Full wwPDB EM Validation Report (i)

Jul 9, 2024 – 09:45 pm BST

PDB ID	:	7YYH
EMDB ID	:	EMD-14375
Title	:	Structure of the human CCANdeltaT CENP-A alpha-satellite complex
Authors	:	Yatskevich, S.; Muir, K.W.; Bellini, D.; Zhang, Z.; Yang, J.; Tischer, T.; Predin, M.; Dendooven, T.; McLaughlin, S.H.; Barford, D.
Deposited on	:	2022-02-17
Resolution	:	8.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

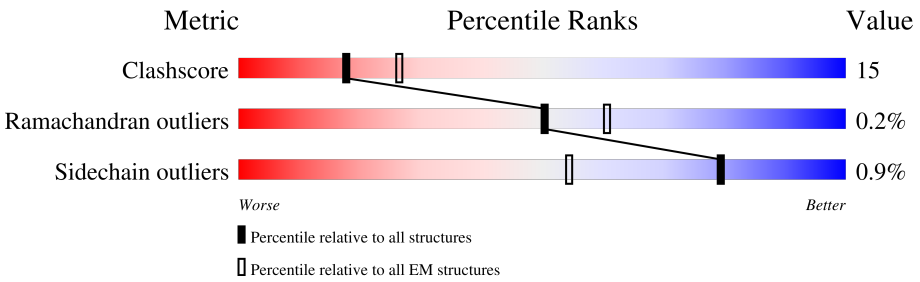
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	140	10% 59% 11% 29%
1	E	140	5% 58% 9% 33%
2	B	103	6% 68% 7% • 24%
2	F	103	7% 61% 17% 22%
3	C	130	6% 63% 12% • 25%
3	G	130	7% 72% 8% 21%
4	D	126	5% 64% 9% 27%
4	h	126	• 71% • 27%

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Mol	Chain	Length	Quality of chain
5	H	247	11% 50% 19% 31%
6	I	756	17% 54% 18% 28%
7	J	171	40% 45% 11%
8	K	269	30% 66% 14% 19%
9	L	344	61% 25% 14%
10	M	180	58% 38%
11	N	339	56% 31% 12%
12	O	300	47% 23% 30%
13	P	288	7% 55% 21% 24%
14	Q	268	10% 49% 22% 29%
15	R	177	24% 23% 22% 55%
16	U	418	28% 12% 61%
17	k	544	96%
17	l	544	7% 90%
18	i	171	87% 11%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 33344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3-like centromeric protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	99	799	518	147	133	1	0	0
1	E	94	770	501	141	127	1	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	78	622	393	120	108	1	0	0
2	F	80	641	405	125	110	1	0	0

- Molecule 3 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	98	755	474	149	132	0	0
3	G	103	784	491	155	138	0	0

- Molecule 4 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	92	719	452	129	136	2	0	0
4	h	92	719	452	129	136	2	0	0

- Molecule 5 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	171	1384	874	236	266	8	0	0

- Molecule 6 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	543	4402	2897	709	770	26	0	0

- Molecule 7 is a DNA chain called DNA (171-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	153	3133	1501	557	922	153	0	0

- Molecule 8 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	217	1793	1139	297	347	10	0	0

- Molecule 9 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	297	2397	1563	392	428	14	0	0

- Molecule 10 is a protein called Centromere protein M.

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

- Molecule 11 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	297	2452	1581	425	436	10	0	0

- Molecule 12 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	210	1642	1060	277	298	7	0	0

- Molecule 13 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	219	1732	1107	293	324	8	0	0

- Molecule 14 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	189	1506	943	253	299	11	0	0

- Molecule 15 is a protein called Centromere protein R.

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

- Molecule 16 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	165	1346	851	234	256	5	0	0

- Molecule 17 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	k	21	178	111	37	30	0	0
17	l	57	476	298	85	93	0	0

- Molecule 18 is a DNA chain called DNA (171-MER).

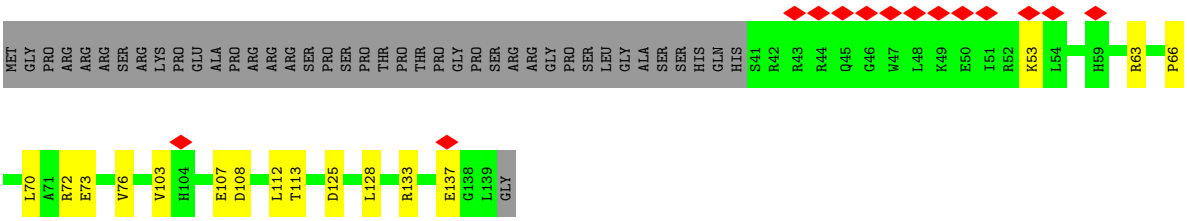
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	i	152	3120	1492	569	907	152	0	0

3 Residue-property plots (i)

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.

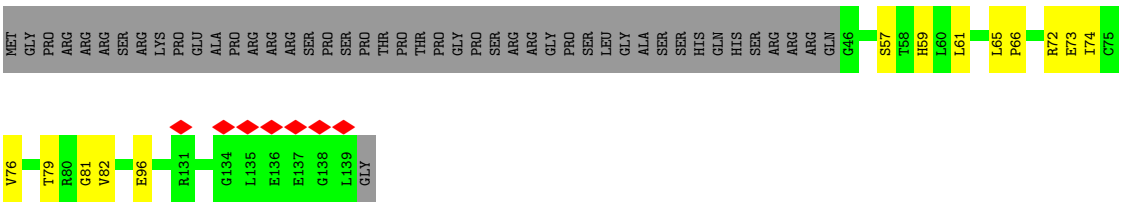
• Molecule 1: Histone H3-like centromeric protein A

Chain A:



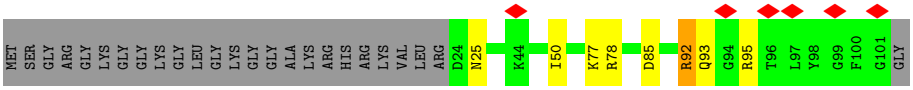
• Molecule 1: Histone H3-like centromeric protein A

Chain E:



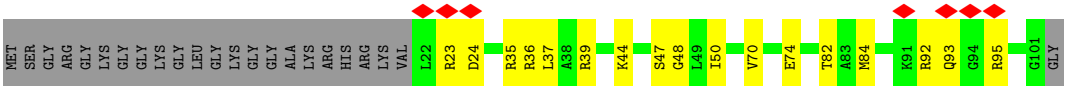
• Molecule 2: Histone H4

Chain B:



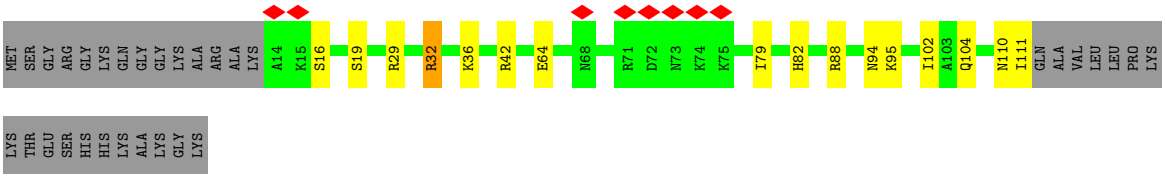
• Molecule 2: Histone H4

Chain F:



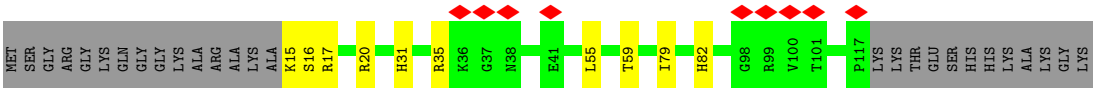
• Molecule 3: Histone H2A type 1-C

Chain C:



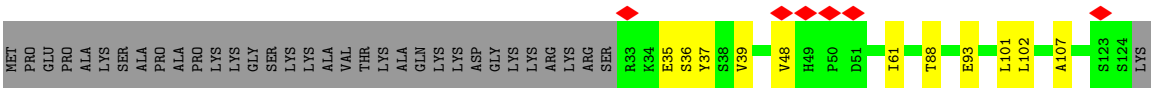
- Molecule 3: Histone H2A type 1-C

Chain G:



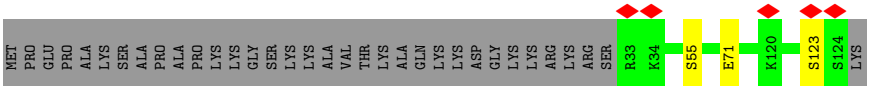
- Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain D:



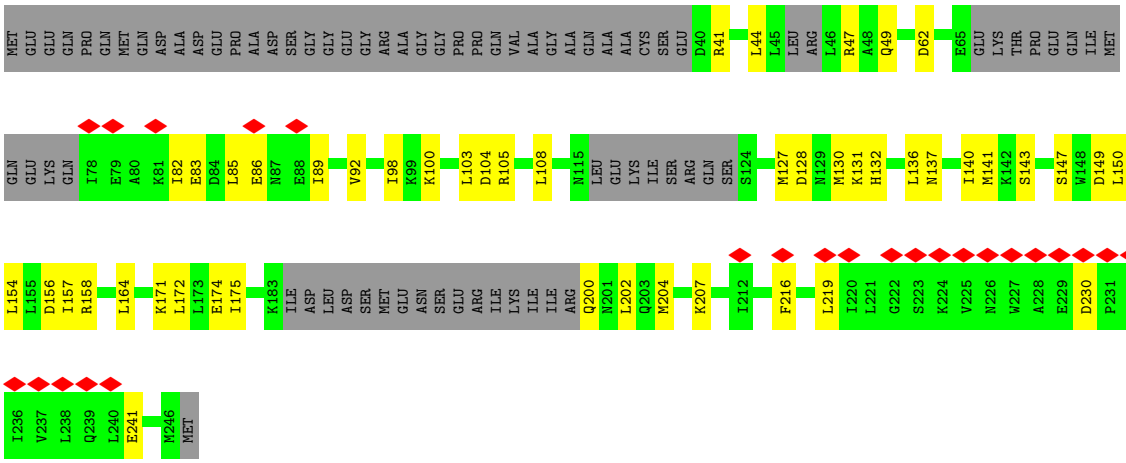
- Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain h:



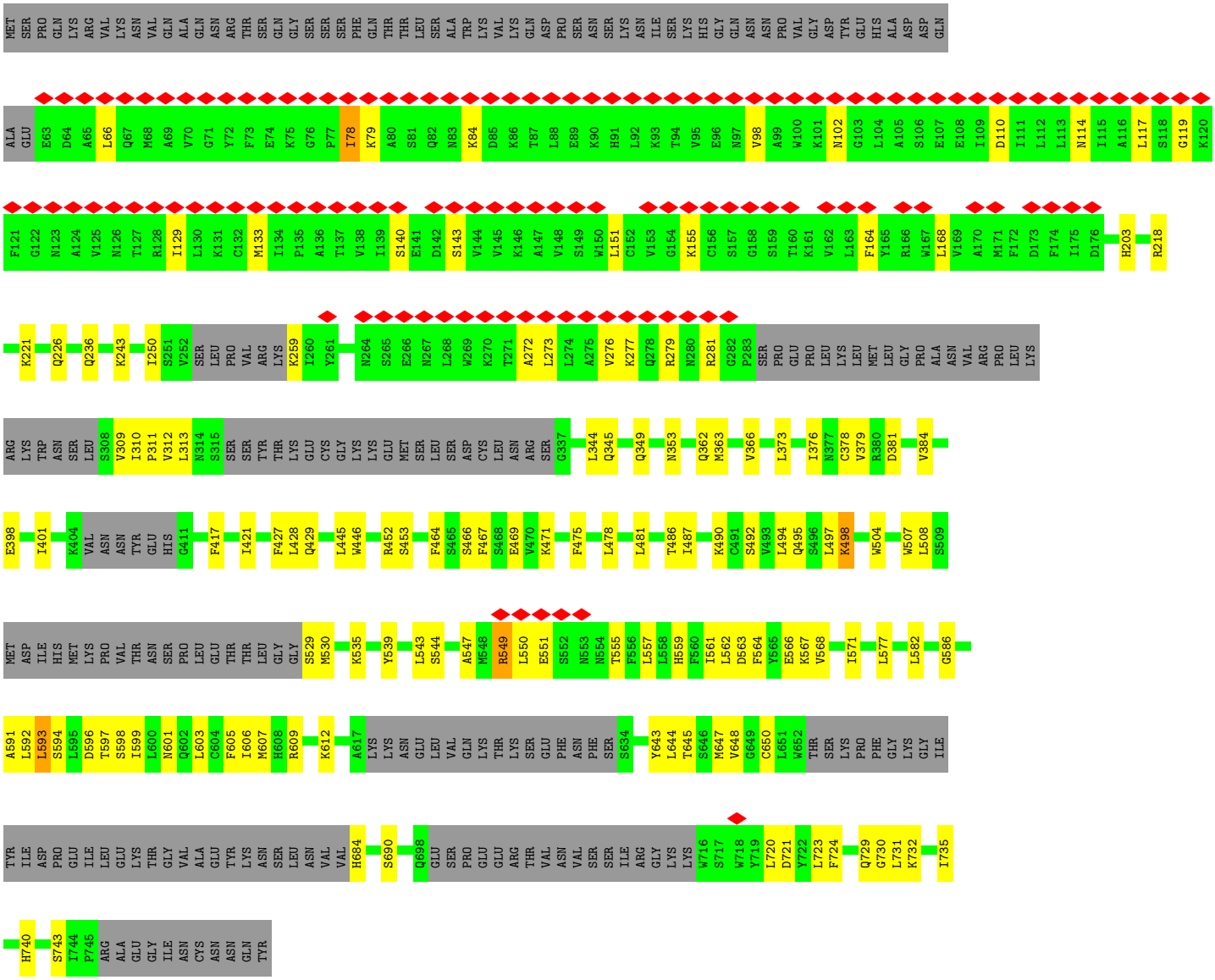
- Molecule 5: Centromere protein H

Chain H:



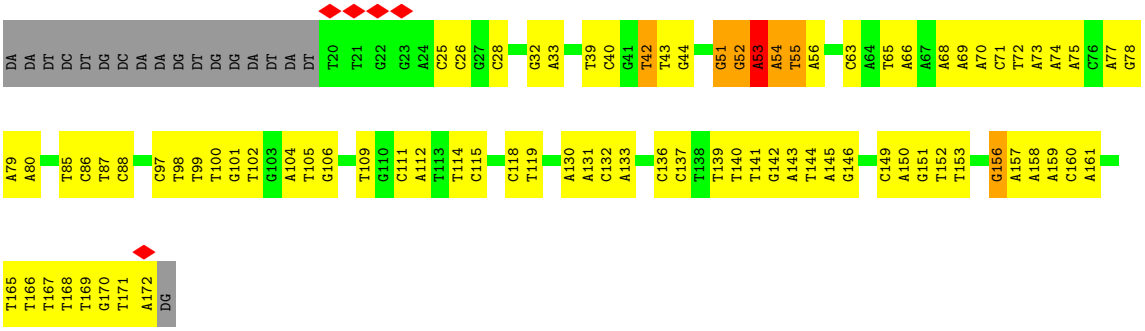
- Molecule 6: Centromere protein I

Chain I:



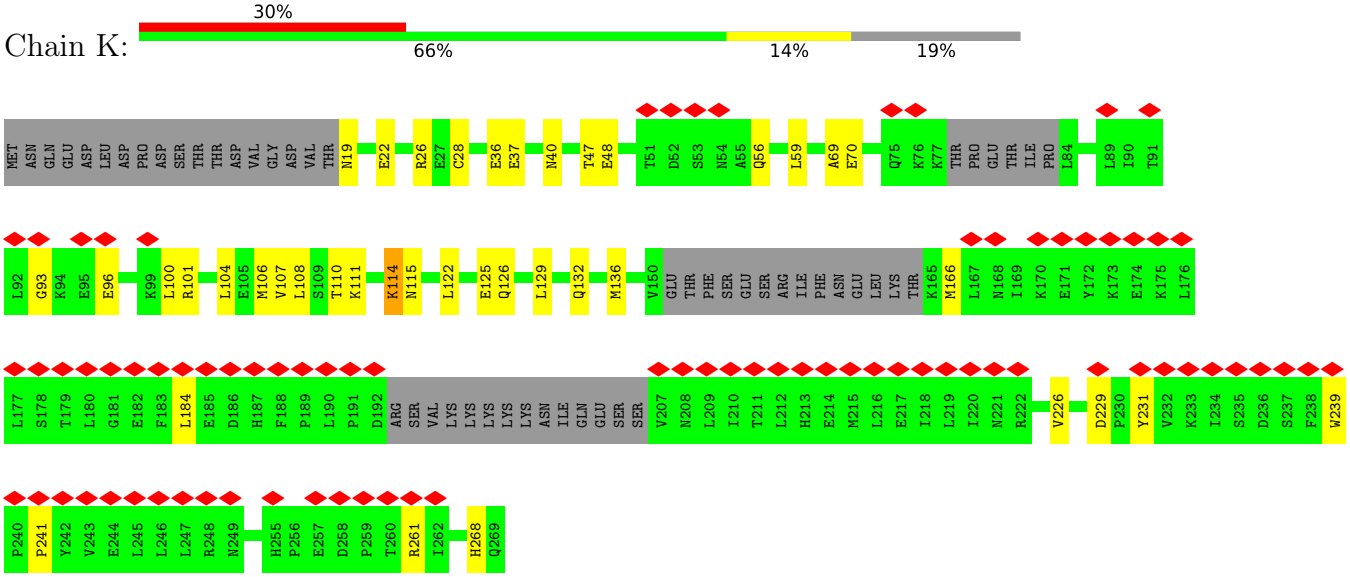
• Molecule 7: DNA (171-MER)

Chain J:



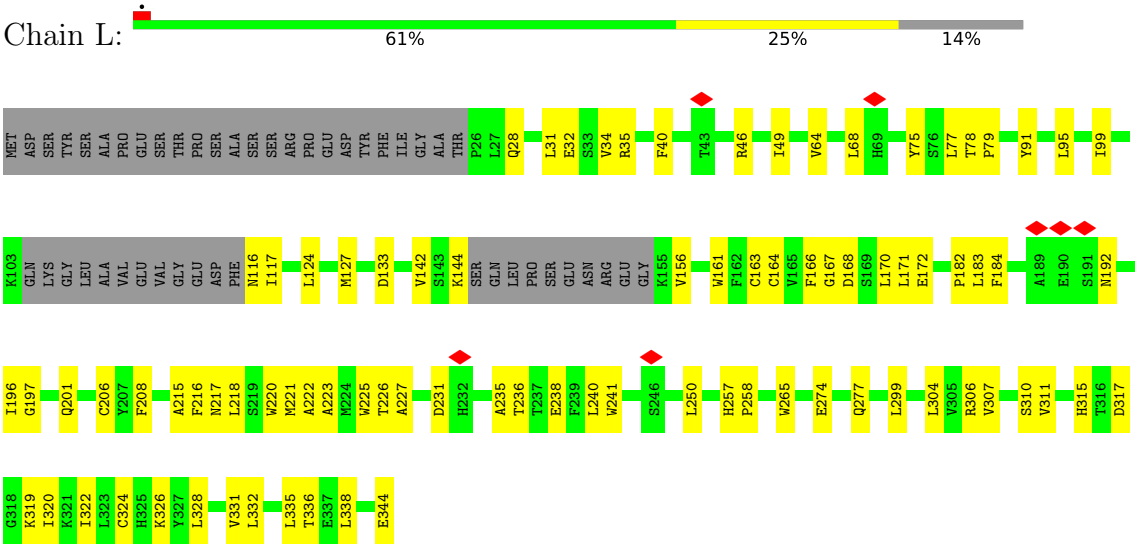
• Molecule 8: Centromere protein K

Chain K:



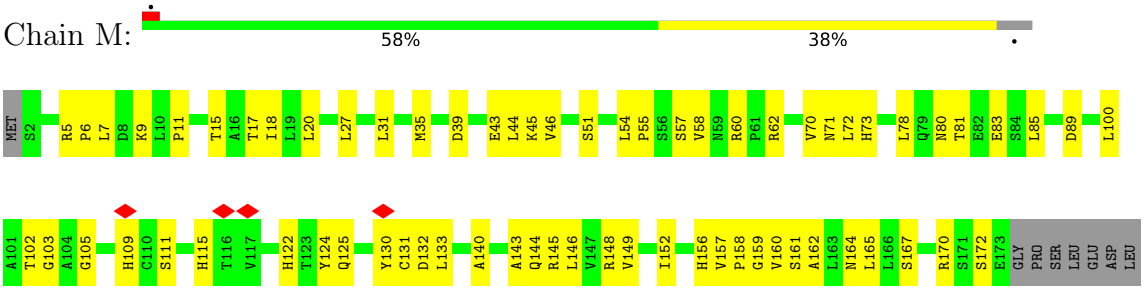
• Molecule 9: Centromere protein L

Chain L:



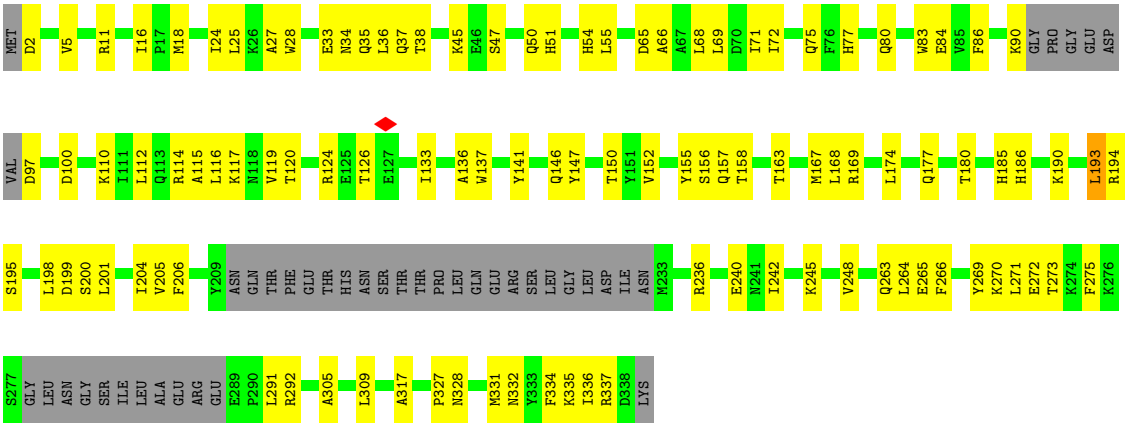
• Molecule 10: Centromere protein M

Chain M:



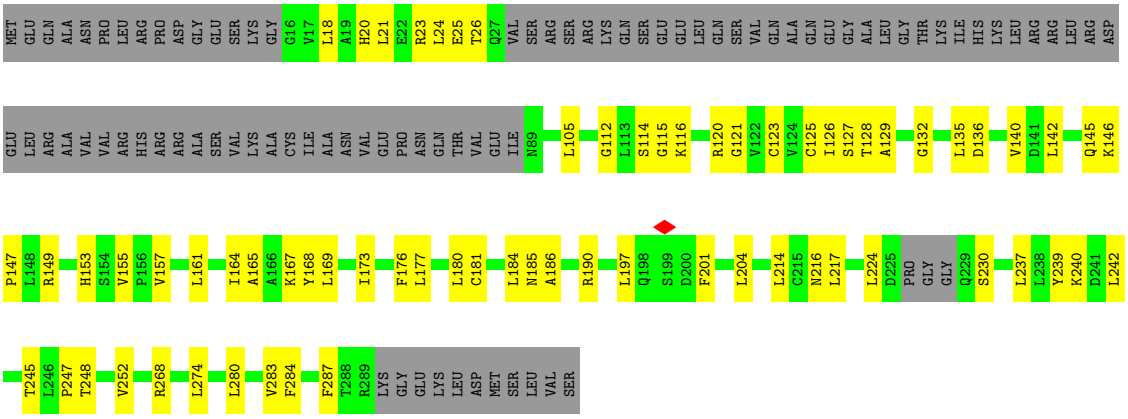
• Molecule 11: Centromere protein N

Chain N:



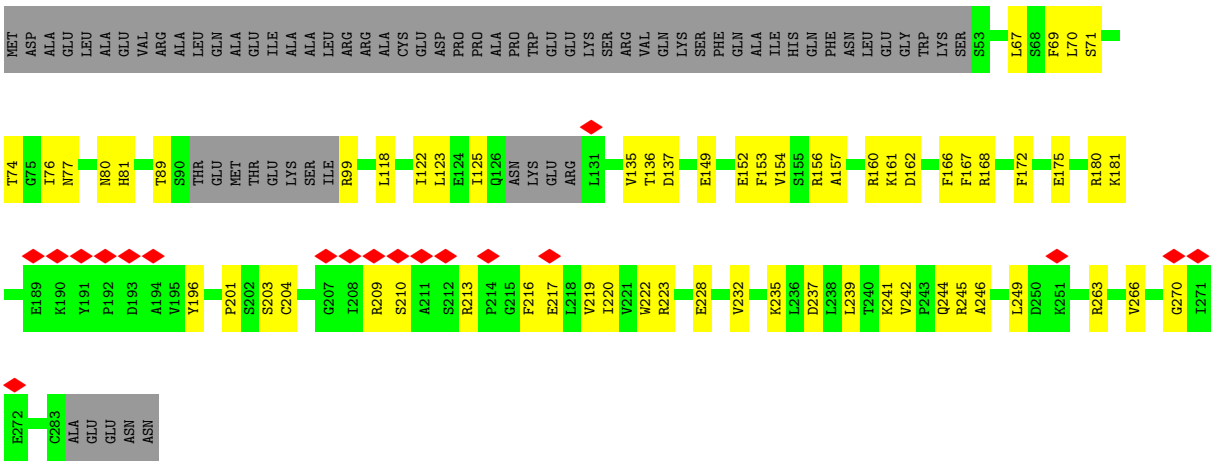
• Molecule 12: Centromere protein O

Chain O: 47% 23% 30%



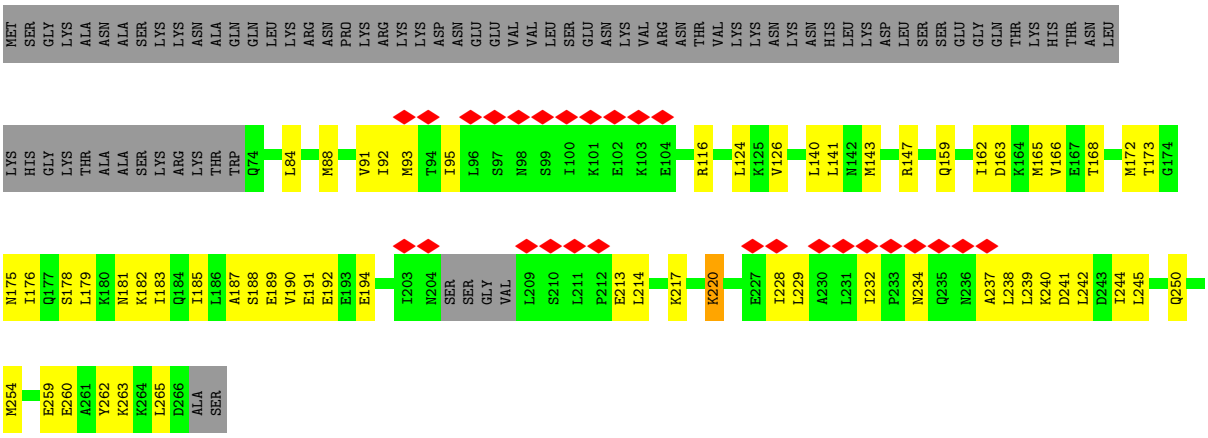
• Molecule 13: Centromere protein P

Chain P: 7% 55% 21% 24%



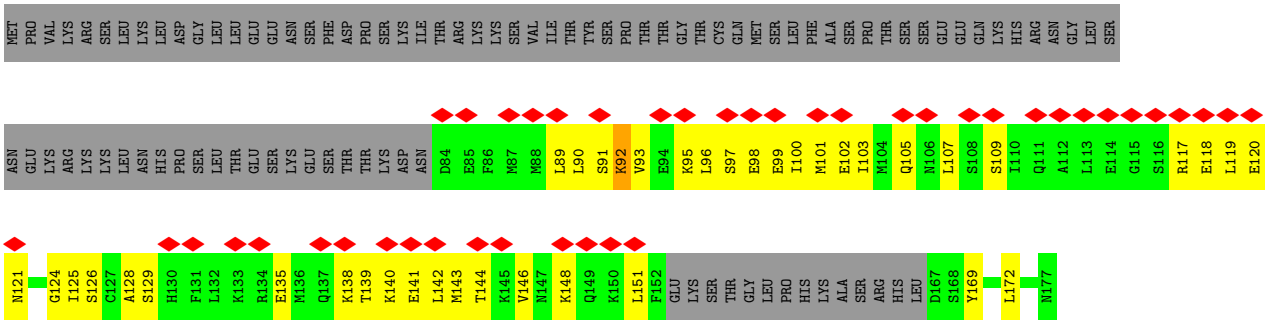
• Molecule 14: Centromere protein Q

Chain Q: 10% 49% 22% 29%



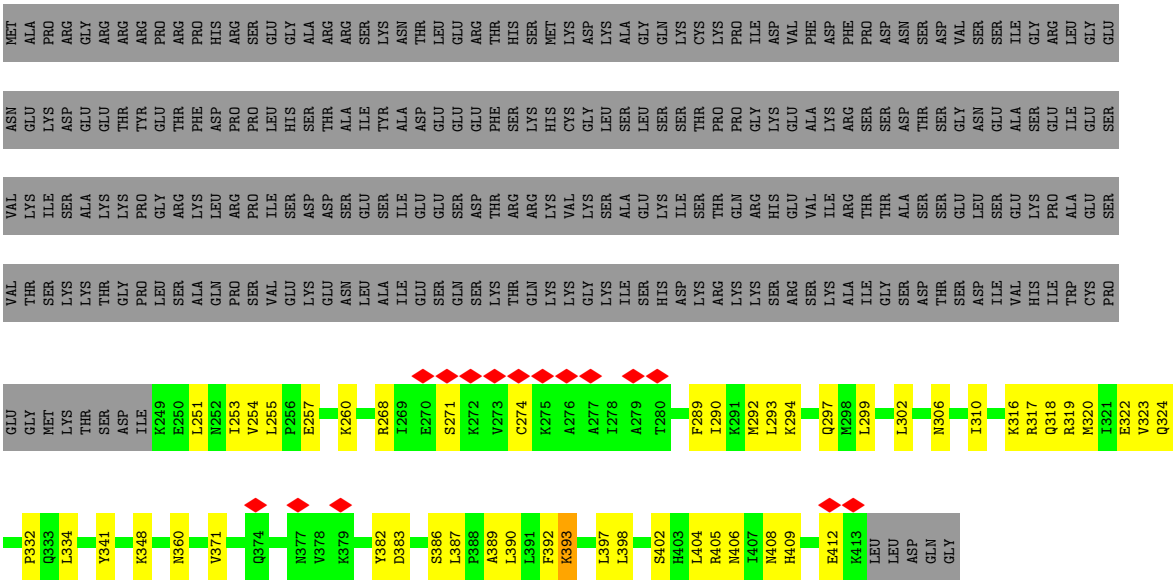
• Molecule 15: Centromere protein R

Chain R:



• Molecule 16: Centromere protein U

Chain U:



• Molecule 17: Centromere protein C

Chain k: 96%

MET ALA ALA SER GLY LEU ASP HIS LEU LYS ASN GLY TYR ARG ARG ARG PHE CYS ARG PRO SER ARG ALA ARG ASP ILE ASN THR GLU GLN GLY GLN ASN VAL LEU GLU ILE LEU GLN ASP CYS PHE GLU GLU LYS SER LEU ALA ASN ASP PHE SER THR ASN SER THR LYS SER VAL PRO

ASN SER THR ARG LYS ILE LYS ASP THR CYS ILE GLN SER PRO SER LYS GLU CYS GLN LYS SER HIS PRO LYS SER VAL PRO VAL SER SER LYS LYS LYS GLU ALA SER LEU GLN PHE VAL VAL GLU PRO SER GLU ALA THR ASN ARG SER VAL GLN ALA HIS GLU VAL HIS GLN LYS ILE

LEU ALA THR ASP VAL SER SER LYS ASN THR PRO ASP SER LYS LYS ILE SER SER SER VAL SER ARG ASN ILE ASN ASP THR HIS HIS SER GLU ALA ASP GLU GLU PHE TYR LEU SER VAL GLY SER PRO SER VAL LEU LEU ASP ALA LYS THR SER VAL SER GLN ASN VAL ILE PRO SER SER GLU GLY GLN LYS

ARG GLU THR TYR THR PHE GLU ASN SER VAL ASN MET LEU PRO SER SER THR GLU VAL SER VAL LYS THR LYS LYS ARG LEU ASN PHE ASP ASP LYS VAL MET LEU LYS LYS ILE GLU ILE ASP ASN LYS VAL SER ASP GLU GLU ASP LYS THR GLU GLU GLY GLN GLU GLU PRO SER

GLY SER SER GLN ASN ARG ILE ARG ASP SER GLU TYR GLU ILE GLN ARG GLN ALA LYS LYS SER PHE SER THR LEU PHE LEU GLU THR VAL LYS ARG LYS SER SER GLU SER SER PRO ILE VAL ARG HIS ALA ALA THR ALA PRO PRO HIS SER CYS PRO PRO ASP ASP THR LYS LEU ILE GLU

ASP GLU PHE ILE ILE ASP GLU SER ASP GLN SER PHE ALA SER ARG SER TRP ILE THR ILE ILE PRO ARG LYS ALA GLY SER LEU LYS GLN ARG THR ILE SER PRO ALA GLU SER THR ALA LEU LEU GLN GLY ARG LYS SER ARG GLU LYS HIS HIS ASN ILE LEU PRO LYS LYS THR

ASP LYS HIS SER HIS LYS PRO HIS PRO VAL GLU THR SER GLN PRO SER SER ASP LYS THR VAL ALA LEU ASP THR SER TYR ALA LEU ILE GLY GLU THR VAL ASN ASN TYR ARG SER THR LYS TYR GLU MET TYR SER LYS ASN ALA GLU LYS PRO SER ARG SER LYS ARG THR ILE LYS GLN LYS

GLN ARG ARG LYS PHE MET ALA LYS PRO ALA GLU GLU GLN LEU ASP VAL GLY GLN SER LYS ASP GLU ASN ILE HIS THR GLN ASP GLU PHE GLN ARG ASN SER ASP ARG ASN MET GLU GLU HIS GLU GLU MET GLY ASN ASP CYS VAL SER LYS LYS GLN MET PRO PRO

VAL GLY SER LYS LYS SER SER THR ARG LYS ASP LYS GLU GLU SER LYS LYS LYS ARG PHE SER SER GLU SER LYS ASN LYS LEU VAL PRO GLU GLU VAL THR S515 S535 GLU GLU SER PRO VAL TYR SER ASN SER

- Molecule 17: Centromere protein C

Chain l: 7% 90%

MET ALA ALA SER GLY LEU ASP HIS LEU LYS ASN GLY TYR ARG ARG ARG PHE CYS ARG PRO SER ARG ALA ARG ASP ILE ASN THR GLU GLN GLY GLN ASN VAL LEU GLU ILE LEU GLN ASP CYS PHE GLU GLU LYS SER LEU ALA ASN ASP PHE SER THR ASN SER THR LYS SER VAL PRO

ASN SER THR ARG LYS ILE LYS ASP THR CYS ILE GLN SER PRO SER LYS GLU CYS GLN LYS SER HIS PRO LYS SER VAL PRO VAL SER SER LYS LYS LYS GLU ALA SER LEU GLN PHE VAL VAL GLU PRO SER GLU ALA THR ASN ARG SER VAL GLN ALA HIS GLU VAL HIS GLN LYS ILE

LEU ALA THR ASP VAL SER SER LYS ASN THR PRO ASP SER LYS LYS ILE SER SER SER ARG ASN ILE ASN ASP HIS HIS SER GLU ALA ASP GLU GLU PHE TYR LEU SER VAL GLY SER PRO SER VAL LEU LEU ASP ALA LYS THR SER VAL SER GLN ASN VAL ILE PRO SER SER GLU GLY GLN LYS

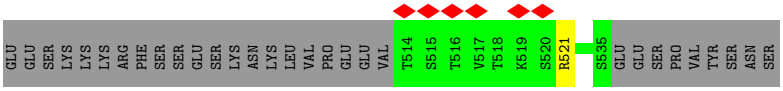
ARG GLU THR TYR THR PHE GLU ASN SER VAL ASN MET LEU PRO SER SER THR GLU VAL SER VAL LYS THR LYS LYS ARG LEU ASN PHE ASP ASP LYS VAL MET LEU LYS LYS ILE GLU ILE ASP ASN LYS VAL SER ASP GLU GLU ASP LYS THR SER GLU GLU GLY GLN GLU ARG LYS PRO SER

GLY SER SER GLN ASN ARG ILE ARG ASP SER GLU TYR GLU ILE GLN R256 Q257 A258 K259 K260 S261 T269 R272 K273 S274 E275 SER SER PRO ILE VAL ARG HIS ALA ALA THR ALA PRO PRO HIS SER CYS PRO PRO ASP D295 T296 K297 L298 I299 E300 D301 S308 D309 GLN SER PHE

ALA SER ARG SER TRP ILE THR THR ILE PRO ARG LYS ALA GLY SER LEU LYS GLN ARG THR ILE SER PRO ALA GLU SER THR ALA LEU LEU GLN GLY ARG LYS SER ARG GLU LYS HIS HIS ASN ILE LEU PRO LYS THR LEU ALA ASN ASP LYS HIS SER HIS PRO VAL GLU THR

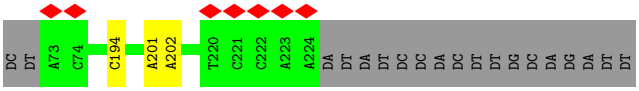
SER GLN PRO SER ASP LYS THR VAL LEU ASP THR SER ARG THR VAL ASN ASN ARG SER THR LYS TYR GLU MET TYR SER LYS ASN ALA GLU LYS PRO SER ARG SER LYS ARG THR ILE LYS GLN LYS ARG ARG LYS PHE MET ALA LYS PRO HIS PRO VAL GLU GLU

GLN LEU ASP VAL GLY GLN SER LYS ASP GLU ASN ILE HIS THR SER GLU PHE GLN ARG ASN SER ASP ARG ASN MET GLU GLU HIS GLU GLU MET GLY ASN ASP CYS VAL SER LYS LYS GLN MET PRO PRO VAL GLY SER LYS LYS SER SER THR ARG LYS ASP LYS



- Molecule 18: DNA (171-MER)

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.745	Depositor
Minimum map value	-0.777	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.239	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	312.456, 312.456, 312.456	wwPDB
Map dimensions	188, 188, 188	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.662, 1.662, 1.662	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/814	0.45	0/1097
1	E	0.50	0/785	0.50	0/1057
2	B	0.58	0/629	0.55	0/843
2	F	0.56	0/648	0.54	0/868
3	C	0.47	0/764	0.49	0/1030
3	G	0.48	0/793	0.46	0/1070
4	D	0.49	0/730	0.47	0/982
4	h	0.49	0/730	0.45	0/982
5	H	0.26	0/1390	0.46	0/1856
6	I	0.25	0/4515	0.41	1/6118 (0.0%)
7	J	0.82	10/3512 (0.3%)	1.21	18/5418 (0.3%)
8	K	0.28	0/1820	0.42	0/2450
9	L	0.26	0/2462	0.43	0/3340
10	M	0.25	0/1347	0.46	0/1827
11	N	0.32	1/2505 (0.0%)	0.49	2/3380 (0.1%)
12	O	0.26	0/1678	0.47	0/2280
13	P	0.28	0/1763	0.46	0/2377
14	Q	0.26	0/1518	0.44	0/2036
15	R	0.24	0/653	0.49	0/865
16	U	0.25	0/1364	0.43	0/1831
17	k	0.49	0/182	0.52	0/245
17	l	0.81	4/481 (0.8%)	1.62	8/641 (1.2%)
18	i	0.72	2/3502 (0.1%)	1.09	5/5403 (0.1%)
All	All	0.47	17/34585 (0.0%)	0.70	34/47996 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	J	0	1
17	l	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	14

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	54	DA	O3'-P	-10.81	1.48	1.61
17	l	301	ASP	C-N	7.50	1.51	1.34
18	i	194	DC	O3'-P	7.49	1.70	1.61
7	J	156	DG	C1'-N9	-7.11	1.37	1.47
7	J	44	DG	C1'-N9	-7.00	1.37	1.47
7	J	40	DC	C1'-N1	6.29	1.57	1.49
18	i	201	DA	C3'-O3'	-6.13	1.35	1.44
17	l	300	GLU	C-N	6.11	1.48	1.34
7	J	63	DC	O3'-P	6.04	1.68	1.61
17	l	296	THR	C-N	5.64	1.47	1.34
11	N	331	MET	C-N	-5.64	1.21	1.34
17	l	299	ILE	C-N	5.38	1.46	1.34
7	J	39	DT	C1'-N1	5.10	1.55	1.49
7	J	26	DC	C1'-N1	5.08	1.55	1.49
7	J	28	DC	C1'-N1	5.07	1.55	1.49
7	J	42	DT	C1'-N1	5.03	1.55	1.49
7	J	25	DC	C1'-N1	5.01	1.55	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	51	DG	O5'-P-OP1	-18.23	88.82	110.70
7	J	55	DT	O5'-P-OP1	-17.54	89.65	110.70
17	l	274	SER	O-C-N	-16.93	95.61	122.70
17	l	256	ARG	O-C-N	-16.31	96.60	122.70
7	J	54	DA	O5'-P-OP1	-15.98	91.32	105.70
17	l	258	ALA	O-C-N	-15.04	98.64	122.70
7	J	51	DG	O5'-P-OP2	14.50	128.09	110.70
17	l	257	GLN	O-C-N	-13.14	101.68	122.70
7	J	52	DG	O5'-P-OP1	-12.34	94.60	105.70
18	i	201	DA	O3'-P-O5'	-11.56	82.04	104.00
7	J	51	DG	N9-C1'-C2'	11.43	134.32	112.60
18	i	202	DA	O5'-P-OP1	11.25	124.20	110.70
17	l	273	LYS	O-C-N	-11.17	104.83	122.70
7	J	54	DA	O5'-P-OP2	8.64	121.06	110.70
11	N	331	MET	O-C-N	-8.48	109.12	122.70
7	J	51	DG	C4-N9-C1'	-8.43	115.54	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	i	202	DA	P-O5'-C5'	-7.91	108.25	120.90
7	J	51	DG	C1'-O4'-C4'	-7.57	102.53	110.10
7	J	51	DG	P-O5'-C5'	7.55	132.97	120.90
7	J	51	DG	C8-N9-C1'	7.31	136.50	127.00
17	l	259	LYS	O-C-N	-6.91	111.64	122.70
7	J	52	DG	O5'-C5'-C4'	-6.52	94.70	111.00
7	J	51	DG	O4'-C1'-N9	-5.92	103.85	108.00
7	J	51	DG	P-O3'-C3'	5.85	126.72	119.70
7	J	55	DT	P-O5'-C5'	-5.84	111.55	120.90
17	l	272	ARG	O-C-N	-5.78	113.45	122.70
7	J	53	DA	C8-N9-C1'	-5.70	117.45	127.70
11	N	331	MET	CA-C-N	5.64	129.60	117.20
7	J	53	DA	O5'-P-OP2	5.62	117.44	110.70
18	i	201	DA	C2'-C3'-O3'	-5.53	94.36	112.60
6	I	593	LEU	CA-CB-CG	5.35	127.60	115.30
17	l	296	THR	O-C-N	-5.28	114.25	122.70
7	J	55	DT	OP1-P-OP2	5.15	127.33	119.60
18	i	202	DA	C3'-C2'-C1'	-5.05	96.44	102.50

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	J	53	DA	Sidechain
17	l	256	ARG	Mainchain
17	l	257	GLN	Mainchain
17	l	258	ALA	Mainchain
17	l	259	LYS	Mainchain
17	l	260	LYS	Mainchain
17	l	273	LYS	Mainchain
17	l	274	SER	Mainchain
17	l	296	THR	Mainchain
17	l	297	LYS	Mainchain
17	l	298	LEU	Mainchain
17	l	300	GLU	Mainchain
17	l	301	ASP	Mainchain
17	l	308	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	799	0	823	10	0
1	E	770	0	807	9	0
2	B	622	0	660	6	0
2	F	641	0	684	11	0
3	C	755	0	800	14	0
3	G	784	0	815	7	0
4	D	719	0	738	9	0
4	h	719	0	738	0	0
5	H	1384	0	1447	47	0
6	I	4402	0	4398	128	0
7	J	3133	0	1734	107	0
8	K	1793	0	1795	35	0
9	L	2397	0	2395	67	0
10	M	1325	0	1370	54	0
11	N	2452	0	2480	109	0
12	O	1642	0	1616	62	0
13	P	1732	0	1715	48	0
14	Q	1506	0	1561	76	0
15	R	649	0	673	103	0
16	U	1346	0	1367	78	0
17	k	178	0	185	0	0
17	l	476	0	483	0	0
18	i	3120	0	1718	0	0
All	All	33344	0	31002	783	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (783) 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)
6:I:259:LYS:CD	6:I:312:VAL:HG12	1.29	1.55
15:R:151:LEU:HG	16:U:412:GLU:CB	1.11	1.54
14:Q:250:GLN:CB	15:R:96:LEU:HD21	1.38	1.53
6:I:259:LYS:HD3	6:I:312:VAL:CG1	1.34	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:151:LEU:CD2	16:U:412:GLU:HB3	1.33	1.52
14:Q:250:GLN:CG	15:R:96:LEU:HD21	1.28	1.51
11:N:271:LEU:CD2	11:N:336:ILE:HD13	1.38	1.49
15:R:151:LEU:CG	16:U:412:GLU:HB3	1.38	1.46
15:R:135:GLU:CG	16:U:398:LEU:HD23	1.45	1.45
14:Q:254:MET:CE	15:R:93:VAL:HG12	1.48	1.42
15:R:151:LEU:CG	16:U:412:GLU:CB	1.87	1.41
11:N:271:LEU:HD21	11:N:336:ILE:CD1	1.53	1.37
14:Q:250:GLN:HG2	15:R:96:LEU:CD2	1.48	1.35
15:R:135:GLU:CG	16:U:398:LEU:CD2	2.06	1.34
14:Q:254:MET:CE	15:R:93:VAL:CG1	2.06	1.31
14:Q:254:MET:HE1	15:R:93:VAL:CG1	1.63	1.27
15:R:135:GLU:HG2	16:U:398:LEU:CD2	1.65	1.23
14:Q:250:GLN:CG	15:R:96:LEU:CD2	2.06	1.20
7:J:33:DA:OP1	11:N:18:MET:HG3	1.43	1.19
11:N:271:LEU:CD2	11:N:336:ILE:CD1	2.16	1.16
6:I:259:LYS:CD	6:I:313:LEU:O	1.95	1.14
14:Q:241:ASP:OD2	15:R:107:LEU:CD2	1.95	1.13
15:R:135:GLU:HG3	16:U:398:LEU:CD2	1.77	1.13
15:R:151:LEU:HD23	16:U:412:GLU:HB3	1.29	1.12
14:Q:241:ASP:OD2	15:R:107:LEU:HD21	1.47	1.11
6:I:259:LYS:HD2	6:I:313:LEU:O	1.49	1.10
14:Q:254:MET:HE1	15:R:93:VAL:HG11	1.20	1.09
14:Q:241:ASP:CG	15:R:107:LEU:HD21	1.73	1.09
7:J:43:DT:H4'	11:N:169:ARG:NE	1.58	1.09
15:R:151:LEU:HD21	16:U:412:GLU:OE1	1.54	1.08
7:J:43:DT:H2"	11:N:169:ARG:NH1	1.59	1.07
14:Q:250:GLN:CB	15:R:96:LEU:CD2	2.27	1.07
7:J:43:DT:H4'	11:N:169:ARG:CD	1.84	1.07
14:Q:250:GLN:HB3	15:R:96:LEU:HD21	1.30	1.07
7:J:33:DA:OP1	11:N:18:MET:CG	2.02	1.06
14:Q:250:GLN:HB3	15:R:96:LEU:CD2	1.85	1.06
14:Q:254:MET:HE3	15:R:93:VAL:CG1	1.77	1.06
15:R:151:LEU:CG	16:U:412:GLU:HB2	1.64	1.04
7:J:32:DG:H5"	11:N:45:LYS:NZ	1.72	1.04
15:R:151:LEU:CD2	16:U:412:GLU:CB	2.24	1.03
15:R:151:LEU:HD11	16:U:412:GLU:OE1	1.58	1.03
15:R:142:LEU:CB	16:U:405:ARG:HE	1.70	1.03
6:I:259:LYS:CE	6:I:313:LEU:O	2.07	1.01
15:R:151:LEU:HD23	16:U:408:ASN:O	1.61	1.01
6:I:259:LYS:CE	6:I:312:VAL:HG12	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:254:MET:HE3	15:R:93:VAL:HG12	0.99	0.96
14:Q:250:GLN:HG2	15:R:96:LEU:HD21	1.06	0.95
15:R:135:GLU:HG3	16:U:398:LEU:HD21	1.45	0.95
7:J:32:DG:H3'	11:N:45:LYS:HE2	1.50	0.94
6:I:259:LYS:HE3	6:I:313:LEU:O	1.70	0.92
7:J:42:DT:H2"	7:J:43:DT:H72	1.54	0.90
6:I:259:LYS:HD3	6:I:312:VAL:HG11	1.53	0.90
7:J:43:DT:H4'	11:N:169:ARG:HD3	1.51	0.90
7:J:43:DT:C4'	11:N:169:ARG:NE	2.31	0.90
7:J:32:DG:C5'	11:N:45:LYS:NZ	2.35	0.89
7:J:32:DG:C5'	11:N:45:LYS:HZ3	1.86	0.89
6:I:281:ARG:NH1	6:I:345:GLN:HB3	1.88	0.89
6:I:259:LYS:CE	6:I:312:VAL:CG1	2.48	0.88
7:J:53:DA:H1'	7:J:54:DA:O5'	1.75	0.86
7:J:43:DT:H2"	11:N:169:ARG:HH12	1.39	0.85
14:Q:250:GLN:HG2	15:R:96:LEU:HD22	1.55	0.85
7:J:32:DG:H5"	11:N:45:LYS:HZ1	1.43	0.84
6:I:259:LYS:CD	6:I:312:VAL:CG1	2.13	0.83
6:I:729:GLN:HA	6:I:732:LYS:HE2	1.59	0.83
14:Q:241:ASP:CG	15:R:107:LEU:CD2	2.41	0.82
7:J:43:DT:H5'	11:N:167:MET:HE1	1.62	0.82
15:R:151:LEU:HD21	16:U:412:GLU:CD	2.00	0.82
6:I:281:ARG:HH12	6:I:345:GLN:HB3	1.45	0.80
7:J:32:DG:H5"	11:N:45:LYS:HZ3	1.42	0.80
15:R:142:LEU:HB2	16:U:405:ARG:HE	1.46	0.79
15:R:151:LEU:CD2	16:U:412:GLU:OE1	2.29	0.79
12:O:21:LEU:HA	12:O:24:LEU:HD12	1.65	0.79
15:R:142:LEU:HD12	16:U:409:HIS:NE2	1.96	0.79
13:P:69:PHE:CE1	15:R:172:LEU:HD11	2.18	0.78
6:I:487:ILE:HD11	6:I:557:LEU:HB2	1.64	0.78
7:J:43:DT:C2'	11:N:169:ARG:NH1	2.41	0.78
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.31	0.77
9:L:311:VAL:HG23	9:L:324:CYS:HB3	1.65	0.77
15:R:151:LEU:CD1	16:U:412:GLU:OE1	2.32	0.77
5:H:219:LEU:HD13	8:K:184:LEU:HD21	1.68	0.76
11:N:269:TYR:CE1	11:N:334:PHE:CD1	2.74	0.76
15:R:135:GLU:HG2	16:U:398:LEU:HD23	0.78	0.76
11:N:270:LYS:O	11:N:335:LYS:HA	1.86	0.76
11:N:272:GLU:O	11:N:337:ARG:HA	1.86	0.76
6:I:259:LYS:NZ	6:I:312:VAL:CG1	2.49	0.75
10:M:9:LYS:NZ	10:M:58:VAL:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:90:LYS:HG3	11:N:186:HIS:HD2	1.52	0.73
11:N:271:LEU:HD22	11:N:336:ILE:CD1	2.17	0.73
11:N:271:LEU:CG	11:N:336:ILE:HD13	2.07	0.73
7:J:43:DT:H5'	11:N:167:MET:CE	2.19	0.72
6:I:487:ILE:HD13	6:I:551:GLU:HG3	1.69	0.72
9:L:225:TRP:HE1	9:L:331:VAL:HG22	1.55	0.72
15:R:151:LEU:HG	16:U:412:GLU:HB2	0.72	0.72
6:I:720:LEU:HA	6:I:723:LEU:HD12	1.71	0.72
14:Q:262:TYR:HB3	16:U:404:LEU:HD21	1.73	0.71
10:M:6:PRO:O	10:M:62:ARG:NH1	2.23	0.71
9:L:164:CYS:HB2	9:L:182:PRO:HD2	1.72	0.71
15:R:90:LEU:HD21	15:R:140:LYS:HD2	1.72	0.71
11:N:271:LEU:HD21	11:N:336:ILE:HD13	0.71	0.70
13:P:69:PHE:HE1	15:R:172:LEU:CD1	2.05	0.70
14:Q:241:ASP:CB	15:R:107:LEU:HD21	2.21	0.70
6:I:549:ARG:HH22	10:M:157:VAL:HG13	1.56	0.69
7:J:54:DA:H1'	7:J:55:DT:OP2	1.92	0.69
15:R:151:LEU:HD21	16:U:412:GLU:HB3	1.65	0.69
14:Q:213:GLU:HG3	14:Q:217:LYS:H	1.58	0.69
13:P:69:PHE:CZ	15:R:172:LEU:HD11	2.28	0.69
11:N:18:MET:HG2	11:N:45:LYS:HE3	1.75	0.69
6:I:644:LEU:HA	6:I:647:MET:HE3	1.74	0.68
11:N:120:THR:HB	11:N:136:ALA:HB3	1.74	0.68
16:U:251:LEU:HA	16:U:254:VAL:HG22	1.75	0.68
10:M:122:HIS:O	10:M:125:GLN:NE2	2.27	0.67
15:R:142:LEU:HD12	16:U:409:HIS:CE1	2.29	0.67
12:O:197:LEU:HD22	12:O:280:LEU:HD21	1.77	0.67
15:R:151:LEU:HG	16:U:412:GLU:CA	2.16	0.67
6:I:259:LYS:HD3	6:I:312:VAL:HG12	0.69	0.67
6:I:467:PHE:HB3	6:I:535:LYS:HE2	1.76	0.67
14:Q:183:ILE:HD13	16:U:341:TYR:HA	1.75	0.67
15:R:117:ARG:HD2	15:R:120:GLU:HB2	1.77	0.66
7:J:53:DA:H2"	7:J:54:DA:C8	2.30	0.66
6:I:312:VAL:O	6:I:362:GLN:NE2	2.27	0.66
6:I:603:LEU:HB3	6:I:607:MET:HE1	1.78	0.66
7:J:51:DG:H8	7:J:51:DG:OP2	1.78	0.66
10:M:7:LEU:HD23	10:M:62:ARG:HH12	1.60	0.66
6:I:562:LEU:O	6:I:566:GLU:HG3	1.95	0.66
15:R:118:GLU:HG3	15:R:119:LEU:HD12	1.78	0.66
6:I:549:ARG:HE	10:M:159:GLY:HA3	1.61	0.66
11:N:47:SER:O	11:N:51:HIS:ND1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:259:LYS:CE	6:I:312:VAL:HG13	2.24	0.66
10:M:161:SER:N	10:M:164:ASN:OD1	2.29	0.65
11:N:116:LEU:HD12	11:N:117:LYS:H	1.61	0.65
13:P:263:ARG:NH2	14:Q:220:LYS:O	2.21	0.65
15:R:146:VAL:HA	15:R:151:LEU:HD13	1.78	0.65
12:O:237:LEU:HD23	12:O:247:PRO:HG3	1.77	0.65
11:N:328:ASN:HB3	12:O:149:ARG:HH22	1.59	0.65
13:P:239:LEU:HD21	16:U:386:SER:HA	1.78	0.65
9:L:31:LEU:HG	9:L:35:ARG:HH21	1.61	0.65
1:E:61:LEU:O	2:F:36:ARG:NH1	2.30	0.65
9:L:40:PHE:HB3	10:M:115:HIS:HB2	1.79	0.65
12:O:146:LYS:HE2	15:R:169:TYR:CE1	2.33	0.64
11:N:112:LEU:HB3	11:N:119:VAL:HG11	1.79	0.64
6:I:544:SER:HB2	6:I:561:ILE:HD12	1.80	0.64
11:N:77:HIS:ND1	11:N:80:GLN:OE1	2.31	0.64
5:H:164:LEU:HD11	8:K:136:MET:HG3	1.80	0.64
7:J:143:DA:H2"	7:J:144:DT:H5'	1.80	0.64
11:N:97:ASP:O	12:O:216:ASN:ND2	2.31	0.64
11:N:2:ASP:HB3	11:N:5:VAL:HG22	1.80	0.63
10:M:71:ASN:OD1	10:M:102:THR:OG1	2.17	0.63
13:P:69:PHE:CE1	15:R:172:LEU:CD1	2.80	0.63
2:F:82:THR:HG22	2:F:84:MET:H	1.63	0.63
10:M:9:LYS:O	10:M:62:ARG:NE	2.31	0.63
7:J:43:DT:H73	7:J:43:DT:OP2	1.99	0.63
7:J:51:DG:H2"	7:J:52:DG:H2'	1.80	0.62
11:N:271:LEU:CD2	11:N:336:ILE:HD12	2.24	0.62
16:U:389:ALA:O	16:U:392:PHE:HB3	1.99	0.62
16:U:402:SER:O	16:U:406:ASN:ND2	2.28	0.62
9:L:235:ALA:HB3	9:L:310:SER:HA	1.80	0.62
12:O:116:LYS:NZ	12:O:125:CYS:SG	2.68	0.62
12:O:120:ARG:NH1	12:O:120:ARG:HA	2.15	0.62
6:I:102:ASN:HA	6:I:273:LEU:HD22	1.81	0.62
16:U:251:LEU:HB2	16:U:293:LEU:HD21	1.82	0.62
2:F:36:ARG:NH2	7:J:109:DT:OP1	2.32	0.62
9:L:46:ARG:HH11	9:L:274:GLU:HG2	1.64	0.62
11:N:195:SER:HB3	11:N:201:LEU:HD21	1.82	0.62
5:H:241:GLU:OE1	6:I:218:ARG:NH2	2.33	0.61
5:H:158:ARG:HH21	6:I:429:GLN:HG2	1.66	0.61
6:I:490:LYS:NZ	6:I:551:GLU:OE2	2.33	0.61
6:I:529:SER:OG	6:I:530:MET:N	2.33	0.61
11:N:50:GLN:O	11:N:54:HIS:ND1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:481:LEU:HD22	10:M:145:ARG:HH22	1.65	0.61
11:N:271:LEU:HD22	11:N:336:ILE:HD12	1.82	0.61
6:I:592:LEU:HD11	6:I:647:MET:HB3	1.81	0.61
16:U:302:LEU:O	16:U:306:ASN:ND2	2.33	0.61
5:H:86:GLU:HA	5:H:89:ILE:HG12	1.81	0.61
6:I:486:THR:HA	10:M:148:ARG:HH12	1.64	0.61
1:E:57:SER:HG	1:E:59:HIS:HD1	1.48	0.60
7:J:65:DT:H2"	7:J:66:DA:N7	2.16	0.60
6:I:79:LYS:HB2	6:I:84:LYS:HE3	1.83	0.60
6:I:445:LEU:HD13	10:M:105:GLY:HA2	1.82	0.60
7:J:143:DA:H2'	7:J:144:DT:H71	1.83	0.60
15:R:142:LEU:CB	16:U:405:ARG:NE	2.50	0.60
9:L:40:PHE:O	10:M:115:HIS:ND1	2.35	0.60
9:L:163:CYS:SG	9:L:164:CYS:N	2.74	0.60
9:L:183:LEU:HD21	9:L:336:THR:HA	1.82	0.60
10:M:70:VAL:HG12	10:M:81:THR:HG21	1.83	0.60
14:Q:245:LEU:CD2	15:R:103:ILE:HB	2.31	0.60
7:J:54:DA:H1'	7:J:55:DT:P	2.42	0.60
7:J:51:DG:H1'	7:J:52:DG:N9	2.17	0.60
16:U:382:TYR:HD2	16:U:386:SER:HB2	1.67	0.60
12:O:23:ARG:O	12:O:26:THR:OG1	2.19	0.60
6:I:596:ASP:OD2	6:I:598:SER:OG	2.19	0.59
7:J:42:DT:H2"	7:J:43:DT:C7	2.28	0.59
10:M:170:ARG:HH22	10:M:172:SER:HA	1.67	0.59
3:C:29:ARG:NH1	4:D:36:SER:O	2.34	0.59
14:Q:172:MET:HB2	16:U:334:LEU:HD21	1.82	0.59
5:H:128:ASP:HA	5:H:131:LYS:HE3	1.85	0.59
10:M:73:HIS:HE1	10:M:103:GLY:HA3	1.67	0.59
15:R:91:SER:O	15:R:95:LYS:HG2	2.03	0.59
6:I:259:LYS:NZ	6:I:312:VAL:HG12	2.14	0.58
7:J:33:DA:OP1	11:N:18:MET:SD	2.60	0.58
12:O:181:CYS:O	12:O:185:ASN:ND2	2.35	0.58
6:I:724:PHE:HE1	6:I:731:LEU:HD22	1.68	0.58
9:L:68:LEU:HD21	9:L:328:LEU:HD22	1.85	0.58
12:O:128:THR:OG1	12:O:136:ASP:O	2.18	0.58
7:J:51:DG:H1'	7:J:52:DG:O4'	2.03	0.58
2:F:93:GLN:HE21	2:F:95:ARG:HH21	1.52	0.58
11:N:120:THR:HG21	11:N:146:GLN:HE22	1.67	0.58
12:O:177:LEU:HD13	12:O:180:LEU:HD21	1.84	0.58
13:P:74:THR:HG23	13:P:76:ILE:H	1.68	0.58
13:P:153:PHE:HA	13:P:156:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:582:LEU:HD21	6:I:643:TYR:HE1	1.68	0.58
11:N:11:ARG:HH12	11:N:147:TYR:HA	1.69	0.58
11:N:84:GLU:HG2	11:N:194:ARG:HG3	1.86	0.58
11:N:240:GLU:O	11:N:245:LYS:NZ	2.35	0.57
6:I:311:PRO:HB2	6:I:362:GLN:HG3	1.85	0.57
12:O:114:SER:HB2	12:O:125:CYS:HB2	1.86	0.57
6:I:724:PHE:CG	6:I:732:LYS:HD2	2.38	0.57
7:J:51:DG:H1'	7:J:52:DG:C8	2.40	0.57
9:L:142:VAL:HG22	9:L:156:VAL:HG22	1.86	0.57
7:J:51:DG:O4'	7:J:52:DG:H5'	2.05	0.57
12:O:197:LEU:HD12	12:O:201:PHE:HB2	1.85	0.57
5:H:104:ASP:OD1	5:H:105:ARG:N	2.37	0.57
11:N:116:LEU:HD12	11:N:117:LYS:N	2.18	0.57
13:P:210:SER:OG	13:P:213:ARG:O	2.22	0.57
14:Q:173:THR:O	14:Q:176:ILE:HB	2.05	0.57
11:N:25:LEU:HG	11:N:36:LEU:HD13	1.86	0.57
16:U:390:LEU:O	16:U:393:LYS:HG3	2.05	0.57
3:G:55:LEU:O	3:G:59:THR:HG23	2.04	0.57
7:J:52:DG:P	7:J:52:DG:H3'	2.33	0.57
12:O:284:PHE:HD1	12:O:287:PHE:HE1	1.53	0.56
15:R:135:GLU:O	15:R:139:THR:HG23	2.05	0.56
12:O:145:GLN:HG3	12:O:147:PRO:HD2	1.86	0.56
15:R:151:LEU:CD1	16:U:412:GLU:HB2	2.33	0.56
5:H:141:MET:HE1	6:I:730:GLY:H	1.70	0.56
9:L:163:CYS:O	9:L:183:LEU:HB2	2.05	0.56
11:N:180:THR:OG1	11:N:185:HIS:O	2.22	0.56
9:L:322:ILE:HG21	9:L:328:LEU:HD13	1.87	0.56
11:N:16:ILE:HG21	11:N:24:ILE:HG13	1.88	0.56
5:H:105:ARG:HH22	6:I:594:SER:HA	1.71	0.56
9:L:35:ARG:HG2	9:L:344:GLU:HG3	1.86	0.56
3:C:88:ARG:HH11	3:C:94:ASN:HD22	1.54	0.56
7:J:54:DA:H2'	7:J:54:DA:OP2	2.05	0.56
12:O:190:ARG:NH1	12:O:214:LEU:O	2.38	0.56
14:Q:234:ASN:HB2	14:Q:237:ALA:HB3	1.88	0.56
10:M:31:LEU:HB2	10:M:133:LEU:HD11	1.88	0.55
14:Q:228:ILE:HD12	15:R:118:GLU:CD	2.27	0.55
5:H:156:ASP:OD1	5:H:157:ILE:N	2.39	0.55
9:L:306:ARG:HD3	9:L:315:HIS:HD2	1.71	0.55
11:N:328:ASN:HB3	12:O:149:ARG:NH2	2.21	0.55
10:M:39:ASP:OD1	11:N:236:ARG:NH1	2.40	0.55
11:N:273:THR:CG2	11:N:336:ILE:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:51:DG:C3'	7:J:52:DG:H5'	2.35	0.55
8:K:93:GLY:O	8:K:96:GLU:HG3	2.07	0.55
11:N:65:ASP:OD1	11:N:66:ALA:N	2.39	0.55
6:I:487:ILE:HA	6:I:490:LYS:HD2	1.89	0.55
10:M:131:CYS:SG	10:M:132:ASP:N	2.80	0.55
9:L:31:LEU:HG	9:L:35:ARG:HE	1.71	0.55
12:O:161:LEU:O	12:O:165:ALA:N	2.39	0.55
6:I:529:SER:OG	6:I:530:MET:SD	2.65	0.55
6:I:603:LEU:HA	6:I:606:ILE:HG22	1.89	0.55
15:R:144:THR:O	15:R:148:LYS:HG2	2.07	0.54
5:H:207:LYS:HD2	8:K:268:HIS:HB2	1.89	0.54
7:J:71:DC:H1'	7:J:72:DT:H5'	1.88	0.54
13:P:71:SER:OG	13:P:77:ASN:OD1	2.21	0.54
6:I:281:ARG:NH1	6:I:345:GLN:O	2.36	0.54
7:J:51:DG:H1'	7:J:52:DG:C1'	2.37	0.54
15:R:135:GLU:CB	16:U:398:LEU:CD2	2.84	0.54
12:O:18:LEU:O	12:O:21:LEU:HG	2.07	0.54
6:I:591:ALA:HB1	6:I:603:LEU:HD21	1.89	0.54
6:I:547:ALA:HA	6:I:550:LEU:HB2	1.90	0.54
11:N:115:ALA:HB1	11:N:174:LEU:HD21	1.89	0.54
11:N:71:ILE:O	11:N:75:GLN:HG2	2.08	0.54
10:M:146:LEU:HA	10:M:149:VAL:HG12	1.91	0.53
11:N:97:ASP:O	11:N:157:GLN:NE2	2.42	0.53
13:P:172:PHE:HB3	13:P:232:VAL:HG11	1.90	0.53
14:Q:254:MET:CE	15:R:93:VAL:HG11	1.97	0.53
15:R:151:LEU:CG	16:U:412:GLU:OE1	2.56	0.53
6:I:599:ILE:O	6:I:603:LEU:HD23	2.08	0.53
11:N:199:ASP:OD1	11:N:200:SER:N	2.41	0.53
12:O:146:LYS:HE2	15:R:169:TYR:CZ	2.44	0.53
12:O:216:ASN:OD1	12:O:217:LEU:N	2.41	0.53
14:Q:228:ILE:HD12	15:R:118:GLU:OE2	2.07	0.53
6:I:281:ARG:HH22	6:I:345:GLN:HB2	1.73	0.53
6:I:453:SER:HA	12:O:18:LEU:HD21	1.89	0.53
7:J:160:DC:H2"	7:J:161:DA:C8	2.43	0.53
9:L:77:LEU:HD13	9:L:208:PHE:CD1	2.43	0.53
8:K:19:ASN:N	8:K:22:GLU:OE1	2.41	0.53
15:R:151:LEU:CD2	16:U:408:ASN:O	2.46	0.53
9:L:218:LEU:HD23	9:L:304:LEU:HG	1.91	0.53
7:J:87:DT:H2"	7:J:88:DC:C6	2.44	0.53
14:Q:189:GLU:O	14:Q:192:GLU:HG3	2.09	0.53
15:R:117:ARG:HE	15:R:121:ASN:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:228:ILE:HG21	15:R:119:LEU:HG	1.90	0.53
15:R:142:LEU:CD1	16:U:409:HIS:NE2	2.71	0.53
7:J:68:DA:H2"	7:J:69:DA:H8	1.72	0.53
2:F:35:ARG:O	2:F:39:ARG:HG2	2.08	0.53
7:J:32:DG:C5'	11:N:45:LYS:HZ1	2.10	0.53
7:J:55:DT:P	7:J:55:DT:O4'	2.67	0.53
11:N:27:ALA:HB1	11:N:72:ILE:HG12	1.90	0.53
6:I:349:GLN:O	6:I:353:ASN:ND2	2.42	0.52
9:L:225:TRP:HZ2	9:L:331:VAL:HG13	1.75	0.52
5:H:47:ARG:HG2	8:K:28:CYS:HB2	1.91	0.52
3:C:64:GLU:HB2	4:D:48:VAL:HG21	1.91	0.52
9:L:222:ALA:HB2	9:L:307:VAL:HG11	1.91	0.52
9:L:332:LEU:HD13	9:L:335:LEU:HD11	1.90	0.52
7:J:55:DT:C6	7:J:55:DT:OP1	2.62	0.52
7:J:68:DA:H2"	7:J:69:DA:C8	2.44	0.52
11:N:242:ILE:HA	11:N:245:LYS:HE2	1.91	0.52
14:Q:260:GLU:HA	14:Q:263:LYS:HD3	1.91	0.52
7:J:53:DA:OP2	7:J:53:DA:H8	1.92	0.52
9:L:116:ASN:ND2	9:L:144:LYS:O	2.43	0.52
13:P:263:ARG:NH1	14:Q:217:LYS:O	2.42	0.52
6:I:507:TRP:HE3	6:I:508:LEU:HD22	1.74	0.52
10:M:72:LEU:O	10:M:111:SER:N	2.42	0.52
10:M:85:LEU:HD13	10:M:124:TYR:HE2	1.75	0.52
13:P:136:THR:O	13:P:161:LYS:NZ	2.38	0.52
14:Q:191:GLU:O	14:Q:194:GLU:HG3	2.10	0.52
15:R:151:LEU:HD21	16:U:412:GLU:CG	2.40	0.52
8:K:36:GLU:O	8:K:40:ASN:ND2	2.42	0.52
9:L:75:TYR:HB2	9:L:184:PHE:HB3	1.92	0.52
10:M:100:LEU:HD11	10:M:131:CYS:HB3	1.92	0.52
13:P:160:ARG:NH2	13:P:228:GLU:OE1	2.43	0.52
5:H:132:HIS:O	5:H:136:LEU:HD23	2.09	0.52
12:O:240:LYS:NZ	12:O:248:THR:HB	2.26	0.51
13:P:246:ALA:HA	13:P:249:LEU:HD12	1.92	0.51
1:E:79:THR:HG23	1:E:81:GLY:H	1.75	0.51
5:H:137:ASN:OD1	6:I:597:THR:OG1	2.29	0.51
11:N:201:LEU:HA	11:N:204:ILE:HG22	1.92	0.51
11:N:264:LEU:HD21	11:N:332:ASN:OD1	2.10	0.51
1:A:112:LEU:HD13	1:A:128:LEU:HD23	1.92	0.51
11:N:269:TYR:CD1	11:N:334:PHE:CD1	2.99	0.51
6:I:568:VAL:O	6:I:571:ILE:HG13	2.10	0.51
7:J:42:DT:H2"	7:J:43:DT:C5	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:43:DT:OP1	11:N:167:MET:CE	2.58	0.51
11:N:33:GLU:OE2	11:N:37:GLN:NE2	2.43	0.51
13:P:239:LEU:HD22	16:U:389:ALA:HB3	1.90	0.51
14:Q:250:GLN:HB3	15:R:96:LEU:HD23	1.83	0.51
15:R:128:ALA:O	16:U:397:LEU:HD22	2.09	0.51
9:L:317:ASP:OD2	9:L:319:LYS:NZ	2.43	0.51
13:P:122:ILE:HA	13:P:135:VAL:HA	1.93	0.51
15:R:98:GLU:O	15:R:102:GLU:HG2	2.11	0.51
7:J:43:DT:OP2	7:J:43:DT:C7	2.59	0.51
9:L:231:ASP:OD1	9:L:326:LYS:NZ	2.44	0.51
6:I:281:ARG:CZ	6:I:345:GLN:HB3	2.40	0.51
6:I:650:CYS:O	6:I:684:HIS:NE2	2.43	0.51
9:L:32:GLU:CD	9:L:35:ARG:HH22	2.14	0.51
9:L:79:PRO:HG3	9:L:170:LEU:HD21	1.93	0.51
6:I:495:GLN:O	6:I:498:LYS:HG3	2.11	0.50
11:N:114:ARG:NH2	16:U:324:GLN:OE1	2.42	0.50
12:O:284:PHE:HA	12:O:287:PHE:CE1	2.46	0.50
13:P:123:LEU:HD21	13:P:125:ILE:HD11	1.92	0.50
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.93	0.50
6:I:366:VAL:HG11	6:I:376:ILE:HG13	1.94	0.50
6:I:549:ARG:HH21	10:M:158:PRO:C	2.14	0.50
5:H:105:ARG:NH2	6:I:593:LEU:HD12	2.25	0.50
9:L:238:GLU:OE1	9:L:306:ARG:NH2	2.43	0.50
9:L:250:LEU:HD21	11:N:309:LEU:HD21	1.94	0.50
11:N:28:TRP:CD2	11:N:69:LEU:HD12	2.46	0.50
9:L:227:ALA:HA	9:L:265:TRP:NE1	2.26	0.50
14:Q:178:SER:HA	14:Q:181:ASN:HD21	1.76	0.50
6:I:78:ILE:HG13	6:I:84:LYS:HD3	1.93	0.50
6:I:605:PHE:O	6:I:609:ARG:HG2	2.12	0.50
7:J:55:DT:OP1	7:J:55:DT:H6	1.94	0.50
7:J:77:DA:H2"	7:J:78:DG:C8	2.47	0.50
7:J:118:DC:H2'	7:J:119:DT:C6	2.47	0.50
8:K:129:LEU:O	8:K:132:GLN:NE2	2.45	0.50
12:O:284:PHE:CD1	12:O:287:PHE:HE1	2.30	0.50
15:R:101:MET:O	15:R:105:GLN:HG2	2.12	0.50
1:A:63:ARG:HB2	1:A:66:PRO:HD2	1.93	0.50
2:F:47:SER:OG	2:F:48:GLY:N	2.45	0.50
9:L:220:TRP:NE1	9:L:277:GLN:OE1	2.37	0.50
12:O:115:GLY:HA3	13:P:70:LEU:HD11	1.94	0.50
14:Q:242:LEU:HD21	16:U:390:LEU:HD22	1.94	0.50
7:J:55:DT:OP1	7:J:55:DT:H2'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:140:DT:H2'	7:J:141:DT:H71	1.94	0.50
9:L:46:ARG:HD3	9:L:274:GLU:HG2	1.94	0.50
11:N:24:ILE:O	11:N:28:TRP:N	2.44	0.50
11:N:206:PHE:CD1	12:O:157:VAL:HG11	2.46	0.50
12:O:186:ALA:HA	12:O:245:THR:HG22	1.94	0.50
3:C:16:SER:O	3:C:19:SER:OG	2.25	0.50
3:C:110:ASN:O	3:C:111:ILE:C	2.49	0.50
7:J:74:DA:H4'	7:J:75:DA:OP1	2.11	0.49
16:U:257:GLU:HA	16:U:260:LYS:HE3	1.92	0.49
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.47	0.49
4:D:36:SER:OG	4:D:37:TYR:N	2.45	0.49
7:J:98:DT:H2'	7:J:99:DT:H71	1.94	0.49
9:L:223:ALA:HA	9:L:226:THR:HG22	1.93	0.49
7:J:53:DA:C1'	7:J:54:DA:O5'	2.56	0.49
9:L:236:THR:HA	9:L:258:PRO:HG3	1.94	0.49
1:A:108:ASP:OD2	1:A:133:ARG:NH1	2.44	0.49
6:I:563:ASP:O	6:I:567:LYS:HG2	2.12	0.49
13:P:219:VAL:HG21	16:U:389:ALA:HB1	1.94	0.49
6:I:475:PHE:HA	6:I:478:LEU:HD12	1.95	0.49
10:M:73:HIS:CD2	10:M:109:HIS:HB3	2.47	0.49
12:O:112:GLY:O	12:O:127:SER:OG	2.29	0.49
13:P:153:PHE:HB2	13:P:156:ARG:HH21	1.77	0.49
2:B:93:GLN:HE21	2:B:95:ARG:HH21	1.59	0.49
5:H:136:LEU:HD12	8:K:108:LEU:HG	1.94	0.49
6:I:226:GLN:NE2	6:I:236:GLN:OE1	2.35	0.49
6:I:379:VAL:HG22	6:I:381:ASP:HB2	1.93	0.49
7:J:152:DT:H2'	7:J:153:DT:H71	1.94	0.49
7:J:169:DT:H2"	7:J:170:DG:C8	2.48	0.49
10:M:18:ILE:HD11	10:M:46:VAL:HG22	1.94	0.49
12:O:114:SER:O	12:O:125:CYS:N	2.43	0.49
16:U:251:LEU:HD22	16:U:292:MET:HE3	1.94	0.49
7:J:104:DA:C8	7:J:104:DA:H5'	2.47	0.49
7:J:139:DT:H2'	7:J:140:DT:H71	1.95	0.49
15:R:151:LEU:CD2	16:U:412:GLU:CG	2.89	0.49
7:J:51:DG:C1'	7:J:52:DG:O4'	2.61	0.49
11:N:141:TYR:HD2	14:Q:147:ARG:HH11	1.60	0.49
13:P:69:PHE:HE1	15:R:172:LEU:HD12	1.76	0.49
14:Q:93:MET:N	14:Q:93:MET:HE2	2.28	0.49
6:I:557:LEU:O	6:I:561:ILE:HG12	2.12	0.48
14:Q:250:GLN:CA	15:R:96:LEU:HD21	2.29	0.48
1:E:72:ARG:O	1:E:76:VAL:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:11:PRO:HD3	10:M:62:ARG:HD2	1.95	0.48
10:M:15:THR:OG1	10:M:43:GLU:OE2	2.22	0.48
11:N:68:LEU:HG	11:N:124:ARG:HD2	1.94	0.48
11:N:152:VAL:HG23	11:N:163:THR:HG22	1.94	0.48
14:Q:245:LEU:HD22	15:R:103:ILE:HB	1.94	0.48
6:I:129:ILE:O	6:I:133:MET:HG2	2.13	0.48
9:L:221:MET:HB2	9:L:225:TRP:CZ3	2.47	0.48
10:M:54:LEU:HD12	10:M:55:PRO:HD2	1.95	0.48
11:N:83:TRP:CG	11:N:198:LEU:HD13	2.48	0.48
6:I:119:GLY:HA3	6:I:155:LYS:NZ	2.28	0.48
6:I:417:PHE:O	6:I:421:ILE:HG12	2.14	0.48
7:J:43:DT:OP1	11:N:167:MET:HE2	2.13	0.48
14:Q:241:ASP:OD2	15:R:107:LEU:HD22	2.03	0.48
6:I:539:TYR:CZ	6:I:543:LEU:HD11	2.48	0.48
11:N:174:LEU:HD12	11:N:177:GLN:HE21	1.79	0.48
8:K:37:GLU:HA	8:K:40:ASN:HD21	1.78	0.48
8:K:110:THR:HG22	12:O:20:HIS:HD2	1.79	0.48
9:L:192:ASN:O	9:L:196:ILE:HG12	2.14	0.48
9:L:231:ASP:OD1	9:L:231:ASP:N	2.45	0.48
13:P:245:ARG:NH2	16:U:371:VAL:HG12	2.29	0.48
15:R:135:GLU:HB3	16:U:398:LEU:HD22	1.96	0.48
16:U:306:ASN:O	16:U:310:ILE:HG12	2.14	0.48
7:J:55:DT:H1'	7:J:56:DA:H5'	1.96	0.48
13:P:216:PHE:CE1	13:P:242:VAL:HG23	2.49	0.48
14:Q:84:LEU:O	14:Q:88:MET:HG2	2.13	0.48
5:H:127:MET:HA	5:H:130:MET:HG2	1.96	0.48
5:H:230:ASP:HB3	5:H:233:LEU:HB2	1.94	0.48
6:I:363:MET:O	6:I:366:VAL:HB	2.14	0.48
9:L:168:ASP:O	9:L:172:GLU:N	2.47	0.48
10:M:18:ILE:HG12	10:M:44:LEU:HD11	1.95	0.48
10:M:27:LEU:HD22	10:M:133:LEU:HD22	1.94	0.48
11:N:34:ASN:OD1	11:N:35:GLN:N	2.46	0.48
6:I:471:LYS:HA	6:I:475:PHE:HB2	1.96	0.47
8:K:22:GLU:HB3	8:K:26:ARG:HH12	1.79	0.47
9:L:133:ASP:OD2	9:L:166:PHE:N	2.47	0.47
10:M:148:ARG:O	10:M:152:ILE:HG12	2.14	0.47
11:N:269:TYR:CE1	11:N:334:PHE:CE1	3.02	0.47
5:H:141:MET:HE1	6:I:729:GLN:N	2.29	0.47
6:I:475:PHE:HE1	6:I:497:LEU:HD11	1.79	0.47
7:J:97:DC:H2"	7:J:98:DT:H72	1.97	0.47
11:N:248:VAL:HG23	11:N:317:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:105:LEU:HB2	13:P:67:LEU:HD21	1.97	0.47
12:O:214:LEU:HD21	12:O:242:LEU:HD13	1.96	0.47
6:I:140:SER:O	6:I:143:SER:OG	2.26	0.47
11:N:200:SER:OG	11:N:263:GLN:N	2.47	0.47
13:P:152:GLU:O	13:P:156:ARG:HG3	2.14	0.47
14:Q:239:LEU:HD23	16:U:387:LEU:HD13	1.97	0.47
3:C:104:GLN:NE2	1:E:96:GLU:OE2	2.48	0.47
5:H:136:LEU:O	5:H:140:ILE:HG12	2.15	0.47
6:I:281:ARG:HH12	6:I:345:GLN:CB	2.22	0.47
14:Q:241:ASP:HA	14:Q:244:ILE:HG12	1.96	0.47
1:A:72:ARG:O	1:A:76:VAL:HG13	2.14	0.47
3:C:42:ARG:HD2	4:D:88:THR:HB	1.97	0.47
7:J:156:DG:H2"	7:J:157:DA:N7	2.29	0.47
10:M:51:SER:OG	10:M:83:GLU:OE2	2.28	0.47
12:O:181:CYS:SG	13:P:168:ARG:HD3	2.55	0.47
13:P:196:TYR:CE2	13:P:209:ARG:HB3	2.50	0.47
14:Q:175:ASN:O	14:Q:178:SER:OG	2.23	0.47
15:R:100:ILE:HA	15:R:103:ILE:HG12	1.95	0.47
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.96	0.47
9:L:75:TYR:HB3	9:L:208:PHE:HB3	1.97	0.47
10:M:31:LEU:O	10:M:35:MET:HG2	2.15	0.47
14:Q:229:LEU:HD22	16:U:387:LEU:HD23	1.97	0.47
14:Q:254:MET:HE3	15:R:93:VAL:CB	2.42	0.47
4:D:93:GLU:N	4:D:93:GLU:OE2	2.48	0.47
6:I:276:VAL:HG12	6:I:279:ARG:NH2	2.30	0.47
8:K:107:VAL:O	8:K:110:THR:OG1	2.30	0.47
5:H:172:LEU:HA	5:H:175:ILE:HG22	1.96	0.46
6:I:466:SER:OG	6:I:469:GLU:OE1	2.30	0.46
9:L:201:GLN:HG2	9:L:206:CYS:O	2.13	0.46
10:M:78:LEU:O	10:M:81:THR:N	2.48	0.46
1:A:70:LEU:HA	2:B:25:ASN:HB3	1.97	0.46
13:P:137:ASP:OD2	13:P:161:LYS:NZ	2.38	0.46
13:P:203:SER:OG	13:P:204:CYS:N	2.49	0.46
15:R:138:LYS:HB3	15:R:138:LYS:HE2	1.74	0.46
15:R:141:GLU:HG2	15:R:142:LEU:HD22	1.95	0.46
7:J:43:DT:C5'	11:N:167:MET:CE	2.91	0.46
12:O:20:HIS:HA	12:O:23:ARG:HG2	1.96	0.46
12:O:214:LEU:HD22	12:O:216:ASN:HB3	1.96	0.46
2:B:92:ARG:HH22	4:D:101:LEU:HD23	1.81	0.46
6:I:259:LYS:CE	6:I:313:LEU:C	2.79	0.46
13:P:157:ALA:O	13:P:161:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:116:ARG:HH22	16:U:268:ARG:HH22	1.63	0.46
5:H:128:ASP:OD2	8:K:101:ARG:NE	2.48	0.46
5:H:150:LEU:O	5:H:154:LEU:HG	2.16	0.46
5:H:171:LYS:O	5:H:174:GLU:HG2	2.15	0.46
6:I:494:LEU:HD21	6:I:561:ILE:HD13	1.98	0.46
9:L:236:THR:HG22	9:L:258:PRO:HD3	1.98	0.46
2:F:70:VAL:O	2:F:74:GLU:HG2	2.15	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.51	0.46
6:I:731:LEU:O	6:I:735:ILE:HG12	2.16	0.46
11:N:177:GLN:HA	11:N:180:THR:HG22	1.98	0.46
5:H:130:MET:HB2	6:I:690:SER:OG	2.16	0.46
6:I:381:ASP:HB3	6:I:384:VAL:HG22	1.98	0.46
14:Q:88:MET:HA	14:Q:91:VAL:HG22	1.98	0.46
3:C:79:ILE:H	3:C:82:HIS:HD1	1.63	0.46
12:O:155:VAL:HG23	12:O:184:LEU:HD11	1.98	0.46
2:F:39:ARG:NH1	2:F:44:LYS:O	2.49	0.46
6:I:729:GLN:HA	6:I:732:LYS:CE	2.39	0.46
7:J:114:DT:H2"	7:J:115:DC:C5	2.51	0.46
5:H:140:ILE:HD11	8:K:108:LEU:HD22	1.99	0.45
7:J:100:DT:C2	7:J:101:DG:C8	3.03	0.45
8:K:132:GLN:O	8:K:136:MET:HG2	2.16	0.45
9:L:218:LEU:HA	9:L:221:MET:HG2	1.98	0.45
2:B:50:ILE:HD13	2:B:50:ILE:HA	1.84	0.45
11:N:305:ALA:O	11:N:309:LEU:HG	2.16	0.45
12:O:204:LEU:HD23	12:O:204:LEU:H	1.81	0.45
13:P:149:GLU:O	13:P:152:GLU:HG3	2.16	0.45
14:Q:124:LEU:HD23	16:U:254:VAL:HG12	1.99	0.45
6:I:110:ASP:O	6:I:114:ASN:ND2	2.37	0.45
6:I:259:LYS:NZ	6:I:312:VAL:HG13	2.27	0.45
7:J:51:DG:C4	7:J:52:DG:C4	3.04	0.45
11:N:35:GLN:O	11:N:38:THR:OG1	2.29	0.45
16:U:409:HIS:O	16:U:412:GLU:HG2	2.17	0.45
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.48	0.45
3:G:15:LYS:O	3:G:20:ARG:NH2	2.49	0.45
6:I:259:LYS:CG	6:I:313:LEU:O	2.61	0.45
6:I:445:LEU:HD23	10:M:130:TYR:HD2	1.81	0.45
9:L:216:PHE:HE1	9:L:277:GLN:HE22	1.63	0.45
9:L:240:LEU:HB3	9:L:306:ARG:HB3	1.97	0.45
10:M:80:ASN:O	10:M:83:GLU:HG3	2.16	0.45
12:O:240:LYS:HZ3	12:O:248:THR:HB	1.81	0.45
1:E:57:SER:OG	1:E:59:HIS:ND1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:43:DT:C5'	11:N:167:MET:HE3	2.46	0.45
15:R:140:LYS:O	15:R:143:MET:HG3	2.15	0.45
6:I:495:GLN:HG3	6:I:498:LYS:HE3	1.98	0.45
7:J:171:DT:H2"	7:J:172:DA:H5"	1.99	0.45
9:L:28:GLN:O	9:L:32:GLU:HG2	2.17	0.45
9:L:127:MET:HG3	9:L:161:TRP:HZ2	1.81	0.45
9:L:328:LEU:O	9:L:331:VAL:HB	2.16	0.45
14:Q:163:ASP:HA	14:Q:166:VAL:HG22	1.99	0.45
5:H:82:ILE:O	5:H:85:LEU:HB2	2.17	0.45
6:I:582:LEU:HD21	6:I:643:TYR:CE1	2.50	0.45
7:J:78:DG:H2"	7:J:79:DA:H8	1.81	0.45
11:N:72:ILE:HA	11:N:75:GLN:HG2	1.99	0.45
15:R:128:ALA:O	16:U:397:LEU:CD2	2.65	0.45
5:H:136:LEU:CD1	8:K:108:LEU:HG	2.47	0.45
9:L:124:LEU:HB3	9:L:127:MET:HE1	1.99	0.45
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.99	0.45
8:K:100:LEU:O	8:K:104:LEU:HG	2.17	0.45
14:Q:92:ILE:HA	14:Q:95:ILE:HG22	1.97	0.45
14:Q:259:GLU:HA	14:Q:262:TYR:CZ	2.52	0.45
5:H:149:ASP:OD1	5:H:150:LEU:N	2.50	0.44
11:N:193:LEU:HD12	11:N:332:ASN:HB2	1.98	0.44
6:I:272:ALA:O	6:I:276:VAL:HG13	2.17	0.44
6:I:490:LYS:O	6:I:494:LEU:HD13	2.17	0.44
9:L:77:LEU:HG	9:L:78:THR:O	2.17	0.44
6:I:344:LEU:HD23	6:I:344:LEU:HA	1.89	0.44
6:I:549:ARG:NH2	10:M:160:VAL:HG22	2.33	0.44
6:I:555:THR:O	6:I:559:HIS:ND1	2.46	0.44
6:I:596:ASP:HB3	6:I:599:ILE:HG12	1.99	0.44
7:J:52:DG:H2"	7:J:53:DA:OP2	2.17	0.44
11:N:269:TYR:CD1	11:N:334:PHE:HD1	2.35	0.44
12:O:120:ARG:HA	12:O:120:ARG:CZ	2.47	0.44
14:Q:240:LYS:O	14:Q:244:ILE:HG23	2.18	0.44
6:I:492:SER:OG	12:O:21:LEU:HD13	2.17	0.44
7:J:51:DG:O4'	7:J:51:DG:N3	2.49	0.44
9:L:197:GLY:O	9:L:201:GLN:HG3	2.17	0.44
11:N:155:TYR:O	11:N:158:THR:OG1	2.32	0.44
13:P:154:VAL:HG22	13:P:166:PHE:CZ	2.53	0.44
14:Q:185:ILE:O	14:Q:188:SER:OG	2.28	0.44
5:H:89:ILE:HA	5:H:92:VAL:HG22	2.00	0.44
7:J:69:DA:H2"	7:J:70:DA:H8	1.81	0.44
11:N:72:ILE:HD13	11:N:124:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:89:THR:HG22	13:P:99:ARG:HA	2.00	0.44
13:P:266:VAL:O	13:P:270:GLY:N	2.49	0.44
7:J:86:DC:H2"	7:J:87:DT:H71	2.00	0.44
10:M:17:THR:HG22	10:M:45:LYS:HB2	1.99	0.44
12:O:121:GLY:HA3	12:O:142:LEU:O	2.18	0.44
15:R:125:ILE:HG23	15:R:126:SER:H	1.83	0.44
6:I:66:LEU:HD22	6:I:98:VAL:HG11	2.00	0.44
6:I:309:VAL:HG23	6:I:310:ILE:HG12	1.98	0.44
14:Q:126:VAL:HG23	16:U:253:ILE:HD12	1.98	0.44
1:A:113:THR:OG1	1:A:125:ASP:OD2	2.23	0.44
4:D:102:LEU:HB2	4:D:107:ALA:HB2	2.00	0.44
5:H:100:LYS:O	5:H:103:LEU:HG	2.17	0.44
6:I:151:LEU:HD11	6:I:164:PHE:CD2	2.53	0.44
5:H:82:ILE:O	5:H:86:GLU:OE1	2.36	0.44
6:I:427:PHE:O	6:I:428:LEU:HB2	2.18	0.44
7:J:51:DG:OP2	7:J:51:DG:C8	2.66	0.44
11:N:110:LYS:HD3	11:N:110:LYS:HA	1.80	0.44
12:O:140:VAL:HG23	12:O:153:HIS:HB3	1.99	0.44
7:J:55:DT:OP2	7:J:55:DT:O4'	2.36	0.43
12:O:224:LEU:O	12:O:230:SER:HA	2.17	0.43
14:Q:176:ILE:HD11	16:U:334:LEU:HD12	2.00	0.43
7:J:51:DG:C4'	7:J:52:DG:H5'	2.48	0.43
7:J:167:DT:H2"	7:J:168:DT:C6	2.54	0.43
11:N:34:ASN:O	11:N:38:THR:HG23	2.18	0.43
12:O:252:VAL:HG13	12:O:268:ARG:HG3	2.00	0.43
13:P:223:ARG:HH11	15:R:124:GLY:CA	2.31	0.43
15:R:90:LEU:HD22	15:R:143:MET:SD	2.58	0.43
6:I:273:LEU:HB3	6:I:277:LYS:NZ	2.33	0.43
12:O:18:LEU:HA	12:O:21:LEU:HG	2.00	0.43
12:O:173:ILE:H	12:O:173:ILE:HD12	1.83	0.43
8:K:239:TRP:CD1	8:K:241:PRO:HD2	2.53	0.43
9:L:64:VAL:O	9:L:68:LEU:HG	2.18	0.43
11:N:156:SER:O	11:N:158:THR:HG23	2.18	0.43
7:J:53:DA:H2"	7:J:54:DA:H8	1.81	0.43
9:L:257:HIS:CG	11:N:292:ARG:HH21	2.37	0.43
10:M:162:ALA:O	10:M:165:LEU:HG	2.19	0.43
6:I:243:LYS:HA	6:I:250:ILE:HG13	2.01	0.43
6:I:645:THR:HA	6:I:648:VAL:HG12	2.00	0.43
14:Q:237:ALA:HA	14:Q:240:LYS:HD2	2.01	0.43
1:A:73:GLU:HB2	2:B:25:ASN:HD22	1.82	0.43
3:C:32:ARG:HD2	3:C:36:LYS:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:122:LEU:HG	8:K:126:GLN:HE22	1.83	0.43
9:L:31:LEU:HA	9:L:34:VAL:HG12	2.00	0.43
15:R:151:LEU:HD23	16:U:412:GLU:CB	2.21	0.43
8:K:104:LEU:O	8:K:108:LEU:HD23	2.19	0.43
11:N:201:LEU:O	11:N:205:VAL:HG12	2.19	0.43
12:O:274:LEU:HD13	12:O:283:VAL:HB	2.00	0.43
15:R:142:LEU:O	15:R:146:VAL:HG23	2.19	0.43
2:F:23:ARG:NE	2:F:24:ASP:OD2	2.52	0.43
5:H:62:ASP:HB3	8:K:69:ALA:HB1	2.01	0.43
11:N:133:ILE:HB	11:N:152:VAL:CG1	2.49	0.43
12:O:126:ILE:HD11	12:O:181:CYS:SG	2.58	0.43
14:Q:140:LEU:HD23	14:Q:143:MET:HE3	2.01	0.43
3:C:95:LYS:HE3	3:C:95:LYS:HB2	1.79	0.42
6:I:612:LYS:HD3	6:I:612:LYS:HA	1.88	0.42
9:L:241:TRP:CD2	9:L:299:LEU:HD11	2.54	0.42
10:M:20:LEU:HD13	10:M:31:LEU:HD23	2.01	0.42
12:O:216:ASN:HA	12:O:239:TYR:HB2	2.00	0.42
13:P:80:ASN:OD1	13:P:81:HIS:N	2.51	0.42
14:Q:228:ILE:CG2	15:R:119:LEU:HD11	2.49	0.42
7:J:150:DA:H2"	7:J:151:DG:H8	1.84	0.42
9:L:99:ILE:HG21	9:L:117:ILE:HD11	2.01	0.42
14:Q:159:GLN:O	14:Q:162:ILE:HB	2.18	0.42
14:Q:187:ALA:O	14:Q:190:VAL:HG22	2.19	0.42
14:Q:245:LEU:HD21	15:R:103:ILE:HB	2.01	0.42
3:G:15:LYS:HB2	7:J:80:DA:OP1	2.19	0.42
3:G:31:HIS:CE1	3:G:35:ARG:HH11	2.37	0.42
10:M:78:LEU:O	10:M:81:THR:OG1	2.28	0.42
13:P:223:ARG:O	13:P:235:LYS:HG2	2.18	0.42
6:I:117:LEU:HD11	6:I:164:PHE:CD1	2.54	0.42
7:J:43:DT:H5'	11:N:167:MET:HE3	2.01	0.42
7:J:111:DC:H2"	7:J:112:DA:C8	2.55	0.42
10:M:5:ARG:HA	10:M:89:ASP:OD1	2.19	0.42
14:Q:262:TYR:HA	14:Q:265:LEU:HD13	2.02	0.42
16:U:317:ARG:O	16:U:320:MET:HB2	2.19	0.42
16:U:319:ARG:O	16:U:323:VAL:HG22	2.19	0.42
7:J:145:DA:H2'	7:J:146:DG:C8	2.55	0.42
11:N:137:TRP:HE1	11:N:150:THR:HG21	1.85	0.42
14:Q:141:LEU:HD21	16:U:299:LEU:HB2	2.01	0.42
3:G:16:SER:HA	7:J:79:DA:H5"	2.02	0.42
5:H:83:GLU:HA	5:H:86:GLU:OE1	2.20	0.42
9:L:32:GLU:OE2	9:L:35:ARG:NH2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:275:PHE:HB2	11:N:291:LEU:HD13	2.01	0.42
13:P:181:LYS:HE3	13:P:201:PRO:HG2	2.01	0.42
14:Q:179:LEU:O	14:Q:182:LYS:HB2	2.19	0.42
5:H:154:LEU:HD23	5:H:157:ILE:HD11	2.02	0.42
6:I:721:ASP:N	6:I:721:ASP:OD1	2.52	0.42
14:Q:241:ASP:CG	15:R:107:LEU:HD22	2.33	0.42
1:A:133:ARG:HB3	1:A:137:GLU:HB3	2.02	0.42
6:I:273:LEU:O	6:I:276:VAL:HG22	2.20	0.42
7:J:165:DT:H1'	7:J:166:DT:H5'	2.01	0.42
8:K:106:MET:O	8:K:110:THR:HG23	2.19	0.42
11:N:204:ILE:HD11	11:N:327:PRO:HA	2.02	0.42
12:O:181:CYS:SG	12:O:185:ASN:ND2	2.92	0.42
5:H:202:LEU:HD22	8:K:166:MET:HG2	2.02	0.42
6:I:464:PHE:HA	6:I:504:TRP:CE2	2.54	0.42
8:K:111:LYS:O	8:K:114:LYS:HG3	2.20	0.42
9:L:217:ASN:HD21	9:L:338:LEU:HD21	1.84	0.42
10:M:35:MET:HE1	10:M:143:ALA:HA	2.01	0.42
11:N:272:GLU:N	11:N:336:ILE:O	2.42	0.42
13:P:217:GLU:HB3	13:P:241:LYS:HB3	2.02	0.42
16:U:294:LYS:NZ	16:U:297:GLN:OE1	2.35	0.42
6:I:564:PHE:O	6:I:568:VAL:HG23	2.20	0.42
10:M:35:MET:CE	10:M:143:ALA:HA	2.50	0.42
11:N:150:THR:HG21	11:N:168:LEU:HD21	2.02	0.42
14:Q:165:MET:HA	14:Q:168:THR:HG22	2.01	0.42
16:U:290:ILE:HD12	16:U:290:ILE:HA	1.92	0.42
11:N:86:PHE:CE1	11:N:190:LYS:HB2	2.55	0.41
11:N:272:GLU:HG3	11:N:292:ARG:HG2	2.02	0.41
12:O:129:ALA:HA	12:O:135:LEU:HG	2.01	0.41
5:H:172:LEU:HD23	6:I:378:CYS:O	2.21	0.41
6:I:446:TRP:HZ2	6:I:452:ARG:HA	1.84	0.41
8:K:56:GLN:O	8:K:59:LEU:HG	2.20	0.41
9:L:320:ILE:HD13	9:L:320:ILE:HA	1.95	0.41
12:O:176:PHE:HD2	12:O:177:LEU:HD22	1.85	0.41
13:P:180:ARG:NH1	13:P:222:TRP:O	2.53	0.41
13:P:223:ARG:HH11	15:R:124:GLY:HA3	1.85	0.41
14:Q:214:LEU:H	14:Q:214:LEU:HD23	1.85	0.41
7:J:101:DG:C2'	7:J:102:DT:H71	2.50	0.41
7:J:130:DA:H2"	7:J:131:DA:H8	1.84	0.41
9:L:124:LEU:HB3	9:L:127:MET:CE	2.50	0.41
11:N:100:ASP:OD1	11:N:100:ASP:N	2.53	0.41
13:P:122:ILE:HG13	13:P:135:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLU:HG3	1:E:74:ILE:N	2.36	0.41
7:J:85:DT:H2"	7:J:86:DC:C6	2.55	0.41
7:J:105:DT:H2"	7:J:106:DG:C8	2.54	0.41
7:J:141:DT:H2"	7:J:142:DG:H8	1.84	0.41
7:J:158:DA:H2"	7:J:159:DA:C8	2.55	0.41
10:M:140:ALA:O	10:M:144:GLN:OE1	2.37	0.41
5:H:98:ILE:HD11	6:I:586:GLY:HA2	2.03	0.41
6:I:481:LEU:HD22	10:M:145:ARG:NH2	2.33	0.41
7:J:79:DA:H2"	7:J:80:DA:H8	1.84	0.41
7:J:86:DC:H2"	7:J:87:DT:C7	2.50	0.41
8:K:47:THR:OG1	8:K:48:GLU:N	2.54	0.41
5:H:89:ILE:HG21	8:K:70:GLU:OE2	2.21	0.41
6:I:78:ILE:HB	6:I:79:LYS:H	1.74	0.41
10:M:57:SER:HG	10:M:60:ARG:HB2	1.85	0.41
15:R:89:LEU:O	15:R:92:LYS:HG3	2.20	0.41
1:A:53:LYS:HE2	1:A:53:LYS:HB3	1.89	0.41
1:A:103:VAL:O	1:A:107:GLU:HG3	2.20	0.41
5:H:200:GLN:O	5:H:204:MET:HG2	2.20	0.41
6:I:373:LEU:HD23	6:I:373:LEU:HA	1.93	0.41
7:J:73:DA:H4'	7:J:74:DA:OP1	2.20	0.41
7:J:132:DC:N3	7:J:133:DA:N6	2.68	0.41
9:L:216:PHE:HB2	10:M:111:SER:O	2.19	0.41
12:O:116:LYS:HE2	12:O:123:CYS:SG	2.61	0.41
12:O:164:ILE:HG22	12:O:176:PHE:CD1	2.55	0.41
12:O:165:ALA:HA	12:O:169:LEU:HB2	2.02	0.41
15:R:129:SER:HB3	16:U:397:LEU:CD2	2.51	0.41
8:K:231:TYR:HB3	8:K:261:ARG:HB3	2.02	0.41
9:L:167:GLY:O	9:L:171:LEU:HD12	2.21	0.41
11:N:35:GLN:HB3	11:N:55:LEU:HD13	2.03	0.41
11:N:265:GLU:OE1	11:N:266:PHE:HB2	2.21	0.41
15:R:97:SER:HA	15:R:100:ILE:HG12	2.02	0.41
5:H:49:GLN:HG2	10:M:156:HIS:HA	2.02	0.41
5:H:105:ARG:NH2	6:I:594:SER:HA	2.36	0.41
5:H:143:SER:HA	8:K:115:ASN:HD21	1.86	0.41
6:I:724:PHE:CE1	6:I:731:LEU:HD22	2.54	0.41
7:J:52:DG:H1'	7:J:53:DA:O5'	2.21	0.41
7:J:136:DC:H2"	7:J:137:DC:C5	2.56	0.41
7:J:157:DA:H2"	7:J:158:DA:C8	2.56	0.41
9:L:91:TYR:O	9:L:95:LEU:HD23	2.19	0.41
10:M:140:ALA:O	10:M:143:ALA:HB3	2.21	0.41
10:M:167:SER:O	10:M:170:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:11:ARG:NH2	11:N:146:GLN:O	2.44	0.41
6:I:221:LYS:HA	6:I:221:LYS:HD3	1.87	0.41
6:I:609:ARG:HA	6:I:609:ARG:HD2	1.98	0.41
7:J:54:DA:H2"	7:J:55:DT:OP1	2.21	0.41
9:L:215:ALA:HB3	10:M:111:SER:HA	2.02	0.41
11:N:186:HIS:CD2	16:U:332:PRO:HB3	2.56	0.41
13:P:244:GLN:HE22	16:U:383:ASP:H	1.68	0.41
15:R:135:GLU:CG	16:U:398:LEU:HD22	2.30	0.41
6:I:740:HIS:ND1	6:I:743:SER:OG	2.50	0.40
8:K:129:LEU:HA	8:K:132:GLN:HE21	1.86	0.40
9:L:49:ILE:HD13	9:L:227:ALA:HB1	2.03	0.40
16:U:255:LEU:HD11	16:U:289:PHE:HB3	2.03	0.40
16:U:316:LYS:O	16:U:320:MET:HG2	2.21	0.40
2:F:50:ILE:HD13	2:F:50:ILE:HA	1.93	0.40
8:K:22:GLU:HB3	8:K:26:ARG:NH1	2.36	0.40
13:P:220:ILE:HD12	13:P:237:ASP:O	2.20	0.40
14:Q:190:VAL:HG12	16:U:348:LYS:HB2	2.03	0.40
14:Q:238:LEU:HD12	15:R:109:SER:HB2	2.02	0.40
15:R:96:LEU:HD12	15:R:99:GLU:HG3	2.02	0.40
16:U:271:SER:HB3	16:U:274:CYS:HB3	2.03	0.40
3:C:29:ARG:HD3	4:D:35:GLU:OE1	2.21	0.40
5:H:105:ARG:HA	5:H:108:LEU:HB3	2.03	0.40
12:O:239:TYR:CZ	12:O:247:PRO:HD3	2.55	0.40
13:P:118:LEU:HD21	13:P:167:PHE:HZ	1.86	0.40
5:H:41:ARG:O	5:H:44:LEU:HG	2.22	0.40
5:H:147:SER:HB3	8:K:114:LYS:NZ	2.37	0.40
5:H:157:ILE:HD12	8:K:125:GLU:HB3	2.04	0.40
7:J:78:DG:H2"	7:J:79:DA:C8	2.56	0.40
7:J:149:DC:H2"	7:J:150:DA:C8	2.56	0.40
8:K:226:VAL:HG12	8:K:229:ASP:H	1.87	0.40
9:L:77:LEU:HD13	9:L:208:PHE:CE1	2.56	0.40
12:O:167:LYS:HB3	12:O:168:TYR:CD2	2.56	0.40
12:O:177:LEU:HA	12:O:180:LEU:HG	2.02	0.40
13:P:235:LYS:HD2	14:Q:220:LYS:HE2	2.03	0.40
14:Q:232:ILE:HD12	14:Q:232:ILE:HA	1.99	0.40
3:C:88:ARG:HA	3:C:88:ARG:HD3	1.91	0.40
6:I:398:GLU:HA	6:I:401:ILE:HG22	2.03	0.40
6:I:571:ILE:HG22	6:I:577:LEU:HB2	2.04	0.40
12:O:21:LEU:O	12:O:25:GLU:OE1	2.40	0.40
12:O:132:GLY:N	13:P:162:ASP:OD1	2.48	0.40
16:U:318:GLN:O	16:U:322:GLU:OE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/140 (69%)	95 (98%)	2 (2%)	0	100	100
1	E	92/140 (66%)	88 (96%)	4 (4%)	0	100	100
2	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
2	F	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	96/130 (74%)	92 (96%)	4 (4%)	0	100	100
3	G	101/130 (78%)	97 (96%)	4 (4%)	0	100	100
4	D	90/126 (71%)	86 (96%)	4 (4%)	0	100	100
4	h	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
5	H	163/247 (66%)	161 (99%)	2 (1%)	0	100	100
6	I	525/756 (69%)	505 (96%)	19 (4%)	1 (0%)	47	81
8	K	209/269 (78%)	205 (98%)	4 (2%)	0	100	100
9	L	291/344 (85%)	282 (97%)	9 (3%)	0	100	100
10	M	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
11	N	289/339 (85%)	277 (96%)	12 (4%)	0	100	100
12	O	204/300 (68%)	196 (96%)	8 (4%)	0	100	100
13	P	213/288 (74%)	209 (98%)	4 (2%)	0	100	100
14	Q	185/268 (69%)	179 (97%)	6 (3%)	0	100	100
15	R	76/177 (43%)	72 (95%)	4 (5%)	0	100	100
16	U	163/418 (39%)	162 (99%)	1 (1%)	0	100	100
17	k	19/544 (4%)	14 (74%)	5 (26%)	0	100	100
17	l	51/544 (9%)	44 (86%)	3 (6%)	4 (8%)	1	13
All	All	3278/5672 (58%)	3169 (97%)	104 (3%)	5 (0%)	50	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	l	257	GLN
17	l	258	ALA
17	l	259	LYS
17	l	273	LYS
6	I	78	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	80/118 (68%)	80 (100%)	0	100	100
1	E	79/118 (67%)	78 (99%)	1 (1%)	69	81
2	B	64/79 (81%)	62 (97%)	2 (3%)	40	62
2	F	66/79 (84%)	65 (98%)	1 (2%)	65	80
3	C	76/99 (77%)	75 (99%)	1 (1%)	69	81
3	G	77/99 (78%)	77 (100%)	0	100	100
4	D	79/106 (74%)	78 (99%)	1 (1%)	69	81
4	h	79/106 (74%)	76 (96%)	3 (4%)	33	57
5	H	156/224 (70%)	155 (99%)	1 (1%)	86	92
6	I	490/691 (71%)	485 (99%)	5 (1%)	76	86
8	K	205/260 (79%)	204 (100%)	1 (0%)	88	93
9	L	267/306 (87%)	267 (100%)	0	100	100
10	M	151/158 (96%)	151 (100%)	0	100	100
11	N	270/311 (87%)	268 (99%)	2 (1%)	84	90
12	O	177/263 (67%)	177 (100%)	0	100	100
13	P	191/259 (74%)	190 (100%)	1 (0%)	88	93
14	Q	176/248 (71%)	175 (99%)	1 (1%)	86	92
15	R	75/166 (45%)	74 (99%)	1 (1%)	69	81
16	U	149/379 (39%)	147 (99%)	2 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	k	21/508 (4%)	21 (100%)	0	100	100
17	l	56/508 (11%)	53 (95%)	3 (5%)	22	47
All	All	2984/5085 (59%)	2958 (99%)	26 (1%)	79	87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	77	LYS
2	B	92	ARG
3	C	32	ARG
4	D	39	VAL
1	E	82	VAL
2	F	92	ARG
5	H	216	PHE
6	I	168	LEU
6	I	203	HIS
6	I	498	LYS
6	I	549	ARG
6	I	601	ASN
8	K	114	LYS
11	N	126	THR
11	N	193	LEU
13	P	175	GLU
14	Q	220	LYS
15	R	92	LYS
16	U	360	ASN
16	U	393	LYS
4	h	55	SER
4	h	71	GLU
4	h	123	SER
17	l	269	THR
17	l	296	THR
17	l	521	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	GLN
3	C	94	ASN
4	D	49	HIS

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Mol	Chain	Res	Type
1	E	87	GLN
1	E	115	HIS
2	F	93	GLN
3	G	31	HIS
3	G	94	ASN
8	K	40	ASN
10	M	73	HIS
11	N	186	HIS
12	O	185	ASN
12	O	212	ASN
15	R	147	ASN
16	U	288	GLN
4	h	63	ASN
4	h	95	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (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.

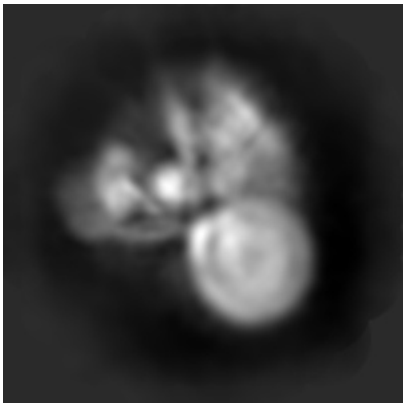
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14375. These allow visual inspection of the internal detail of the map and identification of artifacts.

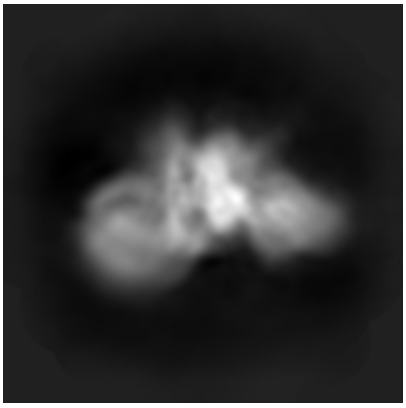
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



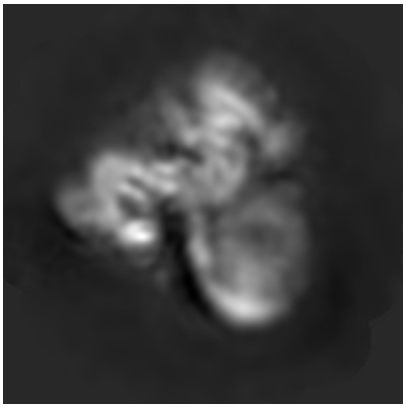
Y

Z

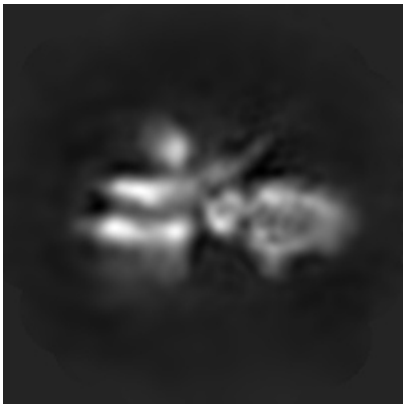
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

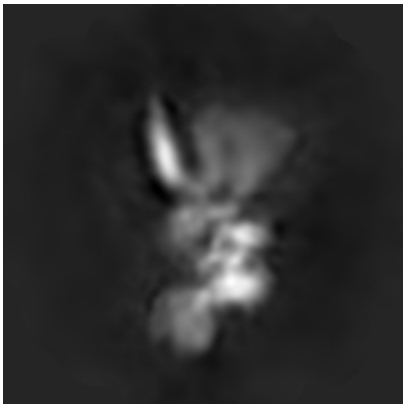
6.2.1 Primary map



X Index: 94



Y Index: 94

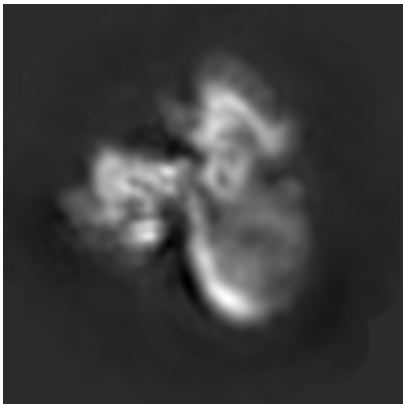


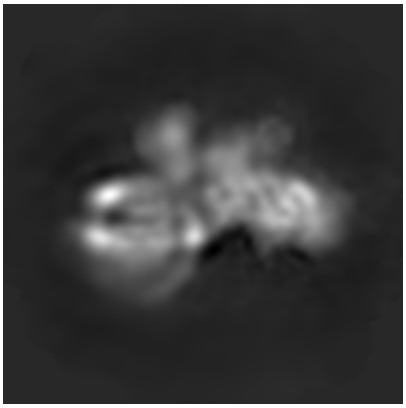
Z Index: 94

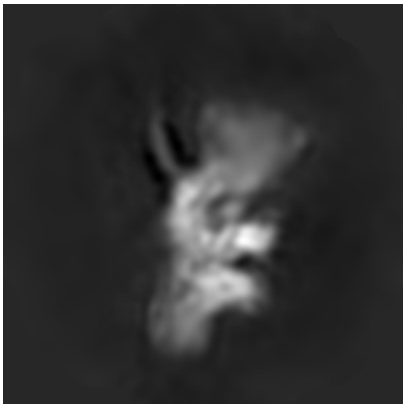
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 97

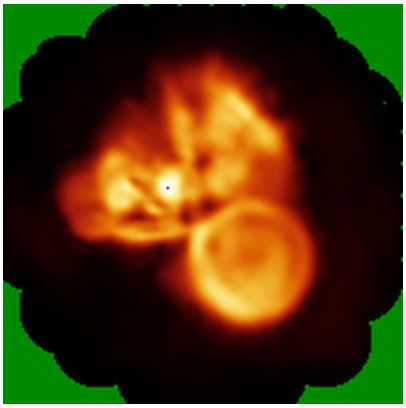

Y Index: 105


Z Index: 101

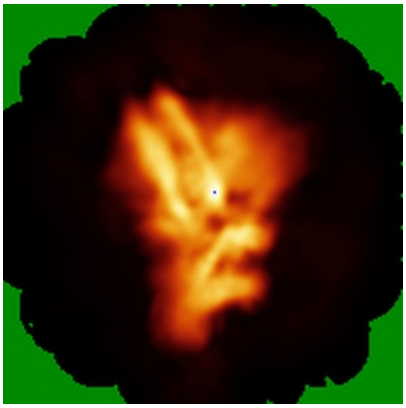
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

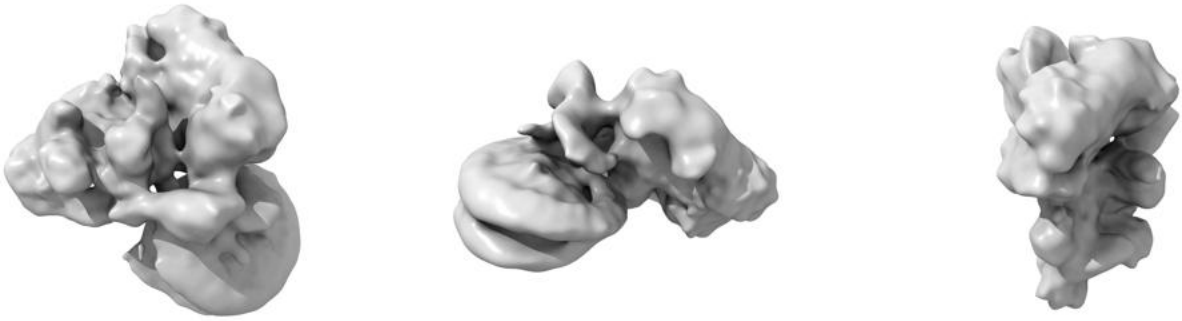
Y


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

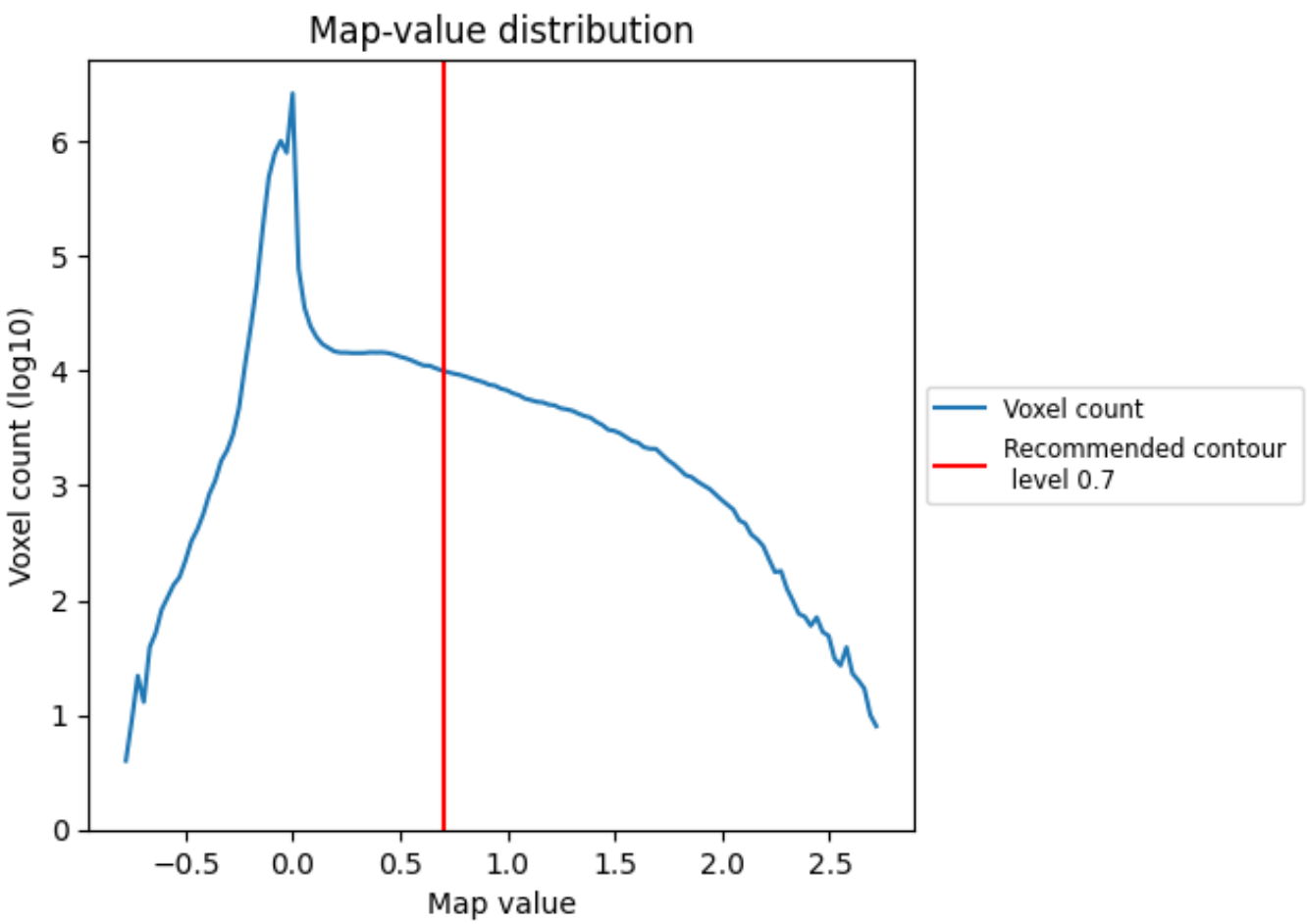
6.6 Mask visualisation (i)

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

7 Map analysis (i)

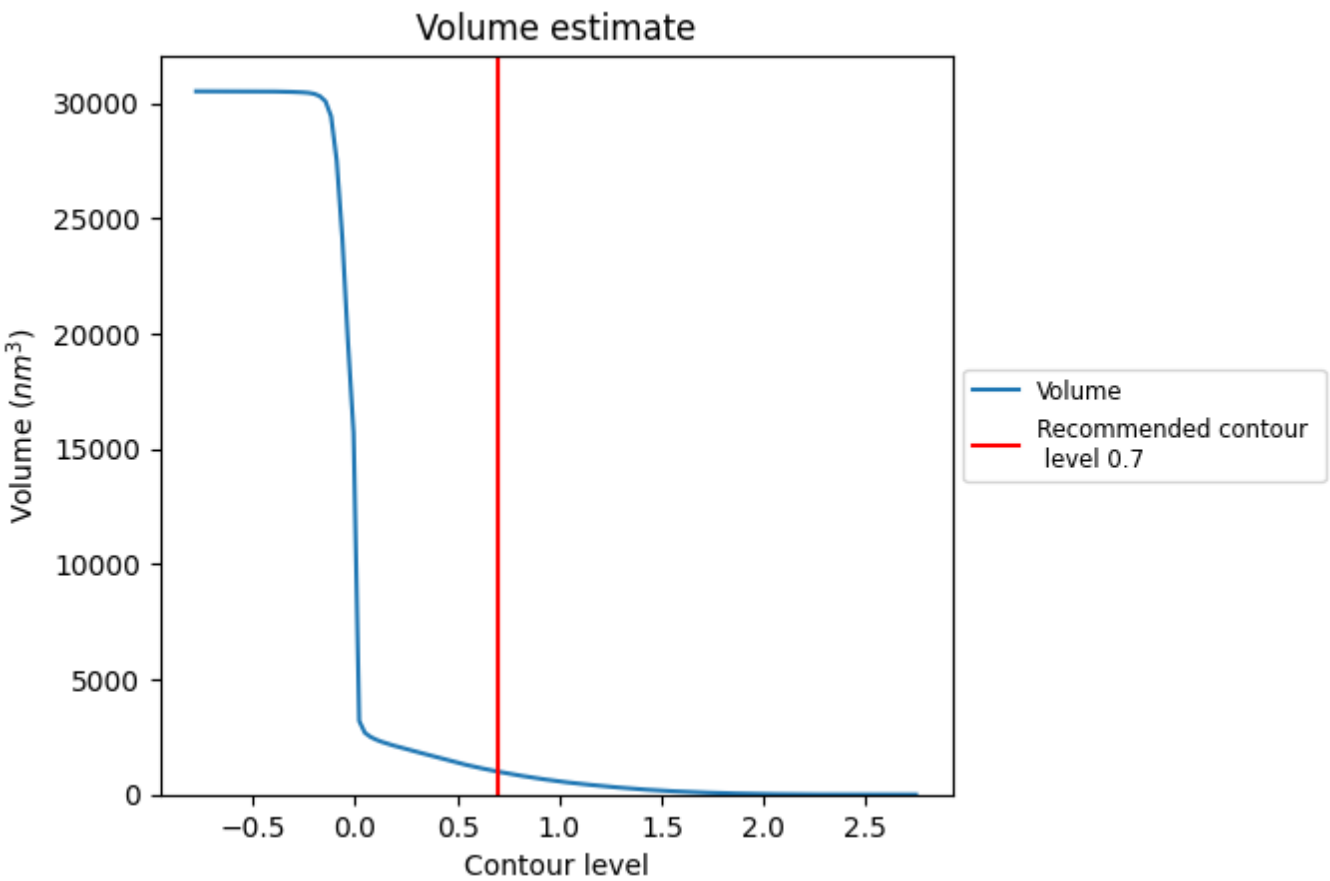
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

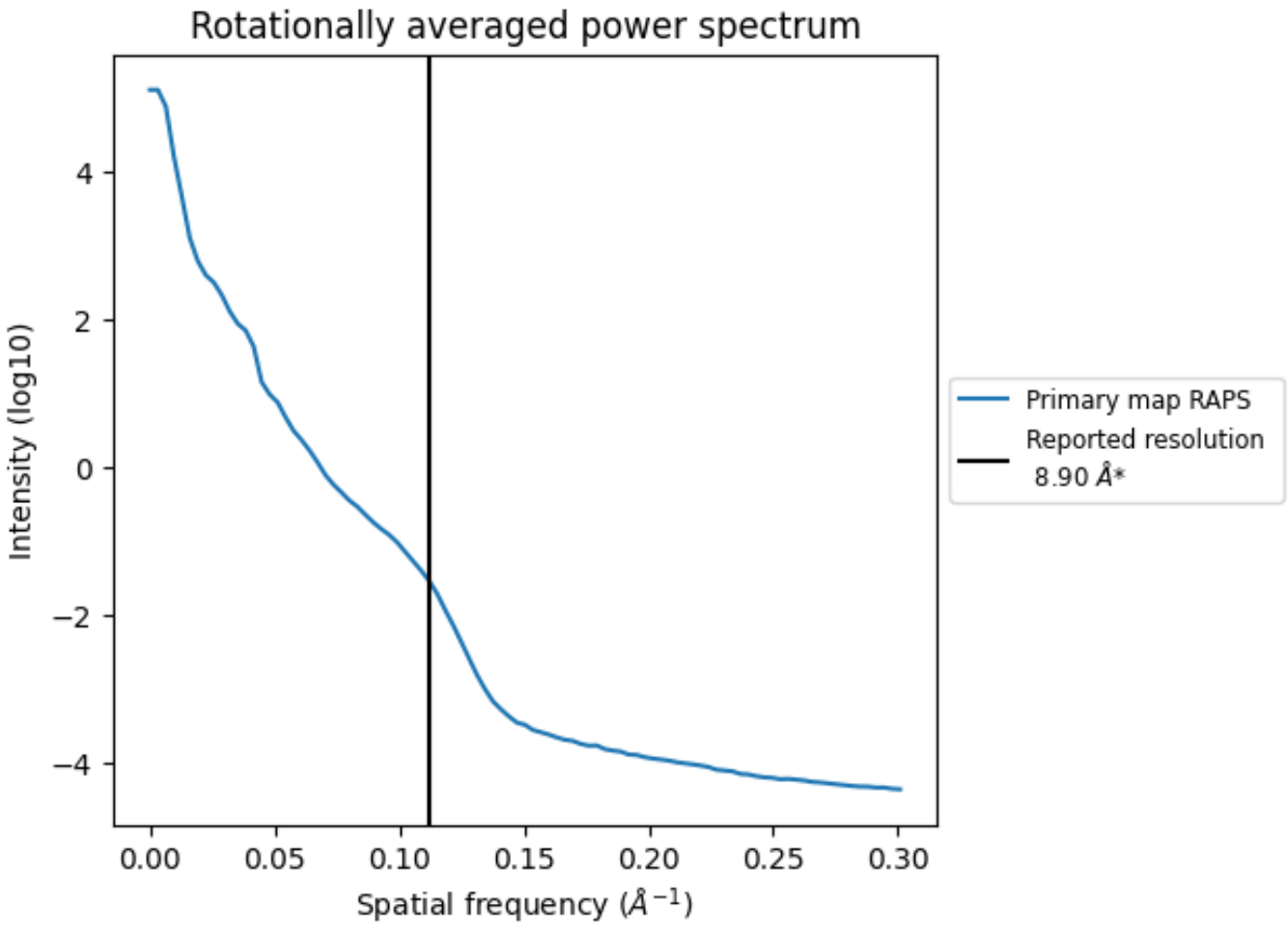
7.2 Volume estimate (i)



The volume at the recommended contour level is 995 nm^3; this corresponds to an approximate mass of 899 kDa.

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

7.3 Rotationally averaged power spectrum (i)

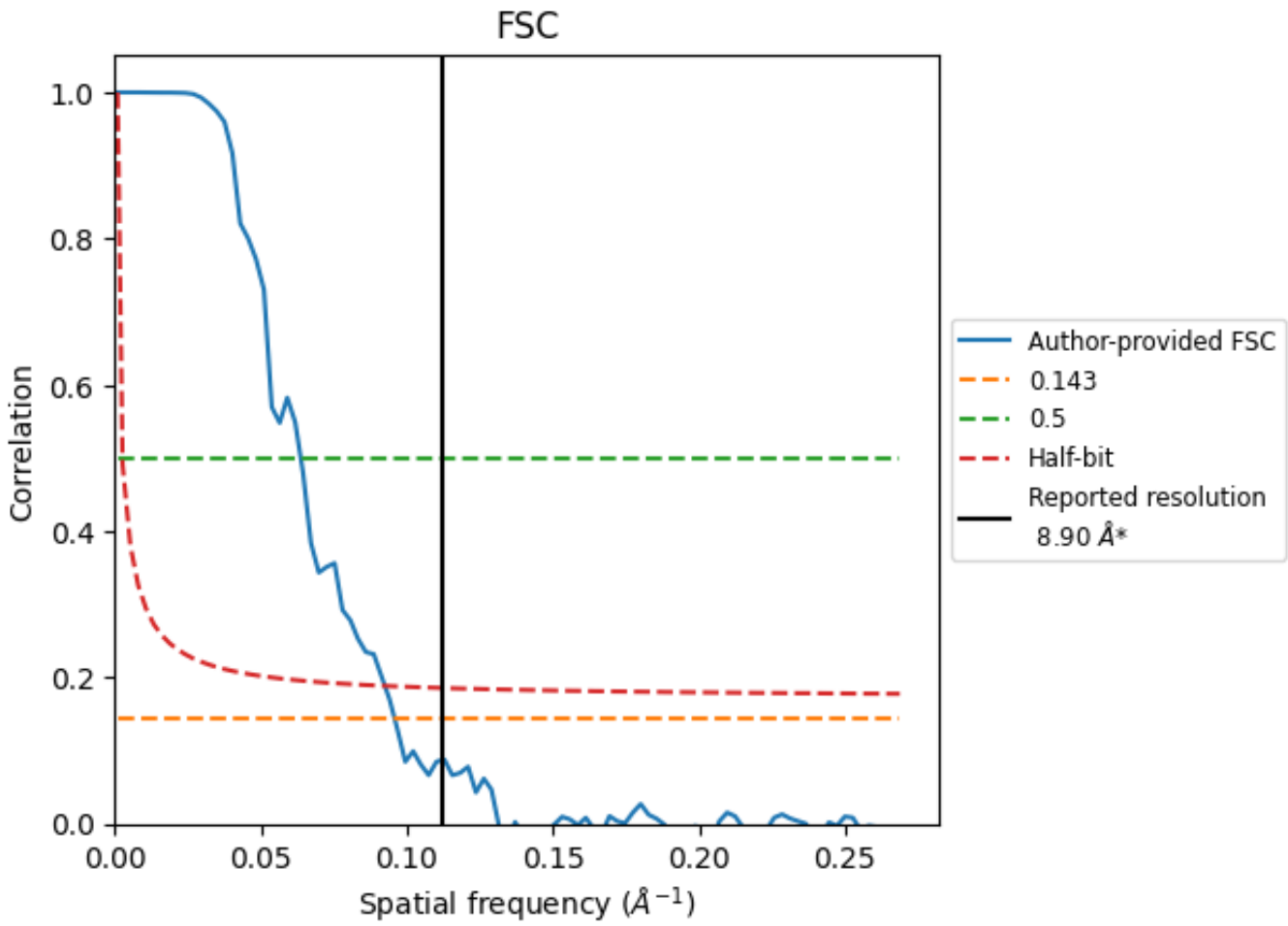


*Reported resolution corresponds to spatial frequency of 0.112 Å^{-1}

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 0.112 Å^{-1}

8.2 Resolution estimates (i)

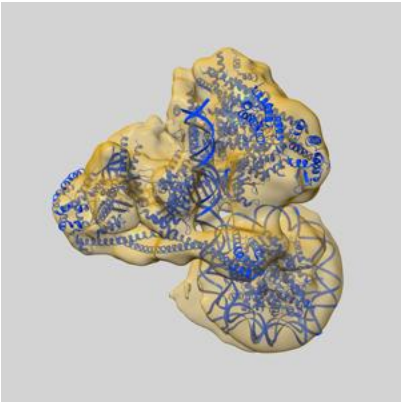
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	10.44	15.70	10.81
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 10.44 differs from the reported value 8.9 by more than 10 %

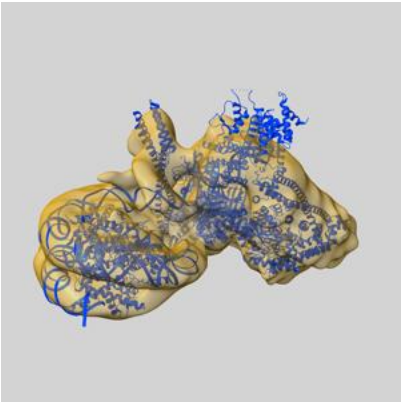
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14375 and PDB model 7YYH. Per-residue inclusion information can be found in section 3 on page 7.

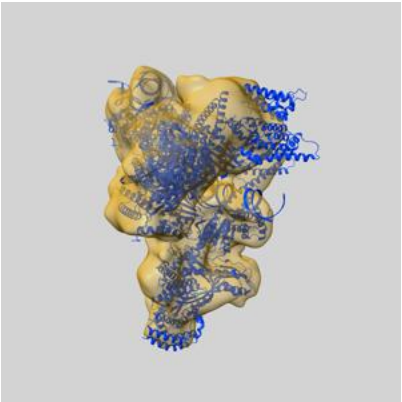
9.1 Map-model overlay (i)



X



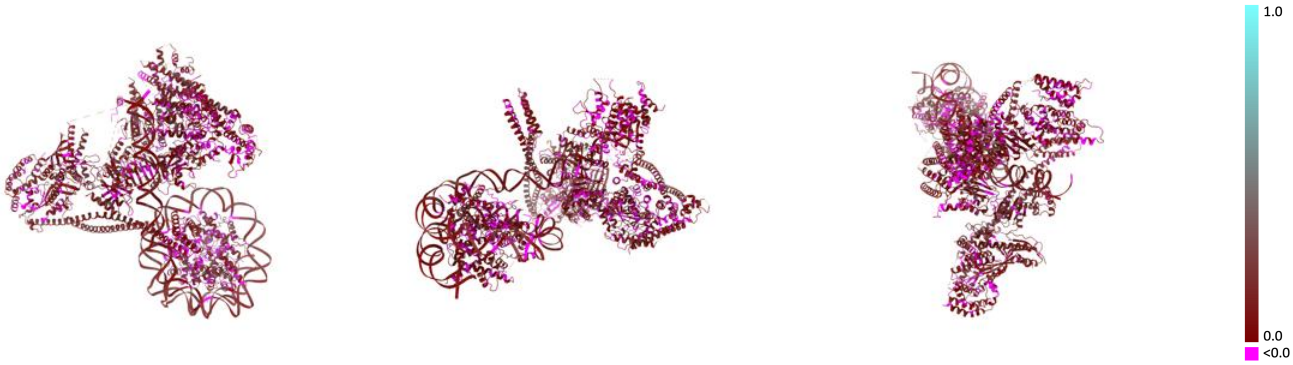
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

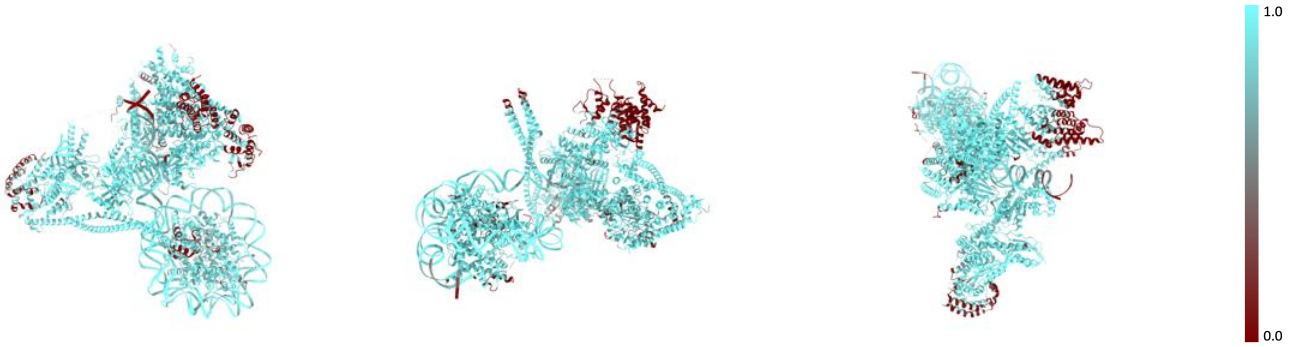
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

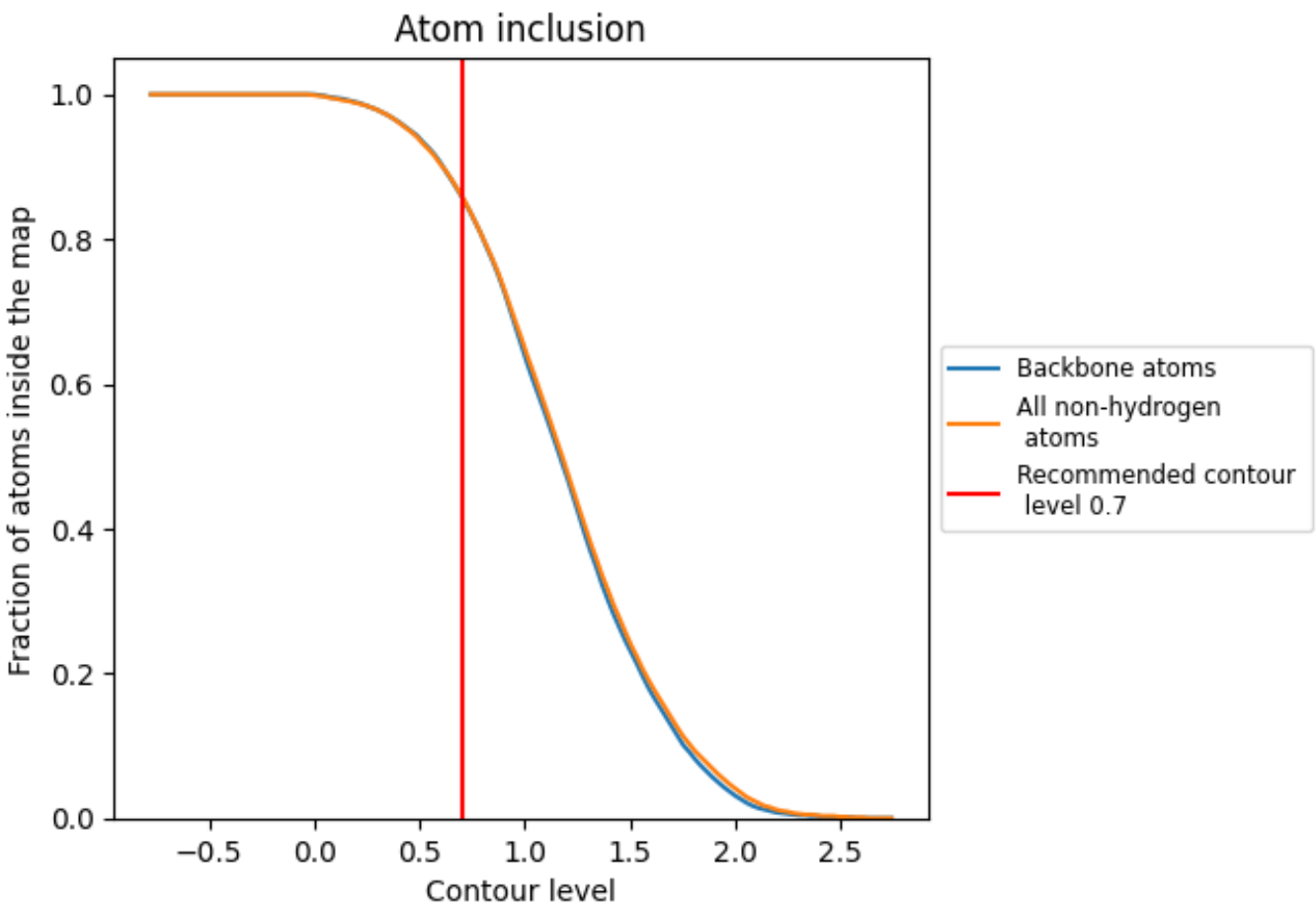
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.0750
A	0.8480	0.0280
B	0.8910	0.0440
C	0.8900	0.0550
D	0.9300	0.0670
E	0.9210	0.0290
F	0.8860	0.0200
G	0.8870	0.0550
H	0.8100	0.0740
I	0.7550	0.0460
J	0.9040	0.1020
K	0.6040	0.0710
L	0.9630	0.0800
M	0.9380	0.0640
N	0.9800	0.0990
O	0.9850	0.1140
P	0.8930	0.0750
Q	0.8240	0.1050
R	0.4320	0.0640
U	0.8920	0.1080
h	0.9130	0.0380
i	0.8890	0.1000
k	0.8810	0.0180
l	0.7340	0.0260