



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 11:46 AM JST

PDB ID : 6KW4
EMDB ID : EMD-0778
Title : The ClassB RSC-Nucleosome Complex
Authors : Ye, Y.P.; Wu, H.; Chen, K.J.; Verma, N.; Cairns, B.; Gao, N.; Chen, Z.C.
Deposited on : 2019-09-06
Resolution : 7.55 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

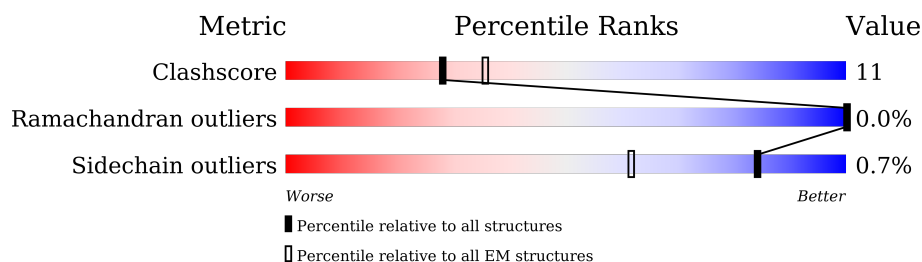
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.55 Å.

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






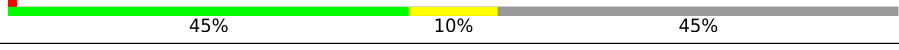


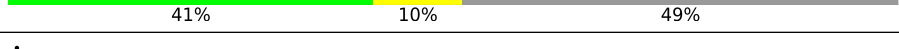
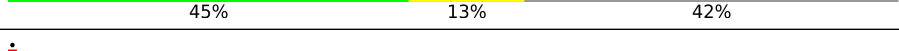
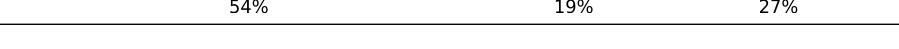
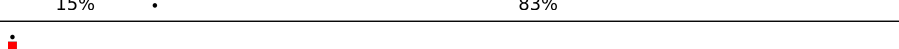
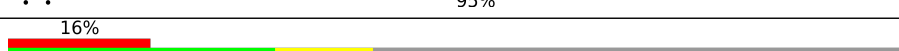


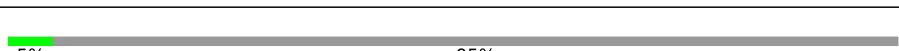






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	N	136	
1	Q	136	
2	B	103	
2	R	103	
3	O	130	
3	S	130	
4	U	167	
5	W	167	

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Mol	Chain	Length	Quality of chain
6	f	477	
7	h	157	
8	F	435	
9	D	557	
9	H	557	
10	M	581	
11	I	483	
12	G	426	
13	A	502	
14	J	1359	
14	V	1359	
14	Y	1359	
15	E	78	
16	C	883	
17	K	885	
18	X	625	
19	L	889	
20	P	126	
20	T	126	
21	g	467	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 45924 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	98	Total	C	N	O	S	0	0
			810	511	157	139	3		
1	Q	95	Total	C	N	O	S	0	0
			784	494	151	136	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
2	R	87	Total	C	N	O	S	0	0
			703	443	142	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	107	Total	C	N	O	0	0
			823	519	161	143		
3	S	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 4 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	156	Total	C	N	O	P	0	0
			3183	1512	579	936	156		

- Molecule 5 is a DNA chain called DNA 167.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	156	Total	C	N	O	P	0	0
			3213	1522	599	936	156		

- Molecule 6 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	398	Total	C	N	O	S	3	0
			3219	2075	527	602	15		

- Molecule 7 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 8 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	118	Total	C	N	O	S	0	0
			964	601	164	197	2		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	393	Total	C	N	O	S	0	0
			3215	2036	552	613	14		
9	D	305	Total	C	N	O	S	0	0
			2510	1613	416	471	10		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	384	Total	C	N	O	S	0	0
			3058	1970	497	574	17		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	244	Total	C	N	O	S	0	0
			1944	1234	328	377	5		

- Molecule 12 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	246	Total	C	N	O	S	0	0
			1996	1271	337	380	8		

- Molecule 13 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	365	Total	C	N	O	S	0	0
			3007	1942	509	547	9		

- Molecule 14 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	235	Total	C	N	O	S	0	0
			1814	1136	327	349	2		
14	V	69	Total	C	N	O	S	0	0
			592	364	121	105	2		
14	Y	548	Total	C	N	O	S	0	0
			4503	2873	780	832	18		

- Molecule 15 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	58	Total	C	N	O	S	0	0
			477	295	86	92	4		

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	33	Total	C	N	O	S	0	0
			269	177	39	52	1		

- Molecule 17 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	42	Total	C	N	O	S	0	0
			347	225	57	63	2		

- Molecule 18 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	147	Total	C	N	O	S	0	0
			1220	776	202	234	8		

- Molecule 19 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	85	Total	C	N	O	S	0	0
			669	428	120	119	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	93	Total	C	N	O	S	0	0
			717	450	128	137	2		
20	T	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 21 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	395	Total	C	N	O	S	1	0
			3191	2048	522	614	7		

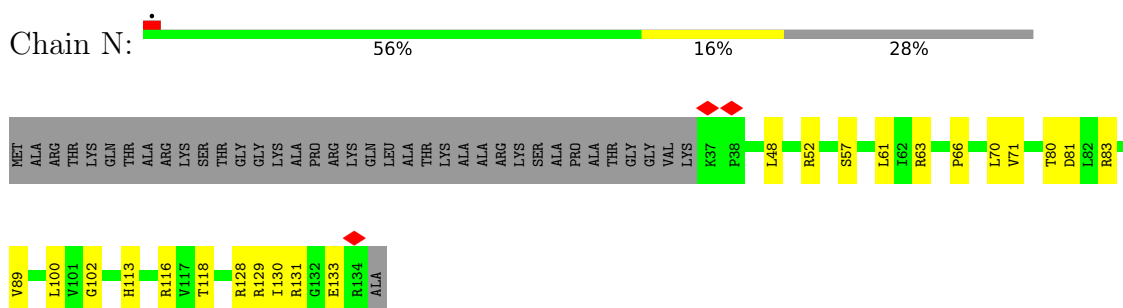
- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	H	1	Total	Zn	0
			1	1	

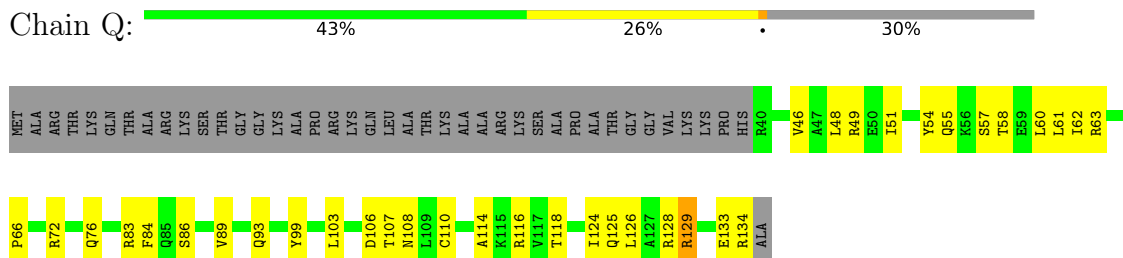
3 Residue-property plots [i](#)

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.

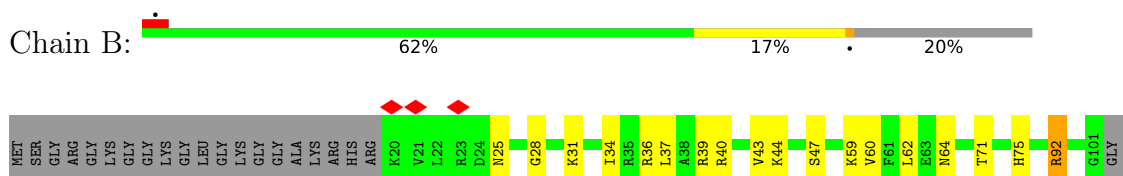
• Molecule 1: Histone H3.2



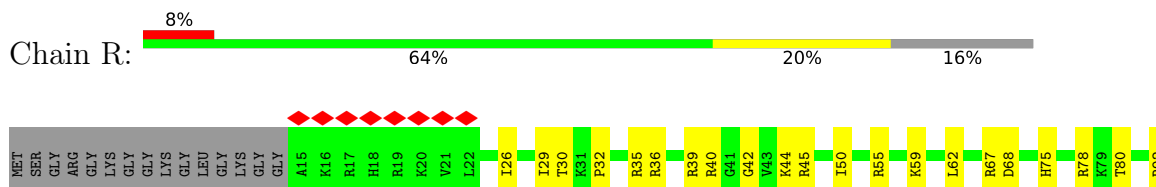
• Molecule 1: Histone H3.2



• Molecule 2: Histone H4



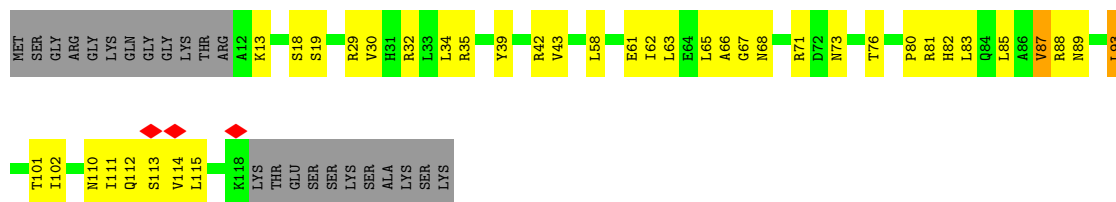
• Molecule 2: Histone H4





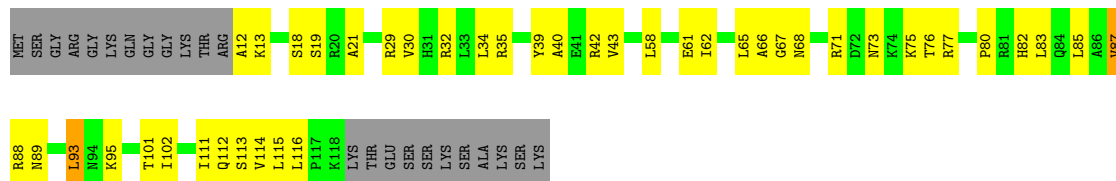
- Molecule 3: Histone H2A

Chain O: 52% 28% 18%



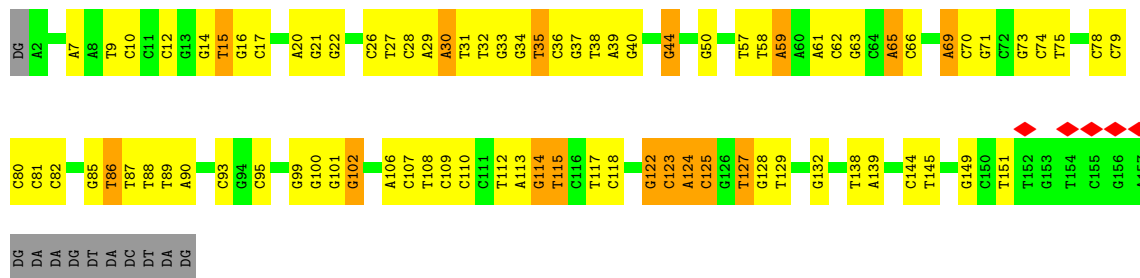
- Molecule 3: Histone H2A

Chain S: 49% 32% 18%



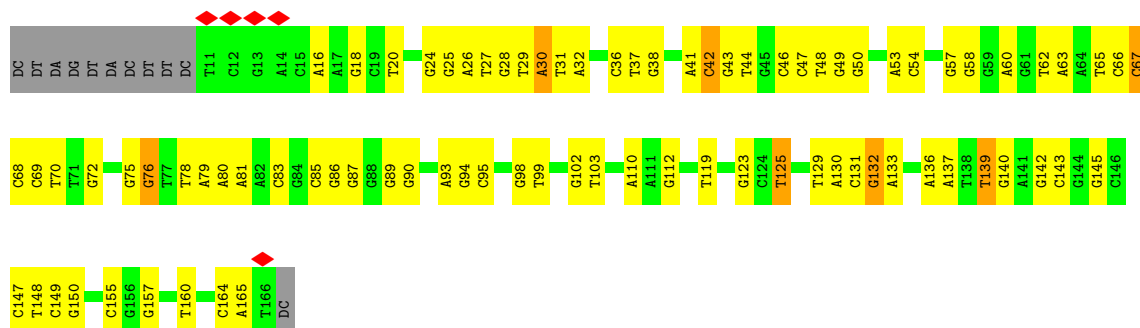
- Molecule 4: DNA 167

Chain U: 43% 41% 10% 7%



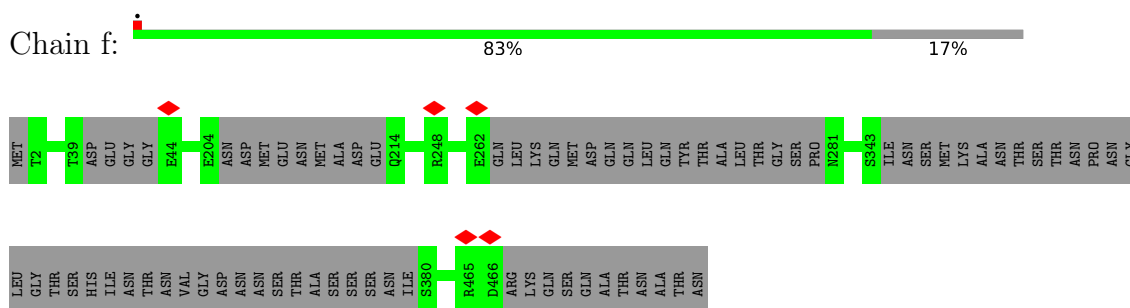
- Molecule 5: DNA 167

Chain W: 44% 46% 7%



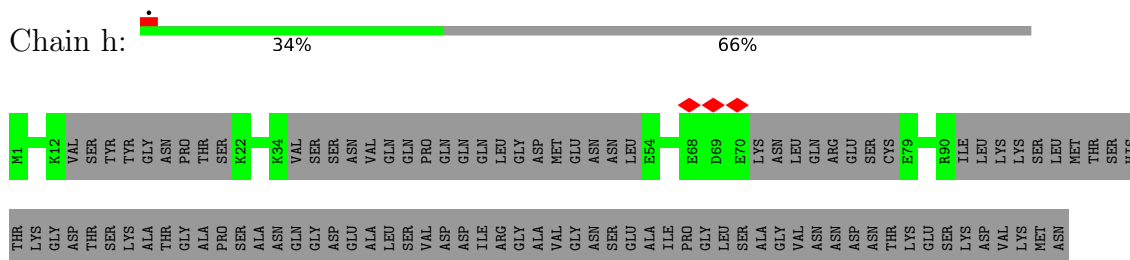
- Molecule 6: Actin-related protein 7

Chain f:



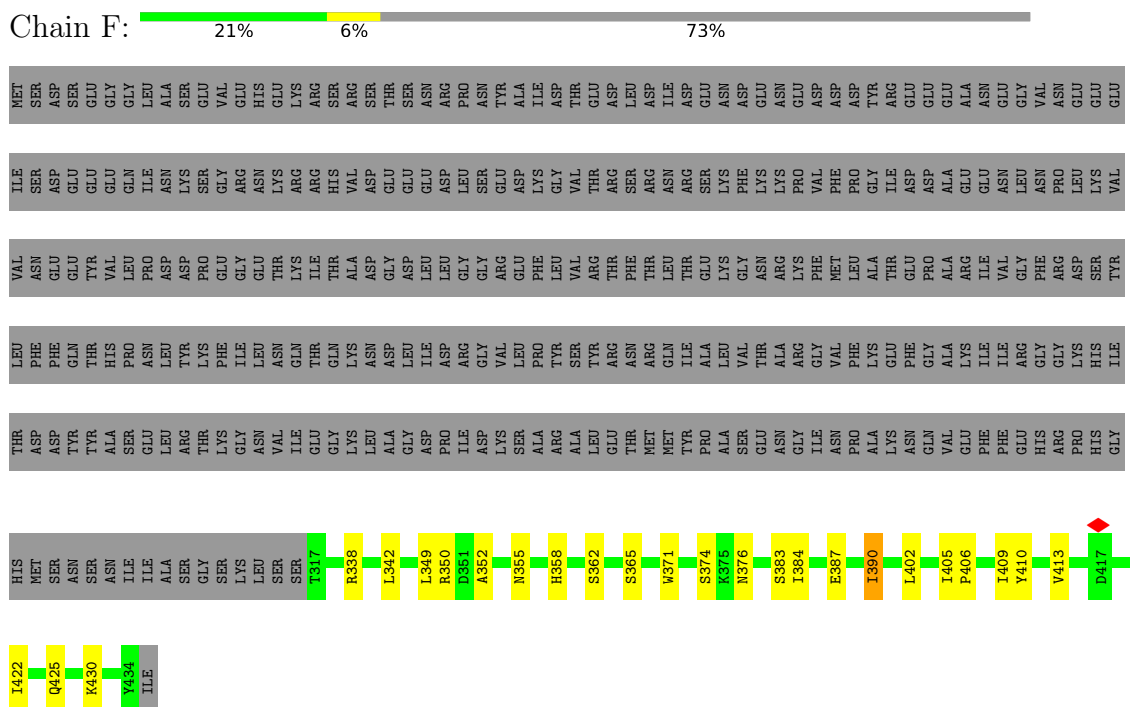
● Molecule 7: Regulator of Ty1 transposition protein 102

Chain h:



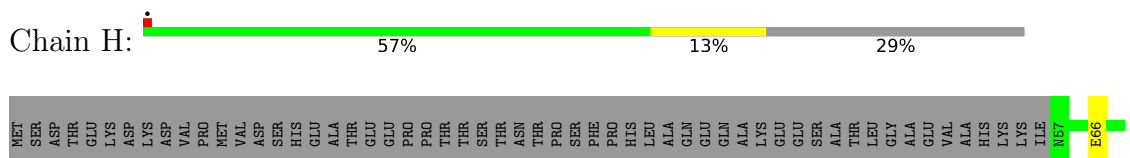
- Molecule 8: Chromatin structure-remodeling complex subunit RSC7

Chain F:



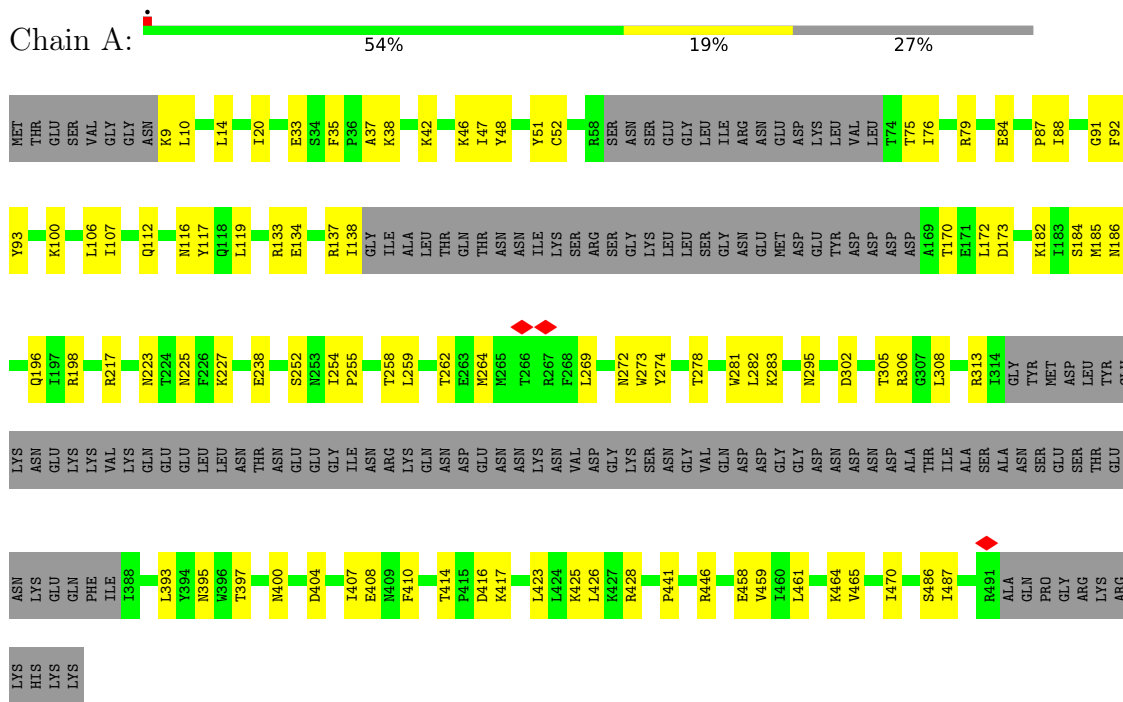
- Molecule 9: Chromatin structure-remodeling complex protein RSC8

Chain H:

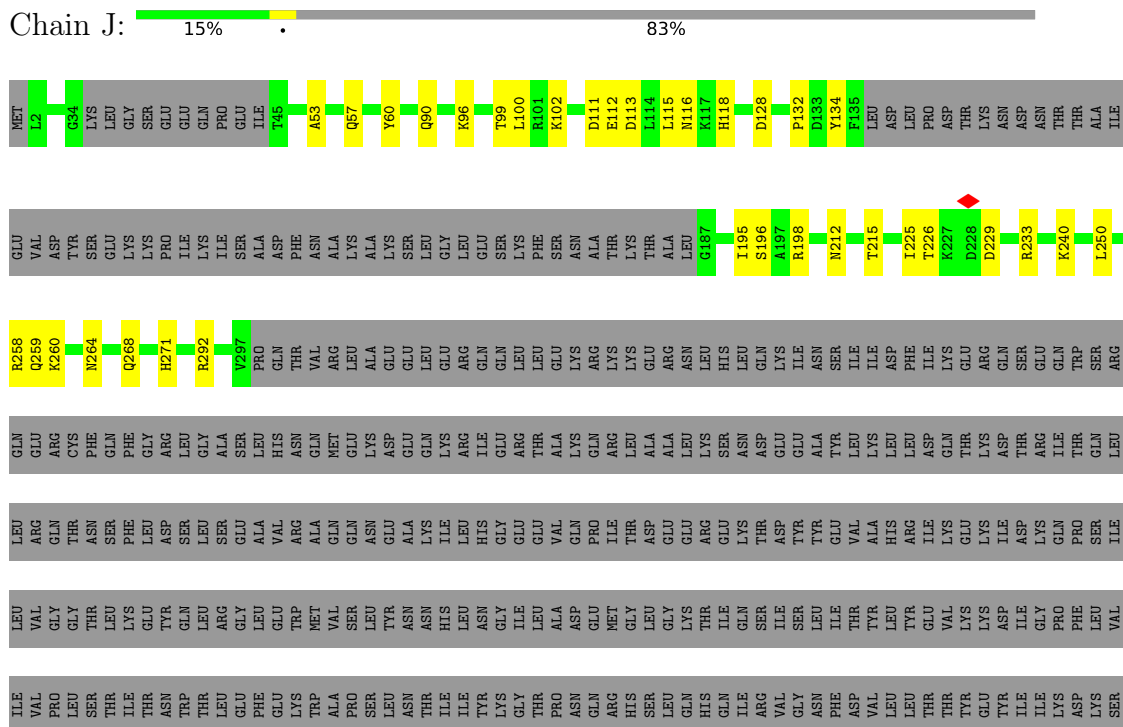




- Molecule 13: Chromatin structure-remodeling complex protein RSC58



- Molecule 14: Nuclear protein STH1/NPS1



GLU	LYS	THR	ALA	ALA	LYS	GLY	ASN	SER	LYS	ARG	VAL	LYS	ASP	ILE	ASN	LEU	GLN	THR	MET	LYS	ARG	LEU	GLY	VAL	ASN	GLN	THR	GLY	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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● Molecule 14: Nuclear protein STH1/NPS1

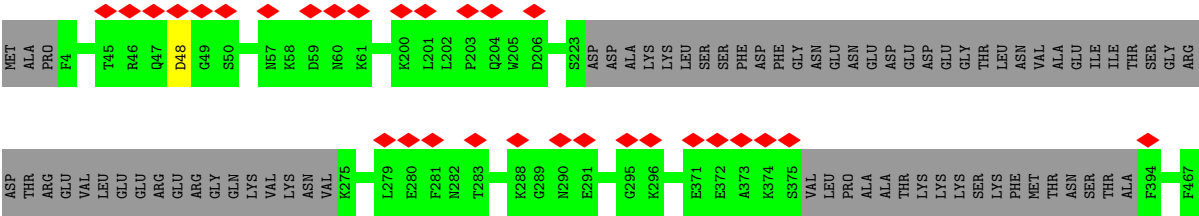












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.14, 2.14, 2.14	Depositor

5 Model quality

5.1 Standard geometry

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

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	N	0.30	0/822	0.53	0/1102
1	Q	0.29	0/794	0.49	0/1064
2	B	0.31	0/664	0.55	0/889
2	R	0.30	0/711	0.52	0/950
3	O	0.29	0/833	0.56	0/1124
3	S	0.29	0/833	0.56	0/1124
4	U	1.07	9/3567 (0.3%)	1.20	18/5499 (0.3%)
5	W	1.13	4/3607 (0.1%)	1.18	12/5569 (0.2%)
6	f	0.28	0/3295	0.49	0/4454
7	h	0.26	0/501	0.49	0/669
8	F	0.27	0/983	0.53	0/1337
9	D	0.26	0/2557	0.46	0/3442
9	H	0.27	0/3275	0.46	0/4409
10	M	0.29	0/3113	0.53	2/4215 (0.0%)
11	I	0.25	0/1976	0.48	0/2685
12	G	0.27	0/2039	0.53	1/2769 (0.0%)
13	A	0.28	0/3077	0.48	0/4169
14	J	0.25	0/1836	0.46	0/2480
14	V	0.24	0/598	0.37	0/789
14	Y	0.28	0/4580	0.54	0/6167
15	E	0.26	0/480	0.50	0/643
16	C	0.25	0/272	0.41	0/366
17	K	0.27	0/356	0.50	0/483
18	X	0.28	0/1243	0.55	0/1672
19	L	0.27	0/681	0.51	0/921
20	P	0.30	0/728	0.46	0/983
20	T	0.29	0/736	0.45	0/991
21	g	0.28	0/3261	0.50	0/4421
All	All	0.50	13/47418 (0.0%)	0.67	33/65386 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	53	DA	N9-C4	-8.46	1.32	1.37
4	U	65	DA	N9-C4	-6.03	1.34	1.37
4	U	99	DG	N9-C4	-5.90	1.33	1.38
5	W	32	DA	N9-C4	-5.74	1.34	1.37
4	U	124	DA	N9-C4	-5.65	1.34	1.37
5	W	76	DG	N9-C4	-5.64	1.33	1.38
4	U	59	DA	N9-C4	-5.54	1.34	1.37
4	U	99	DG	C2-N3	-5.43	1.28	1.32
4	U	44	DG	N9-C4	-5.43	1.33	1.38
5	W	125	DT	N1-C2	-5.34	1.33	1.38
4	U	129	DT	N1-C2	-5.32	1.33	1.38
4	U	114	DG	N9-C4	-5.13	1.33	1.38
4	U	69	DA	N9-C4	-5.13	1.34	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	127	DT	O4'-C1'-N1	7.24	113.07	108.00
5	W	67	DC	O4'-C1'-N1	6.60	112.62	108.00
5	W	30	DA	O4'-C4'-C3'	-6.43	101.93	104.50
5	W	27	DT	O4'-C1'-N1	6.43	112.50	108.00
12	G	300	LEU	CA-CB-CG	6.16	129.47	115.30
5	W	42	DC	O4'-C1'-N1	6.11	112.28	108.00
5	W	123	DG	O4'-C1'-N9	6.11	112.28	108.00
4	U	102	DG	O4'-C1'-N9	6.08	112.25	108.00
4	U	86	DT	O4'-C1'-N1	5.88	112.11	108.00
4	U	44	DG	C3'-C2'-C1'	-5.83	95.50	102.50
4	U	93	DC	O4'-C1'-N1	5.78	112.04	108.00
4	U	100	DG	O4'-C4'-C3'	-5.77	102.19	104.50
10	M	124	LEU	CA-CB-CG	5.75	128.53	115.30
10	M	317	LEU	CA-CB-CG	5.63	128.24	115.30
4	U	108	DT	C3'-C2'-C1'	-5.62	95.75	102.50
4	U	35	DT	N3-C4-O4	5.59	123.26	119.90
4	U	127	DT	C1'-O4'-C4'	-5.59	104.51	110.10
4	U	15	DT	O4'-C4'-C3'	-5.56	102.28	104.50
4	U	122	DG	O4'-C1'-N9	5.53	111.87	108.00
5	W	132	DG	O4'-C1'-N9	5.51	111.86	108.00
4	U	123	DC	O4'-C1'-N1	5.41	111.79	108.00
5	W	67	DC	C1'-O4'-C4'	-5.30	104.80	110.10
4	U	30	DA	OP2-P-O3'	5.29	116.84	105.20
4	U	125	DC	O4'-C1'-N1	5.18	111.63	108.00
5	W	139	DT	O5'-P-OP1	-5.18	101.04	105.70
4	U	115	DT	N3-C4-O4	5.14	122.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	143	DC	O4'-C1'-N1	5.14	111.60	108.00
5	W	139	DT	O5'-P-OP2	5.12	116.84	110.70
5	W	145	DG	O4'-C1'-N9	5.06	111.54	108.00
5	W	132	DG	C1'-O4'-C4'	-5.04	105.06	110.10
4	U	35	DT	C5-C4-O4	-5.02	121.39	124.90
4	U	99	DG	N3-C4-N9	-5.02	122.99	126.00
4	U	100	DG	C4'-C3'-C2'	-5.02	98.58	103.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	810	0	851	18	0
1	Q	784	0	824	30	0
2	B	657	0	706	16	0
2	R	703	0	757	23	0
3	O	823	0	882	33	0
3	S	823	0	882	32	0
4	U	3183	0	1752	74	0
5	W	3213	0	1752	67	0
6	f	3219	0	3240	0	0
7	h	490	0	467	0	0
8	F	964	0	919	24	0
9	D	2510	0	2542	48	0
9	H	3215	0	3196	73	0
10	M	3058	0	3127	53	0
11	I	1944	0	1964	42	0
12	G	1996	0	1948	36	0
13	A	3007	0	3045	70	0
14	J	1814	0	1777	26	0
14	V	592	0	610	4	0
14	Y	4503	0	4573	97	0
15	E	477	0	491	14	0
16	C	269	0	279	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	K	347	0	342	3	0
18	X	1220	0	1192	22	0
19	L	669	0	693	12	0
20	P	717	0	723	26	0
20	T	725	0	745	21	0
21	g	3191	0	3179	0	0
22	H	1	0	0	0	0
All	All	45924	0	43458	661	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (661) 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)
14:Y:710:VAL:CG2	14:Y:912:ILE:H	1.60	1.15
14:Y:710:VAL:HG21	14:Y:912:ILE:H	1.17	1.05
14:Y:710:VAL:HG21	14:Y:912:ILE:N	1.74	1.02
14:Y:710:VAL:O	14:Y:712:LYS:HG2	1.77	0.85
14:Y:710:VAL:O	14:Y:712:LYS:N	2.10	0.85
14:Y:710:VAL:O	14:Y:711:GLU:C	2.21	0.75
2:B:44:LYS:HB2	3:S:115:LEU:HD22	1.74	0.70
4:U:107:DC:N3	5:W:60:DA:N6	2.39	0.70
4:U:113:DA:N6	5:W:54:DC:N3	2.38	0.69
3:O:29:ARG:HH22	20:T:37:TYR:HE1	1.41	0.69
4:U:79:DC:O2	5:W:90:DG:N2	2.26	0.68
4:U:27:DT:O2	5:W:142:DG:N2	2.26	0.68
4:U:82:DC:O2	5:W:87:DG:N2	2.26	0.68
14:Y:880:ASP:HB2	14:Y:910:VAL:HA	1.76	0.68
4:U:44:DG:N2	5:W:125:DT:O2	2.27	0.67
8:F:387:GLU:HG3	9:H:188:GLN:HB3	1.76	0.67
12:G:295:ASN:HB2	12:G:376:TRP:HB2	1.75	0.67
8:F:376:ASN:H	9:H:184:THR:HB	1.59	0.67
9:H:83:PRO:HA	9:D:192:ASP:HB3	1.77	0.67
13:A:404:ASP:H	14:J:96:LYS:HD3	1.59	0.67
4:U:50:DG:N2	5:W:119:DT:O2	2.28	0.66
4:U:124:DA:H2''	4:U:125:DC:H2'	1.76	0.66
5:W:36:DC:H4'	5:W:37:DT:H5'	1.77	0.66
4:U:7:DA:N6	5:W:160:DT:O4	2.29	0.66
14:Y:710:VAL:HA	14:Y:712:LYS:HE2	1.77	0.65
14:Y:763:CYS:HG	14:Y:920:SER:HG	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:447:ASP:HB2	13:A:272:ASN:HD22	1.62	0.65
13:A:186:ASN:HB3	18:X:433:GLU:HB3	1.78	0.65
3:O:88:ARG:HH22	3:O:101:THR:HA	1.62	0.64
3:S:88:ARG:HH22	3:S:101:THR:HA	1.62	0.64
4:U:144:DC:O2	5:W:25:DG:N2	2.30	0.64
2:B:60:VAL:O	2:B:64:ASN:ND2	2.31	0.64
9:H:175:LYS:HG2	10:M:77:ARG:HH21	1.63	0.64
13:A:258:THR:HG23	14:J:196:SER:HB2	1.80	0.63
2:R:75:HIS:HD1	20:P:96:THR:HG1	1.46	0.63
14:Y:710:VAL:CG2	14:Y:912:ILE:N	2.40	0.63
8:F:384:ILE:HB	9:H:235:TYR:HB2	1.80	0.63
2:R:75:HIS:HB2	20:P:96:THR:HG21	1.81	0.62
9:H:433:VAL:HG11	9:D:429:ILE:HG23	1.80	0.62
14:Y:799:VAL:HA	14:Y:802:LYS:HD2	1.81	0.62
18:X:493:GLN:NE2	18:X:614:THR:O	2.32	0.62
2:R:26:ILE:HA	2:R:29:ILE:HD12	1.81	0.62
14:Y:809:ARG:HA	14:Y:861:PHE:HB3	1.80	0.62
14:Y:702:VAL:HG12	14:Y:703:GLU:HG3	1.82	0.61
9:H:272:TYR:HB2	9:H:282:LEU:HB2	1.82	0.61
9:H:275:LEU:HD11	9:H:302:ILE:HG13	1.82	0.61
14:Y:479:GLU:HA	14:Y:482:VAL:HB	1.81	0.61
3:O:83:LEU:HB3	3:O:102:ILE:HD13	1.82	0.61
8:F:413:VAL:HG13	9:D:88:TRP:HB3	1.83	0.61
14:Y:474:GLN:NE2	14:Y:499:LEU:O	2.34	0.61
11:I:27:VAL:HG12	11:I:29:ASN:H	1.64	0.61
1:N:52:ARG:HG3	3:S:111:ILE:HD11	1.83	0.60
2:R:39:ARG:NH1	2:R:44:LYS:O	2.33	0.60
9:H:279:ASP:HB2	10:M:41:ARG:HH11	1.66	0.60
3:S:83:LEU:HB3	3:S:102:ILE:HD13	1.82	0.60
14:Y:812:MET:HB2	14:Y:864:LEU:HA	1.82	0.60
2:B:71:THR:HG22	20:T:96:THR:HG23	1.82	0.60
2:B:39:ARG:NH1	2:B:43:VAL:O	2.34	0.60
4:U:36:DC:H4'	4:U:37:DG:H5'	1.84	0.60
4:U:40:DG:N2	5:W:129:DT:O2	2.34	0.60
4:U:80:DC:O2	5:W:89:DG:N2	2.35	0.60
3:S:85:LEU:O	3:S:89:ASN:ND2	2.35	0.59
9:H:426:GLN:HB2	9:D:422:ILE:HD11	1.84	0.59
13:A:9:LYS:HE2	13:A:138:ILE:HG12	1.83	0.59
14:Y:802:LYS:HE3	14:Y:982:ASN:HD21	1.66	0.59
3:S:87:VAL:HB	3:S:93:LEU:HD23	1.85	0.59
4:U:132:DG:N2	5:W:37:DT:O2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:338:ARG:NH1	12:G:317:ASP:OD1	2.35	0.59
1:N:57:SER:OG	2:B:40:ARG:NH2	2.36	0.59
15:E:20:THR:H	15:E:23:ASN:HB2	1.68	0.59
3:O:87:VAL:HB	3:O:93:LEU:HD23	1.85	0.59
5:W:65:DT:H4'	5:W:66:DC:H5'	1.85	0.59
13:A:254:ILE:HG21	14:J:250:LEU:HD23	1.85	0.59
3:O:85:LEU:O	3:O:89:ASN:ND2	2.35	0.59
10:M:294:SER:HB2	11:I:45:LEU:HD11	1.84	0.58
13:A:112:GLN:HE21	13:A:217:ARG:HD2	1.68	0.58
18:X:604:PHE:HB3	18:X:617:MET:HB2	1.84	0.58
4:U:29:DA:H4'	4:U:30:DA:H5'	1.84	0.58
4:U:101:DG:N2	5:W:68:DC:O2	2.36	0.58
14:Y:710:VAL:O	14:Y:712:LYS:CG	2.49	0.58
4:U:73:DG:H1'	4:U:74:DC:H5'	1.86	0.58
9:H:94:ILE:HD11	9:H:119:LYS:HB2	1.85	0.58
14:J:115:LEU:HA	14:J:118:HIS:HB2	1.85	0.58
3:O:42:ARG:HH22	5:W:58:DG:H21	1.52	0.57
9:D:327:ILE:HG23	13:A:470:ILE:HD13	1.85	0.57
8:F:365:SER:H	9:H:194:PRO:HB3	1.69	0.57
12:G:315:VAL:HG13	12:G:320:LEU:HB2	1.87	0.57
13:A:33:GLU:HG3	13:A:106:LEU:HD11	1.86	0.57
4:U:151:DT:O2	5:W:18:DG:N2	2.38	0.57
14:Y:683:ILE:HA	14:Y:686:LEU:HB2	1.87	0.57
1:N:48:LEU:HD21	3:S:116:LEU:HA	1.86	0.57
18:X:375:GLU:HB2	18:X:514:HIS:HB2	1.87	0.57
8:F:376:ASN:ND2	8:F:383:SER:O	2.38	0.57
14:Y:459:ASP:HB3	14:Y:475:LEU:HD13	1.85	0.57
12:G:337:LEU:HA	12:G:340:LYS:HB2	1.86	0.57
13:A:264:MET:HA	14:J:259:GLN:HE21	1.70	0.57
1:Q:108:ASN:ND2	2:R:42:GLY:O	2.38	0.56
9:D:178:LEU:HB2	12:G:316:GLN:HE21	1.70	0.56
9:D:451:GLU:OE2	11:I:49:ARG:NH2	2.37	0.56
10:M:216:ASN:ND2	13:A:302:ASP:OD1	2.38	0.56
13:A:10:LEU:HB3	13:A:87:PRO:HB3	1.87	0.56
13:A:404:ASP:HB3	13:A:407:ILE:HG22	1.86	0.56
14:Y:763:CYS:SG	14:Y:920:SER:OG	2.59	0.56
2:R:67:ARG:HH22	20:P:100:LEU:HA	1.69	0.56
13:A:35:PHE:HB3	13:A:75:THR:HA	1.88	0.56
13:A:185:MET:HG2	19:L:860:LEU:HD22	1.86	0.56
13:A:410:PHE:HZ	13:A:417:LYS:HB3	1.71	0.56
14:Y:1000:LYS:HA	14:Y:1004:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:227:GLU:O	10:M:268:ARG:NH1	2.38	0.56
14:Y:476:ARG:O	14:Y:480:TRP:N	2.38	0.56
9:D:143:ARG:HH12	12:G:314:ILE:HD11	1.70	0.56
13:A:88:ILE:HG13	13:A:91:GLY:H	1.70	0.56
14:Y:790:ALA:HB3	14:Y:793:PHE:HB2	1.88	0.56
10:M:325:GLU:HA	10:M:328:LYS:HE2	1.86	0.56
4:U:21:DG:N2	5:W:148:DT:O2	2.39	0.56
14:Y:687:HIS:HE1	14:Y:942:ALA:HB1	1.71	0.56
4:U:22:DG:N2	5:W:147:DC:O2	2.39	0.56
10:M:166:ARG:NH1	14:J:292:ARG:O	2.37	0.56
13:A:414:THR:OG1	13:A:416:ASP:OD1	2.24	0.55
20:P:68:ASP:OD2	20:P:72:ARG:NH2	2.39	0.55
14:Y:470:LEU:HD13	14:Y:475:LEU:HD21	1.88	0.55
14:Y:975:GLU:HG2	14:Y:980:GLU:HG3	1.89	0.55
8:F:402:LEU:HA	8:F:405:ILE:HD12	1.88	0.55
9:H:282:LEU:HD11	9:H:292:PHE:HB3	1.88	0.55
2:R:67:ARG:NH2	2:R:68:ASP:OD1	2.40	0.55
4:U:57:DT:O2	5:W:112:DG:N2	2.39	0.55
5:W:67:DC:H4'	5:W:68:DC:H5'	1.89	0.55
18:X:511:LEU:HB2	18:X:591:PHE:HB2	1.89	0.55
4:U:145:DT:O2	5:W:24:DG:N2	2.40	0.55
5:W:46:DC:H4'	5:W:47:DC:H5'	1.88	0.55
10:M:110:LYS:HG3	17:K:164:ILE:HG23	1.87	0.55
14:Y:565:ARG:O	14:Y:589:HIS:NE2	2.40	0.55
5:W:94:DG:H1'	5:W:95:DC:H5'	1.89	0.55
1:Q:72:ARG:O	1:Q:76:GLN:NE2	2.40	0.55
10:M:551:GLN:NE2	10:M:578:THR:O	2.40	0.55
1:Q:48:LEU:HD23	1:Q:51:ILE:HD12	1.88	0.55
9:H:435:LEU:O	11:I:398:LYS:NZ	2.38	0.55
13:A:282:LEU:HD11	13:A:295:ASN:HB2	1.88	0.55
4:U:14:DG:N2	5:W:155:DC:O2	2.40	0.54
9:H:472:ARG:NH2	9:D:464:GLU:O	2.40	0.54
2:R:26:ILE:HG23	2:R:55:ARG:HD3	1.89	0.54
2:R:75:HIS:ND1	20:P:96:THR:OG1	2.41	0.54
4:U:112:DT:O2	5:W:57:DG:N2	2.41	0.54
9:H:271:ARG:NH1	9:H:305:GLU:O	2.40	0.54
14:J:215:THR:OG1	14:J:233:ARG:O	2.24	0.54
3:O:35:ARG:HA	3:O:43:VAL:HG21	1.90	0.54
9:H:236:ASP:OD1	9:H:236:ASP:N	2.39	0.54
11:I:477:LEU:HD22	11:I:482:ARG:HD2	1.88	0.54
5:W:37:DT:H4'	5:W:38:DG:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:267:SER:OG	9:H:306:ASN:ND2	2.41	0.54
1:N:71:VAL:HG11	1:N:89:VAL:HG22	1.90	0.54
3:S:35:ARG:HA	3:S:43:VAL:HG21	1.90	0.54
4:U:65:DA:H1'	4:U:66:DC:H5'	1.89	0.54
9:D:120:ASP:OD2	12:G:366:ARG:NH1	2.41	0.54
9:D:160:LEU:HD22	9:D:165:LEU:HD22	1.90	0.54
3:O:63:LEU:HD11	20:T:41:VAL:HG13	1.90	0.54
9:H:355:LEU:O	14:J:258:ARG:NH1	2.38	0.54
9:H:429:ILE:HA	9:H:432:LEU:HD12	1.89	0.54
12:G:294:ASP:HB3	12:G:378:PRO:HB3	1.88	0.54
13:A:133:ARG:NH2	19:L:870:PRO:O	2.41	0.54
20:P:77:ALA:HA	20:P:80:LEU:HB2	1.89	0.54
1:Q:57:SER:OG	2:R:40:ARG:NH2	2.40	0.54
4:U:78:DC:H4'	4:U:79:DC:H5'	1.89	0.54
3:O:58:LEU:HA	3:O:61:GLU:HB3	1.90	0.53
2:R:75:HIS:HA	20:P:92:ARG:HH21	1.73	0.53
4:U:106:DA:H1'	4:U:107:DC:H5'	1.90	0.53
9:H:127:ASN:ND2	9:D:184:THR:OG1	2.41	0.53
9:D:222:LYS:H	11:I:463:ASN:HD21	1.56	0.53
3:O:29:ARG:HG2	3:O:32:ARG:HH21	1.74	0.53
8:F:349:LEU:HB2	8:F:358:HIS:HB2	1.91	0.53
8:F:350:ARG:NH1	8:F:355:ASN:OD1	2.40	0.53
14:Y:941:GLN:HA	14:Y:944:LYS:HE3	1.90	0.53
11:I:456:ARG:NH1	13:A:262:THR:O	2.41	0.53
9:H:149:ASP:N	9:H:149:ASP:OD1	2.42	0.53
9:H:439:LYS:NZ	11:I:40:ASP:OD2	2.37	0.53
14:V:351:PHE:HA	14:V:354:LEU:HB2	1.89	0.53
9:H:178:LEU:HD11	9:D:195:GLN:HG3	1.91	0.53
14:Y:397:LYS:HE2	14:Y:688:LYS:HB2	1.91	0.53
3:O:80:PRO:HG2	20:T:57:LYS:HG3	1.89	0.53
11:I:441:GLU:HG3	15:E:29:LEU:HD21	1.89	0.53
18:X:524:THR:OG1	18:X:589:GLU:OE1	2.27	0.53
2:R:78:ARG:NH1	2:R:80:THR:O	2.41	0.53
12:G:17:HIS:HA	12:G:20:LEU:HD12	1.91	0.53
12:G:358:ALA:HB1	12:G:365:ILE:H	1.73	0.53
13:A:461:LEU:O	13:A:464:LYS:NZ	2.39	0.53
1:Q:61:LEU:HB3	2:R:36:ARG:HE	1.73	0.52
9:H:406:LYS:NZ	9:D:396:ALA:O	2.31	0.52
3:O:32:ARG:NH2	20:T:35:GLU:OE2	2.42	0.52
13:A:116:ASN:HA	13:A:119:LEU:HB2	1.90	0.52
14:Y:656:GLU:O	14:Y:660:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:61:LEU:O	2:R:36:ARG:NH2	2.39	0.52
3:S:58:LEU:HA	3:S:61:GLU:HB3	1.90	0.52
14:Y:999:ASP:O	14:Y:1004:ASN:ND2	2.42	0.52
3:O:67:GLY:HA2	20:T:52:THR:HG21	1.92	0.52
12:G:294:ASP:N	12:G:294:ASP:OD1	2.42	0.52
14:Y:481:MET:O	14:Y:485:TYR:N	2.40	0.52
12:G:12:TYR:HB3	12:G:180:VAL:HG13	1.92	0.52
2:B:75:HIS:HD1	20:T:96:THR:HG1	1.53	0.52
4:U:34:DG:H3'	4:U:35:DT:H71	1.92	0.52
10:M:143:LYS:O	10:M:211:ASN:ND2	2.39	0.52
9:H:271:ARG:HB2	9:H:281:ASN:HB3	1.91	0.52
12:G:228:ASP:OD1	12:G:228:ASP:N	2.43	0.52
13:A:79:ARG:HD2	13:A:84:GLU:HG3	1.91	0.52
3:O:63:LEU:HD22	20:T:45:LEU:HD13	1.91	0.51
5:W:98:DG:H4'	5:W:99:DT:H5'	1.92	0.51
10:M:323:ILE:HG22	10:M:545:ALA:HB3	1.92	0.51
19:L:867:GLY:O	19:L:869:ARG:NH1	2.43	0.51
3:O:112:GLN:HB2	3:O:115:LEU:HG	1.92	0.51
3:S:29:ARG:HG2	3:S:32:ARG:HH21	1.74	0.51
3:S:42:ARG:HB3	5:W:132:DG:H5''	1.91	0.51
9:H:285:ARG:HE	19:L:763:GLN:HB2	1.75	0.51
12:G:165:ILE:HG12	12:G:171:ILE:HG21	1.92	0.51
14:Y:775:VAL:HG23	14:Y:776:VAL:HG13	1.92	0.51
14:Y:787:PHE:HA	14:Y:793:PHE:HB3	1.92	0.51
9:D:161:GLU:HG3	9:D:167:ASN:HB2	1.92	0.51
10:M:197:CYS:O	10:M:202:ASP:N	2.43	0.51
16:C:214:ASP:O	16:C:218:ASN:ND2	2.44	0.51
8:F:390:ILE:HD12	9:H:228:LEU:HB2	1.93	0.51
9:D:315:TRP:NE1	9:D:349:ASP:OD2	2.43	0.51
9:D:469:LEU:HD22	11:I:258:LYS:HD3	1.93	0.51
3:S:43:VAL:HA	20:P:89:ILE:HG13	1.91	0.51
5:W:75:DG:H2''	5:W:76:DG:H2'	1.92	0.51
9:H:256:LYS:NZ	10:M:46:GLY:O	2.39	0.51
14:Y:481:MET:HA	14:Y:484:LEU:HB2	1.91	0.51
4:U:90:DA:H2	5:W:79:DA:H2	1.57	0.51
9:H:235:TYR:OH	9:D:188:GLN:NE2	2.36	0.51
9:H:259:ILE:HD12	10:M:43:GLN:HB3	1.93	0.51
4:U:86:DT:O4	5:W:81:DA:N6	2.44	0.51
9:H:97:ILE:HG12	9:H:100:ARG:HH21	1.76	0.51
14:J:112:GLU:O	14:J:116:ASN:N	2.37	0.51
13:A:425:LYS:HG2	13:A:428:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:680:LEU:HD22	14:Y:684:ARG:HG3	1.93	0.51
2:R:30:THR:HG21	4:U:61:DA:H5''	1.93	0.51
9:H:311:VAL:O	9:H:314:ASN:ND2	2.44	0.51
18:X:378:LEU:HB2	18:X:484:TYR:HB2	1.93	0.51
14:Y:552:GLY:HA2	14:Y:843:THR:HG21	1.93	0.51
1:N:66:PRO:HB3	2:B:28:GLY:HA3	1.93	0.50
3:O:80:PRO:HA	3:O:83:LEU:HB2	1.93	0.50
9:H:98:GLU:OE1	9:H:122:ARG:NH1	2.44	0.50
20:P:67:ASN:HA	20:P:70:PHE:HB3	1.93	0.50
20:T:81:ALA:O	20:T:86:ARG:N	2.42	0.50
14:Y:800:LEU:HD13	14:Y:830:LYS:HD3	1.92	0.50
14:Y:809:ARG:HH22	14:Y:853:PHE:HA	1.77	0.50
13:A:172:LEU:HB2	18:X:379:LEU:HD12	1.93	0.50
2:B:47:SER:HA	4:U:81:DC:H5''	1.93	0.50
3:S:40:ALA:HB3	20:P:89:ILE:HG12	1.92	0.50
5:W:43:DG:H3'	5:W:44:DT:H71	1.92	0.50
12:G:19:ARG:HA	12:G:22:ASN:HB2	1.92	0.50
1:N:128:ARG:HB3	1:N:133:GLU:HB2	1.93	0.50
3:S:80:PRO:HA	3:S:83:LEU:HB2	1.93	0.50
10:M:327:PHE:HB2	10:M:545:ALA:HB1	1.94	0.50
11:I:417:GLN:HA	11:I:420:HIS:HB3	1.94	0.50
12:G:279:VAL:HG21	12:G:339:ILE:HD13	1.92	0.50
11:I:220:ILE:HB	11:I:351:LEU:HB3	1.94	0.50
14:J:111:ASP:OD1	14:J:111:ASP:N	2.43	0.50
20:T:106:LEU:HA	20:T:109:HIS:HB2	1.93	0.50
4:U:29:DA:H2	5:W:140:DG:H22	1.59	0.50
4:U:90:DA:N6	5:W:78:DT:O4	2.45	0.50
12:G:205:PRO:HA	12:G:222:LEU:HA	1.93	0.50
1:N:116:ARG:NH1	1:N:118:THR:O	2.45	0.50
3:S:112:GLN:HB2	3:S:115:LEU:HG	1.92	0.50
9:H:355:LEU:HD22	14:J:258:ARG:HG3	1.94	0.50
14:Y:495:ASP:OD2	14:Y:697:ARG:NH2	2.45	0.50
14:Y:630:LEU:O	14:Y:892:HIS:NE2	2.45	0.50
3:S:77:ARG:HE	4:U:20:DA:H4'	1.76	0.49
14:Y:525:ILE:HB	14:Y:596:ILE:HA	1.93	0.49
14:Y:535:THR:HA	14:Y:538:PHE:HB2	1.93	0.49
4:U:124:DA:H5'	20:T:33:ARG:HA	1.93	0.49
10:M:551:GLN:NE2	10:M:578:THR:OG1	2.39	0.49
11:I:8:VAL:O	13:A:283:LYS:N	2.45	0.49
12:G:374:SER:OG	12:G:375:ASN:N	2.46	0.49
3:S:43:VAL:N	5:W:133:DA:OP1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:110:ASN:O	1:Q:55:GLN:NE2	2.46	0.49
9:H:110:SER:HB3	12:G:201:ALA:H	1.77	0.49
13:A:42:LYS:O	13:A:93:TYR:OH	2.28	0.49
18:X:433:GLU:HG3	18:X:444:GLU:HB3	1.95	0.49
4:U:151:DT:O4	5:W:16:DA:N6	2.45	0.49
9:H:181:PRO:O	11:I:468:ARG:NH1	2.45	0.49
1:Q:110:CYS:O	1:Q:114:ALA:N	2.45	0.49
3:S:67:GLY:O	3:S:71:ARG:NE	2.42	0.49
4:U:101:DG:H4'	4:U:102:DG:H5'	1.95	0.49
3:S:43:VAL:HG22	20:P:89:ILE:HD11	1.95	0.49
4:U:122:DG:H4'	4:U:123:DC:H5'	1.95	0.49
13:A:305:THR:HA	13:A:308:LEU:HB2	1.94	0.49
14:Y:876:LEU:HD23	14:Y:901:ALA:HA	1.94	0.49
10:M:149:SER:HG	11:I:435:TRP:HE1	1.57	0.49
4:U:30:DA:H1'	4:U:31:DT:H5'	1.95	0.49
1:Q:124:ILE:HD11	2:R:50:ILE:HD12	1.95	0.49
9:H:259:ILE:HB	10:M:44:SER:HA	1.95	0.49
11:I:315:LEU:HB3	11:I:320:GLN:HG3	1.95	0.49
9:H:405:ASP:O	9:H:409:LYS:NZ	2.46	0.48
9:D:348:GLU:HG3	13:A:461:LEU:HD11	1.95	0.48
4:U:89:DT:H4'	4:U:90:DA:H5'	1.95	0.48
12:G:307:PRO:HB3	12:G:332:LEU:HD22	1.95	0.48
14:Y:765:HIS:HD2	14:Y:819:VAL:HB	1.78	0.48
14:Y:885:PHE:HE1	14:Y:915:LEU:HB2	1.77	0.48
8:F:410:TYR:HB3	9:D:163:TRP:HH2	1.78	0.48
9:D:116:LYS:NZ	9:D:120:ASP:OD1	2.46	0.48
12:G:15:ASN:HD22	12:G:174:THR:HG22	1.79	0.48
13:A:397:THR:H	13:A:400:ASN:HD21	1.59	0.48
11:I:260:ILE:HG23	11:I:265:LEU:HD12	1.96	0.48
19:L:874:PHE:O	19:L:878:ARG:N	2.44	0.48
3:S:21:ALA:HB1	20:P:117:ALA:HB1	1.96	0.48
13:A:182:LYS:HD2	18:X:431:GLN:HG3	1.95	0.48
13:A:196:GLN:N	13:A:227:LYS:O	2.43	0.48
14:Y:451:ALA:O	14:Y:487:ASN:ND2	2.46	0.48
10:M:115:ILE:HG13	10:M:168:LEU:HD21	1.95	0.48
12:G:158:GLN:O	12:G:164:ASN:ND2	2.44	0.48
14:Y:408:THR:HG22	14:Y:487:ASN:HB3	1.95	0.48
1:N:70:LEU:HD13	2:B:25:ASN:HB2	1.96	0.48
1:Q:99:TYR:O	1:Q:103:LEU:N	2.46	0.48
4:U:28:DC:H4'	4:U:29:DA:H5'	1.94	0.48
20:P:56:SER:HA	20:P:59:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:524:VAL:HB	14:Y:573:LEU:HD23	1.96	0.48
14:Y:594:MET:HB2	14:Y:622:ARG:HA	1.95	0.48
8:F:352:ALA:HB1	12:G:25:ASP:HB3	1.96	0.48
10:M:141:LEU:HB3	10:M:205:TRP:HZ2	1.78	0.48
14:J:260:LYS:O	14:J:264:ASN:ND2	2.47	0.48
20:P:51:ASP:OD1	20:P:51:ASP:N	2.47	0.48
1:N:130:ILE:HG23	1:Q:106:ASP:HB3	1.95	0.48
8:F:374:SER:HB2	9:H:186:HIS:H	1.79	0.48
10:M:94:PRO:HA	10:M:97:ILE:HB	1.95	0.48
13:A:107:ILE:HG23	13:A:117:TYR:HE1	1.78	0.48
13:A:458:GLU:HA	13:A:461:LEU:HB2	1.95	0.48
1:Q:116:ARG:HD3	4:U:71:DG:H3'	1.96	0.47
9:D:425:SER:HA	15:E:62:LEU:HD13	1.96	0.47
10:M:550:CYS:HB3	10:M:574:TYR:HE1	1.79	0.47
13:A:223:ASN:HD21	13:A:225:ASN:HB2	1.78	0.47
3:O:73:ASN:HB2	3:O:82:HIS:HE2	1.79	0.47
12:G:27:ILE:HG22	12:G:29:ILE:H	1.80	0.47
13:A:133:ARG:NH2	13:A:134:GLU:OE2	2.47	0.47
14:J:225:ILE:HG23	14:J:229:ASP:HB3	1.96	0.47
5:W:130:DA:H4'	5:W:131:DC:H5'	1.96	0.47
9:D:462:VAL:HG11	10:M:555:PRO:HB3	1.95	0.47
4:U:9:DT:H4'	4:U:10:DC:H5'	1.96	0.47
14:J:128:ASP:OD2	14:J:198:ARG:NH2	2.47	0.47
15:E:59:ARG:NH1	15:E:63:GLU:OE2	2.47	0.47
3:O:67:GLY:O	3:O:71:ARG:NE	2.42	0.47
4:U:62:DC:H2''	4:U:63:DG:C8	2.50	0.47
10:M:192:LEU:HB3	10:M:245:THR:HG21	1.95	0.47
10:M:314:GLN:HA	10:M:317:LEU:HD23	1.95	0.47
10:M:569:LEU:HD13	11:I:310:LEU:HB2	1.96	0.47
1:Q:83:ARG:HE	4:U:50:DG:H4'	1.79	0.47
20:P:58:ALA:HA	20:P:61:ILE:HD12	1.97	0.47
20:T:56:SER:HA	20:T:59:MET:HB3	1.96	0.47
14:Y:457:LYS:HA	14:Y:479:GLU:HG2	1.96	0.47
14:Y:945:PHE:HE1	14:Y:957:PHE:HB2	1.79	0.47
3:S:39:TYR:HB2	20:P:89:ILE:HD13	1.95	0.47
4:U:85:DG:N1	5:W:83:DC:O2	2.36	0.47
9:H:414:SER:HB3	15:E:39:LEU:HD21	1.96	0.47
10:M:80:ASP:OD1	10:M:80:ASP:N	2.46	0.47
18:X:378:LEU:HD22	18:X:509:LEU:HD13	1.97	0.47
14:Y:695:LEU:HD12	14:Y:947:ASN:HB3	1.97	0.47
1:N:61:LEU:HB3	2:B:36:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:83:ARG:HD3	5:W:70:DT:H4'	1.97	0.47
8:F:406:PRO:HG2	8:F:409:ILE:HG12	1.97	0.47
14:Y:811:LEU:HB2	14:Y:882:VAL:HG22	1.95	0.47
14:Y:909:GLU:HB3	14:Y:987:ARG:HD2	1.97	0.47
3:O:62:ILE:HD12	3:O:65:LEU:HB2	1.96	0.46
20:P:81:ALA:O	20:P:86:ARG:N	2.37	0.46
14:Y:564:ILE:O	14:Y:567:GLY:N	2.42	0.46
1:N:80:THR:OG1	1:N:81:ASP:N	2.49	0.46
3:S:73:ASN:HB2	3:S:82:HIS:HE2	1.79	0.46
5:W:85:DC:H1'	5:W:86:DG:C5	2.51	0.46
10:M:224:ASP:OD1	10:M:257:TYR:OH	2.30	0.46
11:I:440:ASN:HB2	15:E:29:LEU:HD13	1.96	0.46
13:A:408:GLU:OE2	14:J:99:THR:OG1	2.33	0.46
14:Y:535:THR:O	14:Y:539:GLU:N	2.47	0.46
14:Y:876:LEU:O	14:Y:906:GLN:NE2	2.48	0.46
3:S:62:ILE:HD12	3:S:65:LEU:HB2	1.96	0.46
9:D:101:SER:OG	9:D:102:ASN:N	2.49	0.46
18:X:528:ILE:HA	18:X:602:LEU:HD12	1.97	0.46
3:S:12:ALA:HB3	4:U:32:DT:H4'	1.97	0.46
10:M:134:LEU:HD12	10:M:137:ILE:HD12	1.95	0.46
9:H:180:GLY:HA3	9:D:198:LYS:HE2	1.96	0.46
12:G:276:ASP:OD1	12:G:301:ASN:ND2	2.42	0.46
13:A:14:LEU:HD13	13:A:92:PHE:HE1	1.79	0.46
20:P:110:ALA:HA	20:P:113:GLU:HB2	1.97	0.46
9:H:430:GLN:HG2	9:D:429:ILE:HD11	1.98	0.46
14:Y:809:ARG:HG2	14:Y:861:PHE:HD1	1.80	0.46
3:S:76:THR:O	20:P:53:GLY:N	2.49	0.46
4:U:33:DG:H1'	4:U:34:DG:C8	2.50	0.46
8:F:342:LEU:HD22	9:D:179:ILE:HD13	1.98	0.46
9:H:390:MET:HG3	15:E:33:ARG:HD2	1.97	0.46
9:H:454:LEU:HB3	9:D:454:LEU:HD11	1.97	0.46
9:D:193:THR:HG22	9:D:195:GLN:H	1.81	0.46
10:M:93:ILE:HB	10:M:96:GLU:HB2	1.98	0.46
13:A:486:SER:O	18:X:622:ASN:ND2	2.49	0.46
3:O:43:VAL:N	4:U:113:DA:OP1	2.49	0.46
10:M:95:GLU:HA	10:M:98:LYS:HB2	1.98	0.46
10:M:547:SER:HA	10:M:550:CYS:HB2	1.98	0.46
11:I:260:ILE:HG12	11:I:319:LEU:HD21	1.97	0.46
1:Q:86:SER:HA	1:Q:89:VAL:HB	1.97	0.46
2:R:32:PRO:O	2:R:36:ARG:N	2.45	0.46
19:L:745:ALA:HB1	19:L:793:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:874:PHE:HA	19:L:877:HIS:HB3	1.98	0.46
14:Y:731:LYS:HA	14:Y:735:LEU:HD12	1.98	0.46
10:M:72:PRO:HB2	10:M:75:THR:HG22	1.98	0.45
1:N:48:LEU:HG	3:S:111:ILE:HG21	1.98	0.45
4:U:16:DG:H1'	4:U:17:DC:H5'	1.97	0.45
4:U:149:DG:N2	5:W:20:DT:O2	2.49	0.45
9:H:66:GLU:HB2	9:H:228:LEU:HD13	1.98	0.45
1:Q:63:ARG:HB2	1:Q:66:PRO:HD2	1.99	0.45
11:I:430:LEU:HA	11:I:433:TYR:HB3	1.97	0.45
12:G:355:ASN:N	12:G:355:ASN:OD1	2.48	0.45
13:A:170:THR:HG22	13:A:173:ASP:H	1.81	0.45
14:Y:490:ASN:ND2	14:Y:644:VAL:O	2.49	0.45
14:Y:769:PHE:HB2	14:Y:772:VAL:HG23	1.98	0.45
2:B:59:LYS:HA	2:B:62:LEU:HD12	1.99	0.45
13:A:37:ALA:O	13:A:79:ARG:NH2	2.45	0.45
20:P:86:ARG:HA	20:P:86:ARG:HD3	1.78	0.45
14:Y:916:ILE:HG13	14:Y:926:LEU:HD22	1.98	0.45
14:Y:925:ILE:HA	14:Y:928:ARG:HB2	1.98	0.45
9:H:414:SER:OG	11:I:423:SER:OG	2.30	0.45
9:D:434:LYS:HE3	9:D:434:LYS:HB2	1.71	0.45
13:A:47:ILE:HD13	13:A:100:LYS:HB3	1.97	0.45
13:A:134:GLU:HA	13:A:137:ARG:HD3	1.99	0.45
18:X:434:MET:O	18:X:443:MET:N	2.46	0.45
14:Y:991:GLU:HA	14:Y:994:LEU:HB3	1.99	0.45
9:H:161:GLU:HG3	9:H:167:ASN:HB2	1.99	0.45
9:H:178:LEU:HB2	9:D:198:LYS:HB3	1.99	0.45
13:A:423:LEU:HD23	13:A:426:LEU:HD12	1.98	0.45
14:Y:929:ALA:HA	14:Y:932:LYS:HE2	1.98	0.45
2:B:31:LYS:HA	2:B:34:ILE:HD12	1.98	0.45
3:O:102:ILE:HG23	20:T:61:ILE:HD12	1.98	0.45
1:Q:125:GLN:HA	1:Q:128:ARG:HB2	1.98	0.45
8:F:371:TRP:HZ3	9:H:187:PHE:HB3	1.81	0.45
9:D:73:LEU:O	9:D:77:THR:OG1	2.30	0.45
10:M:140:GLY:O	10:M:145:SER:OG	2.30	0.45
14:Y:612:THR:O	14:Y:616:TYR:N	2.45	0.45
2:B:92:ARG:HG3	20:T:79:ARG:HH22	1.82	0.45
1:Q:116:ARG:NH1	1:Q:118:THR:O	2.50	0.45
4:U:37:DG:H4'	4:U:38:DT:H5'	1.99	0.45
9:D:227:ASN:HD21	14:J:240:LYS:HE2	1.82	0.45
13:A:255:PRO:HB2	13:A:259:LEU:HD22	1.99	0.45
15:E:62:LEU:O	15:E:66:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:374:THR:O	18:X:488:GLY:N	2.50	0.45
14:Y:462:PRO:HG2	14:Y:465:LEU:HG	1.99	0.45
4:U:12:DC:O2	5:W:157:DG:N2	2.50	0.44
9:H:426:GLN:HA	9:H:429:ILE:HD12	2.00	0.44
13:A:252:SER:HB3	13:A:254:ILE:HG12	1.98	0.44
19:L:878:ARG:HA	19:L:881:MET:HB2	1.99	0.44
1:Q:62:ILE:HG23	2:R:29:ILE:HG12	1.98	0.44
9:D:330:TYR:O	9:D:333:GLN:NE2	2.50	0.44
11:I:27:VAL:O	11:I:29:ASN:ND2	2.50	0.44
13:A:393:LEU:O	14:J:60:TYR:OH	2.35	0.44
18:X:377:TYR:HB2	18:X:512:GLN:HB3	1.99	0.44
14:Y:465:LEU:HD22	14:Y:541:TRP:HE3	1.83	0.44
14:Y:696:ARG:O	14:Y:947:ASN:ND2	2.48	0.44
3:O:81:ARG:HD3	1:Q:58:THR:HB	1.98	0.44
1:Q:125:GLN:O	1:Q:129:ARG:N	2.49	0.44
4:U:109:DC:H1'	4:U:110:DC:C2	2.52	0.44
1:N:102:GLY:O	1:N:131:ARG:NH2	2.44	0.44
8:F:384:ILE:O	9:H:235:TYR:N	2.46	0.44
20:P:90:THR:OG1	20:P:93:GLU:OE1	2.29	0.44
2:R:59:LYS:HA	2:R:62:LEU:HD12	1.99	0.44
4:U:102:DG:N2	5:W:67:DC:O2	2.51	0.44
9:H:401:LEU:HD22	11:I:427:ARG:HD2	1.99	0.44
1:Q:46:VAL:HG12	1:Q:49:ARG:HH12	1.83	0.44
4:U:87:DT:H6	4:U:87:DT:H2'	1.68	0.44
1:Q:128:ARG:HB3	1:Q:133:GLU:HB2	1.99	0.44
9:H:450:LEU:HD13	11:I:50:ARG:HG2	2.00	0.44
14:Y:553:THR:HG22	14:Y:555:ASN:H	1.83	0.44
4:U:26:DC:H2''	4:U:27:DT:C5	2.51	0.44
9:H:401:LEU:O	11:I:427:ARG:NH2	2.51	0.44
11:I:237:ASN:HB3	11:I:322:VAL:HG12	2.00	0.44
1:N:113:HIS:ND1	1:Q:126:LEU:HD13	2.32	0.44
5:W:25:DG:H2''	5:W:26:DA:C8	2.53	0.44
5:W:102:DG:H1'	5:W:103:DT:H5'	2.00	0.44
13:A:269:LEU:HG	13:A:274:TYR:HE1	1.83	0.44
1:N:100:LEU:HD12	2:B:37:LEU:HD22	2.00	0.43
4:U:88:DT:H2''	4:U:89:DT:C6	2.53	0.43
10:M:105:LEU:HD21	10:M:163:LEU:HD23	2.00	0.43
13:A:281:TRP:CH2	13:A:306:ARG:HG3	2.53	0.43
14:Y:896:GLN:HG3	14:Y:900:ARG:HH22	1.83	0.43
3:S:30:VAL:O	3:S:34:LEU:N	2.50	0.43
4:U:58:DT:H4'	4:U:59:DA:H5'	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:147:CYS:HG	11:I:431:THR:HG1	1.53	0.43
13:A:313:ARG:HD3	15:E:16:TYR:HB3	2.00	0.43
14:Y:937:GLY:HA2	14:Y:941:GLN:HB2	1.99	0.43
1:Q:118:THR:HA	2:R:45:ARG:HB3	1.99	0.43
5:W:48:DT:H4'	5:W:49:DG:H5'	2.00	0.43
5:W:139:DT:H2''	5:W:140:DG:C5	2.54	0.43
13:A:459:VAL:O	13:A:464:LYS:N	2.50	0.43
20:T:94:ILE:H	20:T:94:ILE:HG13	1.66	0.43
14:Y:938:LYS:HG2	14:Y:961:LEU:HD21	2.01	0.43
8:F:362:SER:OG	9:H:195:GLN:O	2.31	0.43
9:H:472:ARG:HH21	9:D:468:MET:HG2	1.82	0.43
14:V:350:GLN:O	14:V:354:LEU:N	2.43	0.43
14:Y:472:GLU:HA	14:Y:475:LEU:HB2	2.01	0.43
3:O:30:VAL:O	3:O:34:LEU:N	2.50	0.43
2:R:35:ARG:HH21	2:R:39:ARG:HH21	1.66	0.43
8:F:358:HIS:HB3	9:D:179:ILE:HG13	1.99	0.43
9:H:93:LYS:HB3	9:H:93:LYS:HE2	1.82	0.43
10:M:203:ASN:HD22	10:M:206:GLN:HE21	1.67	0.43
4:U:127:DT:H2''	4:U:128:DG:C8	2.53	0.43
12:G:208:LEU:HD11	12:G:254:ILE:HG12	2.01	0.43
14:Y:473:TYR:O	14:Y:697:ARG:NH1	2.51	0.43
8:F:402:LEU:HD12	8:F:425:GLN:HB3	2.01	0.43
9:H:249:ARG:HH22	9:H:346:ARG:HD2	1.83	0.43
14:Y:835:MET:SD	14:Y:835:MET:N	2.92	0.43
9:H:407:LEU:HD22	11:I:426:PRO:HB2	2.00	0.43
9:D:319:GLU:HB3	9:D:341:VAL:HG13	2.01	0.43
10:M:341:PRO:O	10:M:560:LYS:NZ	2.51	0.43
18:X:502:LEU:HD23	18:X:502:LEU:HA	1.91	0.43
14:Y:841:THR:OG1	14:Y:842:LYS:N	2.51	0.43
3:S:65:LEU:HD23	3:S:68:ASN:HD22	1.84	0.43
5:W:46:DC:H1'	5:W:47:DC:C2	2.54	0.43
5:W:129:DT:H2''	5:W:130:DA:C5	2.53	0.43
8:F:402:LEU:HD13	8:F:422:ILE:HG23	2.01	0.43
12:G:20:LEU:HD23	12:G:27:ILE:HG21	2.01	0.43
13:A:20:ILE:HD11	19:L:875:THR:HB	2.01	0.43
20:P:46:LYS:HA	20:P:46:LYS:HD3	1.84	0.43
14:Y:699:LYS:NZ	14:Y:705:ASP:OD1	2.52	0.43
4:U:117:DT:H2''	4:U:118:DC:H2'	2.01	0.43
5:W:28:DG:H1'	5:W:29:DT:H5'	2.01	0.43
10:M:109:ASN:HA	14:J:292:ARG:HD3	2.01	0.43
14:Y:682:ILE:O	14:Y:686:LEU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:401:LEU:HD23	9:H:407:LEU:HD21	2.01	0.42
14:Y:876:LEU:HD12	14:Y:878:THR:H	1.83	0.42
5:W:93:DA:H2''	5:W:94:DG:H8	1.84	0.42
9:D:316:SER:HB2	19:L:807:GLY:HA3	2.01	0.42
13:A:38:LYS:HZ3	13:A:51:TYR:HE1	1.67	0.42
18:X:447:PRO:HB3	18:X:480:ASN:HD22	1.83	0.42
14:Y:698:LEU:HD21	14:Y:944:LYS:HD3	2.01	0.42
3:O:83:LEU:HD13	20:T:61:ILE:HG21	2.01	0.42
10:M:286:HIS:HA	10:M:289:LEU:HB3	2.02	0.42
14:J:268:GLN:HB3	14:J:271:HIS:HD2	1.84	0.42
20:P:116:LYS:HB3	20:P:116:LYS:HE2	1.83	0.42
3:O:42:ARG:HH22	5:W:58:DG:N2	2.16	0.42
3:O:76:THR:O	20:T:53:GLY:N	2.53	0.42
1:Q:54:TYR:HB3	2:R:40:ARG:HE	1.83	0.42
4:U:59:DA:H2	5:W:110:DA:H2	1.67	0.42
9:D:116:LYS:HD2	9:D:116:LYS:HA	1.81	0.42
13:A:487:ILE:HG21	19:L:747:SER:HB2	2.01	0.42
18:X:435:GLN:HA	18:X:442:THR:HA	2.01	0.42
14:Y:630:LEU:HB2	14:Y:634:LEU:HD12	2.01	0.42
3:O:65:LEU:HD23	3:O:68:ASN:HD22	1.84	0.42
4:U:69:DA:H4'	4:U:70:DC:H5'	2.02	0.42
5:W:149:DC:H2''	5:W:150:DG:N7	2.35	0.42
11:I:419:PHE:O	11:I:423:SER:N	2.47	0.42
18:X:376:ASP:O	18:X:486:PHE:N	2.49	0.42
14:Y:522:PHE:HE1	14:Y:592:ALA:HB3	1.83	0.42
1:Q:134:ARG:O	3:S:95:LYS:NZ	2.48	0.42
4:U:39:DA:H2	5:W:130:DA:H2	1.66	0.42
13:A:273:TRP:HA	15:E:20:THR:HB	2.01	0.42
16:C:194:ALA:N	17:K:164:ILE:O	2.52	0.42
14:Y:499:LEU:HD22	14:Y:702:VAL:HG11	2.01	0.42
10:M:323:ILE:HD13	10:M:540:ASP:HB2	2.02	0.42
14:Y:475:LEU:HD23	14:Y:475:LEU:HA	1.89	0.42
4:U:123:DC:O2	20:T:33:ARG:NH1	2.53	0.42
9:H:179:ILE:HG22	11:I:468:ARG:HH12	1.85	0.42
9:H:428:ILE:HD13	9:H:428:ILE:HA	1.90	0.42
20:P:71:GLU:HA	20:P:74:ALA:HB3	2.01	0.42
14:Y:453:ARG:H	14:Y:453:ARG:HG2	1.62	0.42
14:Y:496:GLU:O	14:Y:501:LYS:NZ	2.43	0.42
12:G:211:GLU:HA	12:G:216:THR:HA	2.02	0.42
13:A:48:TYR:O	13:A:52:CYS:N	2.40	0.42
4:U:15:DT:H2'	4:U:16:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:41:SER:O	11:I:45:LEU:N	2.52	0.42
14:Y:894:ASP:O	14:Y:898:GLN:N	2.51	0.42
11:I:245:GLN:HG2	11:I:246:THR:HG22	2.02	0.41
13:A:198:ARG:HD2	13:A:198:ARG:HA	1.87	0.41
13:A:278:THR:HB	13:A:306:ARG:HG2	2.01	0.41
16:C:197:ASP:O	17:K:160:GLN:NE2	2.53	0.41
14:Y:779:SER:O	14:Y:779:SER:OG	2.38	0.41
4:U:95:DC:N4	5:W:72:DG:O6	2.53	0.41
9:H:325:GLU:HB3	9:H:329:MET:HE3	2.03	0.41
15:E:54:ASN:HB3	15:E:57:ARG:HE	1.84	0.41
1:N:63:ARG:HH11	5:W:81:DA:H5''	1.86	0.41
1:Q:103:LEU:O	1:Q:107:THR:OG1	2.30	0.41
3:S:34:LEU:HA	3:S:39:TYR:HE2	1.85	0.41
8:F:430:LYS:HA	8:F:430:LYS:HD2	1.83	0.41
9:H:363:TYR:HB3	14:J:195:ILE:HG23	2.01	0.41
9:H:426:GLN:HG2	11:I:27:VAL:HA	2.03	0.41
10:M:64:ASN:OD1	10:M:64:ASN:N	2.52	0.41
10:M:330:LYS:HB2	10:M:330:LYS:HE2	1.83	0.41
11:I:220:ILE:HD12	11:I:351:LEU:HD22	2.01	0.41
11:I:248:SER:OG	11:I:249:VAL:N	2.53	0.41
13:A:395:ASN:O	14:J:90:GLN:NE2	2.53	0.41
3:O:111:ILE:HG23	1:Q:51:ILE:HG21	2.03	0.41
4:U:75:DT:H6	4:U:75:DT:H2'	1.63	0.41
5:W:41:DA:H1'	5:W:42:DC:H5'	2.02	0.41
14:J:53:ALA:HB1	14:J:57:GLN:HG2	2.02	0.41
14:J:132:PRO:HG2	14:J:134:TYR:HE1	1.86	0.41
20:P:36:SER:OG	20:P:37:TYR:N	2.54	0.41
14:V:334:ILE:O	14:V:338:GLN:N	2.49	0.41
4:U:113:DA:H2''	4:U:114:DG:H8	1.84	0.41
5:W:30:DA:H2'	5:W:31:DT:C2	2.55	0.41
5:W:155:DC:H6	5:W:155:DC:H2'	1.61	0.41
8:F:350:ARG:NH2	12:G:25:ASP:OD1	2.42	0.41
9:H:414:SER:HB2	11:I:419:PHE:HB3	2.03	0.41
13:A:238:GLU:OE1	14:J:212:ASN:ND2	2.53	0.41
14:V:337:ARG:HA	14:V:340:GLU:HB2	2.02	0.41
2:B:71:THR:HG21	20:T:100:LEU:HD21	2.03	0.41
3:O:63:LEU:HB3	20:T:48:VAL:HG21	2.03	0.41
4:U:118:DC:O2	5:W:50:DG:N1	2.47	0.41
10:M:61:SER:O	10:M:61:SER:OG	2.38	0.41
14:Y:485:TYR:OH	14:Y:622:ARG:O	2.36	0.41
5:W:69:DC:H1'	5:W:70:DT:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:421:GLU:HA	11:I:424:LEU:HB2	2.01	0.41
18:X:602:LEU:HB3	18:X:619:PHE:HB2	2.02	0.41
20:T:74:ALA:O	20:T:78:SER:OG	2.33	0.41
14:Y:723:GLN:HA	14:Y:726:TYR:HD2	1.86	0.41
3:O:62:ILE:O	3:O:66:ALA:N	2.48	0.41
2:R:92:ARG:HD3	20:P:79:ARG:HH22	1.86	0.41
3:S:62:ILE:O	3:S:66:ALA:N	2.48	0.41
9:H:246:ASP:OD2	12:G:160:HIS:NE2	2.53	0.41
9:H:409:LYS:HB3	9:D:399:THR:HA	2.03	0.41
9:D:112:PHE:HB3	12:G:361:TYR:CG	2.56	0.41
9:D:312:LYS:HD3	9:D:312:LYS:HA	1.91	0.41
13:A:76:ILE:HA	13:A:79:ARG:HG2	2.02	0.41
14:Y:502:THR:OG1	14:Y:537:GLU:OE1	2.27	0.41
1:N:128:ARG:HH22	2:B:60:VAL:HG21	1.85	0.41
3:S:75:LYS:HA	3:S:75:LYS:HD3	1.85	0.41
4:U:109:DC:H6	4:U:109:DC:H2'	1.76	0.41
4:U:114:DG:H1'	4:U:115:DT:H5'	2.03	0.41
5:W:79:DA:H2''	5:W:80:DA:C8	2.56	0.41
9:H:104:ASP:HB3	9:H:113:LYS:HD3	2.03	0.41
9:D:155:LYS:HE2	9:D:155:LYS:HB3	1.76	0.41
9:D:192:ASP:O	10:M:84:ARG:NH2	2.52	0.41
9:D:465:SER:HA	9:D:468:MET:HB2	2.03	0.41
10:M:118:ARG:HD2	10:M:118:ARG:HA	1.91	0.41
11:I:7:PRO:HB2	13:A:282:LEU:HB3	2.03	0.41
13:A:273:TRP:HE1	15:E:22:LYS:HD2	1.86	0.41
14:Y:936:ASP:HB3	14:Y:940:ILE:HG23	2.02	0.41
5:W:62:DT:H2''	5:W:63:DA:N7	2.36	0.41
9:D:103:PRO:HA	9:D:106:PHE:HD2	1.86	0.41
12:G:20:LEU:HB3	12:G:30:PHE:HD2	1.86	0.41
14:J:113:ASP:HA	14:J:116:ASN:HB2	2.03	0.41
1:Q:72:ARG:HG2	1:Q:84:PHE:CD2	2.56	0.40
9:D:88:TRP:O	9:D:95:HIS:NE2	2.54	0.40
10:M:189:LEU:HD11	10:M:241:HIS:HB3	2.03	0.40
10:M:270:LEU:HD13	10:M:280:ALA:HB2	2.03	0.40
11:I:320:GLN:NE2	11:I:327:ALA:O	2.51	0.40
15:E:66:LYS:HB2	15:E:66:LYS:HE3	1.86	0.40
18:X:602:LEU:HD22	18:X:621:ILE:HD11	2.02	0.40
14:Y:495:ASP:OD1	14:Y:697:ARG:N	2.49	0.40
1:Q:60:LEU:HD13	1:Q:93:GLN:HG2	2.03	0.40
9:H:304:LEU:HD22	9:H:318:GLN:HG3	2.02	0.40
10:M:246:LEU:HG	10:M:262:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:119:LEU:HD23	13:A:119:LEU:HA	1.94	0.40
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.96	0.40
5:W:136:DA:N7	5:W:137:DA:N6	2.69	0.40
5:W:164:DC:H2''	5:W:165:DA:C8	2.56	0.40
10:M:148:ASP:OD1	10:M:148:ASP:N	2.53	0.40
11:I:460:ILE:HG23	11:I:470:LEU:HD21	2.04	0.40
13:A:46:LYS:HA	13:A:46:LYS:HD3	1.90	0.40
13:A:459:VAL:HG12	13:A:465:VAL:HG22	2.02	0.40
3:O:34:LEU:HA	3:O:39:TYR:HE2	1.85	0.40
4:U:138:DT:H2''	4:U:139:DA:C8	2.56	0.40
9:H:72:PHE:HA	12:G:155:LEU:HD22	2.03	0.40
9:H:154:VAL:HG11	12:G:230:ILE:HD12	2.02	0.40
10:M:62:LEU:HD11	12:G:163:PHE:HD1	1.86	0.40
13:A:184:SER:HB2	19:L:857:LYS:HG2	2.03	0.40
13:A:407:ILE:HG23	14:J:100:LEU:HD13	2.03	0.40
13:A:441:PRO:HG2	13:A:446:ARG:HH21	1.85	0.40
14:Y:553:THR:HA	14:Y:554:PRO:HD3	1.94	0.40
10:M:65:PHE:HB2	10:M:68:PHE:HD2	1.86	0.40
10:M:142:ASN:OD1	10:M:142:ASN:N	2.54	0.40
15:E:57:ARG:O	15:E:61:SER:N	2.44	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	N	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	Q	93/136 (68%)	90 (97%)	3 (3%)	0	100	100
2	B	80/103 (78%)	78 (98%)	2 (2%)	0	100	100
2	R	85/103 (82%)	81 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
3	S	105/130 (81%)	98 (93%)	7 (7%)	0	100	100
6	f	391/477 (82%)	382 (98%)	9 (2%)	0	100	100
7	h	46/157 (29%)	44 (96%)	2 (4%)	0	100	100
8	F	116/435 (27%)	104 (90%)	12 (10%)	0	100	100
9	D	295/557 (53%)	282 (96%)	13 (4%)	0	100	100
9	H	387/557 (70%)	360 (93%)	27 (7%)	0	100	100
10	M	378/581 (65%)	349 (92%)	29 (8%)	0	100	100
11	I	236/483 (49%)	220 (93%)	16 (7%)	0	100	100
12	G	238/426 (56%)	221 (93%)	17 (7%)	0	100	100
13	A	357/502 (71%)	332 (93%)	25 (7%)	0	100	100
14	J	229/1359 (17%)	203 (89%)	26 (11%)	0	100	100
14	V	67/1359 (5%)	67 (100%)	0	0	100	100
14	Y	536/1359 (39%)	483 (90%)	52 (10%)	1 (0%)	47	81
15	E	56/78 (72%)	54 (96%)	2 (4%)	0	100	100
16	C	31/883 (4%)	31 (100%)	0	0	100	100
17	K	40/885 (4%)	37 (92%)	3 (8%)	0	100	100
18	X	139/625 (22%)	124 (89%)	15 (11%)	0	100	100
19	L	79/889 (9%)	68 (86%)	11 (14%)	0	100	100
20	P	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
20	T	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
21	g	390/467 (84%)	377 (97%)	13 (3%)	0	100	100
All	All	4757/13069 (36%)	4458 (94%)	298 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	711	GLU

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	N	86/111 (78%)	85 (99%)	1 (1%)	71	83
1	Q	83/111 (75%)	82 (99%)	1 (1%)	71	83
2	B	68/79 (86%)	67 (98%)	1 (2%)	65	80
2	R	72/79 (91%)	72 (100%)	0	100	100
3	O	84/102 (82%)	77 (92%)	7 (8%)	11	34
3	S	84/102 (82%)	77 (92%)	7 (8%)	11	34
6	f	356/420 (85%)	356 (100%)	0	100	100
7	h	53/140 (38%)	53 (100%)	0	100	100
8	F	111/388 (29%)	110 (99%)	1 (1%)	78	87
9	D	285/500 (57%)	283 (99%)	2 (1%)	84	90
9	H	363/500 (73%)	362 (100%)	1 (0%)	92	95
10	M	349/521 (67%)	349 (100%)	0	100	100
11	I	223/435 (51%)	222 (100%)	1 (0%)	91	94
12	G	226/384 (59%)	225 (100%)	1 (0%)	91	94
13	A	343/462 (74%)	343 (100%)	0	100	100
14	J	187/1228 (15%)	185 (99%)	2 (1%)	73	84
14	V	63/1228 (5%)	62 (98%)	1 (2%)	62	79
14	Y	502/1228 (41%)	500 (100%)	2 (0%)	91	94
15	E	56/75 (75%)	55 (98%)	1 (2%)	59	77
16	C	32/824 (4%)	32 (100%)	0	100	100
17	K	39/832 (5%)	39 (100%)	0	100	100
18	X	141/578 (24%)	141 (100%)	0	100	100
19	L	77/810 (10%)	77 (100%)	0	100	100
20	P	77/105 (73%)	77 (100%)	0	100	100
20	T	79/105 (75%)	79 (100%)	0	100	100
21	g	362/423 (86%)	361 (100%)	1 (0%)	92	95
All	All	4401/11770 (37%)	4371 (99%)	30 (1%)	84	90

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	129	ARG
2	B	92	ARG
3	O	13	LYS
3	O	18	SER
3	O	19	SER
3	O	87	VAL
3	O	93	LEU
3	O	113	SER
3	O	114	VAL
1	Q	129	ARG
3	S	13	LYS
3	S	18	SER
3	S	19	SER
3	S	87	VAL
3	S	93	LEU
3	S	113	SER
3	S	114	VAL
8	F	390	ILE
9	H	346	ARG
9	D	111	ARG
9	D	440	LEU
11	I	246	THR
12	G	274	MET
14	J	102	LYS
14	J	226	THR
15	E	67	LYS
21	g	48	ASP
14	V	368	LYS
14	Y	460	LYS
14	Y	947	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	O	31	HIS
1	Q	125	GLN
2	R	18	HIS
2	R	64	ASN
3	S	31	HIS
6	f	12	ASN
6	f	53	ASN
6	f	79	ASN
6	f	86	GLN

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Mol	Chain	Res	Type
6	f	237	GLN
6	f	406	GLN
9	H	123	ASN
9	H	127	ASN
9	H	167	ASN
9	H	186	HIS
9	H	239	GLN
9	H	242	ASN
9	H	281	ASN
9	H	314	ASN
9	D	107	ASN
9	D	188	GLN
9	D	227	ASN
9	D	318	GLN
9	D	394	ASN
9	D	483	ASN
10	M	203	ASN
10	M	521	GLN
10	M	551	GLN
11	I	29	ASN
11	I	337	GLN
12	G	220	GLN
12	G	297	GLN
12	G	316	GLN
13	A	22	ASN
13	A	112	GLN
13	A	223	ASN
13	A	225	ASN
13	A	272	ASN
13	A	400	ASN
13	A	412	ASN
14	J	66	GLN
14	J	204	ASN
14	J	259	GLN
14	J	271	HIS
14	J	290	GLN
16	C	218	ASN
17	K	160	GLN
17	K	183	ASN
19	L	800	ASN
19	L	810	HIS
21	g	192	GLN

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Mol	Chain	Res	Type
21	g	438	GLN
14	V	328	ASN
14	V	360	ASN
14	Y	487	ASN
14	Y	488	HIS
14	Y	600	HIS
14	Y	621	ASN
14	Y	660	ASN
14	Y	854	ASN
14	Y	982	ASN
14	Y	1004	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

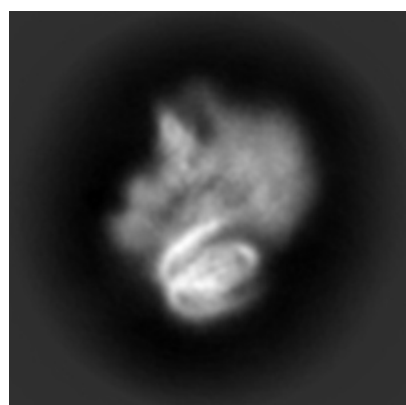
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0778. These allow visual inspection of the internal detail of the map and identification of artifacts.

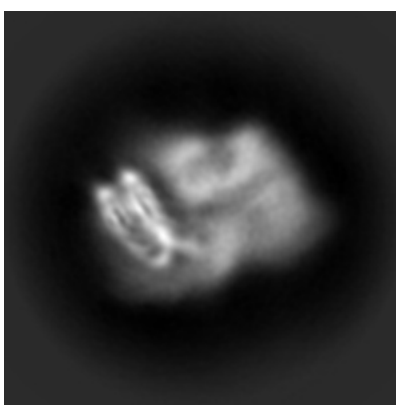
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

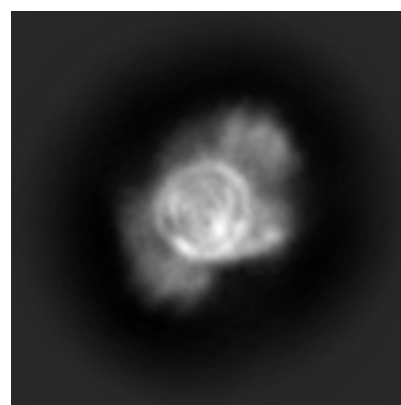
6.1.1 Primary map



X



Y

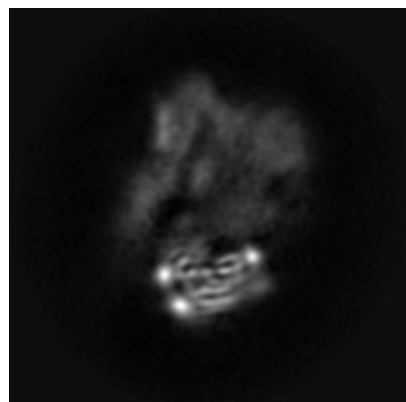


Z

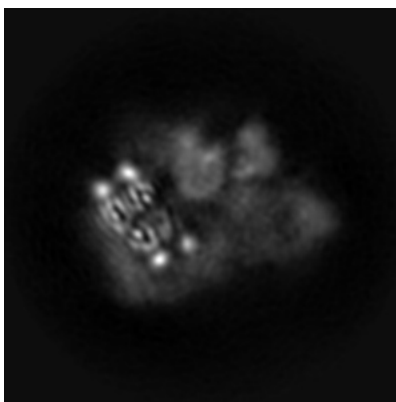
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

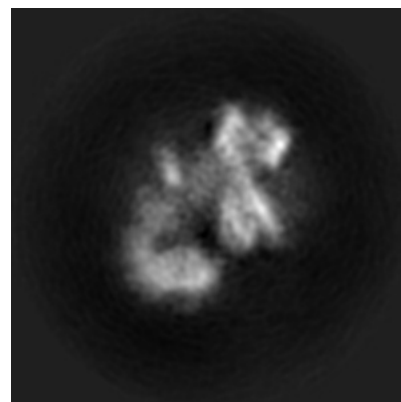
6.2.1 Primary map



X Index: 90



Y Index: 90

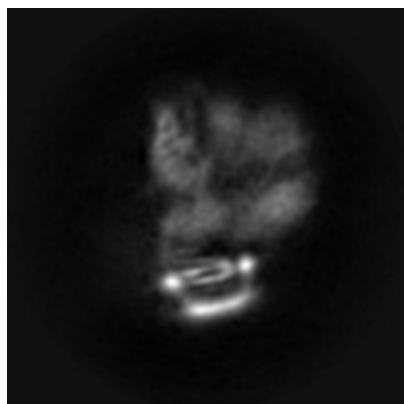


Z Index: 90

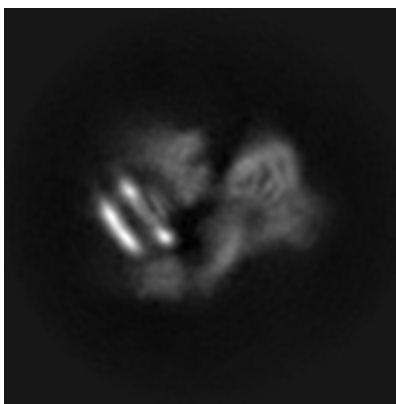
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

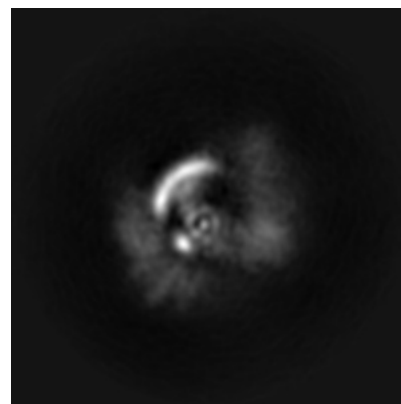
6.3.1 Primary map



X Index: 97



Y Index: 74

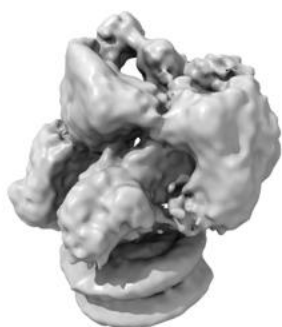


Z Index: 71

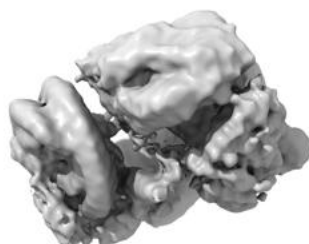
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

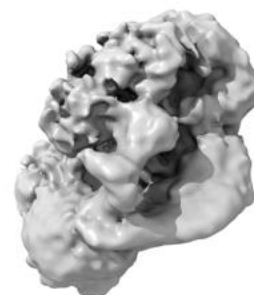
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

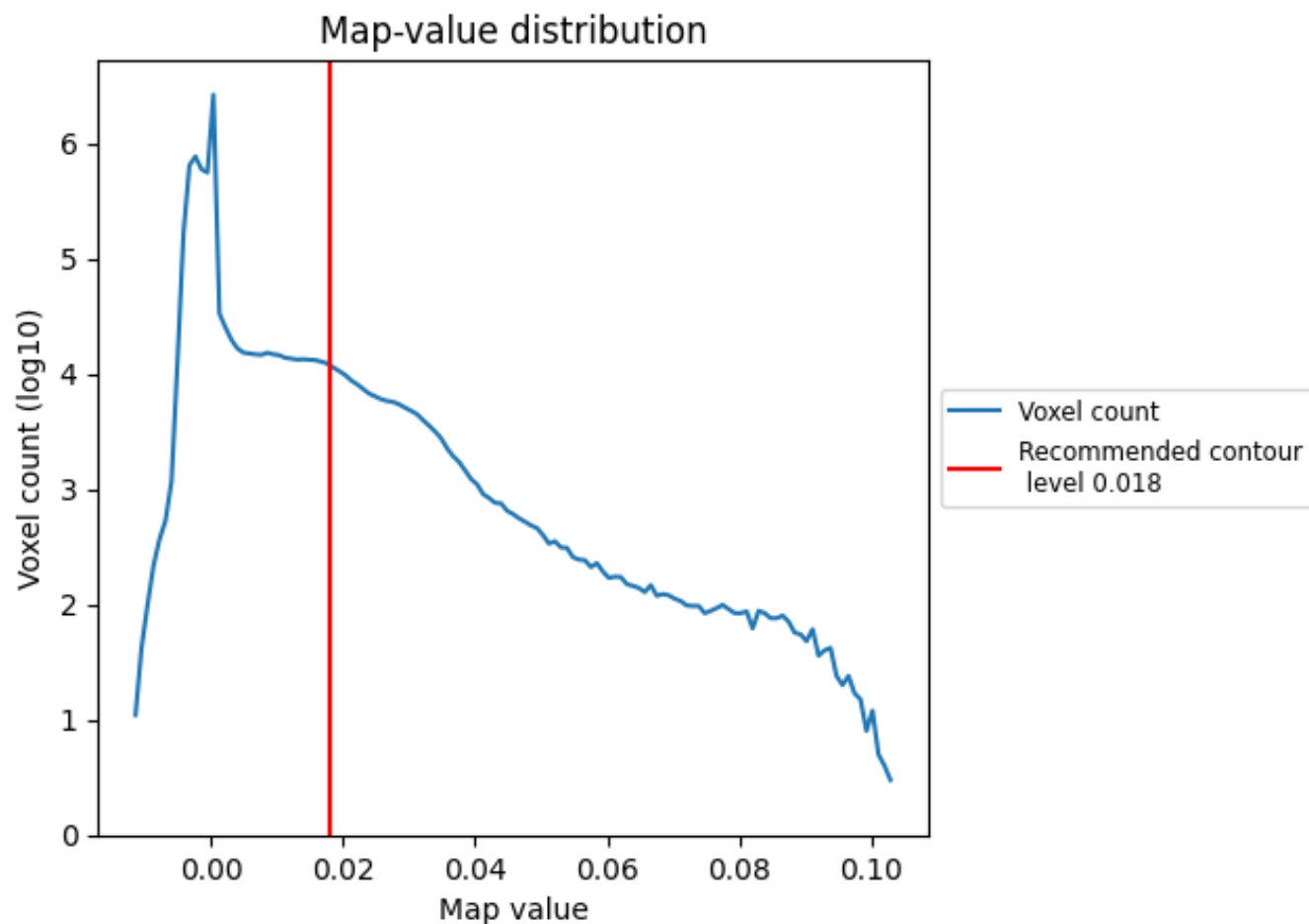
6.5 Mask visualisation

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

7 Map analysis [i](#)

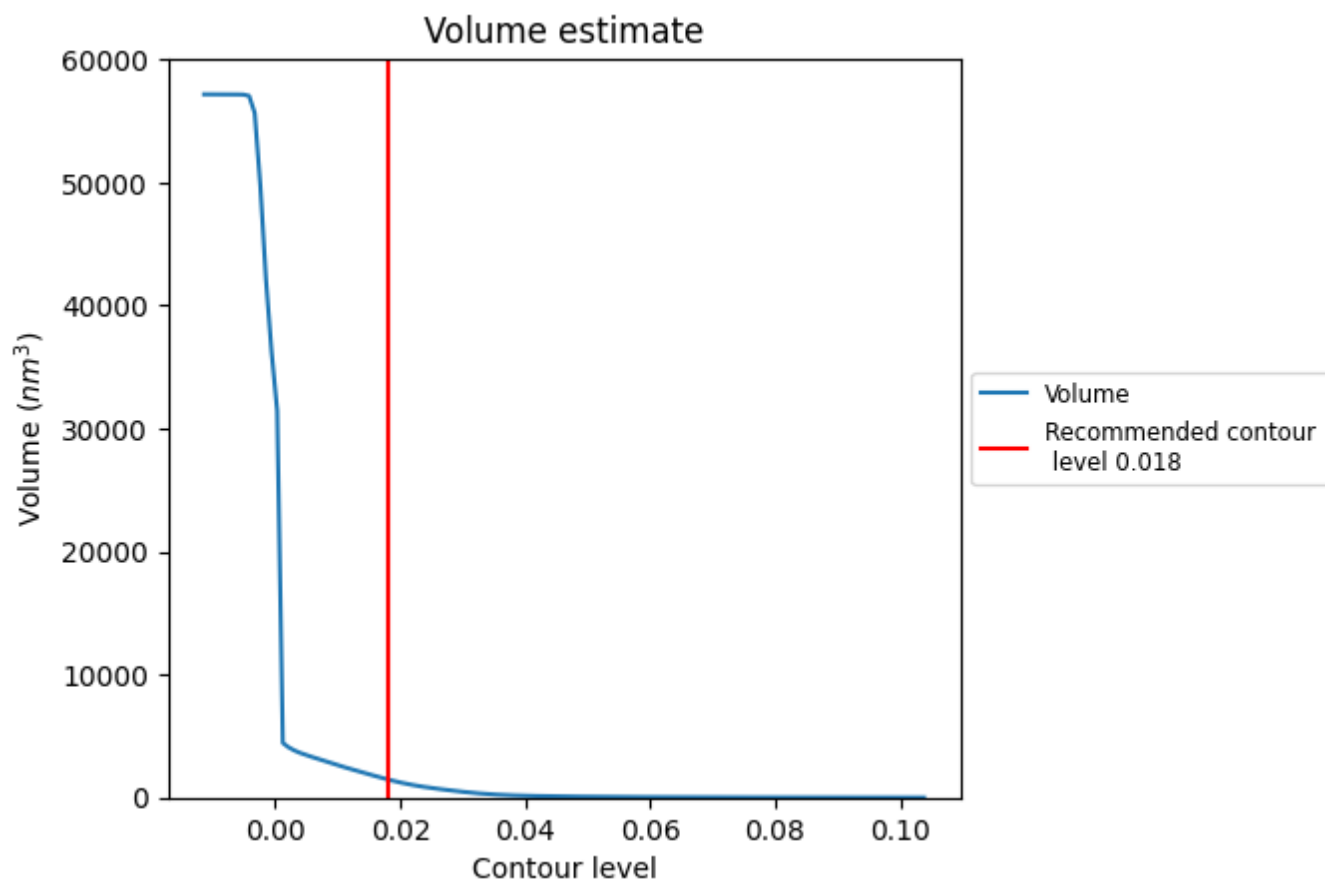
This section contains the results of statistical analysis of the map.

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.

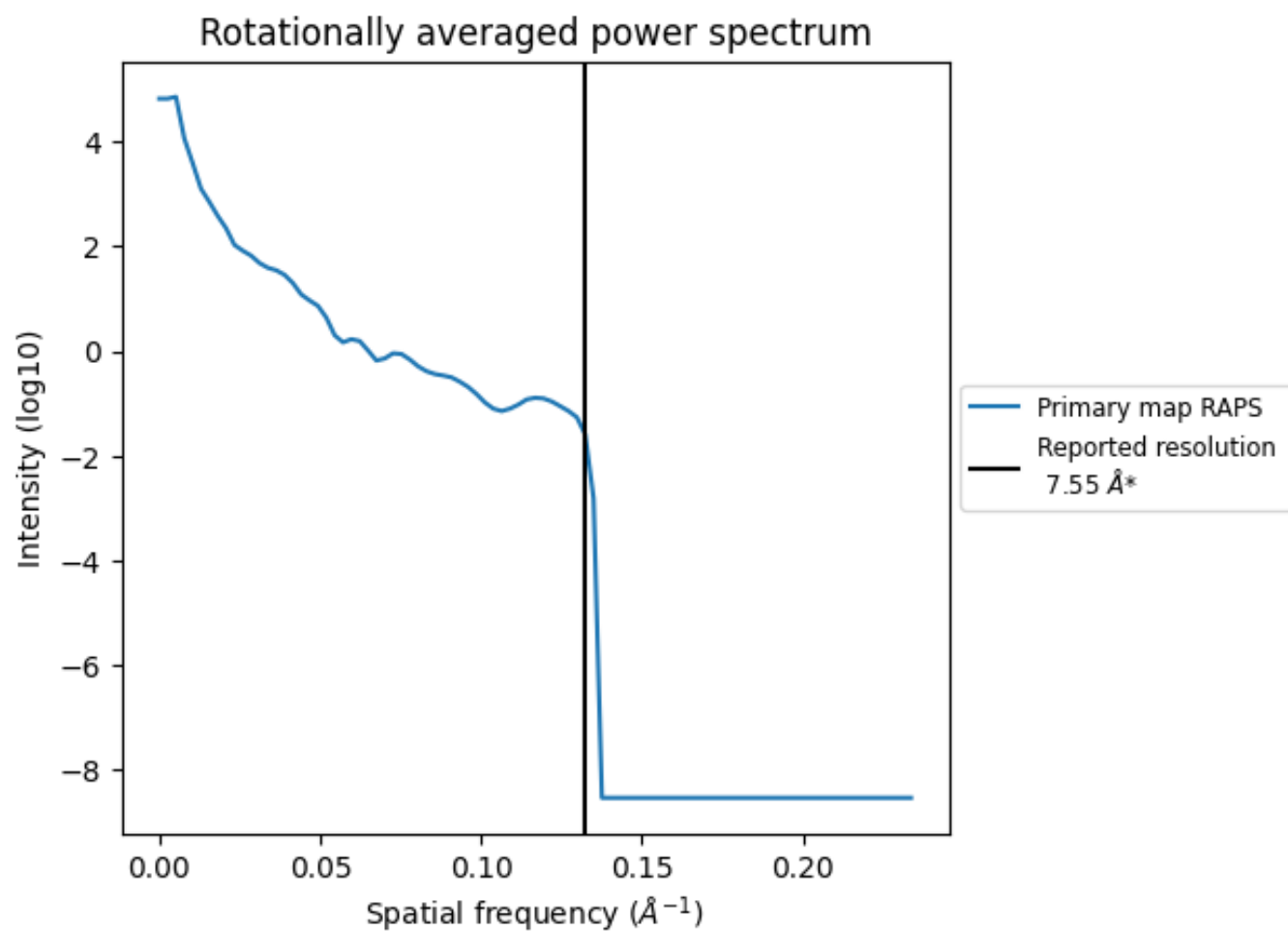
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1474 nm³; this corresponds to an approximate mass of 1331 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 0.132 Å⁻¹

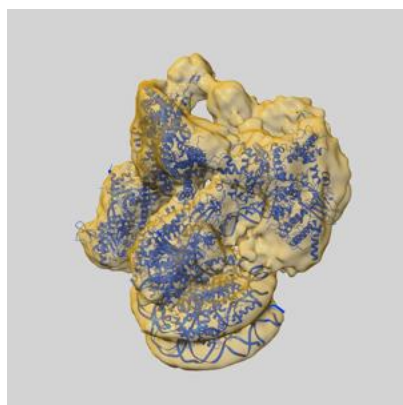
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

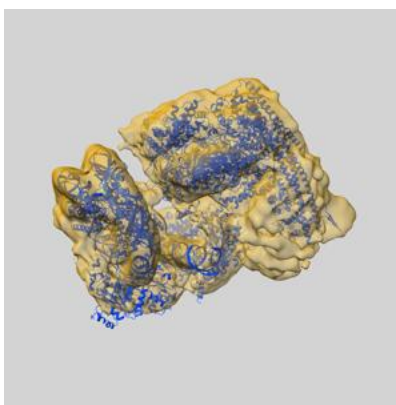
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0778 and PDB model 6KW4. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

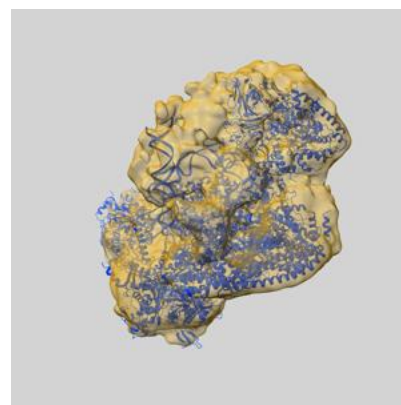
9.1 Map-model overlay [i](#)



X



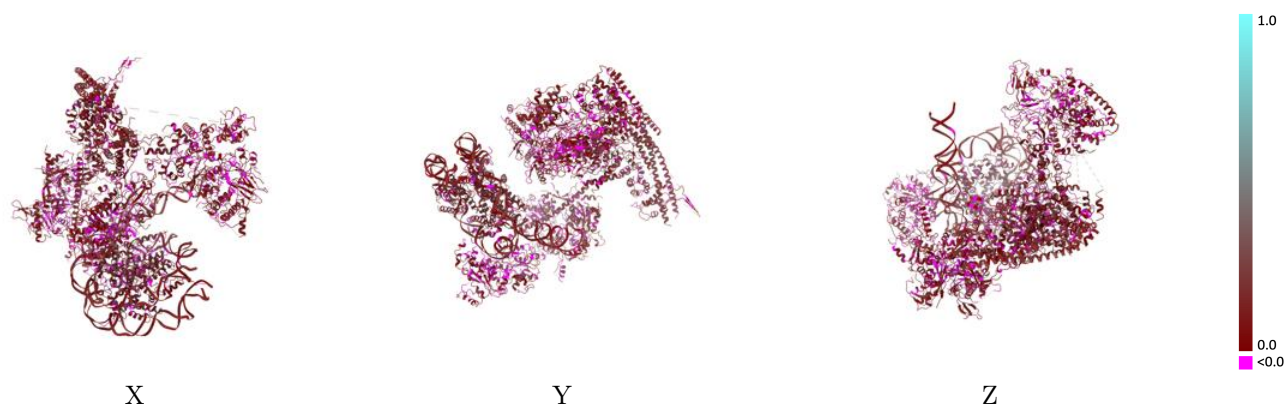
Y



Z

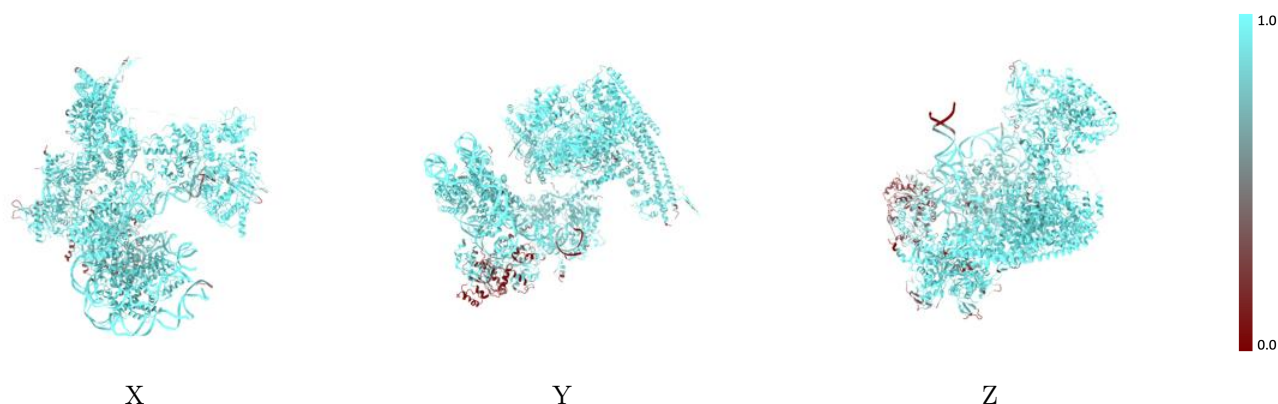
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



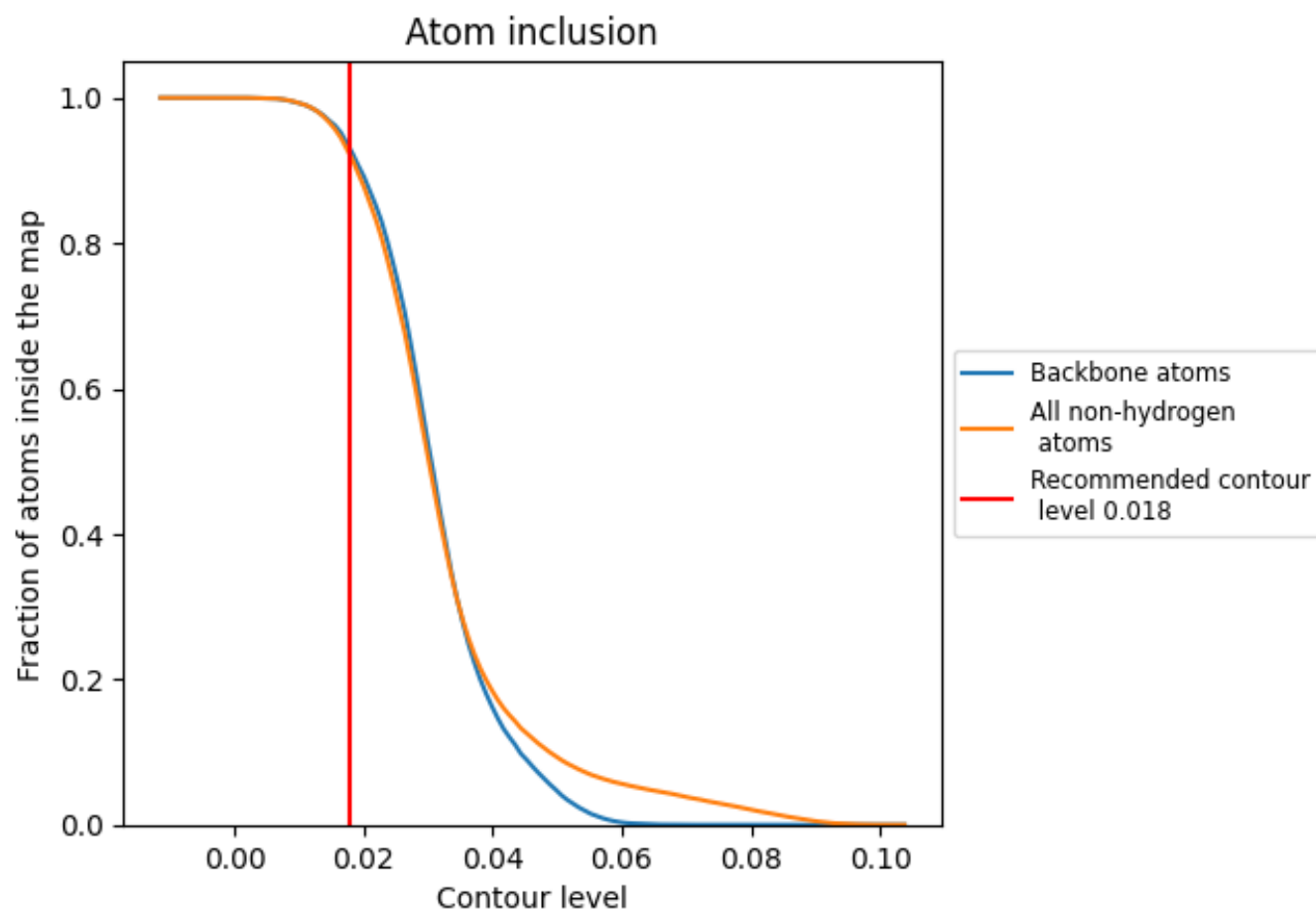
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9205	 0.0990
A	 0.9844	 0.0990
B	 0.9588	 0.1370
C	 0.9703	 0.1140
D	 0.9773	 0.1080
E	 0.9957	 0.1150
F	 0.9725	 0.0990
G	 0.9512	 0.0870
H	 0.9779	 0.1040
I	 0.9727	 0.1180
J	 0.9747	 0.0830
K	 0.9067	 0.1210
L	 0.9465	 0.0440
M	 0.9794	 0.1170
N	 0.9653	 0.1300
O	 0.9361	 0.1150
P	 0.9929	 0.1580
Q	 0.9907	 0.1440
R	 0.9138	 0.1290
S	 0.9962	 0.1360
T	 0.9661	 0.1490
U	 0.9566	 0.1270
V	 0.7435	 0.0870
W	 0.9452	 0.1230
X	 0.9320	 0.0820
Y	 0.5682	 0.0540
f	 0.9768	 0.0780
g	 0.9040	 0.0540
h	 0.9366	 0.0660

