	648	GLU	-	expression tag	UNP Q03188
b	649	SER	-	expression tag	UNP Q03188
b	650	PHE	-	expression tag	UNP Q03188
b	651	THR	-	expression tag	UNP Q03188
b	652	ARG	-	expression tag	UNP Q03188
b	653	GLN	-	expression tag	UNP Q03188
b	654	VAL	-	expression tag	UNP Q03188
b	655	LEU	-	expression tag	UNP Q03188
b	656	TRP	-	expression tag	UNP Q03188
b	657	LYS	-	expression tag	UNP Q03188
b	658	LEU	-	expression tag	UNP Q03188
b	659	LEU	-	expression tag	UNP Q03188
b	660	LYS	-	expression tag	UNP Q03188
b	661	VAL	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
b	662	VAL	-	expression tag	UNP Q03188
b	663	LYS	-	expression tag	UNP Q03188
b	664	PHE	-	expression tag	UNP Q03188
b	665	GLY	-	expression tag	UNP Q03188
b	666	GLU	-	expression tag	UNP Q03188
b	667	VAL	-	expression tag	UNP Q03188
b	668	ILE	-	expression tag	UNP Q03188
b	669	SER	-	expression tag	UNP Q03188
b	670	TYR	-	expression tag	UNP Q03188
b	671	SER	-	expression tag	UNP Q03188
b	672	HIS	-	expression tag	UNP Q03188
b	673	LEU	-	expression tag	UNP Q03188
b	674	ALA	-	expression tag	UNP Q03188
b	675	ALA	-	expression tag	UNP Q03188
b	676	LEU	-	expression tag	UNP Q03188
b	677	ALA	-	expression tag	UNP Q03188
b	678	GLY	-	expression tag	UNP Q03188
b	679	ASN	-	expression tag	UNP Q03188
b	680	PRO	-	expression tag	UNP Q03188
b	681	ALA	-	expression tag	UNP Q03188
b	682	ALA	-	expression tag	UNP Q03188
b	683	THR	-	expression tag	UNP Q03188
b	684	ALA	-	expression tag	UNP Q03188
b	685	ALA	-	expression tag	UNP Q03188
b	686	VAL	-	expression tag	UNP Q03188
b	687	LYS	-	expression tag	UNP Q03188
b	688	THR	-	expression tag	UNP Q03188
b	689	ALA	-	expression tag	UNP Q03188
b	690	LEU	-	expression tag	UNP Q03188
b	691	SER	-	expression tag	UNP Q03188
b	692	GLY	-	expression tag	UNP Q03188
b	693	ASN	-	expression tag	UNP Q03188
b	694	PRO	-	expression tag	UNP Q03188
b	695	VAL	-	expression tag	UNP Q03188
b	696	PRO	-	expression tag	UNP Q03188
b	697	ILE	-	expression tag	UNP Q03188
b	698	LEU	-	expression tag	UNP Q03188
b	699	ILE	-	expression tag	UNP Q03188
b	700	PRO	-	expression tag	UNP Q03188
b	701	CYS	-	expression tag	UNP Q03188
b	702	HIS	-	expression tag	UNP Q03188
b	703	ARG	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
b	704	VAL	-	expression tag	UNP Q03188
b	705	VAL	-	expression tag	UNP Q03188
b	706	GLN	-	expression tag	UNP Q03188
b	707	GLY	-	expression tag	UNP Q03188
b	708	ASP	-	expression tag	UNP Q03188
b	709	LEU	-	expression tag	UNP Q03188
b	710	ASP	-	expression tag	UNP Q03188
b	711	VAL	-	expression tag	UNP Q03188
b	712	GLY	-	expression tag	UNP Q03188
b	713	GLY	-	expression tag	UNP Q03188
b	714	TYR	-	expression tag	UNP Q03188
b	715	GLU	-	expression tag	UNP Q03188
b	716	GLY	-	expression tag	UNP Q03188
b	717	GLY	-	expression tag	UNP Q03188
b	718	LEU	-	expression tag	UNP Q03188
b	719	ALA	-	expression tag	UNP Q03188
b	720	VAL	-	expression tag	UNP Q03188
b	721	LYS	-	expression tag	UNP Q03188
b	722	GLU	-	expression tag	UNP Q03188
b	723	TRP	-	expression tag	UNP Q03188
b	724	LEU	-	expression tag	UNP Q03188
b	725	LEU	-	expression tag	UNP Q03188
b	726	ALA	-	expression tag	UNP Q03188
b	727	HIS	-	expression tag	UNP Q03188
b	728	GLU	-	expression tag	UNP Q03188
b	729	GLY	-	expression tag	UNP Q03188
b	730	HIS	-	expression tag	UNP Q03188
b	731	ARG	-	expression tag	UNP Q03188
b	732	LEU	-	expression tag	UNP Q03188
b	733	GLY	-	expression tag	UNP Q03188
b	734	LYS	-	expression tag	UNP Q03188
b	735	PRO	-	expression tag	UNP Q03188
b	736	GLY	-	expression tag	UNP Q03188
b	737	LEU	-	expression tag	UNP Q03188
b	738	GLY	-	expression tag	UNP Q03188
b	739	GLU	-	expression tag	UNP Q03188
b	740	ASN	-	expression tag	UNP Q03188
b	741	LEU	-	expression tag	UNP Q03188
b	742	TYR	-	expression tag	UNP Q03188
b	743	PHE	-	expression tag	UNP Q03188
b	744	GLN	-	expression tag	UNP Q03188
b	745	SER	-	expression tag	UNP Q03188

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Chain	Residue	Modelled	Actual	Comment	Reference
b	746	SER	-	expression tag	UNP Q03188
b	747	ALA	-	expression tag	UNP Q03188
b	748	TRP	-	expression tag	UNP Q03188
b	749	SER	-	expression tag	UNP Q03188
b	750	HIS	-	expression tag	UNP Q03188
b	751	PRO	-	expression tag	UNP Q03188
b	752	GLN	-	expression tag	UNP Q03188
b	753	PHE	-	expression tag	UNP Q03188
b	754	GLU	-	expression tag	UNP Q03188
b	755	LYS	-	expression tag	UNP Q03188
b	756	GLY	-	expression tag	UNP Q03188
b	757	GLY	-	expression tag	UNP Q03188
b	758	GLY	-	expression tag	UNP Q03188
b	759	SER	-	expression tag	UNP Q03188
b	760	GLY	-	expression tag	UNP Q03188
b	761	GLY	-	expression tag	UNP Q03188
b	762	GLY	-	expression tag	UNP Q03188
b	763	SER	-	expression tag	UNP Q03188
b	764	GLY	-	expression tag	UNP Q03188
b	765	GLY	-	expression tag	UNP Q03188
b	766	SER	-	expression tag	UNP Q03188
b	767	ALA	-	expression tag	UNP Q03188
b	768	TRP	-	expression tag	UNP Q03188
b	769	SER	-	expression tag	UNP Q03188
b	770	HIS	-	expression tag	UNP Q03188
b	771	PRO	-	expression tag	UNP Q03188
b	772	GLN	-	expression tag	UNP Q03188
b	773	PHE	-	expression tag	UNP Q03188
b	774	GLU	-	expression tag	UNP Q03188
b	775	LYS	-	expression tag	UNP Q03188

- Molecule 19 is a protein called Histone H3-like centromeric protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	99	Total	C	N	O	S	0	0
			816	526	156	133	1		
19	g	98	Total	C	N	O	S	0	0
			811	523	155	132	1		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
20	h	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 21 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	107	Total	C	N	O		0	0
			822	517	163	142			
21	i	107	Total	C	N	O		0	0
			822	517	163	142			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-23	MET	-	initiating methionine	UNP Q93077
e	-22	GLY	-	expression tag	UNP Q93077
e	-21	SER	-	expression tag	UNP Q93077
e	-20	SER	-	expression tag	UNP Q93077
e	-19	HIS	-	expression tag	UNP Q93077
e	-18	HIS	-	expression tag	UNP Q93077
e	-17	HIS	-	expression tag	UNP Q93077
e	-16	HIS	-	expression tag	UNP Q93077
e	-15	HIS	-	expression tag	UNP Q93077
e	-14	HIS	-	expression tag	UNP Q93077
e	-13	SER	-	expression tag	UNP Q93077
e	-12	PRO	-	expression tag	UNP Q93077
e	-11	GLY	-	expression tag	UNP Q93077
e	-10	LEU	-	expression tag	UNP Q93077
e	-9	GLU	-	expression tag	UNP Q93077
e	-8	VAL	-	expression tag	UNP Q93077
e	-7	LEU	-	expression tag	UNP Q93077
e	-6	PHE	-	expression tag	UNP Q93077
e	-5	GLN	-	expression tag	UNP Q93077
e	-4	GLY	-	expression tag	UNP Q93077
e	-3	PRO	-	expression tag	UNP Q93077
e	-2	ARG	-	expression tag	UNP Q93077
e	-1	GLY	-	expression tag	UNP Q93077
i	-23	MET	-	initiating methionine	UNP Q93077
i	-22	GLY	-	expression tag	UNP Q93077
i	-21	SER	-	expression tag	UNP Q93077
i	-20	SER	-	expression tag	UNP Q93077

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Chain	Residue	Modelled	Actual	Comment	Reference
i	-19	HIS	-	expression tag	UNP Q93077
i	-18	HIS	-	expression tag	UNP Q93077
i	-17	HIS	-	expression tag	UNP Q93077
i	-16	HIS	-	expression tag	UNP Q93077
i	-15	HIS	-	expression tag	UNP Q93077
i	-14	HIS	-	expression tag	UNP Q93077
i	-13	SER	-	expression tag	UNP Q93077
i	-12	PRO	-	expression tag	UNP Q93077
i	-11	GLY	-	expression tag	UNP Q93077
i	-10	LEU	-	expression tag	UNP Q93077
i	-9	GLU	-	expression tag	UNP Q93077
i	-8	VAL	-	expression tag	UNP Q93077
i	-7	LEU	-	expression tag	UNP Q93077
i	-6	PHE	-	expression tag	UNP Q93077
i	-5	GLN	-	expression tag	UNP Q93077
i	-4	GLY	-	expression tag	UNP Q93077
i	-3	PRO	-	expression tag	UNP Q93077
i	-2	ARG	-	expression tag	UNP Q93077
i	-1	GLY	-	expression tag	UNP Q93077

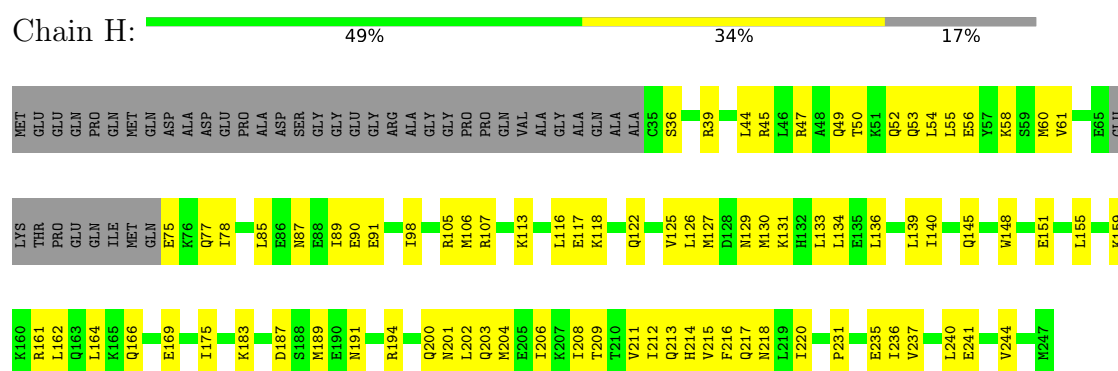
- Molecule 22 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	95	Total	C	N	O	S	0	0
			745	467	136	140	2		
22	j	94	Total	C	N	O	S	0	0
			736	461	134	139	2		

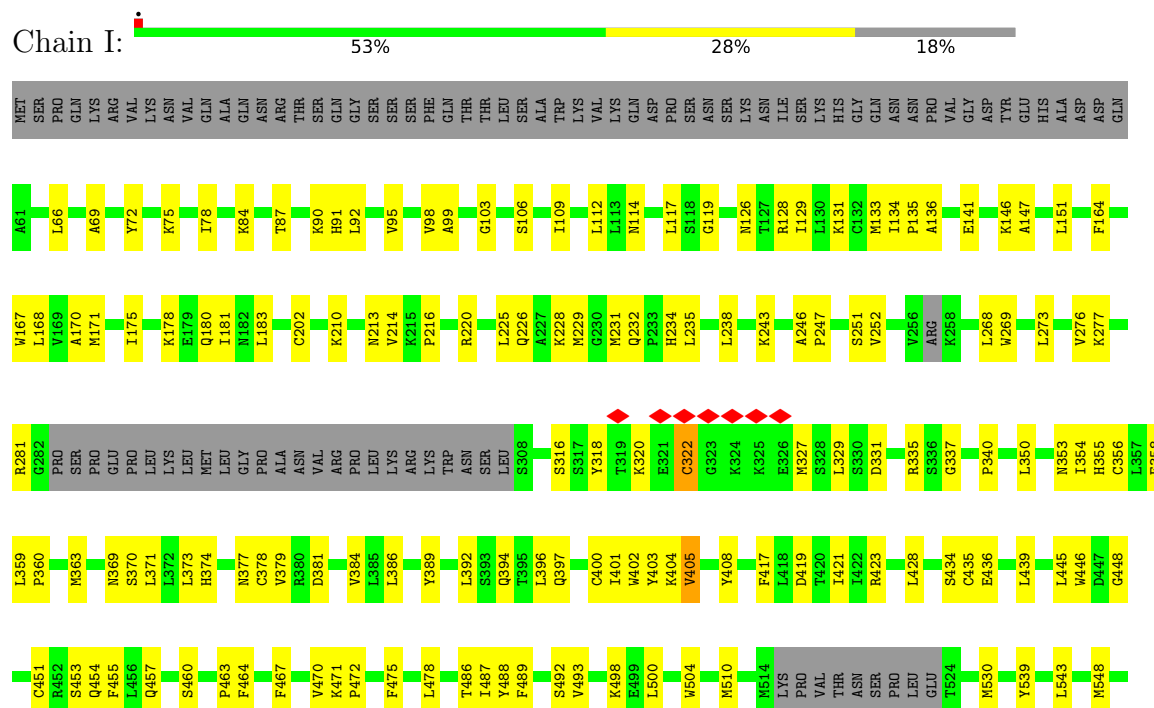
3 Residue-property plots

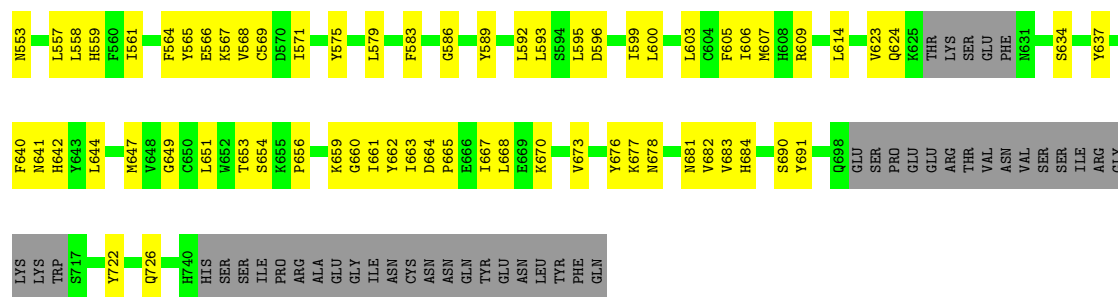
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Centromere protein H



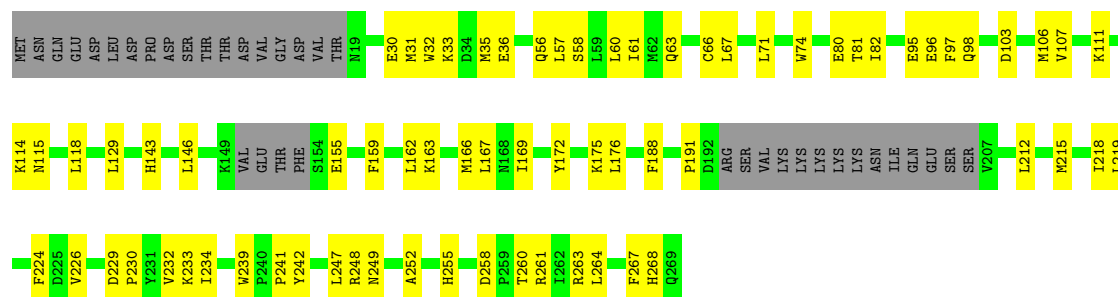
• Molecule 2: Centromere protein I





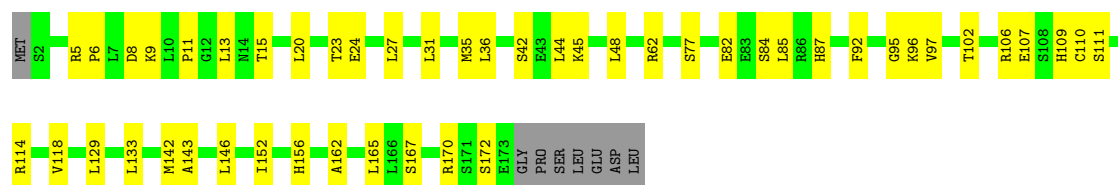
• Molecule 3: Centromere protein K

Chain K: 60% 26% 13%



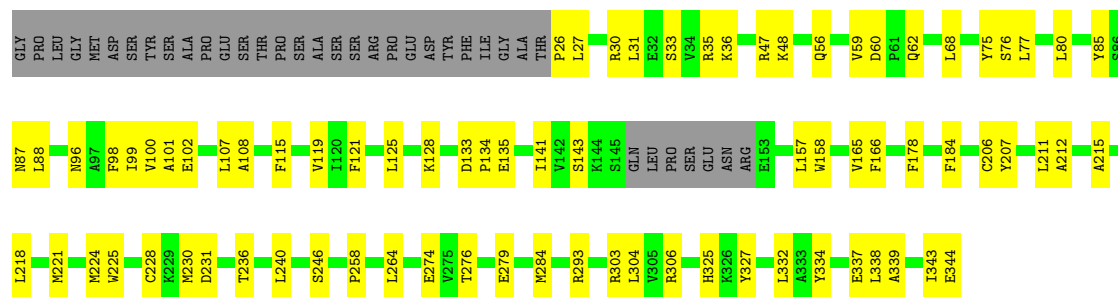
• Molecule 4: Centromere protein M

Chain M: 69% 27% .



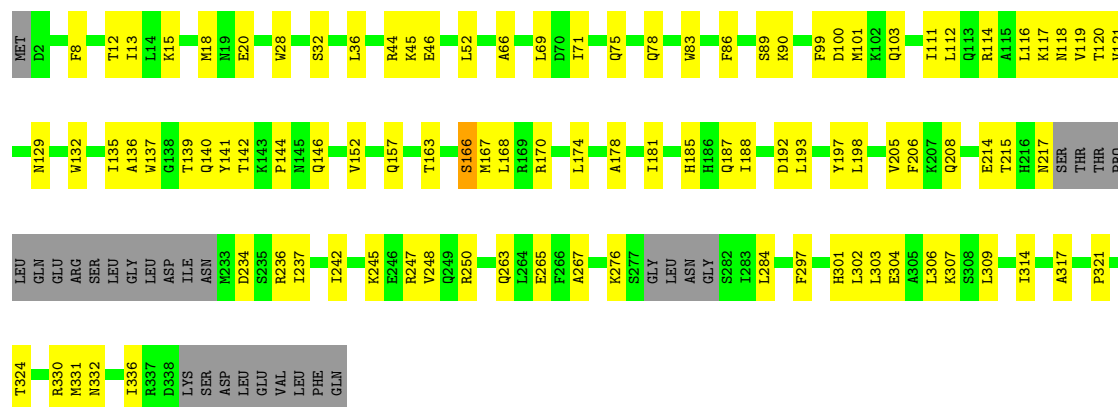
• Molecule 5: Centromere protein L

Chain L: 67% 23% 10%

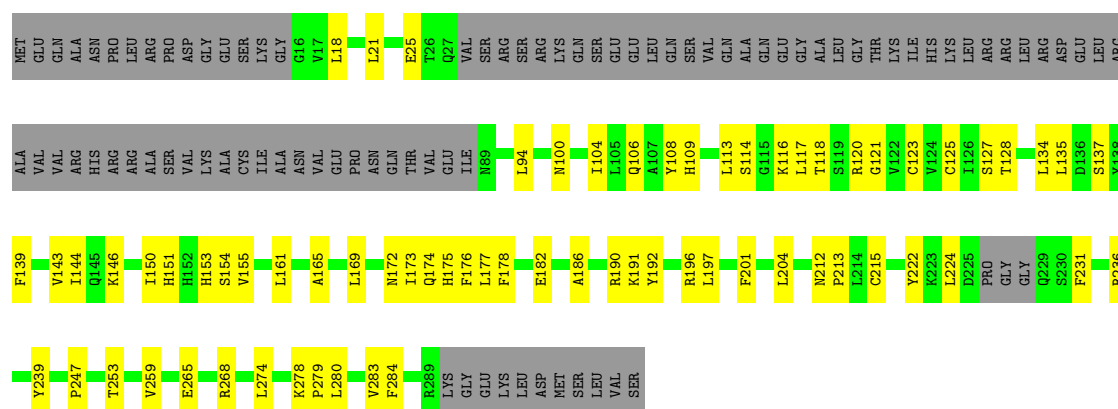


• Molecule 6: Isoform 3 of Centromere protein N

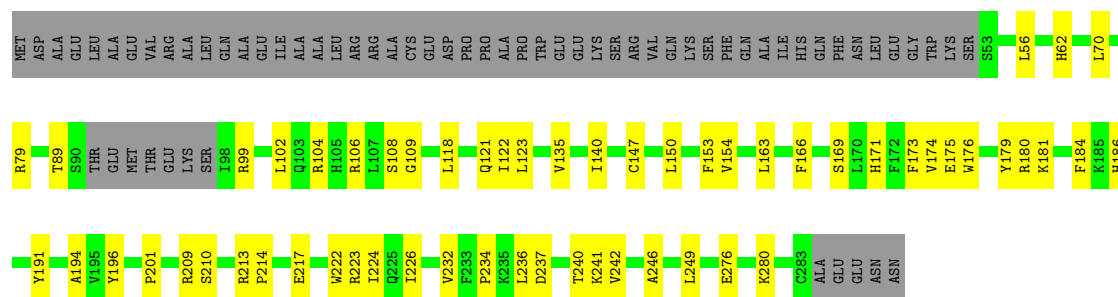
Chain N: 63% 28% 9%



• Molecule 7: Centromere protein O

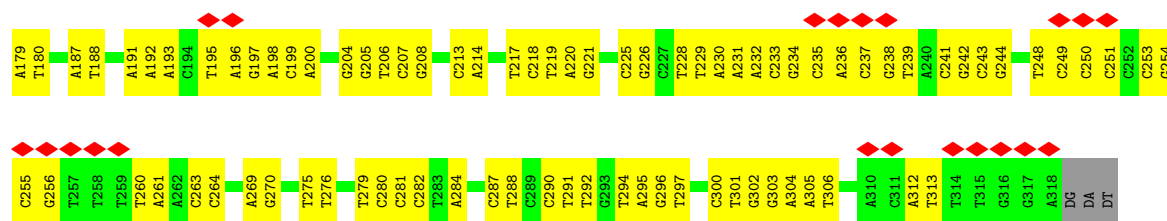


• Molecule 8: Centromere protein P

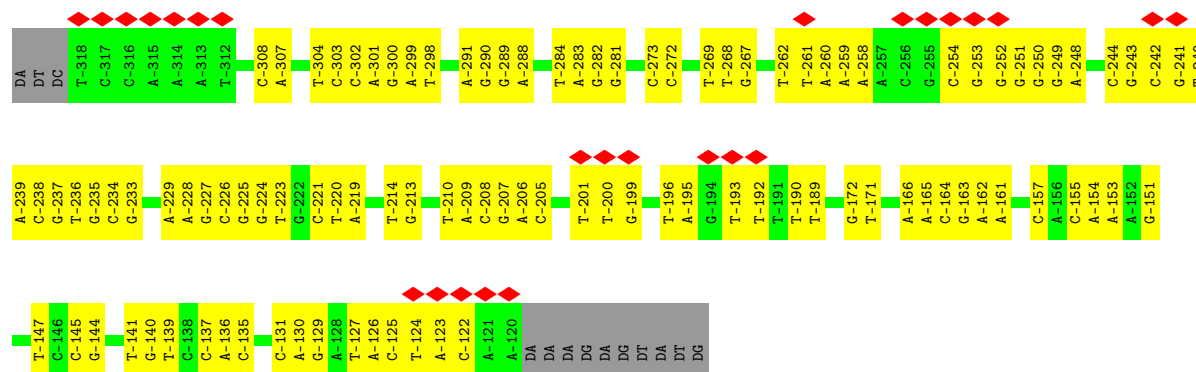


• Molecule 9: Centromere protein Q

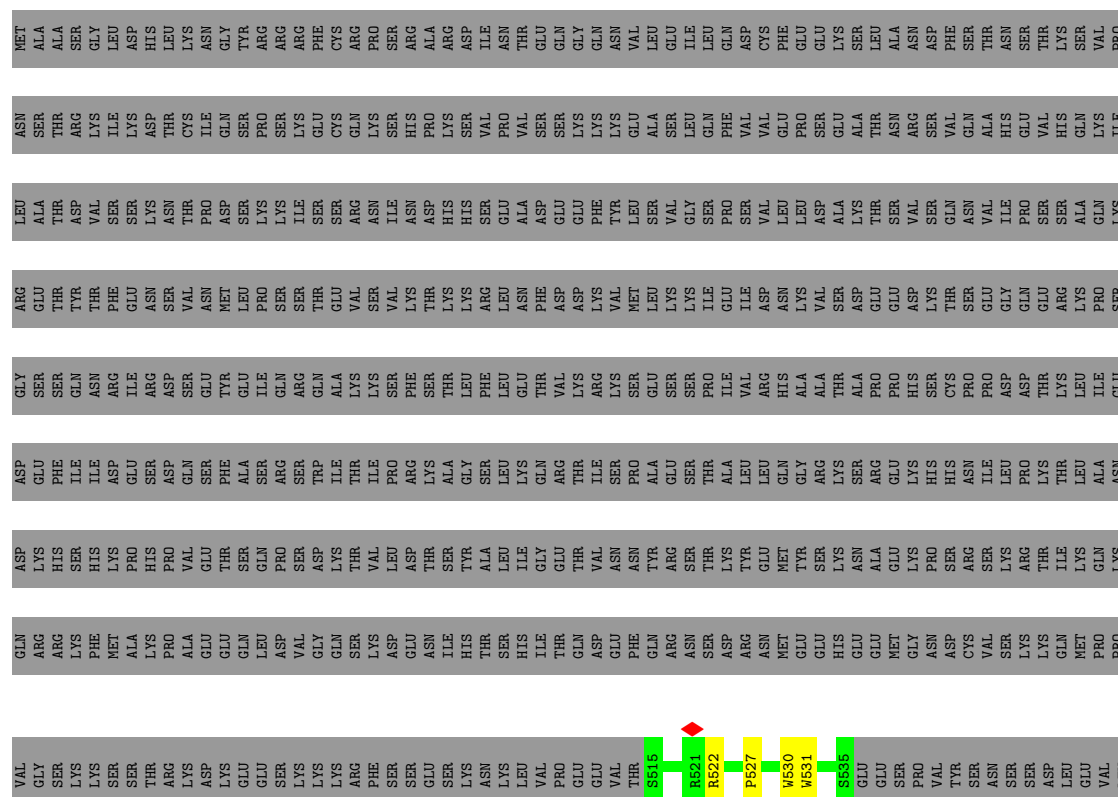




• Molecule 17: DNA (199-MER)



• Molecule 18: Centromere protein C



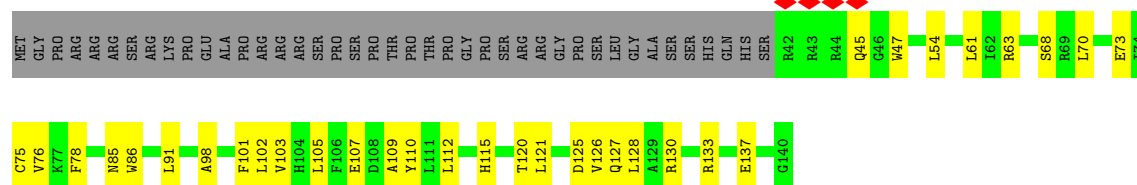
[illegible]

- Molecule 18: Centromere protein C

[illegible]

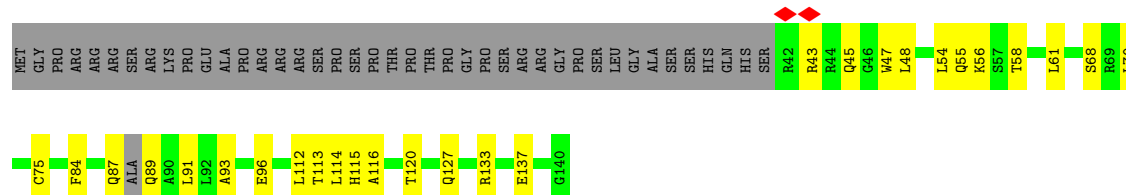
- Molecule 19: Histone H3-like centromeric protein A

Chain c: 



- Molecule 19: Histone H3-like centromeric protein A

Chain g: 



- Molecule 20: Histone H4

Chain d: 



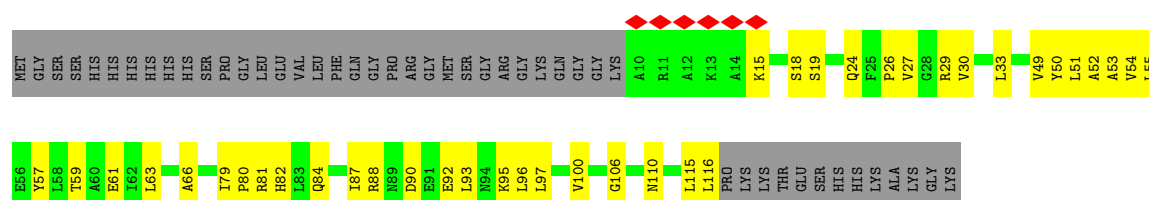
- Molecule 20: Histone H4

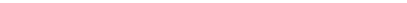
Chain h: 

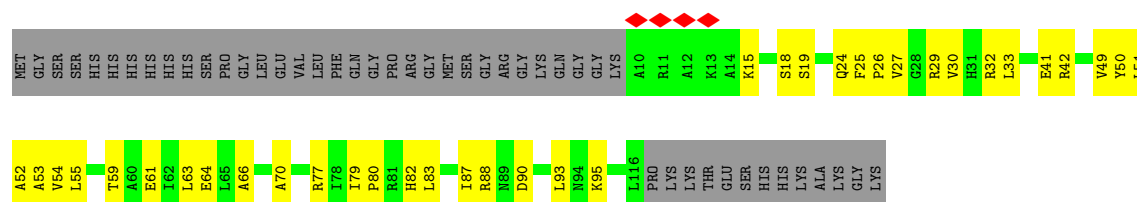


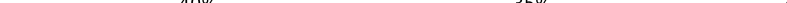
- Molecule 21: Histone H2A type 1-C

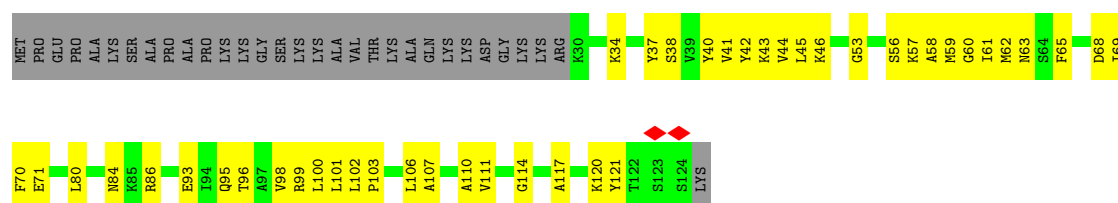
Chain e: 

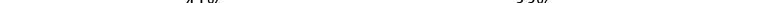


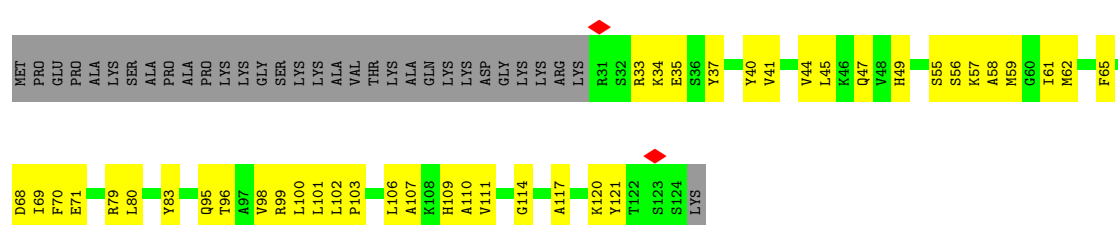
Chain i:  46% 24% 30%



Chain f: 



Chain j: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39306	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.017	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0016	Depositor
Map size (Å)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	H	0.22	0/1686	0.39	0/2247
2	I	0.22	0/5176	0.40	1/7003 (0.0%)
3	K	0.22	0/1967	0.35	0/2651
4	M	0.25	0/1347	0.37	0/1827
5	L	0.26	0/2573	0.38	0/3490
6	N	0.27	0/2688	0.42	0/3626
7	O	0.20	0/1717	0.39	0/2329
8	P	0.16	0/1851	0.36	0/2488
9	Q	0.17	0/1542	0.34	0/2067
10	U	0.17	0/1395	0.36	0/1869
11	R	0.17	0/653	0.42	0/865
12	T	0.24	0/937	0.48	0/1263
13	W	0.23	0/698	0.36	0/927
14	S	0.19	0/991	0.35	0/1322
15	X	0.23	0/596	0.33	0/801
16	V	0.20	0/4572	0.41	0/7055
17	Y	0.20	0/4580	0.39	0/7066
18	a	0.11	0/182	0.33	0/245
18	b	0.15	0/481	0.38	0/641
19	c	0.17	0/831	0.43	0/1116
19	g	0.13	0/825	0.31	0/1106
20	d	0.16	0/645	0.34	0/862
20	h	0.14	0/645	0.31	0/862
21	e	0.16	0/831	0.37	0/1120
21	i	0.16	0/831	0.39	0/1120
22	f	0.20	0/756	0.44	0/1015
22	j	0.20	0/747	0.44	0/1004
All	All	0.21	0/41743	0.39	1/57987 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	322	CYS	CB-CA-C	-5.23	110.12	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1678	0	1780	79	0
2	I	5051	0	5093	174	0
3	K	1936	0	1947	69	0
4	M	1325	0	1370	39	0
5	L	2506	0	2496	51	0
6	N	2631	0	2665	82	0
7	O	1681	0	1668	59	0
8	P	1819	0	1848	48	0
9	Q	1530	0	1592	58	0
10	U	1377	0	1422	57	0
11	R	649	0	673	28	0
12	T	915	0	924	47	0
13	W	691	0	772	24	0
14	S	982	0	987	39	0
15	X	590	0	623	20	0
16	V	4078	0	2245	95	0
17	Y	4081	0	2239	79	0
18	a	178	0	185	3	0
18	b	476	0	483	13	0
19	c	816	0	857	35	0
19	g	811	0	851	27	0
20	d	638	0	676	30	0
20	h	638	0	676	20	0
21	e	822	0	880	48	0
21	i	822	0	880	44	0
22	f	745	0	769	54	0
22	j	736	0	756	57	0
All	All	40202	0	37357	1089	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 (1089) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:99:ALA:HB1	2:I:134:ILE:HB	1.57	0.83
20:h:71:THR:HG22	22:j:96:THR:HG23	1.59	0.83
6:N:193:LEU:HD12	6:N:332:ASN:HB2	1.60	0.82
6:N:139:THR:HG23	6:N:141:TYR:H	1.44	0.81
11:R:146:VAL:HG13	11:R:151:LEU:HB2	1.63	0.81
11:R:97:SER:HB3	11:R:136:MET:HE1	1.62	0.80
3:K:188:PHE:HB3	3:K:212:LEU:HD23	1.65	0.78
9:Q:88:MET:HE1	9:Q:114:LYS:HA	1.66	0.77
6:N:71:ILE:HG23	6:N:132:TRP:CD1	2.20	0.76
6:N:303:LEU:H	6:N:306:LEU:HD23	1.51	0.76
9:Q:190:VAL:HG22	10:U:348:LYS:HB2	1.67	0.76
20:d:71:THR:HG22	22:f:96:THR:HG23	1.65	0.76
16:V:191:DA:H2"	16:V:192:DA:H5"	1.69	0.75
1:H:106:MET:HG3	2:I:673:VAL:HG21	1.67	0.75
1:H:127:MET:HG3	1:H:131:LYS:HE3	1.69	0.74
1:H:202:LEU:HG	3:K:166:MET:HE2	1.68	0.73
6:N:86:PHE:HB3	6:N:188:ILE:HD11	1.71	0.73
6:N:214:GLU:HB3	7:O:116:LYS:HB3	1.70	0.73
20:h:71:THR:HG23	22:j:99:ARG:HE	1.52	0.73
6:N:117:LYS:HB3	6:N:140:GLN:HA	1.70	0.72
1:H:54:LEU:HD22	3:K:31:MET:HG3	1.70	0.72
22:f:102:LEU:HD13	22:f:106:LEU:HG	1.71	0.72
12:T:515:LEU:HB3	12:T:519:MET:HE1	1.70	0.71
2:I:353:ASN:HA	2:I:355:HIS:CE1	2.26	0.70
20:d:44:LYS:HD2	20:d:45:ARG:HG2	1.72	0.70
2:I:404:LYS:HD2	2:I:404:LYS:O	1.91	0.70
7:O:172:ASN:HB3	7:O:175:HIS:ND1	2.06	0.70
9:Q:250:GLN:HB3	11:R:100:ILE:HG22	1.72	0.70
19:c:115:HIS:HE1	19:g:113:THR:HA	1.57	0.70
7:O:197:LEU:HD13	7:O:284:PHE:CD2	2.26	0.70
7:O:150:ILE:HD11	7:O:153:HIS:HB3	1.73	0.70
11:R:113:LEU:HD21	11:R:119:LEU:HD23	1.74	0.70
7:O:169:LEU:HA	7:O:176:PHE:HZ	1.56	0.69
14:S:40:MET:HG2	15:X:47:VAL:HG13	1.74	0.69
21:e:63:LEU:HB3	22:f:45:LEU:HD13	1.74	0.69
10:U:299:LEU:HG	10:U:303:LYS:HE3	1.73	0.69
12:T:482:MET:HE1	13:W:76:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:102:LEU:HD13	22:j:106:LEU:HG	1.75	0.69
22:f:41:VAL:HG22	22:f:62:MET:HG2	1.74	0.69
8:P:104:ARG:HH11	8:P:121:GLN:HB2	1.58	0.68
2:I:641:ASN:HA	2:I:644:LEU:HD12	1.76	0.68
1:H:98:ILE:HD11	2:I:586:GLY:HA2	1.75	0.68
2:I:243:LYS:HE3	2:I:251:SER:HA	1.75	0.67
10:U:278:ILE:HA	10:U:281:PHE:CE1	2.29	0.67
21:i:79:ILE:HG12	21:i:82:HIS:CE1	2.29	0.67
2:I:135:PRO:HD3	2:I:167:TRP:HH2	1.60	0.67
2:I:569:CYS:SG	2:I:606:ILE:HG23	2.35	0.67
7:O:173:ILE:HA	7:O:176:PHE:CD2	2.29	0.67
21:i:63:LEU:HB3	22:j:45:LEU:HD13	1.76	0.67
7:O:201:PHE:HB3	7:O:204:LEU:HD12	1.76	0.66
21:e:63:LEU:HD13	22:f:45:LEU:HB2	1.76	0.66
2:I:654:SER:HB3	2:I:677:LYS:HB3	1.78	0.66
21:e:79:ILE:HG12	21:e:82:HIS:CE1	2.30	0.66
6:N:157:GLN:HE22	7:O:213:PRO:HD2	1.60	0.66
8:P:147:CYS:SG	8:P:150:LEU:HD23	2.36	0.66
2:I:66:LEU:HD22	2:I:98:VAL:HG11	1.77	0.66
2:I:487:ILE:HD11	2:I:557:LEU:HB2	1.77	0.66
11:R:133:LYS:HA	11:R:136:MET:HE2	1.78	0.66
12:T:536:GLU:HG2	12:T:544:ARG:HE	1.61	0.66
17:Y:-140:DG:H2'	17:Y:-139:DT:H71	1.78	0.66
21:i:63:LEU:HD13	22:j:45:LEU:HB2	1.77	0.66
2:I:103:GLY:HA3	2:I:136:ALA:HB2	1.78	0.65
9:Q:76:LEU:HG	9:Q:126:VAL:HG21	1.78	0.65
15:X:64:GLU:HA	15:X:67:LEU:HG	1.77	0.65
7:O:173:ILE:HA	7:O:176:PHE:HD2	1.61	0.65
5:L:236:THR:HG22	5:L:258:PRO:HD3	1.78	0.65
4:M:45:LYS:HZ3	6:N:236:ARG:HA	1.61	0.65
12:T:463:TYR:HA	12:T:466:LEU:HD12	1.79	0.65
13:W:57:GLU:HG3	13:W:78:ALA:HB1	1.78	0.65
21:i:30:VAL:HA	21:i:33:LEU:HD12	1.79	0.65
12:T:460:LEU:HD13	12:T:484:GLU:HB2	1.78	0.65
21:i:15:LYS:HE3	21:i:19:SER:HB3	1.79	0.64
10:U:291:LYS:HA	10:U:294:LYS:HE2	1.78	0.64
2:I:405:VAL:HG12	4:M:106:ARG:HA	1.80	0.64
8:P:209:ARG:HB2	8:P:217:GLU:HG3	1.80	0.64
16:V:296:DG:H2''	16:V:297:DT:H5''	1.79	0.64
9:Q:93:MET:HG3	14:S:20:LYS:HE2	1.79	0.64
10:U:342:ASP:HA	10:U:345:LYS:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:134:DA:H2''	16:V:135:DG:C8	2.33	0.64
7:O:236:ARG:HH12	7:O:253:THR:HG22	1.63	0.64
20:h:87:VAL:HG22	20:h:97:LEU:HD23	1.80	0.64
12:T:454:ASP:H	12:T:457:LYS:HZ3	1.44	0.64
16:V:219:DT:H2''	16:V:220:DA:C8	2.33	0.63
11:R:90:LEU:HD22	11:R:140:LYS:HD3	1.80	0.63
3:K:215:MET:HA	3:K:218:ILE:HD12	1.79	0.63
16:V:204:DG:H2''	16:V:205:DG:H5''	1.80	0.63
16:V:218:DC:H2''	16:V:219:DT:H71	1.79	0.63
3:K:172:TYR:HA	3:K:175:LYS:HD2	1.81	0.63
17:Y:-228:DA:H4'	19:c:63:ARG:HD2	1.81	0.63
2:I:78:ILE:HB	2:I:84:LYS:HB3	1.80	0.62
8:P:153:PHE:HZ	8:P:166:PHE:HA	1.65	0.62
3:K:219:LEU:HB3	3:K:264:LEU:HB2	1.80	0.62
20:d:71:THR:HG23	22:f:99:ARG:HE	1.62	0.62
2:I:316:SER:HB2	2:I:359:LEU:O	1.99	0.62
16:V:290:DC:H2''	16:V:291:DT:C5	2.34	0.62
1:H:89:ILE:HD13	3:K:71:LEU:HA	1.81	0.62
22:f:68:ASP:O	22:f:71:GLU:HG3	2.00	0.62
8:P:191:TYR:HB3	8:P:194:ALA:HB3	1.81	0.62
21:e:15:LYS:HE3	21:e:19:SER:HB3	1.81	0.62
2:I:642:HIS:HE1	2:I:660:GLY:H	1.48	0.62
9:Q:126:VAL:HG22	10:U:254:VAL:HB	1.82	0.62
9:Q:148:ASP:HA	10:U:309:MET:HE1	1.80	0.62
16:V:144:DC:H2''	16:V:145:DG:C8	2.35	0.62
12:T:533:VAL:HG12	12:T:537:ARG:HH12	1.65	0.61
12:T:479:ALA:O	12:T:483:VAL:HG23	1.99	0.61
21:i:50:TYR:CZ	22:j:95:GLN:HA	2.34	0.61
9:Q:165:MET:HE1	10:U:320:MET:HG3	1.81	0.61
1:H:117:GLU:HG2	1:H:118:LYS:HG3	1.83	0.61
3:K:103:ASP:HA	3:K:106:MET:HE2	1.81	0.61
2:I:109:ILE:HA	2:I:133:MET:HE1	1.82	0.61
4:M:24:GLU:OE2	4:M:27:LEU:HB2	2.00	0.61
6:N:140:GLN:HE22	10:U:317:ARG:HE	1.47	0.61
9:Q:93:MET:HE1	14:S:24:HIS:CG	2.36	0.61
21:i:61:GLU:HB3	21:i:93:LEU:HD11	1.83	0.61
1:H:126:LEU:HG	1:H:130:MET:HE2	1.83	0.61
7:O:113:LEU:HD11	7:O:177:LEU:HD13	1.81	0.61
5:L:75:TYR:HB2	5:L:184:PHE:HD2	1.65	0.61
10:U:397:LEU:HD21	11:R:104:MET:HB3	1.82	0.60
22:j:68:ASP:O	22:j:71:GLU:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:297:LYS:HE2	18:b:300:GLU:HG3	1.82	0.60
19:c:68:SER:HA	19:c:91:LEU:HD22	1.83	0.60
5:L:284:MET:HE3	5:L:284:MET:HA	1.82	0.60
2:I:106:SER:HA	2:I:109:ILE:HD12	1.82	0.60
12:T:454:ASP:HB3	12:T:457:LYS:HG2	1.83	0.60
6:N:248:VAL:HG22	6:N:317:ALA:HB2	1.84	0.60
21:i:49:VAL:HG12	22:j:117:ALA:HB1	1.83	0.60
17:Y:-225:DG:H2'	17:Y:-224:DG:H8	1.67	0.60
16:V:269:DA:H2''	16:V:270:DG:C8	2.36	0.60
15:X:31:MET:HA	15:X:34:LEU:HG	1.83	0.60
2:I:109:ILE:HD11	2:I:135:PRO:HA	1.84	0.60
2:I:488:TYR:HB2	7:O:25:GLU:OE1	2.02	0.60
17:Y:-240:DT:H2''	17:Y:-239:DA:C8	2.36	0.60
9:Q:251:MET:HE1	10:U:397:LEU:HD22	1.84	0.59
2:I:678:ASN:O	2:I:684:HIS:HB2	2.02	0.59
21:i:33:LEU:HB3	22:j:70:PHE:CZ	2.37	0.59
16:V:198:DA:H2''	16:V:199:DC:C5	2.37	0.59
9:Q:239:LEU:HB3	10:U:387:LEU:HD13	1.84	0.59
13:W:18:PRO:HB2	13:W:21:PHE:HB3	1.85	0.59
8:P:280:LYS:HB2	9:Q:202:GLN:HE22	1.68	0.58
11:R:96:LEU:O	11:R:100:ILE:HG23	2.03	0.58
22:j:41:VAL:HA	22:j:62:MET:SD	2.43	0.58
2:I:228:LYS:HZ3	2:I:229:MET:HE3	1.68	0.58
8:P:249:LEU:HD21	10:U:367:ASP:HB2	1.85	0.58
16:V:197:DG:H2''	16:V:198:DA:C8	2.39	0.58
6:N:100:ASP:HB3	6:N:103:GLN:HG3	1.84	0.58
8:P:153:PHE:CZ	8:P:166:PHE:HA	2.39	0.58
16:V:166:DT:H2''	16:V:167:DG:C8	2.39	0.58
22:f:99:ARG:HA	22:f:107:ALA:HB1	1.84	0.58
5:L:293:ARG:HH22	6:N:276:LYS:H	1.51	0.58
13:W:53:ARG:HH22	13:W:85:LYS:HD3	1.68	0.58
14:S:16:GLN:HG2	15:X:14:LEU:HD21	1.85	0.58
14:S:102:GLU:O	14:S:105:GLN:HG2	2.04	0.58
5:L:77:LEU:HD11	5:L:206:CYS:HB2	1.86	0.58
7:O:169:LEU:HA	7:O:176:PHE:CZ	2.36	0.58
4:M:13:LEU:HD11	18:b:265:LEU:HB3	1.86	0.57
14:S:27:VAL:HG12	14:S:47:ILE:HG23	1.86	0.57
16:V:254:DG:H4'	19:g:43:ARG:HD2	1.86	0.57
17:Y:-282:DG:H2''	17:Y:-281:DG:C8	2.39	0.57
1:H:122:GLN:HG2	1:H:127:MET:HG2	1.85	0.57
3:K:159:PHE:HA	3:K:162:LEU:HD12	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:126:DT:H2''	16:V:127:DA:C8	2.38	0.57
6:N:141:TYR:HB2	9:Q:147:ARG:HH11	1.69	0.57
10:U:382:TYR:HB3	10:U:386:SER:HB2	1.86	0.57
21:i:41:GLU:HG2	21:i:42:ARG:HG2	1.84	0.57
9:Q:83:HIS:CD2	9:Q:131:MET:HE1	2.39	0.57
16:V:300:DC:H2''	16:V:301:DT:C5	2.38	0.57
7:O:108:TYR:CZ	8:P:70:LEU:HB3	2.38	0.57
21:i:24:GLN:HB2	22:j:44:VAL:HG22	1.85	0.57
1:H:162:LEU:HB2	2:I:510:MET:HE3	1.87	0.57
2:I:216:PRO:HB2	2:I:220:ARG:HH12	1.70	0.57
2:I:401:ILE:HB	2:I:402:TRP:CE3	2.40	0.57
12:T:535:VAL:HG13	12:T:539:LEU:HD12	1.87	0.57
17:Y:-229:DA:H2''	17:Y:-228:DA:C8	2.39	0.57
19:c:105:LEU:HD11	19:c:126:VAL:HG13	1.87	0.57
4:M:5:ARG:HB3	4:M:8:ASP:HB2	1.87	0.57
16:V:140:DC:H2''	16:V:141:DA:C8	2.40	0.57
4:M:95:GLY:HA3	4:M:162:ALA:HB1	1.86	0.56
4:M:109:HIS:HA	5:L:303:ARG:HE	1.68	0.56
8:P:217:GLU:HB3	8:P:241:LYS:HE3	1.87	0.56
21:i:54:VAL:HG13	22:j:110:ALA:HB1	1.87	0.56
4:M:48:LEU:HG	6:N:237:ILE:HD11	1.87	0.56
14:S:52:GLU:HA	14:S:55:PHE:HD1	1.71	0.56
16:V:124:DA:H2''	16:V:125:DG:C8	2.41	0.56
22:f:57:LYS:HD2	22:f:58:ALA:N	2.20	0.56
2:I:210:LYS:H	2:I:213:ASN:HB2	1.70	0.56
4:M:31:LEU:HD12	4:M:133:LEU:HD11	1.85	0.56
6:N:114:ARG:HG3	10:U:320:MET:HE1	1.88	0.56
6:N:263:GLN:HA	6:N:301:HIS:CD2	2.40	0.56
22:j:79:ARG:HB3	22:j:83:TYR:CZ	2.40	0.56
6:N:90:LYS:HG3	6:N:185:HIS:CD2	2.41	0.56
17:Y:-284:DT:H2''	17:Y:-283:DA:C8	2.40	0.56
19:c:101:PHE:HE2	20:d:57:VAL:HG12	1.70	0.56
22:f:117:ALA:O	22:f:120:LYS:HG3	2.05	0.56
3:K:107:VAL:O	3:K:111:LYS:HG2	2.06	0.56
6:N:18:MET:HE3	6:N:45:LYS:HD2	1.87	0.56
21:i:54:VAL:HG21	22:j:98:VAL:HG21	1.86	0.56
4:M:23:THR:HG21	4:M:77:SER:HA	1.87	0.56
9:Q:127:PRO:HD3	10:U:253:ILE:HG12	1.86	0.56
1:H:54:LEU:O	1:H:58:LYS:HG2	2.05	0.56
2:I:403:TYR:O	2:I:404:LYS:HG3	2.06	0.56
2:I:548:MET:SD	2:I:553:ASN:HA	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:306:ASN:HA	10:U:309:MET:HG2	1.88	0.56
2:I:571:ILE:O	2:I:575:TYR:HB2	2.06	0.55
2:I:600:LEU:HA	2:I:603:LEU:HD12	1.87	0.55
6:N:129:ASN:CG	7:O:213:PRO:HG3	2.30	0.55
8:P:150:LEU:HD22	8:P:226:ILE:HD11	1.88	0.55
9:Q:76:LEU:HD23	9:Q:126:VAL:HG11	1.88	0.55
2:I:202:CYS:HA	2:I:238:LEU:HD11	1.88	0.55
2:I:419:ASP:HB3	2:I:423:ARG:HH12	1.72	0.55
8:P:280:LYS:HB2	9:Q:202:GLN:NE2	2.22	0.55
6:N:12:THR:HA	6:N:15:LYS:HE2	1.87	0.55
8:P:180:ARG:HD3	8:P:222:TRP:CD1	2.42	0.55
11:R:134:ARG:HG2	11:R:138:LYS:HE3	1.87	0.55
18:b:531:TRP:CD1	19:c:127:GLN:HB3	2.41	0.55
1:H:203:GLN:O	1:H:206:ILE:HG22	2.07	0.55
2:I:106:SER:HA	2:I:109:ILE:HB	1.88	0.55
1:H:105:ARG:HG3	2:I:593:LEU:HB3	1.89	0.55
2:I:135:PRO:HG3	2:I:171:MET:SD	2.47	0.55
2:I:670:LYS:HB3	3:K:81:THR:HG21	1.88	0.55
3:K:111:LYS:HA	3:K:114:LYS:HG2	1.89	0.55
7:O:274:LEU:HD22	7:O:278:LYS:HE3	1.89	0.55
20:h:92:ARG:HH22	22:j:101:LEU:HG	1.72	0.55
17:Y:-137:DC:H2"	17:Y:-136:DA:N7	2.22	0.55
6:N:234:ASP:O	6:N:237:ILE:HG22	2.06	0.55
10:U:257:GLU:O	10:U:260:LYS:HG2	2.07	0.55
12:T:540:PRO:HB3	13:W:15:ARG:CZ	2.37	0.55
14:S:86:ALA:HB3	14:S:96:ILE:HG21	1.89	0.55
18:a:522:ARG:HB2	22:j:109:HIS:CD2	2.42	0.55
5:L:218:LEU:HD23	5:L:304:LEU:HG	1.87	0.54
19:c:112:LEU:HD23	19:g:112:LEU:HD23	1.90	0.54
6:N:336:ILE:HG23	18:b:303:PHE:CE1	2.42	0.54
15:X:8:VAL:O	15:X:12:LEU:HG	2.06	0.54
22:j:57:LYS:HD2	22:j:58:ALA:N	2.21	0.54
5:L:211:LEU:HD12	5:L:212:ALA:N	2.23	0.54
21:e:54:VAL:HG13	22:f:110:ALA:HB1	1.89	0.54
21:i:77:ARG:HH21	22:j:55:SER:HA	1.72	0.54
1:H:155:LEU:HD11	1:H:159:LYS:HE3	1.90	0.54
6:N:118:ASN:HB3	6:N:144:PRO:HD3	1.89	0.54
6:N:181:ILE:HD11	10:U:328:LEU:HD11	1.88	0.54
12:T:520:ARG:NH2	12:T:525:VAL:HG12	2.23	0.54
13:W:14:LYS:HD3	13:W:16:LYS:HB3	1.90	0.54
19:c:128:LEU:HD23	19:g:115:HIS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:65:PHE:O	22:j:69:ILE:HG22	2.07	0.54
2:I:595:LEU:HD21	3:K:97:PHE:CD1	2.42	0.54
10:U:265:HIS:CE1	10:U:268:ARG:HH21	2.26	0.54
2:I:682:VAL:HG23	2:I:683:VAL:HG23	1.89	0.54
6:N:192:ASP:HB3	6:N:331:MET:SD	2.47	0.54
9:Q:211:LEU:HD12	9:Q:212:PRO:HD2	1.90	0.54
17:Y:-221:DC:H2''	17:Y:-220:DT:C6	2.42	0.54
2:I:360:PRO:HG2	2:I:363:MET:HA	1.90	0.54
4:M:129:LEU:HB3	4:M:142:MET:HE1	1.90	0.54
6:N:157:GLN:HE22	7:O:212:ASN:HB2	1.73	0.54
16:V:170:DA:H2''	16:V:171:DA:H8	1.72	0.54
17:Y:-200:DT:H2''	17:Y:-199:DG:C8	2.43	0.54
1:H:44:LEU:O	1:H:47:ARG:HG2	2.08	0.54
4:M:84:SER:HA	4:M:87:HIS:HD2	1.72	0.54
14:S:23:VAL:HG13	15:X:7:LEU:HD11	1.90	0.54
21:e:49:VAL:HG21	22:f:121:TYR:CG	2.42	0.54
2:I:92:LEU:HD21	2:I:128:ARG:HB3	1.90	0.54
2:I:131:LYS:HG2	2:I:268:LEU:HD13	1.90	0.54
6:N:83:TRP:CG	6:N:198:LEU:HD13	2.43	0.54
16:V:133:DA:H2''	16:V:134:DA:C8	2.43	0.54
17:Y:-190:DT:H2'	17:Y:-189:DT:H71	1.89	0.54
17:Y:-131:DC:H2''	17:Y:-130:DA:H8	1.72	0.54
17:Y:-123:DA:H2''	17:Y:-122:DC:C5	2.43	0.54
2:I:78:ILE:O	2:I:84:LYS:HG2	2.07	0.53
17:Y:-208:DC:H2''	17:Y:-207:DG:C8	2.43	0.53
1:H:136:LEU:O	1:H:140:ILE:HG12	2.07	0.53
2:I:559:HIS:CE1	3:K:107:VAL:HG21	2.43	0.53
2:I:595:LEU:HD22	3:K:96:GLU:HG2	1.89	0.53
5:L:128:LYS:HB3	5:L:133:ASP:HB2	1.89	0.53
6:N:336:ILE:HG23	18:b:303:PHE:CD1	2.43	0.53
16:V:237:DC:H2''	16:V:238:DG:C8	2.44	0.53
21:e:30:VAL:HA	21:e:33:LEU:HD12	1.89	0.53
21:e:49:VAL:HG12	22:f:117:ALA:HB1	1.89	0.53
2:I:350:LEU:HD22	2:I:371:LEU:HB3	1.90	0.53
2:I:489:PHE:O	2:I:493:VAL:HG23	2.07	0.53
2:I:389:TYR:CE2	5:L:31:LEU:HD21	2.44	0.53
7:O:100:ASN:O	7:O:104:ILE:HG12	2.07	0.53
13:W:25:VAL:O	13:W:28:ARG:HG2	2.09	0.53
21:e:106:GLY:HA2	20:h:40:ARG:HD3	1.91	0.53
14:S:53:LEU:HD21	15:X:67:LEU:HD13	1.90	0.53
17:Y:-141:DT:H2''	17:Y:-140:DG:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:e:26:PRO:HD3	22:f:40:TYR:CG	2.44	0.53
21:e:54:VAL:HG21	22:f:98:VAL:HG21	1.91	0.53
2:I:394:GLN:HB3	5:L:207:TYR:CE2	2.43	0.53
2:I:642:HIS:CE1	2:I:660:GLY:H	2.27	0.53
9:Q:76:LEU:HD22	9:Q:80:THR:HG21	1.91	0.53
1:H:212:ILE:HA	1:H:215:VAL:HG22	1.91	0.53
2:I:178:LYS:HA	2:I:181:ILE:HD12	1.90	0.53
2:I:445:LEU:HD21	4:M:114:ARG:HH12	1.74	0.53
6:N:141:TYR:HB2	9:Q:147:ARG:NH1	2.23	0.53
8:P:122:ILE:HG12	8:P:135:VAL:HG22	1.91	0.53
17:Y:-304:DT:H4'	17:Y:-303:DC:OP1	2.08	0.53
19:c:105:LEU:HD22	20:d:57:VAL:HG11	1.90	0.53
5:L:125:LEU:HD23	5:L:135:GLU:HG2	1.90	0.53
17:Y:-238:DC:H2''	17:Y:-237:DG:C8	2.44	0.53
5:L:240:LEU:HD22	5:L:306:ARG:HH21	1.73	0.53
8:P:240:THR:HB	8:P:242:VAL:HG23	1.90	0.53
14:S:13:PHE:O	14:S:17:GLN:HB2	2.10	0.53
16:V:136:DT:H2''	16:V:137:DG:C8	2.44	0.53
17:Y:-269:DT:H2'	17:Y:-268:DT:H71	1.90	0.53
1:H:148:TRP:O	1:H:151:GLU:HG2	2.09	0.52
7:O:186:ALA:O	7:O:190:ARG:HG3	2.08	0.52
5:L:85:TYR:OH	5:L:134:PRO:HB2	2.09	0.52
17:Y:-229:DA:H2''	17:Y:-228:DA:H8	1.75	0.52
18:b:531:TRP:HD1	19:c:127:GLN:HB3	1.75	0.52
21:e:92:GLU:HG2	22:f:103:PRO:HG2	1.89	0.52
1:H:218:ASN:HB3	3:K:249:ASN:HB3	1.91	0.52
2:I:228:LYS:HG3	2:I:229:MET:HG2	1.92	0.52
16:V:160:DC:H2'	16:V:161:DT:H71	1.91	0.52
2:I:663:ILE:HB	2:I:667:ILE:HG21	1.91	0.52
5:L:221:MET:HE3	5:L:334:TYR:CZ	2.44	0.52
16:V:168:DG:H2''	16:V:169:DA:H8	1.74	0.52
1:H:169:GLU:HA	2:I:378:CYS:HB3	1.90	0.52
2:I:370:SER:HA	2:I:373:LEU:HD12	1.92	0.52
2:I:392:LEU:HD22	2:I:434:SER:OG	2.08	0.52
1:H:161:ARG:HH22	2:I:428:LEU:H	1.57	0.52
1:H:162:LEU:HB3	2:I:510:MET:HG2	1.91	0.52
6:N:167:MET:HE3	6:N:170:ARG:HB2	1.91	0.52
7:O:192:TYR:O	7:O:196:ARG:HG2	2.08	0.52
16:V:170:DA:H2''	16:V:171:DA:C8	2.45	0.52
5:L:141:ILE:HG22	5:L:158:TRP:HB3	1.92	0.52
7:O:197:LEU:HD12	7:O:201:PHE:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:LEU:HD12	2:I:95:VAL:HG22	1.91	0.52
15:X:45:ARG:HG3	15:X:70:LEU:HD21	1.92	0.52
16:V:192:DA:H2''	16:V:193:DA:H5'	1.92	0.52
21:i:49:VAL:HG21	22:j:121:TYR:CG	2.45	0.52
2:I:214:VAL:HG11	2:I:246:ALA:HB3	1.92	0.52
7:O:280:LEU:O	7:O:283:VAL:HG22	2.10	0.52
16:V:192:DA:H2'	16:V:193:DA:C8	2.45	0.52
17:Y:-237:DG:H2'	17:Y:-236:DT:H71	1.92	0.52
22:j:99:ARG:CG	22:j:111:VAL:HG21	2.40	0.52
2:I:446:TRP:CZ3	2:I:448:GLY:HA2	2.45	0.51
9:Q:88:MET:HA	9:Q:91:VAL:HG12	1.92	0.51
12:T:477:ARG:HD3	12:T:480:LEU:HD12	1.92	0.51
2:I:651:LEU:HA	2:I:681:ASN:HA	1.91	0.51
12:T:522:GLN:HG3	13:W:86:SER:HA	1.91	0.51
21:i:51:LEU:HD21	22:j:70:PHE:CD1	2.46	0.51
1:H:194:ARG:HB3	3:K:159:PHE:CE1	2.45	0.51
2:I:464:PHE:HA	2:I:504:TRP:CE2	2.46	0.51
17:Y:-262:DT:H2''	17:Y:-261:DT:C6	2.45	0.51
20:d:26:ILE:HG12	20:d:59:LYS:HG3	1.91	0.51
1:H:75:GLU:HG2	3:K:57:LEU:HD13	1.93	0.51
20:d:88:TYR:HA	20:d:91:LYS:HE3	1.92	0.51
1:H:58:LYS:HA	1:H:61:VAL:HG12	1.92	0.51
22:j:117:ALA:O	22:j:120:LYS:HG3	2.11	0.51
10:U:398:LEU:HD11	11:R:110:ILE:HG12	1.92	0.51
16:V:207:DC:H2''	16:V:208:DG:C8	2.45	0.51
5:L:236:THR:HA	5:L:258:PRO:HG3	1.93	0.51
10:U:315:LYS:O	10:U:319:ARG:HG2	2.11	0.51
16:V:250:DC:H2''	16:V:251:DC:C5	2.45	0.51
8:P:223:ARG:NH1	11:R:122:LEU:HD23	2.26	0.51
9:Q:265:LEU:HD22	10:U:410:GLN:HB3	1.93	0.51
14:S:57:GLN:HG3	14:S:61:PHE:CE2	2.45	0.51
16:V:205:DG:H2'	16:V:206:DT:H71	1.93	0.51
1:H:217:GLN:HG2	1:H:240:LEU:HD13	1.93	0.51
7:O:165:ALA:O	7:O:169:LEU:HB2	2.11	0.51
12:T:472:LYS:O	12:T:473:MET:HE2	2.11	0.51
16:V:221:DG:H4'	19:c:85:ASN:HB3	1.93	0.51
21:i:30:VAL:HG11	21:i:52:ALA:HB2	1.92	0.51
4:M:6:PRO:HB3	4:M:96:LYS:HD2	1.92	0.50
17:Y:-224:DG:H2'	17:Y:-223:DT:H71	1.93	0.50
21:i:55:LEU:HD22	22:j:69:ILE:HG23	1.93	0.50
1:H:214:HIS:CD2	3:K:267:PHE:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:211:LEU:HD12	5:L:212:ALA:H	1.76	0.50
10:U:318:GLN:O	10:U:321:ILE:HG22	2.11	0.50
22:f:65:PHE:O	22:f:69:ILE:HG22	2.12	0.50
2:I:141:GLU:HA	2:I:175:ILE:HD11	1.92	0.50
2:I:247:PRO:HG2	2:I:318:TYR:CD1	2.46	0.50
2:I:668:LEU:HD21	2:I:676:TYR:HB3	1.92	0.50
16:V:233:DC:H2''	16:V:234:DG:C8	2.47	0.50
2:I:565:TYR:CZ	2:I:583:PHE:HA	2.46	0.50
2:I:634:SER:HA	2:I:637:TYR:HD2	1.76	0.50
3:K:258:ASP:OD2	3:K:261:ARG:HG3	2.12	0.50
6:N:140:GLN:NE2	10:U:317:ARG:HE	2.09	0.50
16:V:192:DA:H2'	16:V:193:DA:H8	1.74	0.50
16:V:280:DC:H2''	16:V:281:DC:C5	2.46	0.50
17:Y:-289:DG:P	21:i:32:ARG:HE	2.34	0.50
21:e:51:LEU:HD21	22:f:70:PHE:CD1	2.47	0.50
21:i:51:LEU:O	21:i:55:LEU:HG	2.12	0.50
21:i:80:PRO:N	22:j:57:LYS:HZ1	2.09	0.50
2:I:87:THR:HG23	2:I:90:LYS:HE2	1.93	0.50
6:N:267:ALA:HB3	6:N:297:PHE:HB2	1.93	0.50
16:V:173:DG:C2	17:Y:-172:DG:C2	3.00	0.50
20:d:84:MET:HA	20:d:87:VAL:HG22	1.93	0.50
1:H:49:GLN:HG2	4:M:156:HIS:HA	1.92	0.50
5:L:48:LYS:HA	5:L:274:GLU:HG2	1.92	0.50
8:P:89:THR:HG22	8:P:99:ARG:HG3	1.93	0.50
17:Y:-254:DC:H2''	17:Y:-253:DG:C8	2.47	0.50
1:H:130:MET:HB3	2:I:690:SER:OG	2.12	0.50
2:I:460:SER:HA	2:I:500:LEU:HB2	1.93	0.50
8:P:175:GLU:HG2	8:P:179:TYR:CE2	2.47	0.50
16:V:147:DA:H2''	16:V:148:DG:C8	2.46	0.50
20:d:35:ARG:O	20:d:39:ARG:HG2	2.12	0.50
1:H:105:ARG:HH22	2:I:595:LEU:HB2	1.77	0.50
11:R:97:SER:O	11:R:100:ILE:HG12	2.12	0.50
17:Y:-225:DG:H2'	17:Y:-224:DG:C8	2.46	0.50
1:H:237:VAL:HA	1:H:240:LEU:HD12	1.94	0.49
2:I:277:LYS:HB3	2:I:281:ARG:NH1	2.27	0.49
9:Q:124:LEU:HD22	10:U:257:GLU:HB3	1.94	0.49
17:Y:-155:DC:H2''	17:Y:-154:DA:C8	2.47	0.49
22:j:44:VAL:O	22:j:47:GLN:HG2	2.12	0.49
2:I:649:GLY:HA2	2:I:653:THR:OG1	2.12	0.49
4:M:152:ILE:HG21	4:M:165:LEU:HD21	1.93	0.49
10:U:274:CYS:O	10:U:278:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:135:DG:H1'	16:V:136:DT:OP2	2.12	0.49
16:V:154:DT:H2''	16:V:155:DG:C8	2.47	0.49
19:g:68:SER:HA	19:g:91:LEU:HD22	1.94	0.49
3:K:233:LYS:HG2	3:K:260:THR:HG22	1.94	0.49
7:O:109:HIS:HA	7:O:114:SER:HB3	1.94	0.49
1:H:50:THR:HB	3:K:31:MET:HE3	1.93	0.49
2:I:397:GLN:O	2:I:404:LYS:HE2	2.12	0.49
9:Q:242:LEU:HD11	10:U:394:ALA:HB2	1.95	0.49
11:R:87:MET:HE3	11:R:87:MET:HA	1.95	0.49
14:S:17:GLN:HA	14:S:20:LYS:HB3	1.95	0.49
16:V:217:DT:H2''	16:V:218:DC:C6	2.47	0.49
2:I:112:LEU:HB3	2:I:129:ILE:HD11	1.95	0.49
2:I:656:PRO:HG2	2:I:676:TYR:HD2	1.77	0.49
10:U:320:MET:HG2	10:U:324:GLN:NE2	2.28	0.49
15:X:13:HIS:HA	15:X:16:PHE:CD2	2.48	0.49
17:Y:-166:DA:H2''	17:Y:-165:DA:C8	2.48	0.49
21:e:116:LEU:HD21	19:g:48:LEU:HD22	1.94	0.49
1:H:60:MET:HE1	3:K:66:CYS:HB3	1.95	0.49
2:I:557:LEU:HG	2:I:561:ILE:HD11	1.95	0.49
6:N:8:PHE:CD2	6:N:66:ALA:HB1	2.48	0.49
7:O:143:VAL:HG23	7:O:151:HIS:HB2	1.95	0.49
16:V:218:DC:H2''	16:V:219:DT:C7	2.42	0.49
2:I:530:MET:SD	2:I:579:LEU:HB2	2.52	0.49
5:L:76:SER:OG	5:L:343:ILE:HG23	2.13	0.49
5:L:221:MET:HB3	5:L:225:TRP:CH2	2.47	0.49
6:N:100:ASP:HB3	6:N:103:GLN:CG	2.42	0.49
21:e:50:TYR:CZ	22:f:95:GLN:HA	2.46	0.49
21:i:64:GLU:HA	22:j:49:HIS:CD2	2.48	0.49
1:H:127:MET:HA	1:H:130:MET:HE3	1.94	0.49
6:N:111:ILE:HG21	6:N:178:ALA:HA	1.95	0.49
9:Q:92:ILE:HD12	9:Q:110:LEU:HD22	1.94	0.49
6:N:28:TRP:CE2	6:N:69:LEU:HB2	2.47	0.49
7:O:178:PHE:O	7:O:182:GLU:HG2	2.13	0.49
16:V:153:DT:H2'	16:V:154:DT:C6	2.48	0.49
21:e:29:ARG:HH11	22:f:40:TYR:HE2	1.60	0.49
4:M:92:PHE:O	4:M:96:LYS:HG2	2.13	0.48
4:M:167:SER:HA	4:M:170:ARG:NH1	2.28	0.48
6:N:157:GLN:NE2	7:O:212:ASN:HB2	2.28	0.48
6:N:157:GLN:NE2	7:O:213:PRO:HD2	2.28	0.48
13:W:21:PHE:O	13:W:24:ARG:HG2	2.12	0.48
19:g:61:LEU:HD12	20:h:37:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:377:ASN:HA	2:I:428:LEU:HD13	1.95	0.48
2:I:659:LYS:HA	2:I:662:TYR:HD1	1.79	0.48
3:K:215:MET:HE1	3:K:242:TYR:HD2	1.78	0.48
4:M:13:LEU:O	4:M:15:THR:HG23	2.13	0.48
5:L:68:LEU:HD11	5:L:325:HIS:HB3	1.94	0.48
8:P:153:PHE:CZ	8:P:169:SER:HB2	2.48	0.48
12:T:505:ALA:HB2	14:S:71:HIS:NE2	2.29	0.48
21:e:81:ARG:HG2	19:g:56:LYS:HA	1.95	0.48
2:I:135:PRO:HD3	2:I:167:TRP:CH2	2.46	0.48
2:I:492:SER:HB2	7:O:18:LEU:HD11	1.96	0.48
6:N:139:THR:HG22	6:N:142:THR:OG1	2.14	0.48
6:N:303:LEU:HA	6:N:306:LEU:HB2	1.94	0.48
8:P:196:TYR:CE2	8:P:209:ARG:HB3	2.48	0.48
19:c:112:LEU:HB3	19:g:115:HIS:CD2	2.48	0.48
14:S:40:MET:HE2	15:X:50:ALA:CB	2.44	0.48
17:Y:-289:DG:H2''	17:Y:-288:DA:H8	1.78	0.48
17:Y:-130:DA:H2''	17:Y:-129:DG:H8	1.77	0.48
21:e:30:VAL:HG11	21:e:52:ALA:HB2	1.95	0.48
21:e:95:LYS:HD3	22:f:103:PRO:HG3	1.95	0.48
16:V:169:DA:H2''	16:V:170:DA:C8	2.47	0.48
17:Y:-273:DC:H2''	17:Y:-272:DC:C6	2.49	0.48
19:c:133:ARG:HB3	19:c:137:GLU:HB2	1.95	0.48
2:I:401:ILE:HG23	2:I:408:TYR:HA	1.96	0.48
7:O:239:TYR:HE1	7:O:247:PRO:HB3	1.77	0.48
17:Y:-210:DT:H2''	17:Y:-209:DA:C8	2.48	0.48
22:j:34:LYS:HD2	22:j:34:LYS:O	2.14	0.48
6:N:302:LEU:C	6:N:304:GLU:H	2.22	0.48
10:U:400:ALA:HA	10:U:403:HIS:HB2	1.96	0.48
16:V:163:DC:H2''	16:V:164:DG:N7	2.29	0.48
21:e:97:LEU:HB3	21:e:100:VAL:HB	1.96	0.48
14:S:46:THR:HG23	15:X:63:LEU:HD22	1.95	0.48
16:V:132:DC:H2''	16:V:133:DA:C8	2.48	0.48
17:Y:-302:DC:H2''	17:Y:-301:DA:C8	2.48	0.48
21:i:25:PHE:CG	21:i:26:PRO:HD2	2.49	0.48
6:N:112:LEU:O	6:N:116:LEU:HG	2.13	0.48
16:V:253:DC:H2''	16:V:254:DG:C8	2.48	0.48
18:b:300:GLU:OE2	18:b:305:ILE:HG13	2.14	0.48
4:M:9:LYS:O	4:M:62:ARG:HD3	2.13	0.48
4:M:111:SER:HA	5:L:215:ALA:HB3	1.96	0.48
9:Q:83:HIS:O	9:Q:87:MET:HE3	2.14	0.48
11:R:135:GLU:O	11:R:139:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:248:DT:H2''	16:V:249:DC:C6	2.49	0.48
21:i:59:THR:OG1	22:j:62:MET:HE3	2.14	0.48
2:I:486:THR:HG21	7:O:25:GLU:CD	2.39	0.47
2:I:568:VAL:O	2:I:571:ILE:HG12	2.14	0.47
3:K:111:LYS:HD2	3:K:114:LYS:HE3	1.95	0.47
10:U:265:HIS:O	10:U:269:ILE:HG12	2.14	0.47
12:T:476:GLU:HG3	12:T:479:ALA:H	1.79	0.47
12:T:484:GLU:HA	12:T:487:LEU:HD12	1.94	0.47
14:S:66:GLU:HG2	14:S:70:ARG:NH1	2.29	0.47
16:V:152:DT:H3	17:Y:-151:DG:N2	2.11	0.47
18:a:531:TRP:HD1	19:g:127:GLN:HB3	1.79	0.47
6:N:206:PHE:HB2	6:N:208:GLN:HG2	1.95	0.47
9:Q:76:LEU:HD12	9:Q:121:CYS:HB2	1.95	0.47
16:V:168:DG:H2''	16:V:169:DA:C8	2.49	0.47
2:I:228:LYS:O	2:I:229:MET:HE2	2.13	0.47
15:X:28:LEU:HA	15:X:31:MET:HE3	1.96	0.47
21:e:57:TYR:O	21:e:61:GLU:HG2	2.14	0.47
1:H:136:LEU:HA	1:H:139:LEU:HD12	1.96	0.47
12:T:551:ALA:HB2	12:T:557:VAL:HG22	1.97	0.47
19:c:102:LEU:HD11	20:d:58:LEU:HB2	1.97	0.47
2:I:381:ASP:HB3	2:I:384:VAL:HG22	1.96	0.47
3:K:95:GLU:HA	3:K:98:GLN:OE1	2.15	0.47
14:S:86:ALA:HB1	14:S:92:LEU:HG	1.95	0.47
21:e:33:LEU:HB3	22:f:70:PHE:CZ	2.48	0.47
21:i:26:PRO:HB2	21:i:29:ARG:HB2	1.96	0.47
6:N:99:PHE:HB3	6:N:157:GLN:OE1	2.14	0.47
7:O:118:THR:HG23	7:O:120:ARG:H	1.79	0.47
9:Q:265:LEU:HD11	10:U:407:ILE:HG23	1.95	0.47
21:i:79:ILE:C	22:j:57:LYS:HZ1	2.22	0.47
21:i:87:ILE:HG13	21:i:88:ARG:HG2	1.96	0.47
22:j:37:TYR:O	22:j:41:VAL:HG23	2.15	0.47
2:I:379:VAL:HG12	2:I:381:ASP:H	1.79	0.47
2:I:386:LEU:HD11	5:L:27:LEU:HD13	1.95	0.47
5:L:165:VAL:HG12	5:L:166:PHE:CD2	2.50	0.47
10:U:357:PHE:CZ	10:U:361:LEU:HD11	2.49	0.47
16:V:156:DT:H2''	16:V:157:DG:N7	2.29	0.47
17:Y:-308:DC:H2''	17:Y:-307:DA:H8	1.79	0.47
17:Y:-253:DG:H2''	17:Y:-252:DG:C8	2.50	0.47
17:Y:-201:DT:H2''	17:Y:-200:DT:C6	2.50	0.47
19:c:115:HIS:ND1	19:g:116:ALA:HB2	2.30	0.47
21:e:115:LEU:HB3	19:g:47:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:229:MET:HA	13:W:12:GLN:HB3	1.97	0.47
4:M:167:SER:HA	4:M:170:ARG:HH12	1.80	0.47
5:L:33:SER:HA	5:L:36:LYS:HE2	1.97	0.47
17:Y:-226:DC:H2''	17:Y:-225:DG:H8	1.79	0.47
1:H:175:ILE:HD11	3:K:143:HIS:HB2	1.96	0.47
9:Q:176:ILE:HG13	10:U:334:LEU:HD13	1.96	0.47
21:e:87:ILE:HG13	21:e:88:ARG:HG2	1.97	0.47
22:j:41:VAL:HG11	22:j:59:MET:HA	1.97	0.47
1:H:244:VAL:HG12	3:K:169:ILE:HG12	1.96	0.47
2:I:231:MET:HE2	13:W:10:ARG:HB3	1.97	0.47
2:I:435:CYS:O	2:I:439:LEU:HD23	2.15	0.47
11:R:97:SER:HA	11:R:100:ILE:HG12	1.97	0.47
17:Y:-283:DA:H2''	17:Y:-282:DG:C8	2.50	0.47
3:K:32:TRP:O	3:K:35:MET:HB2	2.14	0.46
3:K:56:GLN:O	3:K:60:LEU:HG	2.16	0.46
3:K:241:PRO:HB2	12:T:551:ALA:N	2.30	0.46
7:O:155:VAL:HB	7:O:161:LEU:HD11	1.97	0.46
12:T:481:GLU:HA	12:T:484:GLU:CD	2.40	0.46
19:c:73:GLU:O	19:c:76:VAL:HG22	2.14	0.46
21:e:59:THR:CG2	22:f:62:MET:HE1	2.44	0.46
21:i:50:TYR:OH	22:j:111:VAL:HG22	2.15	0.46
5:L:230:MET:HE3	5:L:231:ASP:OD1	2.16	0.46
6:N:139:THR:HA	10:U:317:ARG:HH22	1.81	0.46
16:V:235:DC:H2''	16:V:236:DA:C8	2.50	0.46
5:L:228:CYS:HB3	5:L:327:TYR:CZ	2.50	0.46
6:N:214:GLU:HB2	7:O:123:CYS:HB3	1.96	0.46
8:P:240:THR:O	10:U:386:SER:HA	2.15	0.46
16:V:231:DA:H2''	16:V:232:DA:C8	2.50	0.46
19:c:54:LEU:HD12	20:d:39:ARG:HB2	1.97	0.46
22:j:102:LEU:HB2	22:j:107:ALA:HB2	1.97	0.46
1:H:89:ILE:HD11	3:K:74:TRP:CD1	2.51	0.46
2:I:252:VAL:HA	5:L:101:ALA:HB1	1.96	0.46
2:I:454:GLN:CD	2:I:454:GLN:H	2.22	0.46
10:U:368:TYR:HA	10:U:371:VAL:HG22	1.97	0.46
11:R:117:ARG:HA	11:R:120:GLU:HB2	1.96	0.46
12:T:533:VAL:HA	12:T:536:GLU:OE1	2.15	0.46
16:V:145:DG:H2''	16:V:146:DG:C8	2.50	0.46
21:e:80:PRO:HG3	22:f:57:LYS:HZ3	1.80	0.46
22:f:80:LEU:HD13	22:f:96:THR:HB	1.98	0.46
22:j:99:ARG:HA	22:j:107:ALA:HB1	1.96	0.46
1:H:45:ARG:HH21	4:M:42:SER:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:255:HIS:HB3	3:K:258:ASP:O	2.15	0.46
21:e:51:LEU:HD21	22:f:70:PHE:HD1	1.80	0.46
1:H:164:LEU:HD12	3:K:129:LEU:HD12	1.97	0.46
2:I:722:TYR:O	2:I:726:GLN:HG2	2.15	0.46
5:L:56:GLN:HB2	5:L:59:VAL:HG23	1.96	0.46
12:T:467:PHE:HE2	13:W:54:LEU:HG	1.81	0.46
16:V:275:DT:H2'	16:V:276:DT:H71	1.97	0.46
17:Y:-301:DA:H2''	17:Y:-300:DG:C8	2.51	0.46
19:c:107:GLU:CD	20:d:41:GLY:HA2	2.40	0.46
20:h:58:LEU:O	20:h:62:LEU:HG	2.16	0.46
1:H:36:SER:HA	1:H:39:ARG:HG2	1.98	0.46
2:I:226:GLN:CG	5:L:107:LEU:HD22	2.46	0.46
2:I:322:CYS:SG	5:L:87:ASN:HB3	2.56	0.46
2:I:400:CYS:SG	2:I:403:TYR:HB3	2.55	0.46
2:I:539:TYR:CE2	2:I:543:LEU:HD11	2.51	0.46
2:I:595:LEU:HD21	3:K:97:PHE:HD1	1.81	0.46
5:L:143:SER:HB2	5:L:157:LEU:HD11	1.98	0.46
6:N:205:VAL:HA	6:N:330:ARG:HD2	1.98	0.46
7:O:121:GLY:HA3	7:O:144:ILE:HG23	1.98	0.46
16:V:213:DC:H2''	16:V:214:DA:C8	2.51	0.46
21:i:55:LEU:CD2	22:j:69:ILE:HG23	2.45	0.46
22:j:99:ARG:HG2	22:j:111:VAL:HG21	1.97	0.46
2:I:252:VAL:HB	5:L:108:ALA:HA	1.98	0.46
2:I:350:LEU:O	2:I:354:ILE:HG23	2.15	0.46
4:M:36:LEU:HB3	6:N:236:ARG:NH2	2.31	0.46
6:N:166:SER:H	6:N:168:LEU:HD22	1.81	0.46
9:Q:250:GLN:HE21	11:R:96:LEU:HD22	1.81	0.46
17:Y:-196:DT:H2''	17:Y:-195:DA:C8	2.51	0.46
17:Y:-125:DC:H2''	17:Y:-124:DT:C6	2.51	0.46
22:j:56:SER:O	22:j:59:MET:HB3	2.15	0.46
22:j:102:LEU:HD12	22:j:107:ALA:HA	1.97	0.46
1:H:175:ILE:HG23	3:K:146:LEU:HD12	1.97	0.46
3:K:80:GLU:HG3	3:K:82:ILE:HG12	1.97	0.46
5:L:141:ILE:HG23	5:L:157:LEU:HB2	1.97	0.46
8:P:154:VAL:HG22	8:P:166:PHE:HE1	1.80	0.46
17:Y:-157:DC:H6	17:Y:-157:DC:H2'	1.65	0.46
2:I:69:ALA:HA	2:I:91:HIS:CG	2.51	0.45
2:I:665:PRO:HA	2:I:668:LEU:HG	1.97	0.45
5:L:96:ASN:HB2	5:L:119:VAL:HB	1.98	0.45
8:P:176:TRP:CD2	8:P:234:PRO:HG3	2.51	0.45
9:Q:87:MET:HE2	9:Q:87:MET:HB3	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:155:DG:C8	16:V:155:DG:H5'	2.51	0.45
17:Y:-242:DC:H2''	17:Y:-241:DG:C8	2.51	0.45
3:K:172:TYR:CE1	3:K:176:LEU:HD11	2.52	0.45
5:L:276:THR:HG23	5:L:279:GLU:H	1.81	0.45
6:N:121:VAL:HG22	6:N:135:ILE:HG23	1.98	0.45
6:N:152:VAL:HG23	6:N:163:THR:HG22	1.98	0.45
17:Y:-261:DT:H2''	17:Y:-260:DA:C8	2.51	0.45
22:f:61:ILE:HG23	20:h:98:TYR:HB3	1.99	0.45
3:K:248:ARG:NH2	12:T:545:GLN:HA	2.31	0.45
11:R:92:LYS:HA	11:R:95:LYS:NZ	2.31	0.45
18:b:260:LYS:HZ2	18:b:265:LEU:HD23	1.80	0.45
21:e:115:LEU:HD21	19:g:114:LEU:HD21	1.98	0.45
3:K:248:ARG:CB	12:T:544:ARG:HH12	2.30	0.45
6:N:141:TYR:CZ	10:U:310:ILE:HD12	2.51	0.45
9:Q:168:THR:O	9:Q:172:MET:HG2	2.17	0.45
13:W:44:HIS:O	13:W:48:LEU:HG	2.17	0.45
14:S:64:ASP:HA	14:S:67:MET:HE3	1.98	0.45
20:h:92:ARG:CZ	22:j:100:LEU:HB3	2.46	0.45
4:M:107:GLU:HA	4:M:110:CYS:SG	2.56	0.45
6:N:129:ASN:ND2	7:O:213:PRO:HG3	2.32	0.45
7:O:279:PRO:O	7:O:283:VAL:HG13	2.16	0.45
14:S:93:LEU:HA	14:S:96:ILE:HG22	1.97	0.45
1:H:231:PRO:O	1:H:235:GLU:HG2	2.16	0.45
2:I:475:PHE:HA	2:I:478:LEU:HB2	1.98	0.45
5:L:88:LEU:HD22	5:L:121:PHE:HD2	1.81	0.45
8:P:184:PHE:HD2	8:P:201:PRO:HA	1.82	0.45
16:V:195:DT:H2''	16:V:196:DA:C8	2.51	0.45
22:f:84:ASN:O	22:f:86:ARG:HG3	2.17	0.45
1:H:211:VAL:HG23	3:K:268:HIS:HB3	1.98	0.45
4:M:9:LYS:HB2	4:M:62:ARG:HB2	1.98	0.45
16:V:279:DT:H2''	16:V:280:DC:C6	2.51	0.45
19:g:120:THR:HA	20:h:45:ARG:HB2	1.98	0.45
20:h:75:HIS:HB2	22:j:96:THR:OG1	2.17	0.45
1:H:53:GLN:HB2	3:K:35:MET:HE1	1.99	0.45
3:K:30:GLU:O	3:K:33:LYS:HG2	2.16	0.45
6:N:32:SER:O	6:N:36:LEU:HG	2.16	0.45
12:T:543:TYR:HB3	13:W:41:LEU:HD21	1.99	0.45
15:X:61:ASP:O	15:X:64:GLU:HG2	2.17	0.45
19:c:120:THR:HA	20:d:45:ARG:HB2	1.99	0.45
19:g:137:GLU:HA	20:h:95:ARG:NH2	2.31	0.45
1:H:134:LEU:HD22	2:I:691:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:170:ALA:HB1	2:I:273:LEU:HD11	1.99	0.45
5:L:98:PHE:O	5:L:102:GLU:HG2	2.16	0.45
8:P:118:LEU:HB3	8:P:140:ILE:HG13	1.99	0.45
12:T:451:PRO:HG2	17:Y:-144:DG:O4'	2.17	0.45
15:X:4:ARG:HB2	15:X:7:LEU:HB3	1.99	0.45
17:Y:-225:DG:H2''	17:Y:-224:DG:O5'	2.16	0.45
18:b:297:LYS:HG2	18:b:300:GLU:HB3	1.99	0.45
19:c:125:ASP:HA	19:g:115:HIS:HE2	1.82	0.45
1:H:166:GLN:NE2	2:I:510:MET:HG3	2.31	0.45
2:I:141:GLU:CD	2:I:180:GLN:HB2	2.42	0.45
2:I:614:LEU:HD22	2:I:637:TYR:CE1	2.51	0.45
7:O:239:TYR:CD1	7:O:247:PRO:HA	2.52	0.45
8:P:171:HIS:HA	8:P:174:VAL:HG22	1.99	0.45
17:Y:-268:DT:C2	17:Y:-267:DG:C8	3.05	0.45
17:Y:-207:DG:H2''	17:Y:-206:DA:C8	2.52	0.45
17:Y:-155:DC:H4'	17:Y:-154:DA:H5'	1.98	0.45
2:I:119:GLY:HA2	2:I:126:ASN:OD1	2.17	0.44
2:I:498:LYS:HD2	2:I:567:LYS:HG3	1.99	0.44
12:T:521:ARG:HB3	14:S:88:ARG:NH2	2.32	0.44
16:V:229:DT:H2''	16:V:230:DA:N7	2.32	0.44
17:Y:-244:DC:H2''	17:Y:-243:DG:C8	2.51	0.44
22:f:37:TYR:O	22:f:41:VAL:HG23	2.17	0.44
22:f:99:ARG:CG	22:f:111:VAL:HG21	2.47	0.44
2:I:135:PRO:O	2:I:276:VAL:HG11	2.17	0.44
2:I:337:GLY:O	2:I:356:CYS:HB3	2.17	0.44
3:K:188:PHE:HE1	12:T:552:TYR:HA	1.82	0.44
9:Q:157:LEU:O	9:Q:161:GLU:HG2	2.18	0.44
9:Q:186:LEU:HD21	10:U:345:LYS:HB3	1.99	0.44
12:T:510:VAL:HG22	13:W:35:LEU:HA	1.99	0.44
19:c:137:GLU:HA	20:d:95:ARG:HH22	1.82	0.44
22:f:120:LYS:HD2	22:f:121:TYR:N	2.32	0.44
21:i:26:PRO:HD3	22:j:40:TYR:CG	2.51	0.44
1:H:183:LYS:HE2	2:I:335:ARG:HB3	1.99	0.44
2:I:340:PRO:HA	2:I:358:GLU:OE1	2.17	0.44
7:O:174:GLN:HG2	7:O:175:HIS:N	2.32	0.44
12:T:495:CYS:O	12:T:499:GLU:OE1	2.35	0.44
16:V:287:DC:H2'	16:V:288:DT:H71	2.00	0.44
18:a:527:PRO:HB2	18:a:530:TRP:CD1	2.52	0.44
22:f:34:LYS:HD2	22:f:34:LYS:O	2.17	0.44
1:H:201:ASN:CB	3:K:166:MET:HE1	2.47	0.44
2:I:225:LEU:HA	2:I:228:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:20:LEU:HD13	4:M:31:LEU:HD22	1.99	0.44
13:W:25:VAL:HG12	13:W:28:ARG:CZ	2.47	0.44
14:S:33:GLU:O	14:S:36:LEU:HG	2.17	0.44
16:V:260:DT:H2''	16:V:261:DA:C8	2.52	0.44
1:H:191:ASN:ND2	1:H:194:ARG:HE	2.16	0.44
2:I:247:PRO:HG2	2:I:318:TYR:CE1	2.53	0.44
5:L:100:VAL:HG21	5:L:115:PHE:CG	2.53	0.44
6:N:174:LEU:HA	10:U:321:ILE:HD11	1.98	0.44
7:O:265:GLU:HG2	7:O:268:ARG:NH2	2.32	0.44
8:P:173:PHE:HA	8:P:232:VAL:HG11	2.00	0.44
10:U:310:ILE:O	10:U:313:ILE:HG22	2.17	0.44
12:T:478:LYS:HA	12:T:481:GLU:OE1	2.18	0.44
19:c:45:GLN:HB3	19:c:47:TRP:CD1	2.52	0.44
19:c:130:ARG:NH1	20:d:57:VAL:HG22	2.32	0.44
21:e:24:GLN:HB2	22:f:44:VAL:HG22	1.99	0.44
2:I:164:PHE:CE2	2:I:168:LEU:HD11	2.53	0.44
2:I:377:ASN:HB2	2:I:428:LEU:HD22	2.00	0.44
3:K:60:LEU:HA	3:K:63:GLN:OE1	2.17	0.44
8:P:213:ARG:HB3	10:U:372:GLN:NE2	2.33	0.44
12:T:475:MET:HG3	12:T:480:LEU:HD21	1.99	0.44
17:Y:-214:DT:H2''	17:Y:-213:DG:C8	2.53	0.44
17:Y:-127:DT:H2''	17:Y:-126:DA:C8	2.52	0.44
19:c:75:CYS:HB2	19:c:86:TRP:HE1	1.83	0.44
21:e:96:LEU:HD21	22:f:69:ILE:HD13	2.00	0.44
22:j:120:LYS:HD2	22:j:121:TYR:N	2.33	0.44
3:K:248:ARG:HB2	12:T:544:ARG:HH12	1.83	0.44
5:L:165:VAL:HG21	5:L:332:LEU:HB3	2.00	0.44
7:O:191:LYS:HD3	7:O:215:CYS:SG	2.58	0.44
13:W:49:LEU:O	13:W:53:ARG:HG3	2.18	0.44
19:c:70:LEU:HA	19:c:73:GLU:HG2	2.00	0.44
19:c:103:VAL:O	19:c:107:GLU:OE1	2.35	0.44
20:d:75:HIS:CE1	22:f:93:GLU:HG3	2.53	0.44
21:e:18:SER:OG	21:e:26:PRO:HA	2.18	0.44
21:e:55:LEU:CD2	22:f:69:ILE:HG23	2.48	0.44
2:I:405:VAL:HA	4:M:106:ARG:HG2	1.99	0.44
2:I:589:TYR:HA	2:I:592:LEU:HD12	2.00	0.44
5:L:264:LEU:HA	6:N:284:LEU:HD11	1.99	0.44
9:Q:182:LYS:HB3	10:U:341:TYR:CE1	2.52	0.44
16:V:160:DC:H2'	16:V:161:DT:C7	2.47	0.44
16:V:172:DC:C2	16:V:173:DG:N7	2.86	0.44
16:V:305:DA:H2'	16:V:306:DT:H71	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:110:TYR:HB2	20:d:43:VAL:HG22	1.99	0.44
21:e:115:LEU:HB3	19:g:47:TRP:HH2	1.83	0.44
2:I:103:GLY:CA	2:I:136:ALA:HB2	2.45	0.44
2:I:401:ILE:HD12	2:I:451:CYS:SG	2.58	0.44
2:I:640:PHE:CE2	2:I:644:LEU:HD11	2.53	0.44
7:O:117:LEU:HB2	8:P:62:HIS:NE2	2.33	0.44
16:V:155:DG:N2	17:Y:-154:DA:C2	2.86	0.44
16:V:260:DT:H2''	16:V:261:DA:N7	2.33	0.44
22:f:42:TYR:HE1	22:f:53:GLY:HA2	1.82	0.44
21:i:66:ALA:O	21:i:82:HIS:HB3	2.17	0.44
1:H:52:GLN:O	1:H:56:GLU:OE1	2.36	0.43
2:I:234:HIS:CD2	2:I:235:LEU:HD12	2.53	0.43
16:V:292:DT:H6	16:V:292:DT:H2'	1.70	0.43
21:e:110:ASN:H	19:g:55:GLN:HE22	1.66	0.43
1:H:107:ARG:HA	2:I:673:VAL:HG22	1.99	0.43
2:I:316:SER:OG	2:I:320:LYS:HD3	2.18	0.43
6:N:263:GLN:HA	6:N:301:HIS:NE2	2.33	0.43
8:P:222:TRP:CD2	8:P:236:LEU:HD21	2.53	0.43
9:Q:97:SER:HA	14:S:21:ALA:HB1	2.00	0.43
9:Q:193:GLU:HB3	10:U:351:LEU:HD22	2.00	0.43
11:R:90:LEU:HA	11:R:93:VAL:HG22	2.00	0.43
16:V:161:DT:H2'	16:V:162:DT:H71	2.00	0.43
22:f:43:LYS:O	22:f:46:LYS:HB2	2.18	0.43
1:H:50:THR:CG2	3:K:31:MET:HE3	2.48	0.43
2:I:225:LEU:HD23	2:I:228:LYS:HE3	1.99	0.43
5:L:35:ARG:NH1	5:L:344:GLU:HB3	2.33	0.43
6:N:197:TYR:HE2	6:N:265:GLU:HB3	1.83	0.43
12:T:483:VAL:O	12:T:487:LEU:HG	2.17	0.43
13:W:53:ARG:O	13:W:57:GLU:HG2	2.17	0.43
17:Y:-220:DT:H2''	17:Y:-219:DA:N7	2.34	0.43
19:c:107:GLU:OE2	20:d:41:GLY:HA2	2.18	0.43
19:g:93:ALA:O	19:g:96:GLU:HG3	2.18	0.43
21:i:26:PRO:HD3	22:j:40:TYR:CD1	2.54	0.43
1:H:54:LEU:CD2	3:K:31:MET:HG3	2.43	0.43
1:H:145:GLN:HA	1:H:148:TRP:CE3	2.53	0.43
2:I:72:TYR:HA	2:I:75:LYS:HD2	2.01	0.43
2:I:445:LEU:HD21	4:M:114:ARG:NH1	2.33	0.43
2:I:486:THR:HG21	7:O:25:GLU:OE1	2.18	0.43
2:I:492:SER:HB3	7:O:21:LEU:HD23	1.99	0.43
5:L:334:TYR:O	5:L:337:GLU:HG2	2.18	0.43
6:N:247:ARG:HA	6:N:250:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:186:HIS:CE1	9:Q:209:LEU:HD13	2.53	0.43
9:Q:141:LEU:HD21	10:U:298:MET:HG3	2.00	0.43
16:V:172:DC:H2''	16:V:173:DG:H8	1.83	0.43
21:e:53:ALA:HB3	22:f:114:GLY:HA2	1.99	0.43
21:i:95:LYS:HD3	22:j:103:PRO:HG3	2.00	0.43
2:I:353:ASN:HA	2:I:355:HIS:ND1	2.34	0.43
3:K:103:ASP:O	3:K:107:VAL:HG23	2.18	0.43
8:P:276:GLU:HG3	9:Q:202:GLN:NE2	2.33	0.43
17:Y:-226:DC:C2	17:Y:-225:DG:N7	2.86	0.43
1:H:113:LYS:HA	1:H:116:LEU:HG	2.01	0.43
2:I:114:ASN:HD21	2:I:146:LYS:HE3	1.84	0.43
2:I:467:PHE:HA	2:I:470:VAL:HG12	2.01	0.43
4:M:45:LYS:NZ	6:N:236:ARG:HG2	2.33	0.43
6:N:8:PHE:CE1	6:N:146:GLN:HB3	2.53	0.43
6:N:321:PRO:HG3	18:b:296:THR:HB	2.00	0.43
20:d:92:ARG:HH22	22:f:101:LEU:HG	1.82	0.43
21:e:79:ILE:C	22:f:57:LYS:HZ1	2.26	0.43
1:H:236:ILE:O	1:H:240:LEU:HG	2.19	0.43
2:I:471:LYS:HA	2:I:475:PHE:HD1	1.84	0.43
2:I:472:PRO:HB3	4:M:172:SER:HB2	2.01	0.43
2:I:668:LEU:HD11	2:I:676:TYR:CD1	2.54	0.43
3:K:230:PRO:HG2	3:K:263:ARG:HB2	2.00	0.43
16:V:235:DC:H2''	16:V:236:DA:H8	1.83	0.43
17:Y:-259:DA:H2''	17:Y:-258:DA:H8	1.84	0.43
22:f:41:VAL:HG13	22:f:62:MET:SD	2.58	0.43
22:f:80:LEU:HD11	22:f:100:LEU:HD12	2.01	0.43
21:i:27:VAL:HA	21:i:30:VAL:HG12	2.00	0.43
1:H:77:GLN:HG2	1:H:78:ILE:N	2.33	0.43
6:N:215:THR:HB	7:O:125:CYS:SG	2.59	0.43
12:T:450:ARG:NH2	17:Y:-145:DC:H5'	2.34	0.43
12:T:451:PRO:O	17:Y:-144:DG:H4'	2.19	0.43
20:h:84:MET:HB2	20:h:88:TYR:CZ	2.54	0.43
1:H:87:ASN:O	1:H:91:GLU:OE1	2.35	0.43
2:I:369:ASN:O	2:I:373:LEU:HG	2.18	0.43
2:I:377:ASN:CB	2:I:428:LEU:HD22	2.49	0.43
2:I:486:THR:HG21	7:O:25:GLU:OE2	2.18	0.43
3:K:36:GLU:HG2	18:b:259:LYS:HD3	2.01	0.43
10:U:321:ILE:HA	10:U:324:GLN:HE21	1.84	0.43
14:S:8:GLU:HB3	14:S:12:ARG:HH12	1.83	0.43
14:S:13:PHE:O	14:S:17:GLN:CB	2.67	0.43
14:S:19:LEU:O	14:S:23:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:-234:DC:H2''	17:Y:-233:DG:C8	2.54	0.43
20:h:35:ARG:O	20:h:39:ARG:HG2	2.19	0.43
21:i:29:ARG:HH11	22:j:40:TYR:HE2	1.67	0.43
1:H:187:ASP:OD1	2:I:329:LEU:HB3	2.19	0.43
1:H:216:PHE:CD2	1:H:240:LEU:HD11	2.54	0.43
2:I:436:GLU:OE1	2:I:463:PRO:HD2	2.18	0.43
5:L:80:LEU:O	5:L:178:PHE:HA	2.19	0.43
8:P:106:ARG:NH2	8:P:108:SER:HB3	2.34	0.43
9:Q:186:LEU:HD21	10:U:345:LYS:N	2.34	0.43
2:I:117:LEU:HD13	2:I:147:ALA:HA	2.00	0.42
2:I:320:LYS:C	2:I:322:CYS:H	2.27	0.42
7:O:134:LEU:HD11	8:P:122:ILE:HD13	2.00	0.42
8:P:173:PHE:N	8:P:232:VAL:HG21	2.34	0.42
1:H:53:GLN:CB	3:K:35:MET:HE1	2.49	0.42
1:H:209:THR:HG22	1:H:213:GLN:OE1	2.19	0.42
2:I:392:LEU:O	2:I:396:LEU:HD23	2.18	0.42
3:K:248:ARG:CZ	12:T:545:GLN:HA	2.49	0.42
5:L:26:PRO:C	5:L:30:ARG:HE	2.27	0.42
6:N:20:GLU:CD	6:N:20:GLU:H	2.27	0.42
6:N:44:ARG:HB3	6:N:46:GLU:OE1	2.18	0.42
6:N:135:ILE:HG22	6:N:137:TRP:CD1	2.53	0.42
14:S:15:TYR:O	14:S:18:ARG:HG2	2.19	0.42
16:V:138:DG:H2''	16:V:139:DA:H8	1.85	0.42
19:c:61:LEU:HD12	20:d:37:LEU:HD23	1.99	0.42
21:e:26:PRO:HB2	21:e:29:ARG:HB2	2.01	0.42
19:g:75:CYS:SG	19:g:84:PHE:HB2	2.59	0.42
21:i:27:VAL:HG11	21:i:49:VAL:HG22	2.00	0.42
1:H:189:MET:SD	3:K:155:GLU:HB2	2.59	0.42
2:I:596:ASP:HB3	2:I:599:ILE:CG1	2.50	0.42
3:K:226:VAL:HG12	3:K:229:ASP:H	1.82	0.42
4:M:35:MET:HE1	4:M:143:ALA:HA	2.01	0.42
6:N:116:LEU:HD11	6:N:119:VAL:HB	2.01	0.42
7:O:222:TYR:HE2	7:O:224:LEU:HD11	1.84	0.42
11:R:172:LEU:HD12	11:R:173:LYS:N	2.34	0.42
14:S:89:SER:HB3	14:S:92:LEU:HB3	2.01	0.42
16:V:243:DC:H2''	16:V:244:DG:C8	2.55	0.42
17:Y:-193:DT:H4'	17:Y:-192:DT:OP1	2.20	0.42
19:c:98:ALA:HB2	20:d:62:LEU:HD21	2.01	0.42
20:d:98:TYR:CZ	22:j:65:PHE:HA	2.54	0.42
21:e:50:TYR:OH	22:f:95:GLN:HA	2.20	0.42
3:K:163:LYS:O	3:K:166:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:247:LEU:HD23	3:K:252:ALA:O	2.20	0.42
6:N:13:ILE:HD11	6:N:52:LEU:HD13	2.02	0.42
10:U:278:ILE:HA	10:U:281:PHE:CD1	2.54	0.42
11:R:94:GLU:HA	11:R:136:MET:SD	2.59	0.42
20:d:34:ILE:HD11	20:d:55:ARG:HG3	2.02	0.42
21:e:90:ASP:HB3	21:e:93:LEU:HB2	2.00	0.42
19:g:87:GLN:HB3	19:g:89:GLN:NE2	2.34	0.42
20:h:73:THR:OG1	20:h:81:VAL:HA	2.19	0.42
21:i:53:ALA:HB3	22:j:114:GLY:HA2	2.00	0.42
2:I:558:LEU:HA	2:I:561:ILE:HD12	2.01	0.42
4:M:92:PHE:O	4:M:97:VAL:HG23	2.19	0.42
9:Q:114:LYS:O	9:Q:118:LEU:HG	2.19	0.42
20:d:34:ILE:HA	20:d:37:LEU:HD12	2.02	0.42
1:H:85:LEU:HD13	3:K:67:LEU:HB2	2.00	0.42
2:I:87:THR:O	2:I:90:LYS:HG2	2.19	0.42
2:I:661:ILE:HG22	2:I:663:ILE:HG12	2.01	0.42
3:K:163:LYS:O	3:K:167:LEU:HG	2.19	0.42
3:K:191:PRO:HG3	3:K:239:TRP:CE2	2.54	0.42
3:K:234:ILE:HG12	3:K:260:THR:O	2.19	0.42
5:L:99:ILE:HG13	5:L:100:VAL:N	2.34	0.42
6:N:309:LEU:HG	6:N:314:ILE:HD11	2.01	0.42
7:O:259:VAL:HG11	7:O:268:ARG:HH12	1.85	0.42
9:Q:186:LEU:O	9:Q:190:VAL:HG23	2.19	0.42
15:X:12:LEU:HD13	15:X:23:VAL:HG21	2.02	0.42
17:Y:-206:DA:C4	17:Y:-205:DC:C5	3.08	0.42
17:Y:-130:DA:H2''	17:Y:-129:DG:C8	2.54	0.42
22:f:60:GLY:HA2	22:f:63:ASN:HD22	1.84	0.42
19:g:133:ARG:HB3	19:g:137:GLU:HB2	2.02	0.42
21:i:70:ALA:HA	21:i:82:HIS:CE1	2.54	0.42
1:H:200:GLN:O	1:H:203:GLN:HG3	2.19	0.42
6:N:18:MET:HE1	16:V:158:DG:H3'	2.00	0.42
13:W:79:ALA:HA	13:W:82:ILE:HG22	2.01	0.42
16:V:179:DA:H2'	16:V:180:DT:H71	2.02	0.42
16:V:284:DA:H5'	21:i:42:ARG:HD3	2.02	0.42
1:H:216:PHE:HD2	1:H:240:LEU:HD11	1.84	0.42
3:K:58:SER:HA	3:K:61:ILE:HD12	2.01	0.42
4:M:82:GLU:HA	4:M:85:LEU:HD12	2.01	0.42
6:N:321:PRO:HA	6:N:324:THR:OG1	2.20	0.42
7:O:146:LYS:HD2	11:R:169:TYR:CD2	2.54	0.42
9:Q:87:MET:HE1	9:Q:134:LEU:HD11	2.01	0.42
9:Q:251:MET:SD	10:U:397:LEU:HD22	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:103:ILE:HD13	15:X:30:LEU:HG	2.02	0.42
15:X:8:VAL:HG21	15:X:32:VAL:HG22	2.00	0.42
16:V:255:DC:H2''	16:V:256:DG:H8	1.84	0.42
16:V:312:DA:C8	16:V:313:DT:H72	2.55	0.42
17:Y:-163:DG:H2''	17:Y:-162:DA:OP2	2.18	0.42
19:c:125:ASP:HA	19:g:115:HIS:NE2	2.34	0.42
21:e:26:PRO:HD3	22:f:40:TYR:CD2	2.55	0.42
21:i:51:LEU:HD21	22:j:70:PHE:HD1	1.82	0.42
1:H:87:ASN:O	1:H:90:GLU:HB3	2.19	0.42
3:K:188:PHE:CE1	12:T:552:TYR:HA	2.55	0.42
6:N:217:ASN:HA	7:O:106:GLN:HA	2.01	0.42
6:N:242:ILE:HA	6:N:245:LYS:HD2	2.00	0.42
7:O:190:ARG:HD2	7:O:239:TYR:CD2	2.54	0.42
16:V:173:DG:C2	16:V:174:DG:C5	3.08	0.42
16:V:291:DT:H1'	16:V:292:DT:C4	2.55	0.42
17:Y:-164:DC:H2''	17:Y:-163:DG:N7	2.35	0.42
17:Y:-162:DA:H1'	17:Y:-161:DA:H5'	2.02	0.42
1:H:204:MET:O	1:H:208:ILE:HG12	2.19	0.42
2:I:659:LYS:O	2:I:662:TYR:HB2	2.19	0.42
8:P:209:ARG:HD2	8:P:214:PRO:HA	2.01	0.42
11:R:132:LEU:HD12	11:R:132:LEU:HA	1.91	0.42
16:V:304:DA:H2''	16:V:305:DA:H8	1.85	0.42
17:Y:-221:DC:H2''	17:Y:-220:DT:C5	2.55	0.42
21:i:18:SER:OG	21:i:26:PRO:HA	2.19	0.42
22:j:102:LEU:HB3	22:j:106:LEU:HD23	2.02	0.42
1:H:216:PHE:O	1:H:220:ILE:HG12	2.20	0.41
2:I:607:MET:HE2	2:I:647:MET:SD	2.59	0.41
2:I:623:VAL:HG23	2:I:624:GLN:HG3	2.02	0.41
5:L:60:ASP:CG	5:L:62:GLN:HG2	2.45	0.41
5:L:339:ALA:O	5:L:343:ILE:HG12	2.20	0.41
8:P:79:ARG:HG2	8:P:109:GLY:HA2	2.02	0.41
8:P:224:ILE:HA	8:P:234:PRO:HA	2.02	0.41
8:P:237:ASP:HB3	9:Q:224:LEU:HB2	2.01	0.41
9:Q:85:GLN:O	9:Q:88:MET:HG3	2.20	0.41
12:T:456:HIS:HA	13:W:21:PHE:HE1	1.84	0.41
16:V:228:DT:H2''	16:V:229:DT:C6	2.54	0.41
16:V:294:DT:H2''	16:V:295:DA:C8	2.55	0.41
20:d:48:GLY:HA2	20:d:51:TYR:HE2	1.85	0.41
21:e:80:PRO:N	22:f:57:LYS:HZ1	2.18	0.41
1:H:130:MET:HA	1:H:133:LEU:HD12	2.02	0.41
2:I:417:PHE:CE2	2:I:421:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:36:GLU:HB3	18:b:259:LYS:HD3	2.02	0.41
6:N:75:GLN:O	6:N:78:GLN:HG3	2.20	0.41
9:Q:92:ILE:HG23	9:Q:110:LEU:HB3	2.02	0.41
17:Y:-252:DG:H2''	17:Y:-251:DG:C8	2.55	0.41
19:c:109:ALA:HB1	19:c:121:LEU:HD11	2.02	0.41
21:e:50:TYR:OH	22:f:111:VAL:HG22	2.20	0.41
1:H:209:THR:HA	1:H:212:ILE:HG12	2.02	0.41
4:M:102:THR:HG22	4:M:133:LEU:HD23	2.02	0.41
8:P:140:ILE:HD11	8:P:166:PHE:CZ	2.55	0.41
16:V:146:DG:H2''	16:V:147:DA:C8	2.56	0.41
16:V:238:DG:H2''	16:V:239:DT:C6	2.55	0.41
20:d:58:LEU:O	20:d:62:LEU:HG	2.20	0.41
22:f:38:SER:O	22:f:41:VAL:HB	2.20	0.41
1:H:161:ARG:NH2	2:I:428:LEU:H	2.18	0.41
1:H:208:ILE:HD13	3:K:224:PHE:CZ	2.55	0.41
2:I:453:SER:O	2:I:457:GLN:HG3	2.20	0.41
9:Q:110:LEU:O	9:Q:114:LYS:HG3	2.20	0.41
16:V:281:DC:H2''	16:V:282:DC:C5	2.55	0.41
19:c:78:PHE:C	20:d:70:VAL:HG11	2.46	0.41
21:i:90:ASP:HB3	21:i:93:LEU:HB2	2.03	0.41
2:I:371:LEU:O	2:I:374:HIS:HB2	2.20	0.41
2:I:446:TRP:CE2	2:I:455:PHE:HD2	2.39	0.41
2:I:605:PHE:O	2:I:609:ARG:HG2	2.20	0.41
5:L:338:LEU:HD23	5:L:338:LEU:HA	1.82	0.41
8:P:163:LEU:O	8:P:166:PHE:HB3	2.21	0.41
9:Q:113:LEU:HD22	10:U:265:HIS:CG	2.56	0.41
9:Q:251:MET:CE	10:U:397:LEU:HD22	2.49	0.41
12:T:476:GLU:CG	12:T:479:ALA:H	2.33	0.41
12:T:536:GLU:HA	12:T:544:ARG:HD2	2.01	0.41
16:V:161:DT:C2'	16:V:162:DT:H71	2.51	0.41
16:V:241:DC:H2''	16:V:242:DG:N7	2.36	0.41
16:V:255:DC:H2''	16:V:256:DG:C8	2.55	0.41
16:V:302:DG:H2''	16:V:303:DG:C8	2.56	0.41
17:Y:-154:DA:H2''	17:Y:-153:DA:O5'	2.20	0.41
21:e:51:LEU:O	21:e:55:LEU:HG	2.20	0.41
21:e:66:ALA:HA	21:e:82:HIS:HB3	2.02	0.41
21:e:100:VAL:HG22	20:h:96:THR:HB	2.02	0.41
22:f:65:PHE:HA	20:h:98:TYR:CZ	2.56	0.41
4:M:44:LEU:O	4:M:45:LYS:HE2	2.20	0.41
7:O:127:SER:HA	7:O:137:SER:HA	2.02	0.41
8:P:222:TRP:HA	8:P:236:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:245:LEU:O	9:Q:248:SER:HB3	2.20	0.41
10:U:396:THR:O	10:U:400:ALA:HB2	2.21	0.41
16:V:172:DC:C2	16:V:173:DG:C8	3.09	0.41
17:Y:-251:DG:H2''	17:Y:-250:DG:C8	2.55	0.41
17:Y:-147:DT:H6	17:Y:-147:DT:H2'	1.74	0.41
19:c:102:LEU:HD11	20:d:58:LEU:HD22	2.03	0.41
20:d:92:ARG:CZ	22:f:100:LEU:HB3	2.50	0.41
1:H:125:VAL:O	1:H:129:ASN:HB2	2.21	0.41
3:K:232:VAL:HG12	3:K:233:LYS:O	2.20	0.41
10:U:306:ASN:O	10:U:309:MET:HG2	2.20	0.41
12:T:451:PRO:HB3	16:V:145:DG:H21	1.85	0.41
12:T:515:LEU:HD13	13:W:42:LEU:HB2	2.03	0.41
14:S:99:LYS:HG3	15:X:33:GLU:HG2	2.03	0.41
17:Y:-299:DA:H2''	17:Y:-298:DT:C6	2.55	0.41
17:Y:-249:DG:H2''	17:Y:-248:DA:C8	2.56	0.41
1:H:55:LEU:HA	1:H:58:LYS:NZ	2.36	0.41
5:L:47:ARG:HD3	5:L:224:MET:HE1	2.01	0.41
6:N:89:SER:HB2	6:N:187:GLN:HG2	2.03	0.41
11:R:139:THR:O	11:R:143:MET:CB	2.69	0.41
12:T:550:CYS:O	12:T:557:VAL:HA	2.21	0.41
13:W:72:LYS:HA	13:W:75:VAL:HG22	2.01	0.41
20:d:98:TYR:HB3	22:j:61:ILE:HG23	2.02	0.41
19:g:45:GLN:HB3	19:g:47:TRP:CD1	2.55	0.41
19:g:70:LEU:HD22	20:h:26:ILE:HA	2.02	0.41
2:I:401:ILE:HB	2:I:402:TRP:HE3	1.84	0.41
2:I:564:PHE:O	2:I:568:VAL:HG23	2.20	0.41
2:I:664:ASP:O	2:I:667:ILE:HG22	2.21	0.41
8:P:150:LEU:HD21	8:P:173:PHE:CG	2.55	0.41
9:Q:109:HIS:ND1	10:U:269:ILE:HD12	2.36	0.41
9:Q:141:LEU:HB3	9:Q:145:ARG:NH1	2.35	0.41
11:R:117:ARG:HD2	11:R:120:GLU:OE1	2.21	0.41
14:S:57:GLN:HG3	14:S:61:PHE:HE2	1.85	0.41
14:S:103:ILE:HG21	15:X:30:LEU:HD11	2.03	0.41
16:V:187:DA:H2'	16:V:188:DT:H71	2.02	0.41
16:V:225:DC:H2''	16:V:226:DG:C8	2.56	0.41
16:V:291:DT:H1'	16:V:292:DT:C5	2.56	0.41
17:Y:-291:DA:H2''	17:Y:-290:DG:C8	2.56	0.41
17:Y:-136:DA:H1'	17:Y:-135:DC:H5'	2.03	0.41
19:c:130:ARG:HA	19:c:133:ARG:HD3	2.02	0.41
22:f:57:LYS:HD2	22:f:57:LYS:C	2.46	0.41
20:h:26:ILE:HG12	20:h:59:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:269:TRP:O	2:I:273:LEU:HG	2.21	0.41
3:K:114:LYS:HG3	3:K:115:ASN:N	2.36	0.41
9:Q:193:GLU:O	9:Q:197:VAL:HG13	2.21	0.41
14:S:52:GLU:O	14:S:56:ARG:HG2	2.21	0.41
17:Y:-172:DG:C2	17:Y:-171:DT:C2	3.09	0.41
18:b:297:LYS:O	18:b:297:LYS:HD3	2.20	0.41
21:e:84:GLN:O	21:e:88:ARG:HB2	2.21	0.41
22:f:42:TYR:O	22:f:46:LYS:HG3	2.20	0.41
22:j:80:LEU:HD13	22:j:96:THR:HB	2.03	0.41
2:I:147:ALA:HB1	2:I:164:PHE:CZ	2.56	0.40
2:I:151:LEU:HD11	2:I:164:PHE:HE2	1.86	0.40
2:I:232:GLN:HB2	2:I:235:LEU:HD13	2.03	0.40
2:I:589:TYR:OH	2:I:660:GLY:HA3	2.21	0.40
4:M:11:PRO:HB3	4:M:62:ARG:NH2	2.37	0.40
6:N:120:THR:HB	6:N:136:ALA:HB3	2.03	0.40
6:N:304:GLU:O	6:N:307:LYS:HG2	2.21	0.40
8:P:102:LEU:HD13	8:P:123:LEU:HB2	2.03	0.40
9:Q:85:GLN:HG2	9:Q:118:LEU:HD22	2.03	0.40
9:Q:127:PRO:HA	9:Q:128:PRO:HD3	2.00	0.40
10:U:300:THR:HG22	10:U:304:ARG:HH11	1.86	0.40
13:W:19:ARG:CZ	13:W:41:LEU:HB2	2.51	0.40
15:X:27:ALA:O	15:X:31:MET:HG3	2.20	0.40
16:V:263:DC:H2''	16:V:264:DC:C6	2.56	0.40
22:j:33:ARG:HE	22:j:35:GLU:HB3	1.86	0.40
22:j:99:ARG:HG3	22:j:111:VAL:HG21	2.02	0.40
1:H:129:ASN:O	1:H:133:LEU:HG	2.21	0.40
2:I:327:MET:HE2	2:I:331:ASP:C	2.46	0.40
4:M:142:MET:O	4:M:146:LEU:HD23	2.22	0.40
6:N:18:MET:CE	16:V:158:DG:H3'	2.51	0.40
7:O:125:CYS:HA	7:O:139:PHE:HA	2.02	0.40
8:P:209:ARG:HG2	8:P:210:SER:N	2.35	0.40
8:P:246:ALA:HB2	10:U:368:TYR:CD2	2.57	0.40
16:V:199:DC:H2''	16:V:200:DA:N7	2.36	0.40
21:e:80:PRO:HD2	19:g:58:THR:HG22	2.03	0.40
22:f:56:SER:O	22:f:59:MET:HB3	2.21	0.40
21:i:83:LEU:HD13	22:j:61:ILE:HG21	2.02	0.40
21:i:95:LYS:HB3	22:j:103:PRO:HG3	2.03	0.40
22:j:41:VAL:HG22	22:j:62:MET:SD	2.61	0.40
2:I:566:GLU:HA	2:I:569:CYS:SG	2.61	0.40
4:M:114:ARG:O	4:M:118:VAL:HG23	2.21	0.40
7:O:278:LYS:NZ	7:O:283:VAL:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:133:LYS:HD2	11:R:137:GLN:NE2	2.36	0.40
12:T:468:SER:HB2	13:W:9:GLN:HG2	2.03	0.40
14:S:64:ASP:O	14:S:67:MET:HG2	2.21	0.40
14:S:80:GLU:O	14:S:84:LEU:HG	2.21	0.40
14:S:90:ASN:OD1	14:S:91:SER:N	2.55	0.40
21:e:27:VAL:HA	21:e:30:VAL:HG12	2.04	0.40
19:g:54:LEU:HD12	20:h:39:ARG:HB2	2.02	0.40
1:H:241:GLU:HB3	2:I:183:LEU:HD23	2.04	0.40
3:K:115:ASN:HA	3:K:118:LEU:HD12	2.04	0.40
6:N:8:PHE:CD1	6:N:146:GLN:HB3	2.55	0.40
6:N:101:MET:HE3	6:N:101:MET:HA	2.02	0.40
6:N:111:ILE:HD13	6:N:178:ALA:HA	2.04	0.40
7:O:128:THR:OG1	7:O:135:LEU:HB2	2.21	0.40
8:P:181:LYS:HA	8:P:201:PRO:HB2	2.03	0.40
9:Q:93:MET:HE1	14:S:24:HIS:CD2	2.55	0.40
10:U:266:GLN:NE2	10:U:278:ILE:HG13	2.36	0.40
11:R:86:PHE:CE1	11:R:89:LEU:HD23	2.57	0.40
11:R:100:ILE:HA	11:R:103:ILE:HG12	2.04	0.40
12:T:450:ARG:HH22	17:Y:-145:DC:H5'	1.86	0.40
14:S:87:ARG:HA	14:S:93:LEU:HD22	2.03	0.40
17:Y:-236:DT:H2''	17:Y:-235:DG:C8	2.56	0.40
1:H:169:GLU:HG3	2:I:378:CYS:SG	2.61	0.40
7:O:94:LEU:HD13	8:P:56:LEU:HB2	2.04	0.40
7:O:139:PHE:CE2	7:O:154:SER:HB3	2.57	0.40
7:O:224:LEU:HB2	7:O:231:PHE:HB2	2.03	0.40
14:S:85:LEU:HD23	14:S:85:LEU:HA	1.89	0.40
17:Y:-227:DG:C4	17:Y:-226:DC:C5	3.09	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	H	200/247 (81%)	199 (100%)	1 (0%)	0	100	100
2	I	610/762 (80%)	589 (97%)	20 (3%)	1 (0%)	43	77
3	K	227/269 (84%)	222 (98%)	5 (2%)	0	100	100
4	M	170/180 (94%)	167 (98%)	3 (2%)	0	100	100
5	L	308/348 (88%)	300 (97%)	7 (2%)	1 (0%)	36	71
6	N	312/347 (90%)	300 (96%)	11 (4%)	1 (0%)	36	71
7	O	204/300 (68%)	198 (97%)	6 (3%)	0	100	100
8	P	220/288 (76%)	217 (99%)	3 (1%)	0	100	100
9	Q	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
10	U	164/211 (78%)	164 (100%)	0	0	100	100
11	R	76/177 (43%)	74 (97%)	2 (3%)	0	100	100
12	T	110/777 (14%)	107 (97%)	3 (3%)	0	100	100
13	W	84/88 (96%)	82 (98%)	2 (2%)	0	100	100
14	S	118/138 (86%)	118 (100%)	0	0	100	100
15	X	72/81 (89%)	70 (97%)	2 (3%)	0	100	100
18	a	19/775 (2%)	19 (100%)	0	0	100	100
18	b	51/775 (7%)	46 (90%)	5 (10%)	0	100	100
19	c	97/140 (69%)	96 (99%)	1 (1%)	0	100	100
19	g	94/140 (67%)	93 (99%)	1 (1%)	0	100	100
20	d	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
20	h	78/103 (76%)	78 (100%)	0	0	100	100
21	e	105/153 (69%)	104 (99%)	1 (1%)	0	100	100
21	i	105/153 (69%)	105 (100%)	0	0	100	100
22	f	93/126 (74%)	89 (96%)	4 (4%)	0	100	100
22	j	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
All	All	3874/7022 (55%)	3783 (98%)	88 (2%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	246	SER
6	N	166	SER
2	I	405	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	H	194/224 (87%)	194 (100%)	0	100	100
2	I	568/697 (82%)	568 (100%)	0	100	100
3	K	225/260 (86%)	225 (100%)	0	100	100
4	M	151/158 (96%)	151 (100%)	0	100	100
5	L	278/308 (90%)	278 (100%)	0	100	100
6	N	293/319 (92%)	293 (100%)	0	100	100
7	O	187/263 (71%)	187 (100%)	0	100	100
8	P	206/259 (80%)	206 (100%)	0	100	100
9	Q	180/200 (90%)	180 (100%)	0	100	100
10	U	155/190 (82%)	155 (100%)	0	100	100
11	R	75/166 (45%)	75 (100%)	0	100	100
12	T	100/635 (16%)	100 (100%)	0	100	100
13	W	76/77 (99%)	76 (100%)	0	100	100
14	S	107/121 (88%)	107 (100%)	0	100	100
15	X	65/67 (97%)	65 (100%)	0	100	100
18	a	21/687 (3%)	21 (100%)	0	100	100
18	b	56/687 (8%)	56 (100%)	0	100	100
19	c	83/118 (70%)	83 (100%)	0	100	100
19	g	83/118 (70%)	83 (100%)	0	100	100
20	d	65/79 (82%)	65 (100%)	0	100	100
20	h	65/79 (82%)	65 (100%)	0	100	100
21	e	82/118 (70%)	82 (100%)	0	100	100
21	i	82/118 (70%)	82 (100%)	0	100	100
22	f	82/106 (77%)	82 (100%)	0	100	100
22	j	81/106 (76%)	81 (100%)	0	100	100
All	All	3560/6160 (58%)	3560 (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 (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	191	ASN
1	H	200	GLN
1	H	239	GLN
2	I	91	HIS
2	I	553	ASN
2	I	601	ASN
2	I	698	GLN
2	I	726	GLN
2	I	729	GLN
4	M	87	HIS
5	L	69	HIS
5	L	71	GLN
5	L	232	HIS
6	N	103	GLN
6	N	157	GLN
6	N	177	GLN
7	O	20	HIS
9	Q	83	HIS
10	U	363	GLN
11	R	105	GLN
11	R	111	GLN
11	R	149	GLN
14	S	41	GLN
19	c	59	HIS
20	d	93	GLN
21	e	38	ASN
21	e	73	ASN
22	f	63	ASN
19	g	87	GLN
19	g	89	GLN
20	h	75	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

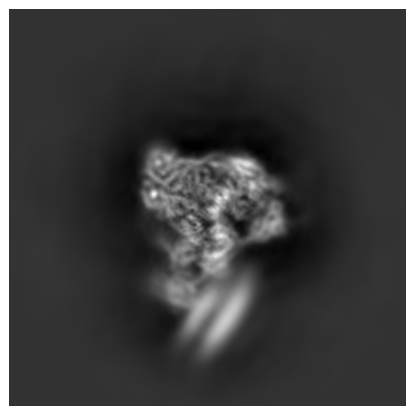
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55758. These allow visual inspection of the internal detail of the map and identification of artifacts.

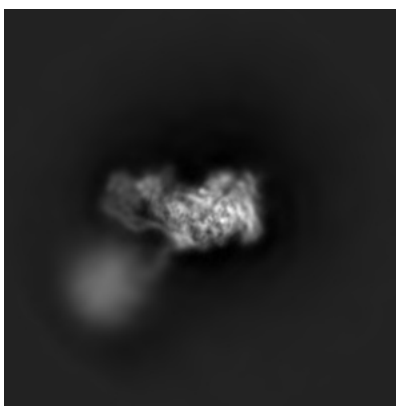
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

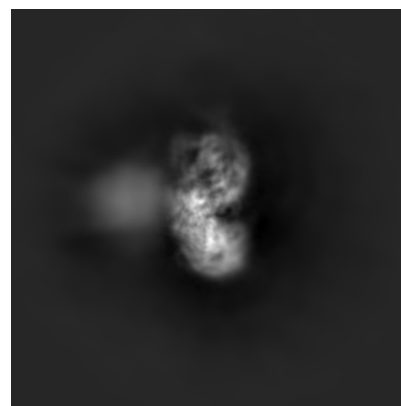
6.1.1 Primary map



X

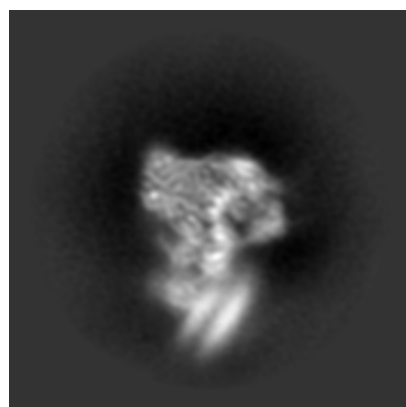


Y

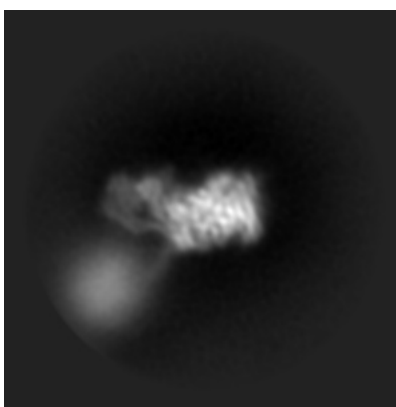


Z

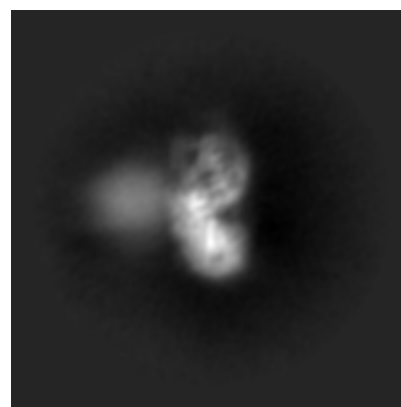
6.1.2 Raw map



X



Y

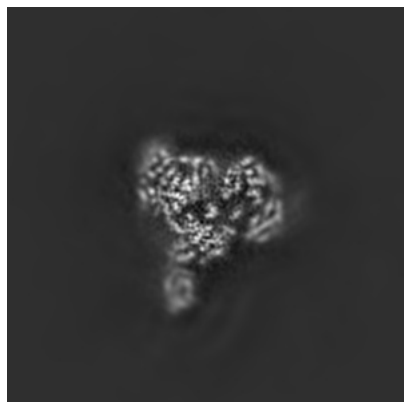


Z

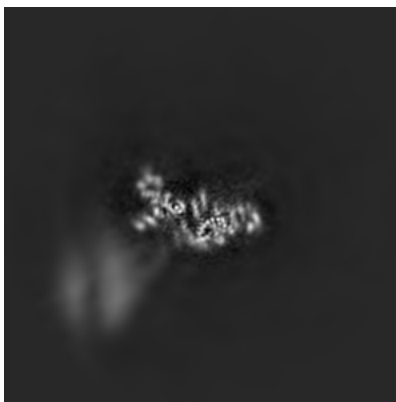
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

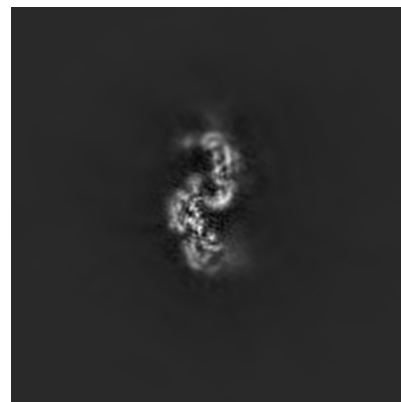
6.2.1 Primary map



X Index: 200

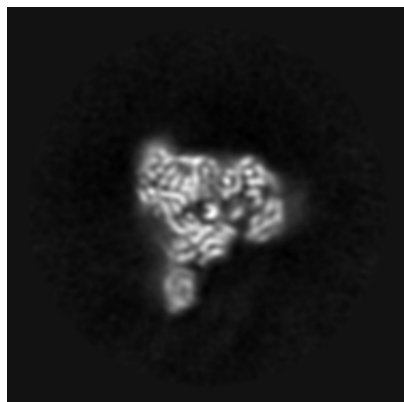


Y Index: 200

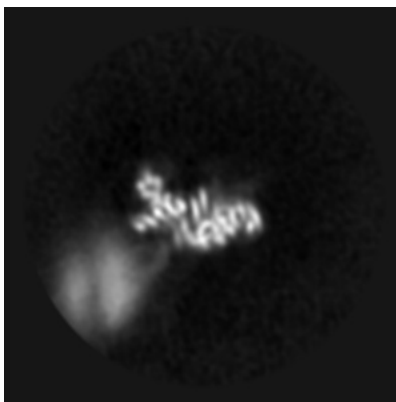


Z Index: 200

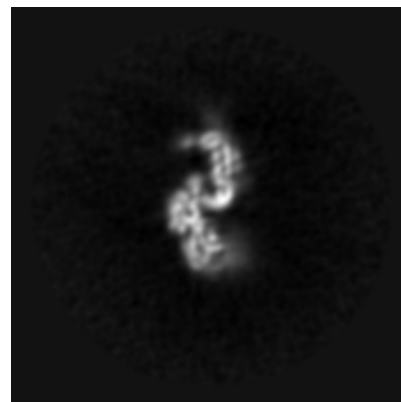
6.2.2 Raw map



X Index: 200



Y Index: 200

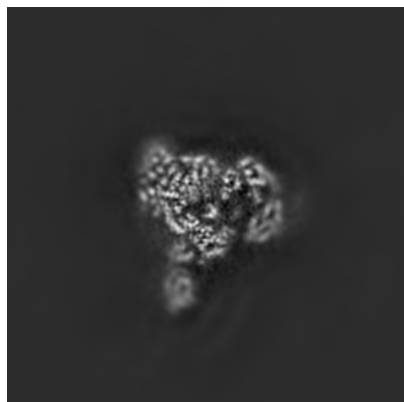


Z Index: 200

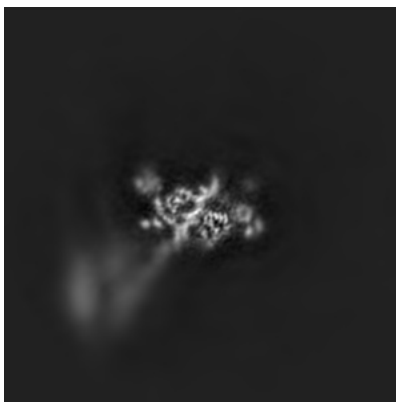
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

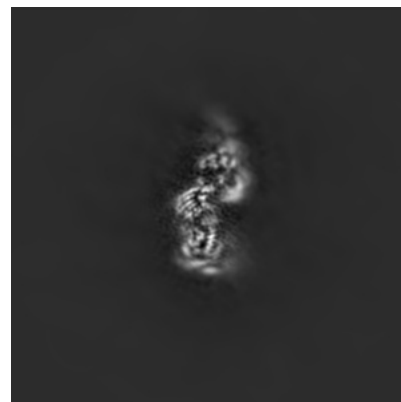
6.3.1 Primary map



X Index: 198

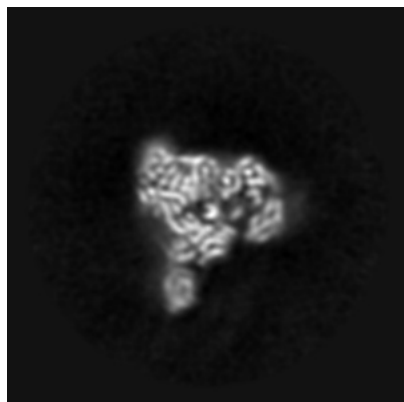


Y Index: 208

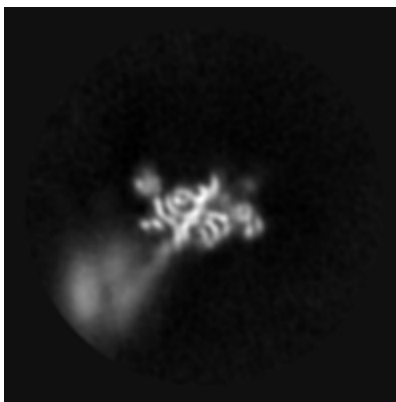


Z Index: 211

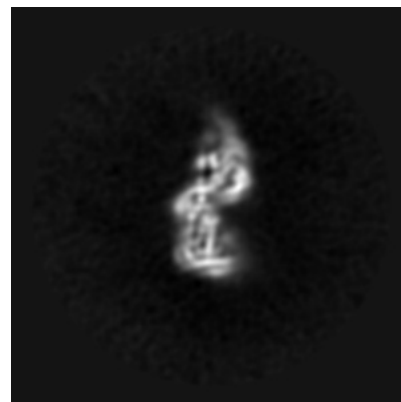
6.3.2 Raw map



X Index: 199



Y Index: 208

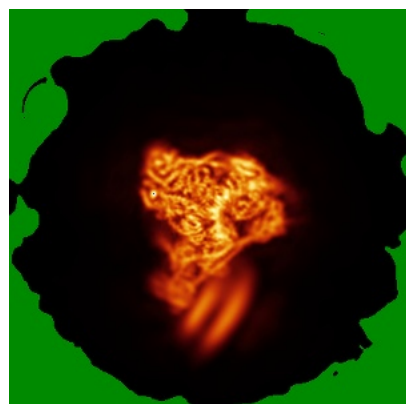


Z Index: 214

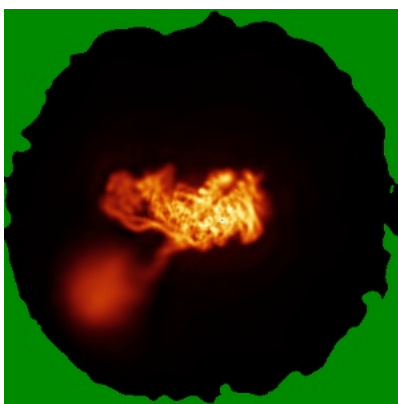
The images above show the largest variance slices of the map in three orthogonal directions.

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

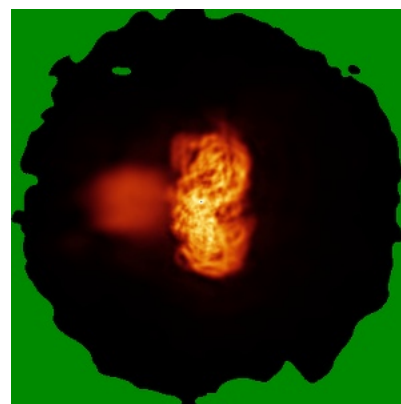
6.4.1 Primary map



X

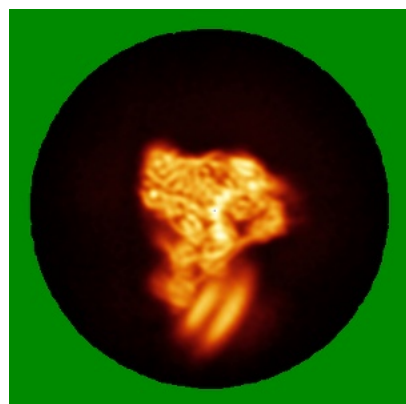


Y



Z

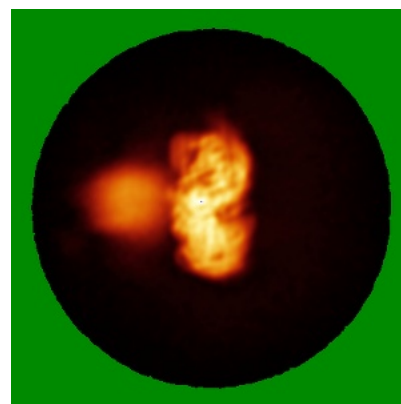
6.4.2 Raw map



X



Y

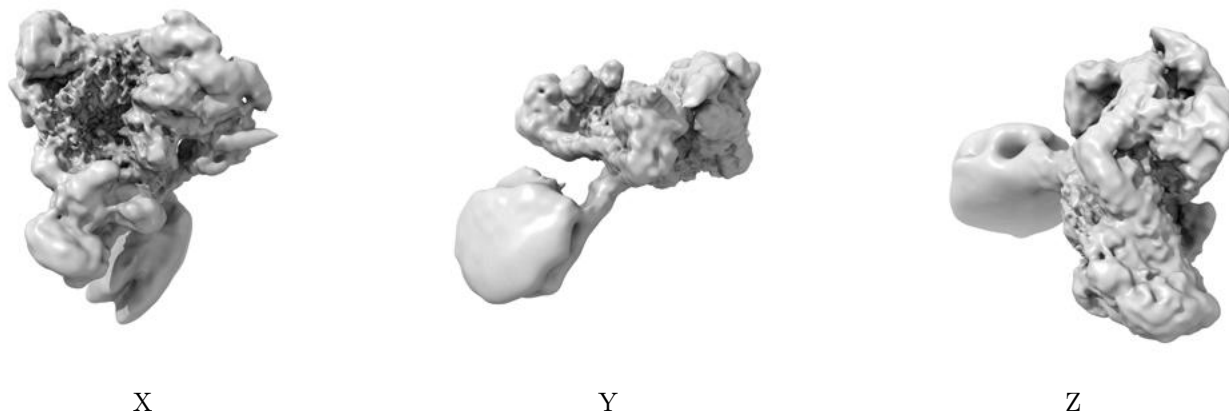


Z

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.

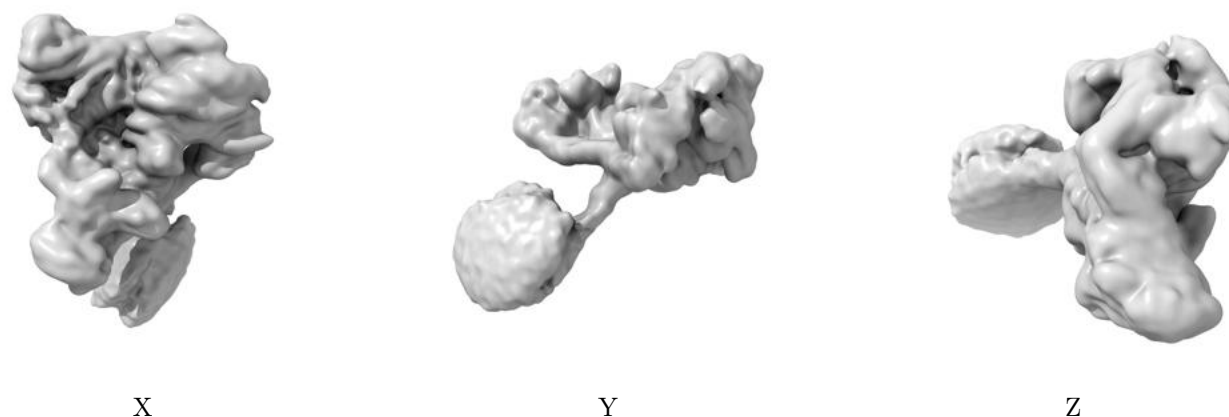
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0016. 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.

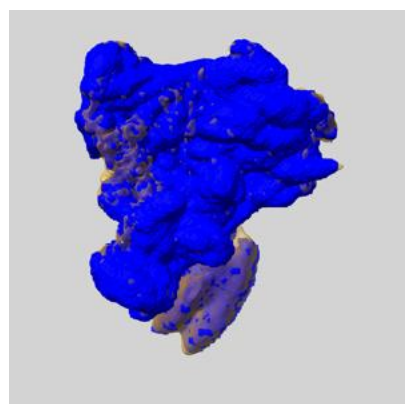
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

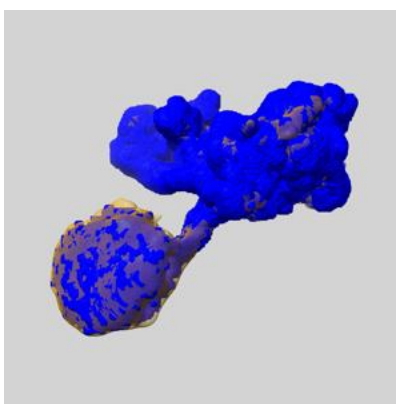
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

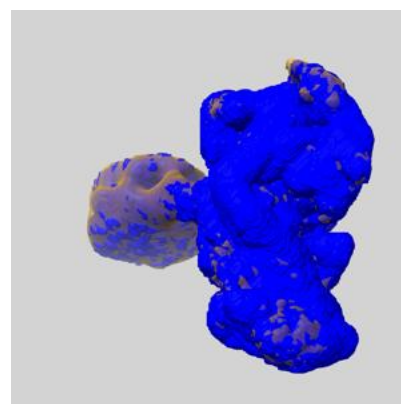
6.6.1 emd_55758_msk_1.map [i](#)



X



Y

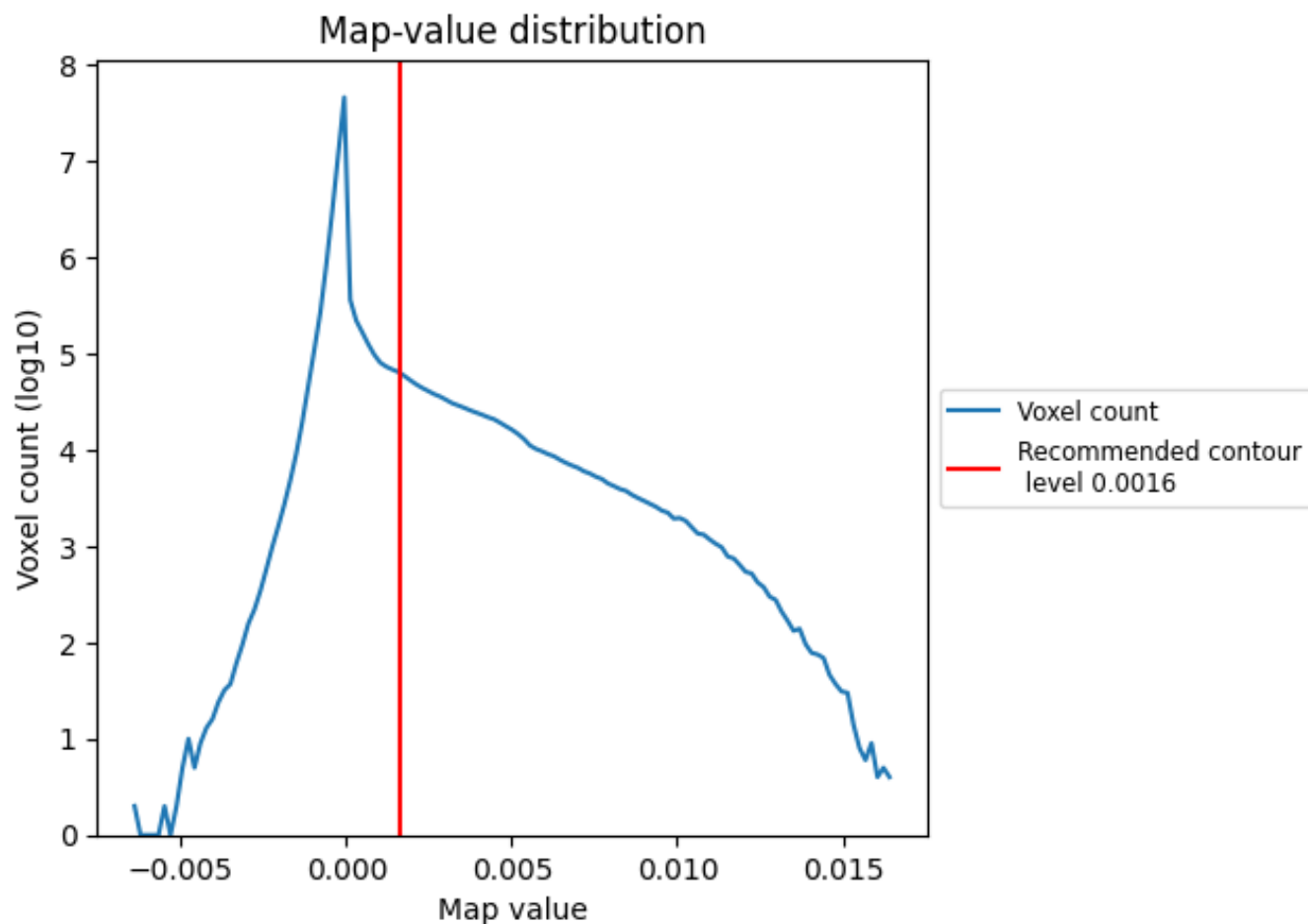


Z

7 Map analysis [i](#)

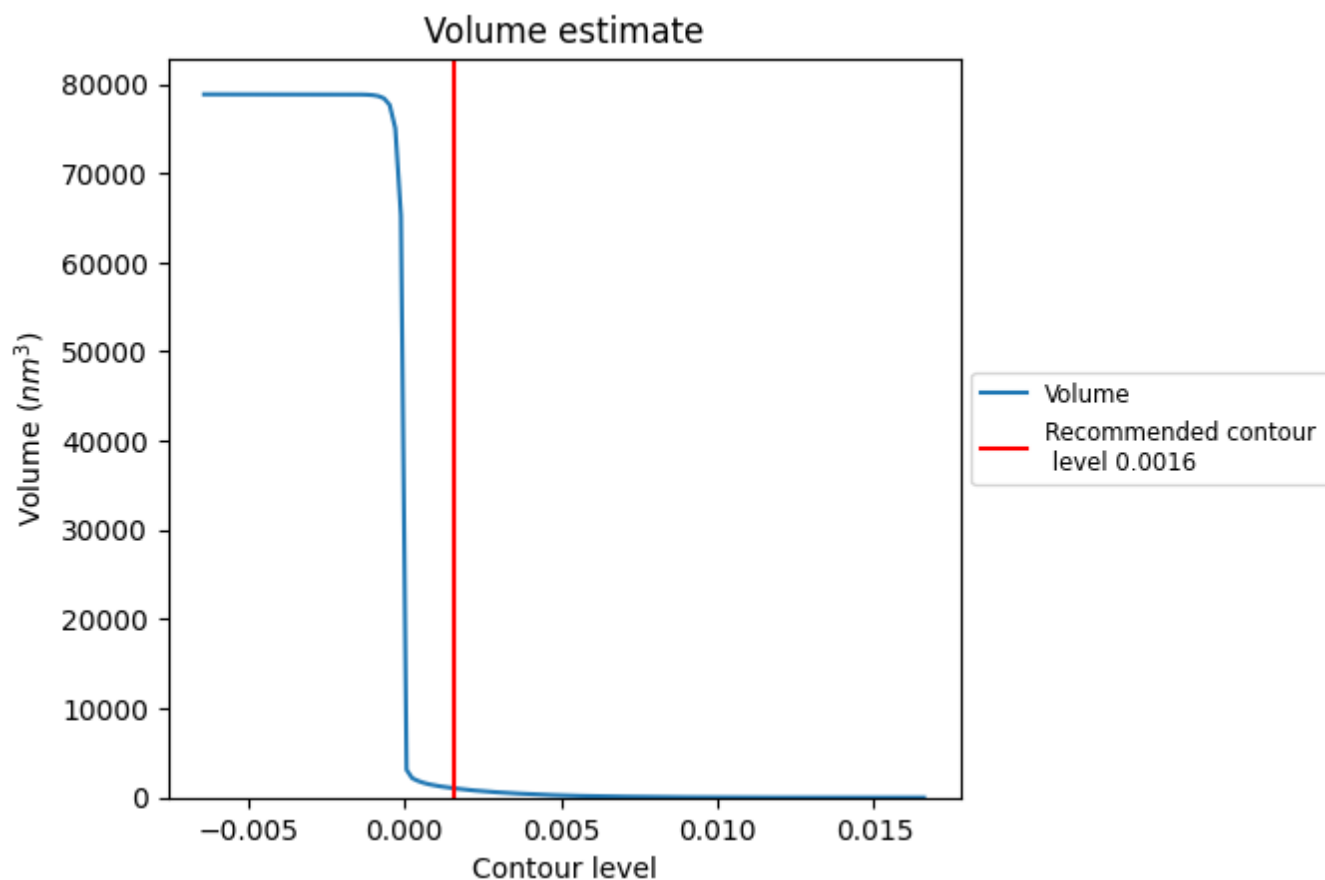
This section contains the results of statistical analysis of the map.

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.

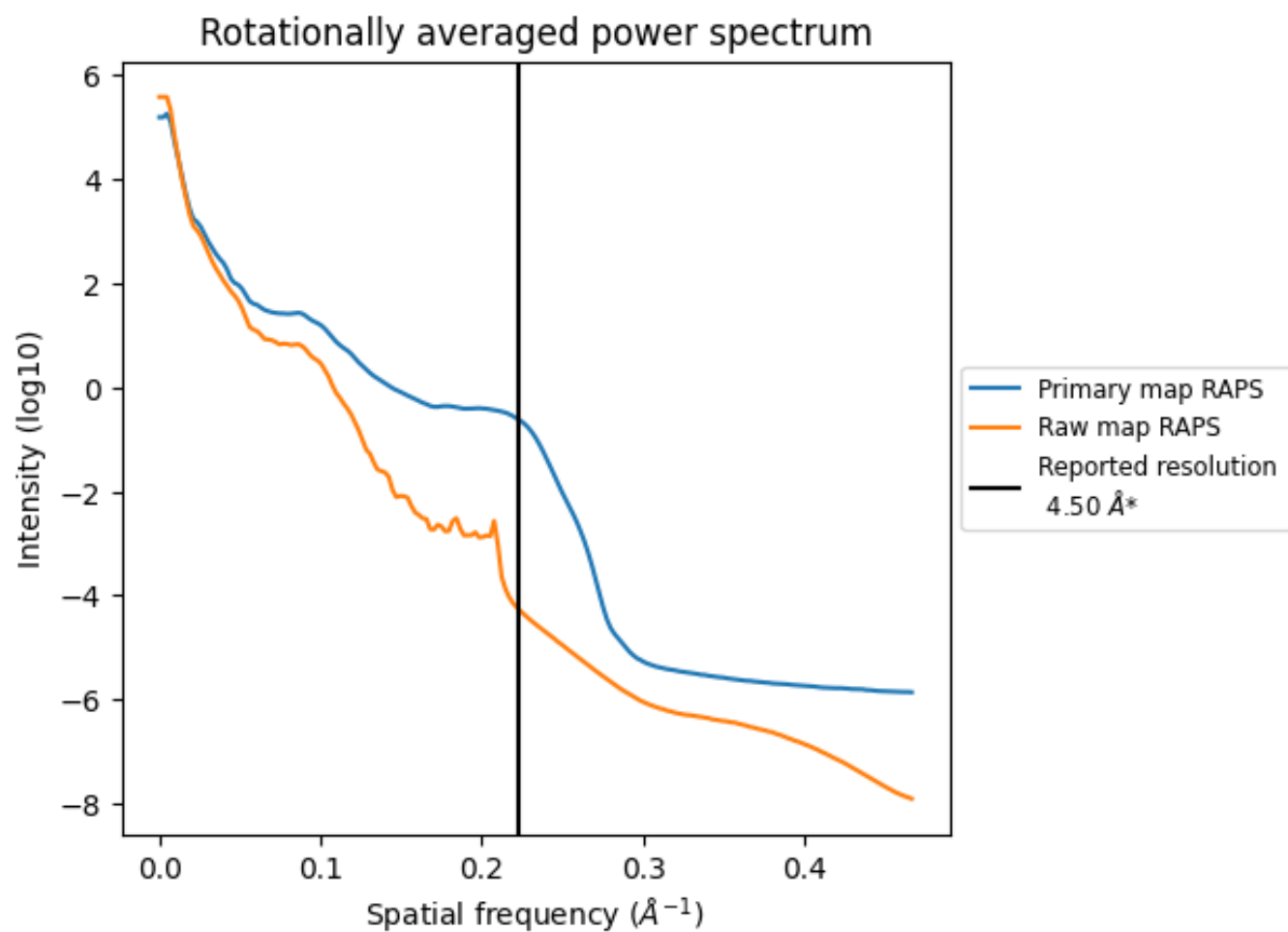
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1036 nm^3 ; this corresponds to an approximate mass of 936 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 ⓘ

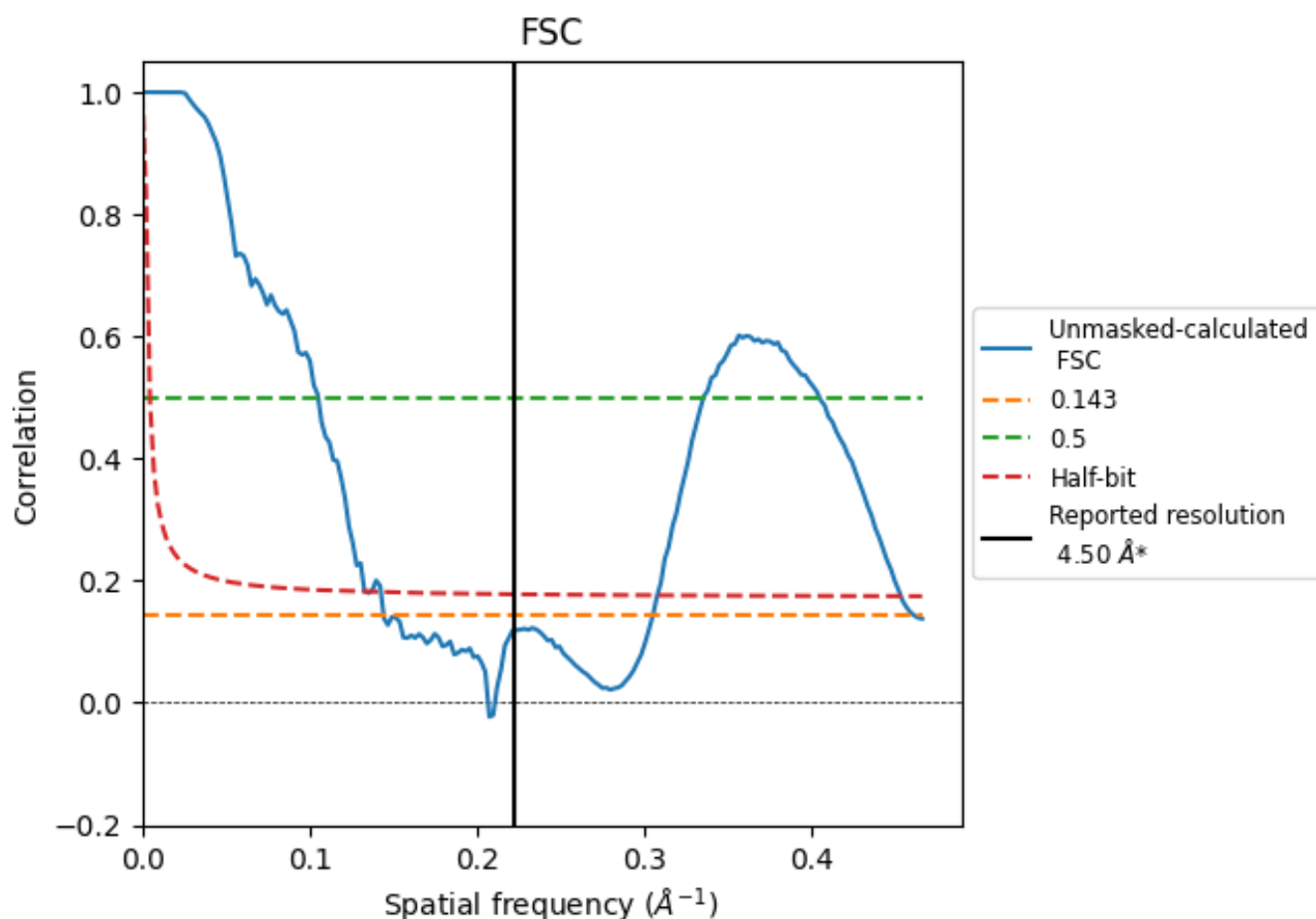


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

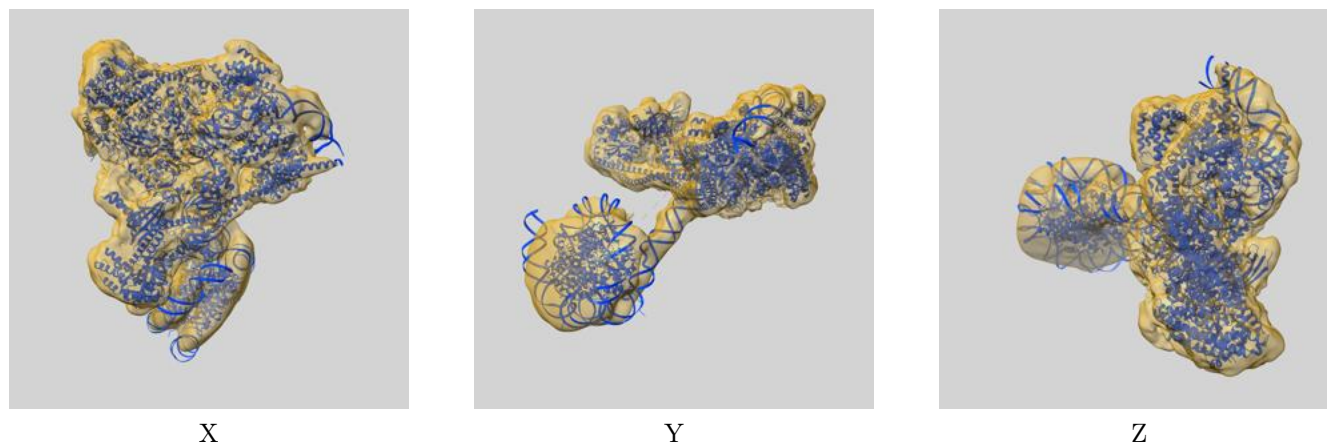
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.93	9.51	7.47

*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 6.93 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

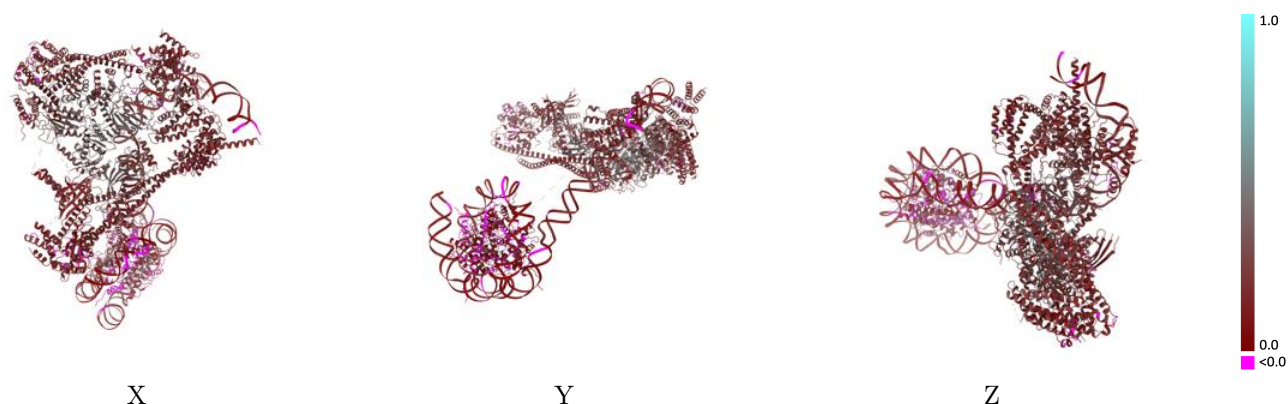
This section contains information regarding the fit between EMDB map EMD-55758 and PDB model 9TAX. Per-residue inclusion information can be found in section 3 on page 28.

9.1 Map-model overlay [i](#)



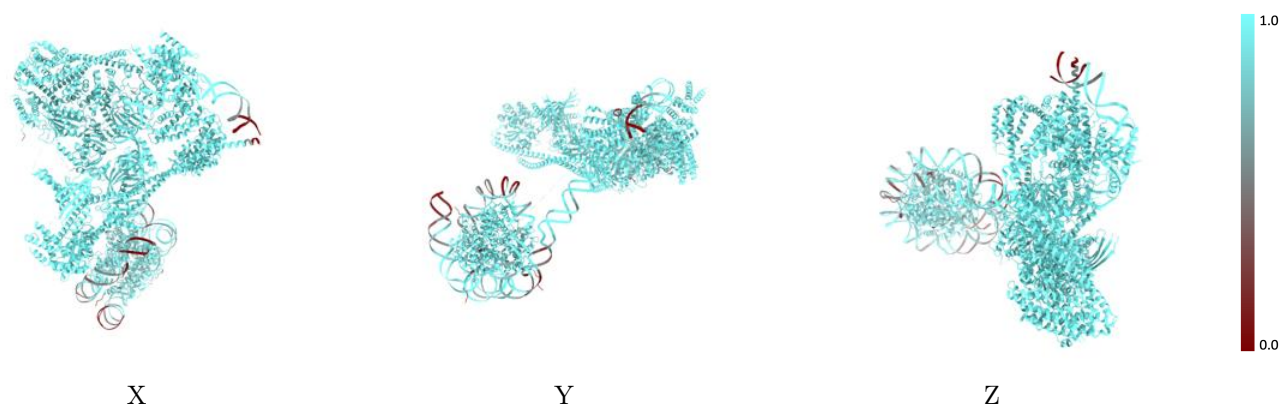
The images above show the 3D surface view of the map at the recommended contour level 0.0016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



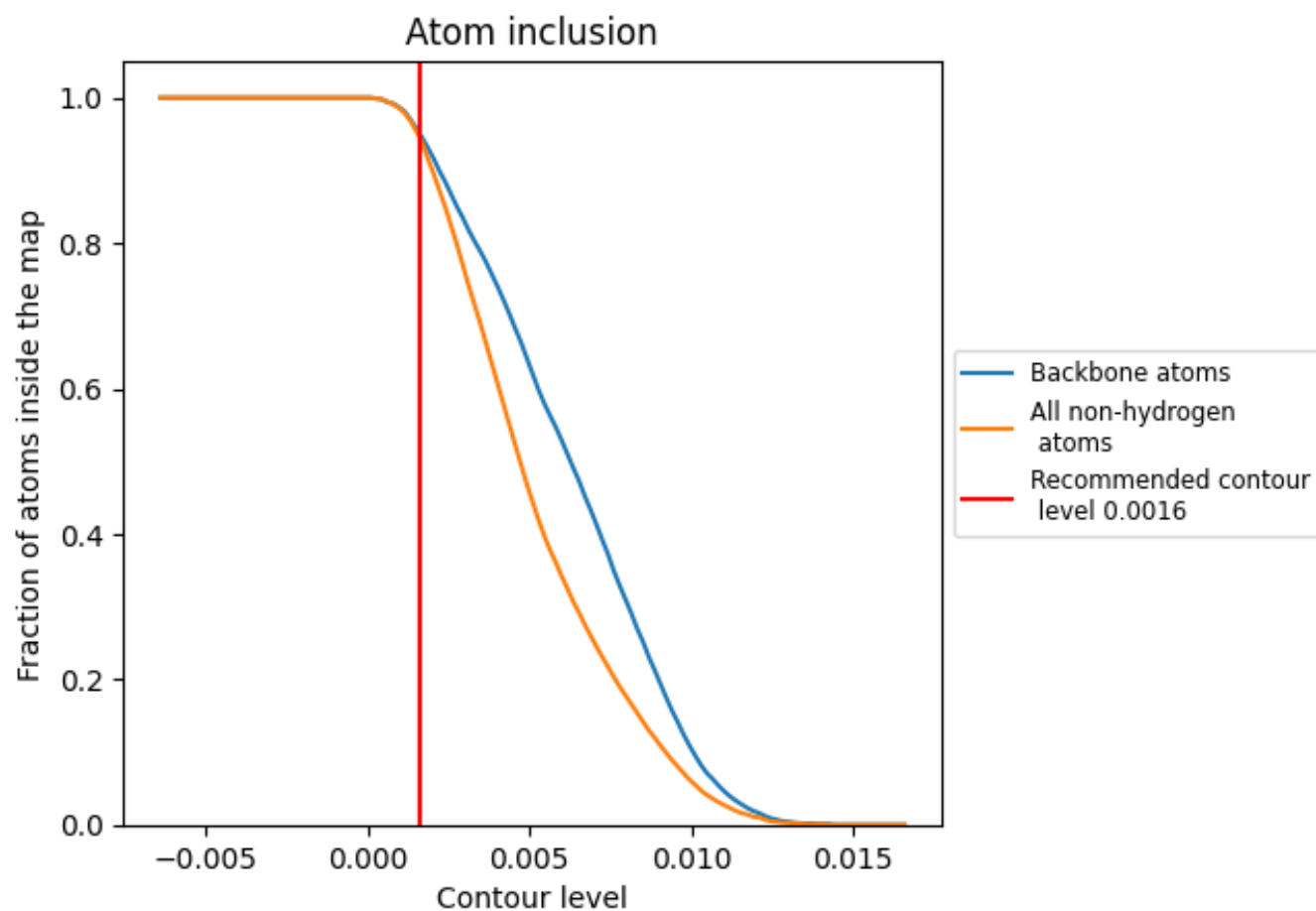
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.0016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.1810
H	 0.9970	 0.1920
I	 0.9810	 0.2320
K	 0.9960	 0.2200
L	 1.0000	 0.3530
M	 0.9940	 0.3400
N	 0.9950	 0.3220
O	 0.9980	 0.2140
P	 0.9990	 0.1630
Q	 0.9970	 0.1810
R	 0.9940	 0.1490
S	 0.9280	 0.1900
T	 0.9970	 0.2290
U	 0.9960	 0.1720
V	 0.8030	 0.1080
W	 0.9960	 0.2500
X	 0.9950	 0.1890
Y	 0.8000	 0.1050
a	 0.9700	 0.0310
b	 0.9030	 0.1410
c	 0.9510	 0.0340
d	 0.9480	 0.0760
e	 0.9470	 0.0520
f	 0.9640	 0.0400
g	 0.9730	 0.0160
h	 0.9980	 0.0580
i	 0.9410	 0.0550
j	 0.9750	 0.0620

