



Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 09:17 AM JST

PDB ID : 7WU0
EMDB ID : EMD-32807
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-B3
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2022-02-05
Resolution : 3.30 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.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

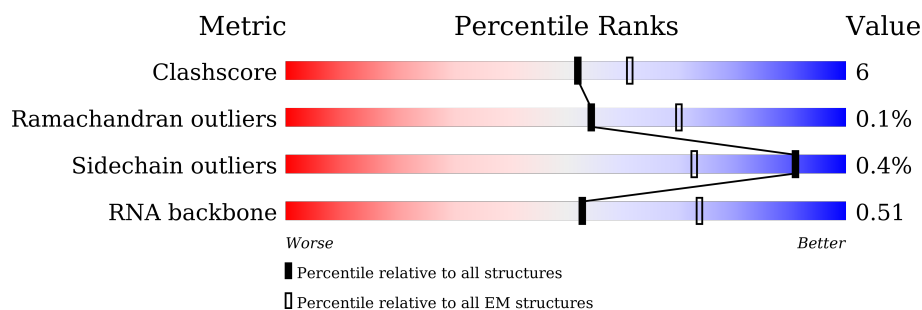
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.




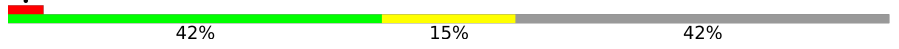

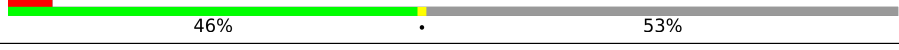


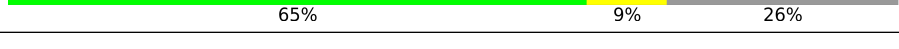
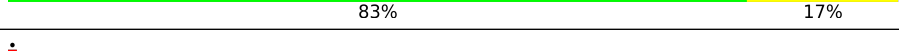
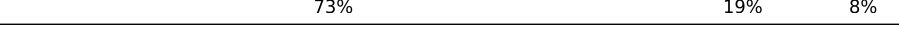
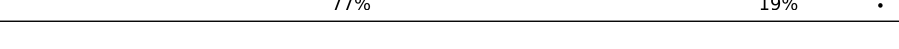
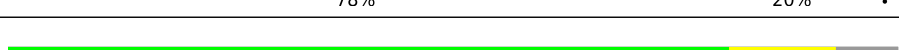

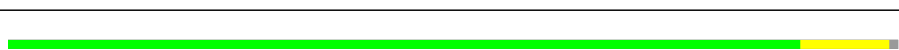

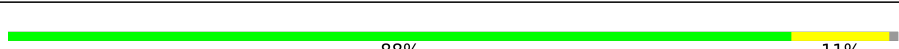



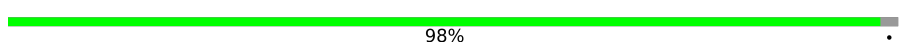
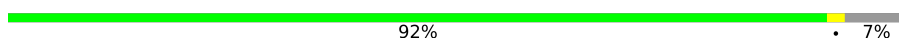
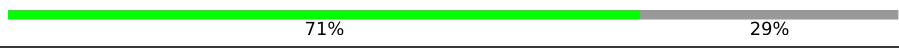
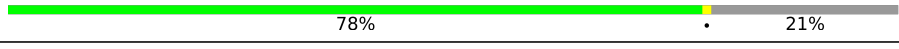



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2	1873	
2	F	204	
3	M	132	
4	P	145	
5	Q	146	
6	R	135	
7	S	152	




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Mol	Chain	Length	Quality of chain
8	T	145	
9	Z	125	
10	c	69	
11	f	156	
12	A	295	
13	B	264	
14	C	293	
15	E	263	
16	G	249	
17	H	194	
18	I	208	
19	J	194	
20	L	158	
21	N	151	
22	O	151	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	b	84	
28	e	59	
29	x	252	
30	y	412	
31	u	804	
32	w	437	

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Mol	Chain	Length	Quality of chain
33	t	475	 26% 73%
34	K	1297	 16% 61% 9% 30%
35	v	552	 58% 41%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 87656 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1624	Total	C	N	O	P	0	0
			34680	15479	6228	11350	1623		

- Molecule 2 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 3 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 4 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 5 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	122	Total	C	N	O	S	0	0
			969	616	180	170	3		

- Molecule 6 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	116	Total	C	N	O	S	0	0
			944	592	174	175	3		

- Molecule 7 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	130	Total	C	N	O	S	0	0
			1083	686	214	182	1		

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 9 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 10 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

- Molecule 11 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	73	Total	C	N	O	S	0	0
			596	375	115	99	7		

- Molecule 12 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 14 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 15 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 16 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 19 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 20 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 22 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 28 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 29 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	178	Total	C	N	O	S	0	0
			1391	891	252	244	4		

- Molecule 30 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	325	Total	C	N	O	S	0	0
			2568	1622	473	463	10		

- Molecule 31 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	629	Total	C	N	O	S	0	0
			5062	3249	902	887	24		

- Molecule 32 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	249	Total	C	N	O	S	0	0
			2027	1322	354	342	9		

- Molecule 33 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	127	Total	C	N	O	S	0	0
			1066	661	204	199	2		

- Molecule 34 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	909	Total	C	N	O	S	0	0
			7047	4520	1216	1266	45		

- Molecule 35 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	324	Total	C	N	O	S	0	0
			2589	1647	459	469	14		

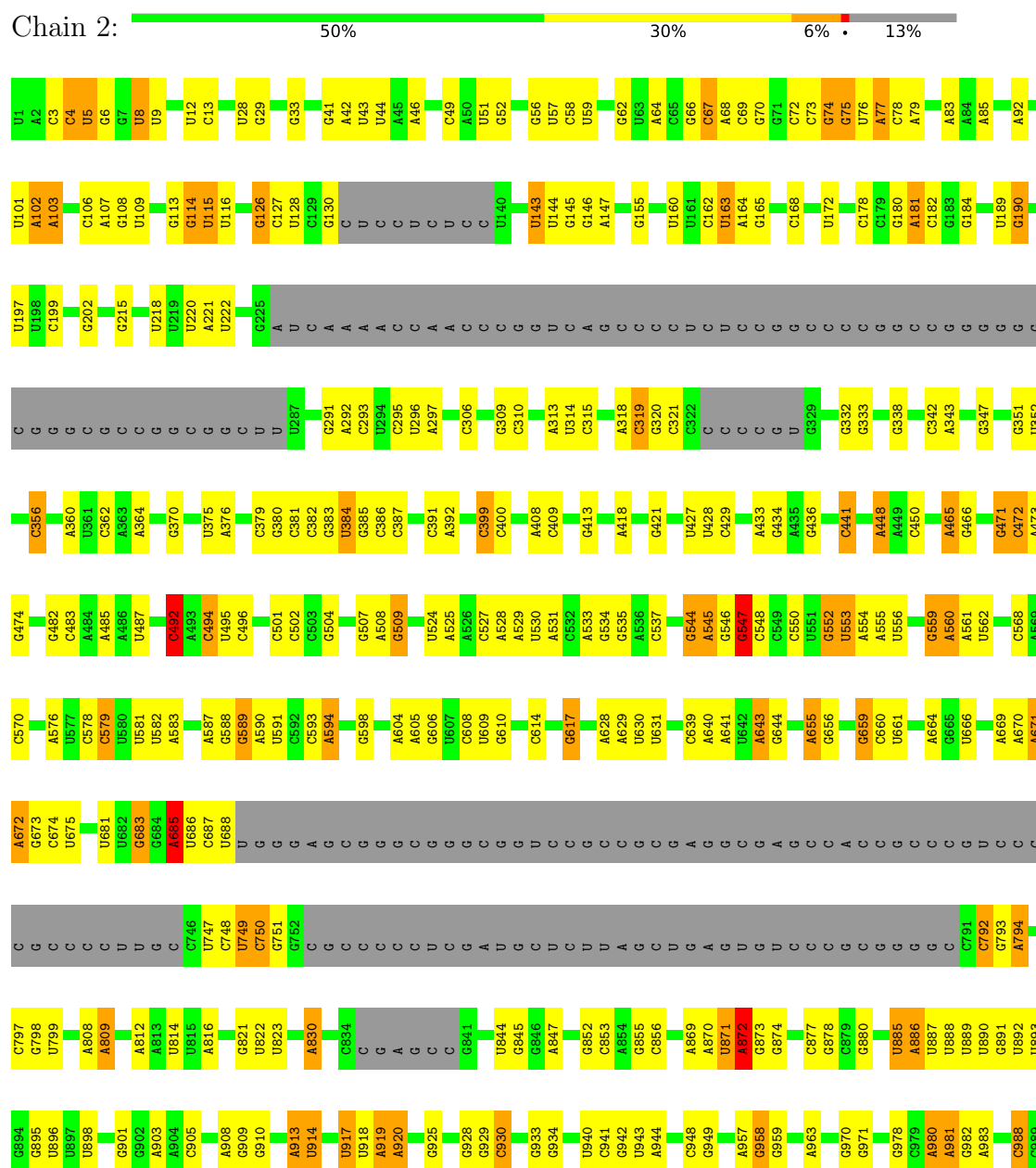
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

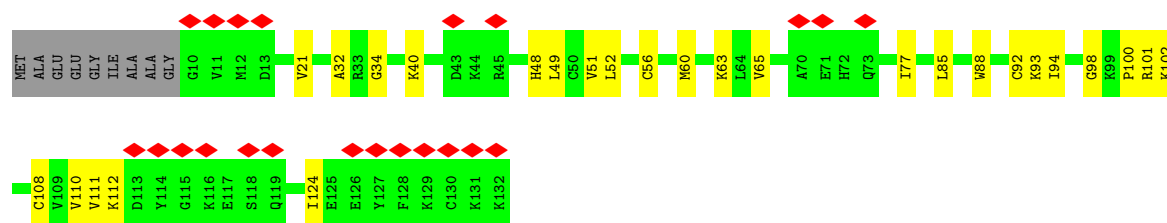
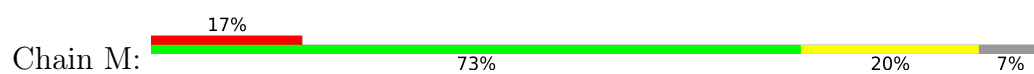
Mol	Chain	Residues	Atoms		AltConf
36	f	1	Total	Zn	0
			1	1	
36	y	1	Total	Zn	0
			1	1	

3 Residue-property plots

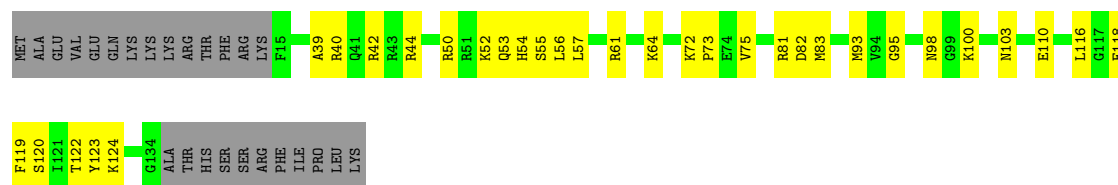
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 18S rRNA

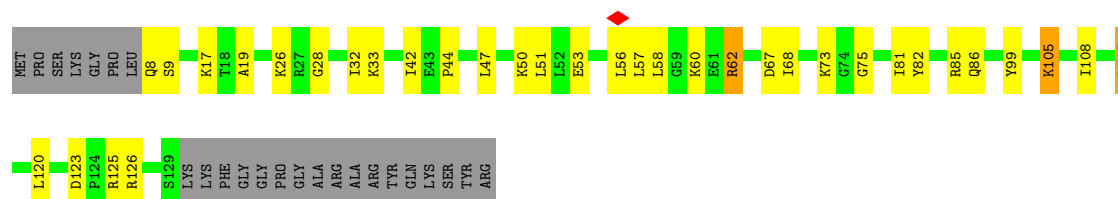




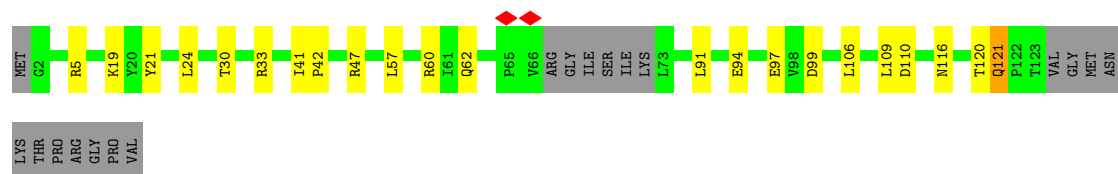
- Molecule 4: 40S ribosomal protein S15



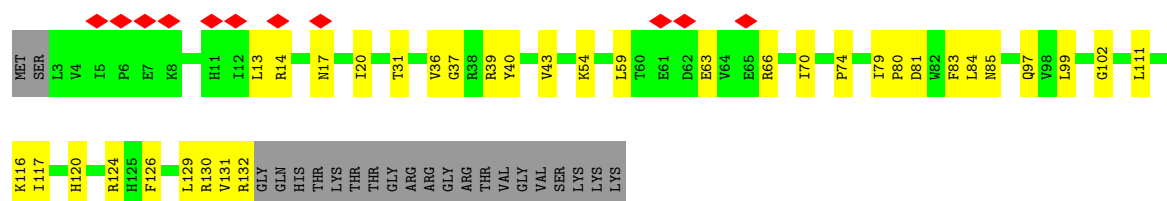
- Molecule 5: 40S ribosomal protein S16



- Molecule 6: 40S ribosomal protein S17



- Molecule 7: 40S ribosomal protein S18



V140	V146	V161	R162	I164	M168	M179	E183	D191	Y206	R213	K219	G233	GLU	GLY	GLY	SER	SER	SER	SER	GLY	GLY	GLY	ALA	LYS	VAL	GLU	ARG	ALA	ASP	GLY	GLY	ALA	LYS	VAL	GLU	PRO	PRO	VAL	GLN	GLY	SER	VAL	V140
MET	ALA	VAL	GLY	LYS	ASN	ARG	LEU	THR	LYS	GLY	LYS	LYS	GLY	ALA	LYS	LYS	V21	W30	V33	K34	A35	R42	M43	I44	S70	R82	L86	I87	T98	H101	D104	I105	T106	R107	D108	K116	I121	H124	T129	L134	V140		

- Chain C:  65% 9% 26%

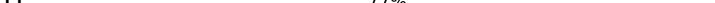
GLN	L78	MET
ALA		ASP
PRO	I81	ASP
ALA		ALA
VAL	I83	GLY
ALA		ALA
THR	I94	GLY
THR		ALA
	K108	GLY
		PRO
	Q115	GLY
		GLY
	Q120	PRO
		GLY
	G131	GLY
		PRO
	N134	GLY
	G135	MET
		GLY
	R166	MET
		ASN
	Y169	ARG
	W170	GLY
		GLY
	G175	PHE
		ARG
	K183	GLY
		GLY
	S190	PHE
	V191	GLY
		SER
	L195	GLY
		ILE
	P199	ARG
	R200	GLY
		ARG
	A207	GLY
		ARG
	M216	GLY
	A217	ARG
	G218	GLY
		ARG
	R227	GLY
		ARG
	L233	GLY
		ARG
	F236	GLY
		ARG
	Y248	GLY
		ALA
	T276	ARG
	HIS	GLY
	THR	GLY
	ARG	LYS
	VAL	ALA
	SER	GLU
	VAL	ASP
	GLN	LYS
	ARG	559

- Chain E: 83% 17%

F172	I173	A187	I192	D212	A213	K233	P234	W235	G243	I244	R245	L256	Q260	C263	E170	P83	I92	P99	R100	L101	I102	T115	E118	V126	T129	F130	V131	G132	L139	V140	T141	H142	D143	T146	D151	F172					
MET	A2	R11	L20	F27	A28	P29	E30	P31	P35	H36	K37	L38	L44	I45	I46	F47	L48	E60	V61	I70	P83	I92	P99	R100	L101	I102	T115	E118	V126	T129	F130	V131	G132	L139	V140	T141	H142	D143	T146	D151	F172

- Chain G:  73% 19% 8%

Category	Item	Value
Top 15	M1	100
	K2	95
	L3	90
	F7	85
	G11	80
	K14	75
	D19	70
	L24	65
	R25	60
	T26	55
	F27	50
	Y28	45
	L41	40
	V49	35
	V50	30
Middle 15	R51	25
	I52	20
	N56	15
	D57	10
	K58	5
	Q65	0
	R72	-5
	L75	-10
	R68	-15
	E91	-20
	R92	-25
	R93	-30
	R94	-35
	K95	-40
	S96	-45
V97	-50	
Bottom 15	R98	-55
	V102	-60
	L106	-65
	S107	-70
	L108	-75
	L109	-80
	N110	-85
	L111	-90
	V112	-95
	V113	-100
	V114	-105
	K115	-110
	V116	-115
	V117	-120
	V118	-125

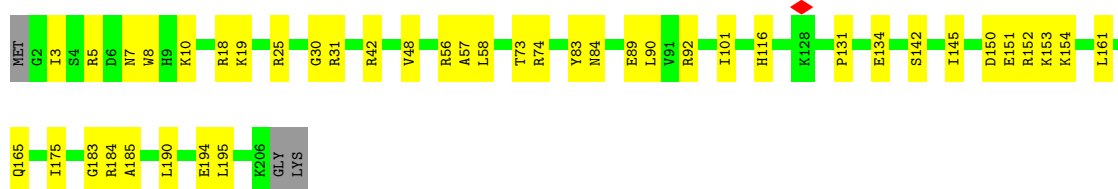
- Chain H:  77% 19% .

MET	PHE	SER	SER	SER	ALA	LYS	I8	D17	E18	F19	L43	A47	E50	I51	K58	A59	I60	F63	V66	P67	Q68	L69	F87	K90	V93	A96	Q97	R98	R99	K103	P104	S108	R109	T110	K111	P117	R118	S119	L120	D132	L133	I144
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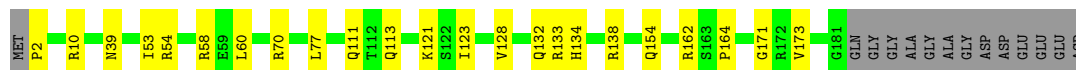
- Molecule 18: 40S ribosomal protein S8

Chain I: 78% 20% .



- Molecule 19: 40S ribosomal protein S9

Chain J: 81% 12% 7% .



- Molecule 20: 40S ribosomal protein S11

Chain L: 80% 15% .



- Molecule 21: 40S ribosomal protein S13

Chain N: 89% 10% .



- Molecule 22: 40S ribosomal protein S14

Chain O: 73% 17% 11% .



- Molecule 23: 40S ribosomal protein S21

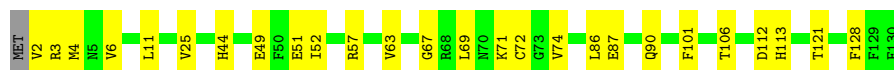
Chain V: 88% 11% .





- Molecule 24: 40S ribosomal protein S15a

Chain W: 79% 20%



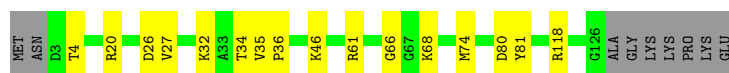
- Molecule 25: 40S ribosomal protein S23

Chain X: 83% 15%



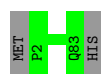
- Molecule 26: 40S ribosomal protein S24

Chain Y: 81% 12% 7%



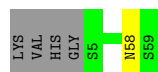
- Molecule 27: 40S ribosomal protein S27

Chain b: 98%



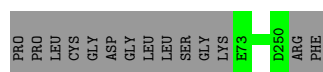
- Molecule 28: 40S ribosomal protein S30

Chain e: 92% 7%



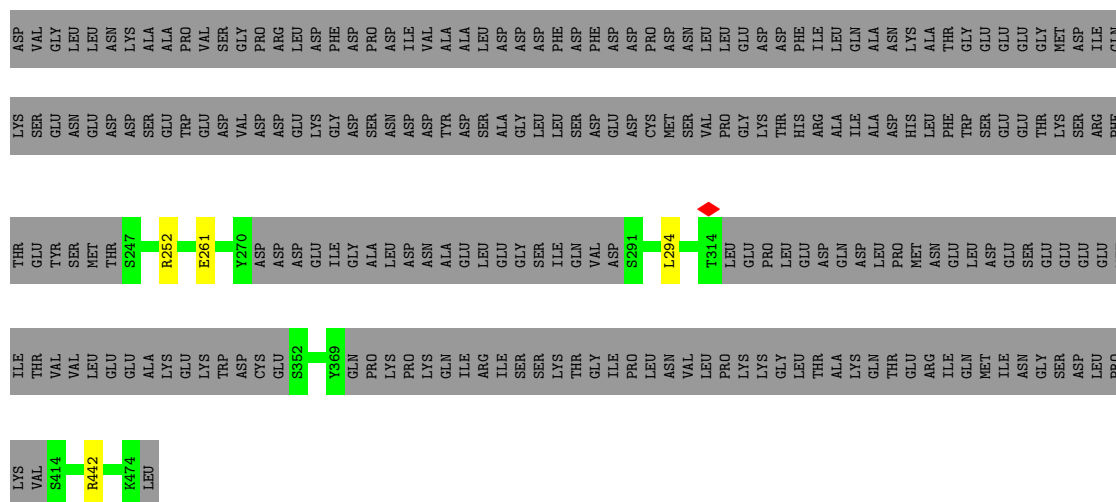
- Molecule 29: RNA-binding protein PNO1

Chain x: 71% 29%

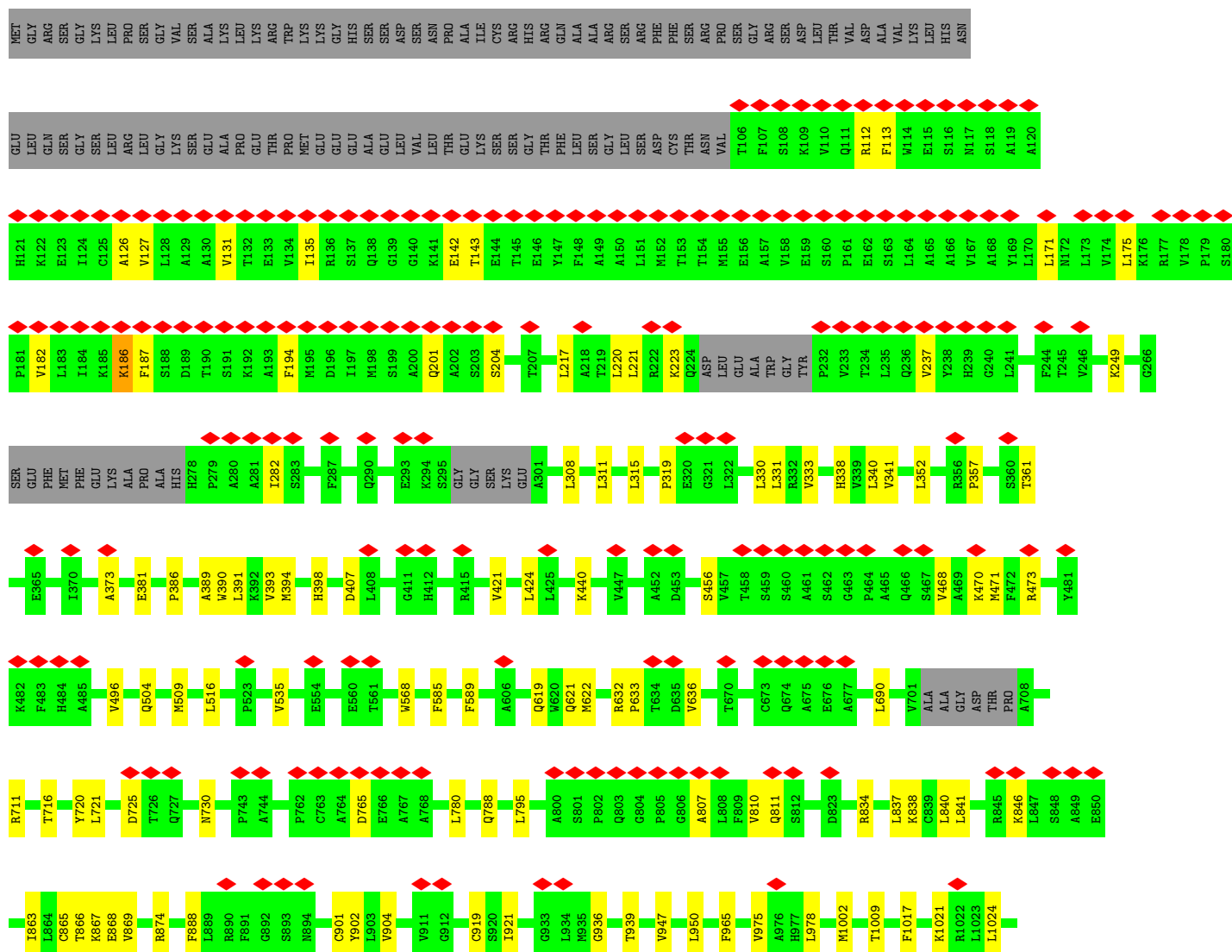


- Molecule 30: RNA-binding protein NOB1

[illegible][illegible][illegible][illegible]



• Molecule 34: RRP12-like protein



- Molecule 35: Serine/threonine-protein kinase RIO2

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.399	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	2	0.29	1/38775 (0.0%)	1.00	158/60417 (0.3%)
2	F	0.27	0/1516	0.60	0/2037
3	M	0.25	0/963	0.53	0/1291
4	P	0.30	0/1003	0.69	0/1341
5	Q	0.27	0/982	0.60	1/1318 (0.1%)
6	R	0.27	0/955	0.66	3/1282 (0.2%)
7	S	0.26	0/1100	0.60	0/1475
8	T	0.32	0/1142	0.60	0/1530
9	Z	0.28	0/580	0.66	0/780
10	c	0.27	0/473	0.71	0/633
11	f	0.25	0/607	0.55	0/802
12	A	0.27	0/1742	0.54	0/2367
13	B	0.28	0/1756	0.56	0/2350
14	C	0.28	0/1726	0.56	0/2332
15	E	0.27	0/2118	0.58	0/2849
16	G	0.26	0/1885	0.61	0/2510
17	H	0.28	0/1524	0.59	0/2042
18	I	0.29	0/1711	0.63	0/2282
19	J	0.26	0/1524	0.60	0/2035
20	L	0.26	0/1250	0.57	0/1673
21	N	0.26	0/1226	0.57	1/1649 (0.1%)
22	O	0.28	0/1022	0.64	0/1372
23	V	0.26	0/631	0.55	0/844
24	W	0.27	0/1051	0.58	0/1406
25	X	0.27	0/1116	0.56	0/1490
26	Y	0.26	0/1031	0.57	0/1370
27	b	0.27	0/653	0.57	0/876
28	e	0.27	0/443	0.60	0/582
29	x	0.26	0/1413	0.56	0/1906
30	y	0.27	0/2618	0.58	0/3536
31	u	0.26	0/5187	0.55	0/7011
32	w	0.28	0/2074	0.57	0/2806

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	t	0.29	0/1075	0.66	1/1424 (0.1%)
34	K	0.27	0/7182	0.58	2/9732 (0.0%)
35	v	0.25	0/2640	0.55	0/3557
All	All	0.28	1/92694 (0.0%)	0.80	166/132907 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	830	A	C6-N1	-5.75	1.31	1.35

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	844	U	C5-C4-O4	22.00	139.10	125.90
1	2	844	U	N3-C4-O4	-20.37	105.14	119.40
1	2	914	U	C5-C4-O4	19.04	137.32	125.90
1	2	914	U	N3-C4-O4	-18.86	106.20	119.40
1	2	917	U	N3-C4-O4	-16.44	107.89	119.40
1	2	917	U	C5-C4-O4	16.00	135.50	125.90
1	2	830	A	N1-C6-N6	-14.65	109.81	118.60
1	2	1453	C	N1-C2-O2	10.77	125.36	118.90
1	2	872	A	N1-C6-N6	-10.68	112.19	118.60
1	2	1453	C	C2-N1-C1'	9.94	129.73	118.80
1	2	830	A	C5-C6-N6	9.64	131.41	123.70
1	2	8	U	N3-C4-O4	-9.30	112.89	119.40
1	2	501	C	N1-C2-O2	8.93	124.26	118.90
1	2	356	C	C2-N1-C1'	8.86	128.55	118.80
1	2	685	A	N1-C6-N6	-8.83	113.30	118.60
1	2	1590	C	N1-C2-O2	8.72	124.13	118.90
1	2	630	U	C2-N1-C1'	8.72	128.16	117.70
1	2	1865	C	N1-C2-O2	8.54	124.03	118.90
1	2	356	C	N1-C2-O2	8.54	124.02	118.90
1	2	630	U	N1-C2-O2	8.49	128.74	122.80
1	2	293	C	N1-C2-O2	8.33	123.90	118.90
1	2	1453	C	N3-C2-O2	-7.99	116.31	121.90
1	2	492	C	N3-C2-O2	-7.99	116.31	121.90
1	2	501	C	C2-N1-C1'	7.95	127.55	118.80
1	2	1774	C	N3-C2-O2	-7.91	116.36	121.90
1	2	630	U	N3-C2-O2	-7.84	116.71	122.20
1	2	853	C	N1-C2-O2	7.83	123.60	118.90
1	2	1865	C	C2-N1-C1'	7.74	127.31	118.80
1	2	1683	C	N1-C2-O2	7.65	123.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	844	U	C2-N3-C4	7.65	131.59	127.00
1	2	1774	C	N1-C2-O2	7.64	123.49	118.90
1	2	1751	C	C2-N1-C1'	7.62	127.19	118.80
1	2	853	C	C2-N1-C1'	7.54	127.09	118.80
1	2	1751	C	N1-C2-O2	7.45	123.37	118.90
1	2	1683	C	C2-N1-C1'	7.40	126.94	118.80
1	2	1624	U	C2-N1-C1'	7.39	126.57	117.70
1	2	1022	U	C2-N1-C1'	7.38	126.56	117.70
1	2	830	A	N1-C2-N3	-7.35	125.62	129.30
1	2	293	C	C2-N1-C1'	7.28	126.80	118.80
1	2	1520	G	C4-N9-C1'	7.23	135.90	126.50
6	R	109	LEU	CA-CB-CG	7.17	131.79	115.30
1	2	1254	C	C2-N1-C1'	7.17	126.69	118.80
1	2	1865	C	N3-C2-O2	-7.12	116.92	121.90
1	2	1590	C	C2-N1-C1'	7.09	126.60	118.80
1	2	501	C	N3-C2-O2	-7.02	116.99	121.90
1	2	1139	C	N1-C2-O2	6.98	123.09	118.90
1	2	1453	C	C6-N1-C1'	-6.95	112.46	120.80
1	2	1590	C	N3-C2-O2	-6.92	117.06	121.90
1	2	1139	C	C2-N1-C1'	6.86	126.35	118.80
1	2	1271	C	N1-C2-O2	6.84	123.00	118.90
1	2	356	C	N3-C2-O2	-6.76	117.17	121.90
1	2	666	U	C2-N1-C1'	6.71	125.75	117.70
1	2	1273	C	N3-C2-O2	-6.64	117.25	121.90
1	2	1254	C	N1-C2-O2	6.62	122.87	118.90
1	2	293	C	N3-C2-O2	-6.62	117.27	121.90
1	2	1196	A	N1-C6-N6	-6.58	114.65	118.60
1	2	1520	G	N3-C4-N9	6.49	129.89	126.00
1	2	1144	A	C6-N1-C2	-6.46	114.72	118.60
1	2	342	C	C2-N1-C1'	6.46	125.90	118.80
1	2	178	C	N1-C2-O2	6.45	122.77	118.90
1	2	853	C	N3-C2-O2	-6.45	117.39	121.90
1	2	547	G	P-O3'-C3'	6.42	127.40	119.70
1	2	844	U	N1-C2-N3	-6.41	111.05	114.90
1	2	1600	G	C4-N9-C1'	6.38	134.79	126.50
1	2	1254	C	C5-C6-N1	6.32	124.16	121.00
6	R	110	ASP	CB-CG-OD1	6.30	123.97	118.30
1	2	1520	G	C8-N9-C1'	-6.29	118.83	127.00
1	2	1600	G	N3-C4-C5	-6.27	125.47	128.60
1	2	685	A	C5-C6-N1	6.25	120.82	117.70
1	2	1453	C	C6-N1-C2	-6.23	117.81	120.30
1	2	356	C	C6-N1-C1'	-6.22	113.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1600	G	N3-C4-N9	6.16	129.70	126.00
1	2	593	C	C2-N1-C1'	6.16	125.58	118.80
1	2	1078	C	C2-N1-C1'	6.16	125.57	118.80
1	2	1337	C	N1-C2-O2	6.16	122.59	118.90
1	2	1590	C	C6-N1-C2	-6.16	117.84	120.30
1	2	427	U	C2-N1-C1'	6.13	125.06	117.70
1	2	1683	C	C6-N1-C2	-6.12	117.85	120.30
1	2	501	C	C6-N1-C2	-6.11	117.86	120.30
1	2	844	U	C4-C5-C6	-6.11	116.04	119.70
1	2	1624	U	N1-C2-O2	6.11	127.08	122.80
1	2	823	U	C2-N1-C1'	6.10	125.02	117.70
1	2	8	U	C5-C4-O4	6.09	129.55	125.90
1	2	1316	C	P-O3'-C3'	6.08	126.99	119.70
1	2	749	U	C2-N1-C1'	6.05	124.96	117.70
1	2	1078	C	N1-C2-O2	6.03	122.52	118.90
1	2	1601	A	P-O3'-C3'	6.00	126.90	119.70
1	2	1618	C	N1-C2-O2	5.96	122.47	118.90
1	2	1558	C	P-O3'-C3'	5.94	126.83	119.70
1	2	441	C	C2-N1-C1'	5.92	125.31	118.80
1	2	1453	C	C5-C6-N1	5.90	123.95	121.00
1	2	1683	C	C5-C6-N1	5.87	123.94	121.00
1	2	856	C	C2-N1-C1'	5.85	125.24	118.80
1	2	1865	C	C6-N1-C2	-5.85	117.96	120.30
1	2	1624	U	N3-C2-O2	-5.84	118.11	122.20
1	2	1520	G	N3-C4-C5	-5.83	125.69	128.60
1	2	1139	C	N3-C2-O2	-5.82	117.83	121.90
1	2	494	C	N1-C2-O2	5.82	122.39	118.90
1	2	823	U	N3-C2-O2	-5.79	118.15	122.20
1	2	1683	C	N3-C2-O2	-5.74	117.88	121.90
1	2	114	G	P-O3'-C3'	5.71	126.55	119.70
1	2	553	U	C5-C6-N1	5.67	125.54	122.70
1	2	4	C	C2-N1-C1'	5.66	125.02	118.80
1	2	823	U	N1-C2-O2	5.65	126.76	122.80
6	R	109	LEU	C-N-CA	5.65	135.82	121.70
1	2	1022	U	N1-C2-O2	5.64	126.75	122.80
1	2	659	G	C4-N9-C1'	5.63	133.82	126.50
1	2	630	U	C6-N1-C1'	-5.63	113.32	121.20
1	2	1272	C	N1-C2-O2	5.59	122.25	118.90
1	2	872	A	C5-C6-N6	5.58	128.16	123.70
1	2	877	C	C2-N1-C1'	5.54	124.90	118.80
1	2	1305	C	N1-C2-O2	5.53	122.22	118.90
1	2	814	U	N1-C2-O2	5.52	126.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1751	C	C6-N1-C1'	-5.51	114.18	120.80
1	2	593	C	N1-C2-O2	5.50	122.20	118.90
1	2	356	C	C6-N1-C2	-5.49	118.10	120.30
34	K	391	LEU	CA-CB-CG	5.49	127.92	115.30
34	K	509	MET	CA-CB-CG	5.49	122.63	113.30
5	Q	116	ASP	CB-CG-OD1	5.48	123.23	118.30
1	2	1271	C	C2-N1-C1'	5.47	124.82	118.80
1	2	509	G	N1-C2-N2	-5.47	111.28	116.20
1	2	465	A	P-O3'-C3'	5.41	126.19	119.70
1	2	1534	C	P-O3'-C3'	5.40	126.18	119.70
1	2	914	U	C4-C5-C6	-5.40	116.46	119.70
1	2	1648	G	P-O3'-C3'	5.40	126.18	119.70
1	2	1271	C	N3-C2-O2	-5.38	118.13	121.90
1	2	1337	C	C2-N1-C1'	5.33	124.67	118.80
1	2	1053	C	C2-N1-C1'	5.32	124.65	118.80
1	2	930	C	N1-C2-O2	5.30	122.08	118.90
1	2	1600	G	C8-N9-C1'	-5.30	120.11	127.00
1	2	1618	C	N3-C2-O2	-5.29	118.19	121.90
1	2	1601	A	OP2-P-O3'	5.28	116.81	105.20
1	2	494	C	C2-N1-C1'	5.27	124.60	118.80
1	2	1304	U	C2-N1-C1'	5.27	124.03	117.70
1	2	143	U	P-O3'-C3'	5.26	126.01	119.70
1	2	853	C	C6-N1-C2	-5.25	118.20	120.30
1	2	814	U	N3-C2-O2	-5.23	118.54	122.20
1	2	102	A	P-O3'-C3'	5.23	125.97	119.70
1	2	1039	C	C2-N1-C1'	5.22	124.54	118.80
1	2	501	C	C6-N1-C1'	-5.21	114.55	120.80
1	2	178	C	C2-N1-C1'	5.21	124.53	118.80
1	2	1016	U	N1-C2-O2	5.20	126.44	122.80
1	2	501	C	C5-C6-N1	5.19	123.59	121.00
1	2	1716	C	C2-N1-C1'	5.18	124.50	118.80
33	t	294	LEU	CA-CB-CG	5.17	127.20	115.30
1	2	1078	C	C6-N1-C2	-5.17	118.23	120.30
1	2	856	C	N1-C2-O2	5.17	122.00	118.90
1	2	750	C	C2-N1-C1'	5.17	124.48	118.80
1	2	178	C	N3-C2-O2	-5.16	118.29	121.90
21	N	45	LEU	CA-CB-CG	5.15	127.15	115.30
1	2	1510	G	N1-C2-N2	-5.14	111.57	116.20
1	2	1139	C	C6-N1-C2	-5.14	118.24	120.30
1	2	1590	C	C5-C6-N1	5.14	123.57	121.00
1	2	579	C	N1-C2-O2	5.11	121.97	118.90
1	2	293	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1259	A	C2-N3-C4	5.11	113.15	110.60
1	2	853	C	C6-N1-C1'	-5.08	114.70	120.80
1	2	199	C	N1-C2-O2	5.07	121.94	118.90
1	2	1865	C	C6-N1-C1'	-5.07	114.72	120.80
1	2	1493	C	P-O3'-C3'	5.07	125.78	119.70
1	2	1022	U	C6-N1-C1'	-5.06	114.11	121.20
1	2	1751	C	N3-C2-O2	-5.06	118.36	121.90
1	2	1618	C	C6-N1-C2	-5.05	118.28	120.30
1	2	578	C	N1-C2-O2	5.05	121.93	118.90
1	2	1016	U	C2-N1-C1'	5.05	123.76	117.70
1	2	886	A	C4-N9-C1'	5.03	135.35	126.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	34680	0	17510	295	0
2	F	1495	0	1549	22	0
3	M	953	0	990	15	0
4	P	984	0	1028	21	0
5	Q	969	0	1030	23	0
6	R	944	0	980	13	0
7	S	1083	0	1140	26	0
8	T	1122	0	1153	15	0
9	Z	574	0	627	14	0
10	c	471	0	499	0	0
11	f	596	0	628	0	0
12	A	1705	0	1706	29	0
13	B	1729	0	1803	23	0
14	C	1690	0	1777	16	0
15	E	2076	0	2177	28	0
16	G	1862	0	2018	32	0
17	H	1501	0	1593	26	0
18	I	1682	0	1769	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	1499	0	1618	19	0
20	L	1229	0	1302	16	0
21	N	1202	0	1289	10	0
22	O	1009	0	1034	16	0
23	V	625	0	628	7	0
24	W	1034	0	1080	17	0
25	X	1098	0	1167	15	0
26	Y	1014	0	1082	11	0
27	b	640	0	665	0	0
28	e	438	0	484	0	0
29	x	1391	0	1467	0	0
30	y	2568	0	2624	0	0
31	u	5062	0	5113	0	0
32	w	2027	0	2126	0	0
33	t	1066	0	1070	0	0
34	K	7047	0	7310	74	0
35	v	2589	0	2548	0	0
36	f	1	0	0	0	0
36	y	1	0	0	0	0
All	All	87656	0	72584	684	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 6.

All (684) 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)
24:W:101:PHE:O	24:W:128:PHE:HA	1.37	1.19
22:O:42:VAL:O	22:O:55:ARG:HA	1.45	1.13
1:2:533:A:H61	1:2:550:C:N4	1.51	1.08
1:2:533:A:N6	1:2:550:C:H42	1.54	1.06
1:2:1710:C:H42	1:2:1823:A:N6	1.63	0.96
1:2:925:G:H1	1:2:1017:U:H3	1.12	0.91
1:2:1236:G:H21	1:2:1522:A:H62	1.18	0.90
1:2:1398:G:H1	1:2:1448:A:H2	1.22	0.87
1:2:1533:A:H62	1:2:1602:U:H3	1.24	0.86
1:2:928:G:H1	1:2:1013:U:H3	1.22	0.84
1:2:1710:C:N4	1:2:1823:A:H61	1.77	0.81
1:2:8:U:N3	1:2:1196:A:N6	2.29	0.81
34:K:716:THR:O	34:K:720:TYR:HB3	1.84	0.78
1:2:1710:C:N4	1:2:1823:A:N6	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:LEU:HD12	5:Q:50:LYS:HG2	1.67	0.76
1:2:1245:G:C6	1:2:1255:G:N2	2.55	0.75
26:Y:20:ARG:NH1	26:Y:74:MET:SD	2.60	0.75
1:2:1726:G:H1	1:2:1808:U:H3	1.35	0.73
1:2:8:U:C4	1:2:1196:A:N6	2.57	0.72
1:2:1260:A:H61	1:2:1617:G:H21	1.38	0.71
2:F:78:MET:HB3	2:F:159:ARG:HH22	1.55	0.71
1:2:533:A:N1	1:2:550:C:N3	2.39	0.70
5:Q:56:LEU:HD23	5:Q:60:LYS:HZ1	1.56	0.70
1:2:1748:G:H1	1:2:1786:U:H3	1.40	0.70
2:F:19:LEU:HB3	2:F:23:TRP:HB2	1.73	0.69
1:2:1215:C:H42	1:2:1220:A:H61	1.40	0.69
6:R:41:ILE:HD12	6:R:47:ARG:HD3	1.73	0.69
14:C:183:LYS:HA	14:C:195:LEU:O	1.93	0.69
1:2:1710:C:N3	1:2:1823:A:N1	2.40	0.69
1:2:1264:C:N4	1:2:1518:C:N3	2.40	0.69
1:2:1091:C:HO2'	24:W:2:VAL:N	1.91	0.68
1:2:164:A:H3'	1:2:165:G:H21	1.60	0.66
4:P:98:ASN:HB3	4:P:120:SER:HB3	1.77	0.66
1:2:957:A:H3'	1:2:958:G:H21	1.61	0.66
1:2:1464:C:HO2'	1:2:1465:A:H8	1.43	0.65
1:2:1143:A:H5'	14:C:190:SER:HB3	1.78	0.65
34:K:690:LEU:HD21	34:K:721:LEU:HD21	1.79	0.65
1:2:533:A:H61	1:2:550:C:H42	0.73	0.65
1:2:1259:A:N6	1:2:1519:U:OP1	2.30	0.64
1:2:1743:G:H21	1:2:1791:A:H62	1.46	0.64
1:2:940:U:H3	1:2:1002:U:H3	1.45	0.64
5:Q:28:GLY:HA3	5:Q:67:ASP:HB2	1.80	0.64
1:2:944:A:H61	1:2:982:G:H1	1.44	0.63
1:2:525:A:N7	1:2:589:G:O6	2.32	0.63
34:K:863:ILE:HG22	34:K:919:CYS:HB3	1.81	0.63
1:2:1674:G:OP1	2:F:51:HIS:NE2	2.31	0.63
1:2:816:A:OP2	19:J:10:ARG:NH2	2.33	0.62
1:2:1606:G:H22	1:2:1632:G:H2'	1.64	0.62
4:P:75:VAL:HA	4:P:93:MET:O	1.99	0.62
14:C:131:GLY:HA3	14:C:216:MET:HB3	1.81	0.62
22:O:85:CYS:HB3	22:O:90:ILE:HB	1.80	0.62
34:K:331:LEU:HD21	34:K:373:ALA:HB1	1.81	0.62
24:W:86:LEU:HD21	24:W:113:HIS:HB2	1.82	0.62
1:2:1854:U:OP1	22:O:147:ARG:NH1	2.33	0.61
5:Q:58:LEU:O	5:Q:62:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:I:31:ARG:HH22	18:I:48:VAL:HA	1.64	0.61
22:O:43:HIS:HE2	22:O:52:THR:HG1	1.45	0.61
1:2:1236:G:N2	1:2:1522:A:H62	1.93	0.61
1:2:1565:C:OP2	8:T:101:ARG:NH1	2.34	0.61
8:T:76:THR:HG22	8:T:94:ARG:HB3	1.82	0.61
17:H:154:ILE:HB	17:H:185:VAL:HG22	1.83	0.61
25:X:51:VAL:HA	25:X:72:VAL:HG12	1.83	0.61
1:2:1614:A:OP2	4:P:42:ARG:NH2	2.34	0.61
1:2:1218:C:H1'	1:2:1683:C:H42	1.65	0.60
1:2:581:U:OP1	19:J:133:ARG:NH2	2.35	0.60
1:2:103:A:OP2	1:2:356:C:N4	2.35	0.60
34:K:807:ALA:O	34:K:811:GLN:NE2	2.34	0.60
1:2:101:U:H5''	18:I:19:LYS:HD2	1.84	0.60
14:C:166:ARG:HB2	14:C:248:TYR:HD1	1.67	0.60
17:H:47:ALA:HB3	17:H:63:PHE:HB2	1.81	0.60
1:2:1542:C:H5''	8:T:62:ARG:HH22	1.66	0.60
1:2:1528:G:O2'	1:2:1666:C:OP1	2.19	0.60
5:Q:53:GLU:O	5:Q:57:LEU:HB2	2.02	0.60
9:Z:111:ARG:NH1	9:Z:113:THR:O	2.34	0.60
22:O:42:VAL:HG11	22:O:81:VAL:HG11	1.84	0.60
6:R:99:ASP:OD2	12:A:42:LYS:NZ	2.34	0.59
3:M:32:ALA:HB2	3:M:112:LYS:HE3	1.83	0.59
22:O:31:CYS:HB2	22:O:93:LEU:HD23	1.85	0.59
1:2:1122:A:N3	13:B:146:ARG:NH1	2.50	0.59
5:Q:58:LEU:HD22	5:Q:62:ARG:HH22	1.68	0.59
4:P:72:LYS:HD3	4:P:73:PRO:HD2	1.85	0.59
34:K:1021:LYS:O	34:K:1029:HIS:NE2	2.36	0.59
5:Q:19:ALA:HB2	5:Q:75:GLY:HA3	1.84	0.59
1:2:928:G:H2'	1:2:929:G:C8	2.38	0.59
1:2:1285:G:H1	3:M:56:CYS:HA	1.68	0.58
1:2:1398:G:N1	1:2:1448:A:C2	2.64	0.58
18:I:8:TRP:HA	18:I:18:ARG:HH11	1.68	0.58
20:L:68:ILE:HG12	20:L:143:LEU:HD21	1.85	0.58
1:2:64:A:H2	1:2:83:A:H62	1.50	0.58
4:P:81:ARG:NH2	4:P:120:SER:O	2.36	0.58
1:2:808:A:HO2'	1:2:809:A:H8	1.50	0.58
17:H:66:VAL:O	17:H:69:LEU:HB3	2.04	0.58
20:L:133:PRO:HB3	20:L:139:ARG:HH11	1.67	0.58
7:S:54:LYS:HE2	7:S:59:LEU:HD23	1.85	0.58
19:J:113:GLN:OE1	19:J:154:GLN:NE2	2.37	0.58
2:F:199:VAL:O	2:F:203:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:124:ARG:HD2	7:S:129:LEU:HB2	1.86	0.57
2:F:28:VAL:O	2:F:42:LYS:NZ	2.37	0.57
1:2:943:U:H2'	1:2:944:A:H8	1.69	0.57
15:E:139:LEU:O	15:E:146:THR:HA	2.04	0.57
16:G:27:PHE:HE2	16:G:41:LEU:HD21	1.69	0.57
7:S:124:ARG:NH1	7:S:130:ARG:O	2.37	0.57
1:2:494:C:H42	1:2:509:G:H21	1.53	0.57
1:2:855:G:O2'	20:L:71:ARG:NH1	2.37	0.57
1:2:925:G:OP1	21:N:121:ARG:NH1	2.37	0.57
1:2:941:C:H2'	1:2:942:G:H8	1.69	0.57
9:Z:103:HIS:H	9:Z:107:VAL:HG22	1.68	0.57
20:L:131:CYS:SG	20:L:132:ARG:N	2.78	0.57
13:B:134:LEU:HB3	13:B:219:LYS:HB2	1.85	0.57
1:2:1215:C:H42	1:2:1220:A:N6	2.03	0.56
17:H:117:PRO:HG2	17:H:120:ARG:HD3	1.85	0.56
1:2:1472:C:OP2	34:K:834:ARG:NH2	2.38	0.56
1:2:1610:G:N2	7:S:85:ASN:OD1	2.36	0.56
1:2:1656:G:H1	1:2:1668:U:H3	1.53	0.56
1:2:1722:G:O6	1:2:1812:U:O2	2.23	0.56
5:Q:8:GLN:N	5:Q:99:TYR:HH	2.03	0.56
1:2:1575:G:O2'	34:K:249:LYS:NZ	2.38	0.56
25:X:101:LEU:HB3	25:X:124:LYS:HB2	1.88	0.56
1:2:1215:C:N4	1:2:1220:A:H61	2.04	0.56
18:I:73:THR:O	18:I:74:ARG:NH1	2.38	0.56
34:K:440:LYS:HG3	34:K:496:VAL:HG21	1.88	0.56
16:G:88:ARG:HB2	16:G:91:GLU:HG2	1.87	0.56
1:2:109:U:O2	20:L:71:ARG:NH2	2.39	0.55
1:2:609:U:H2'	1:2:610:G:H8	1.71	0.55
1:2:683:G:H4'	24:W:4:MET:HG2	1.89	0.55
1:2:1398:G:O6	1:2:1448:A:N1	2.39	0.55
3:M:34:GLY:O	3:M:108:CYS:HB3	2.06	0.55
13:B:129:THR:OG1	13:B:179:ASN:O	2.24	0.55
18:I:101:ILE:HD12	18:I:190:LEU:HD11	1.87	0.55
12:A:66:VAL:HG21	12:A:185:MET:HB3	1.88	0.55
1:2:871:U:H3'	1:2:872:A:H4'	1.88	0.55
1:2:75:G:H1	16:G:155:GLN:HA	1.72	0.55
16:G:52:ILE:HG23	16:G:109:LEU:HD11	1.89	0.55
1:2:492:C:N4	1:2:507:G:OP2	2.28	0.55
1:2:1398:G:N1	1:2:1448:A:H2	1.99	0.55
1:2:1486:A:C6	1:2:1487:A:N6	2.75	0.55
1:2:594:A:H61	1:2:643:A:H5''	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:191:VAL:HG11	14:C:236:PHE:HA	1.87	0.55
26:Y:26:ASP:HB3	26:Y:68:LYS:HE3	1.89	0.55
34:K:338:HIS:HB3	34:K:341:VAL:HG22	1.89	0.55
1:2:189:U:OP1	18:I:152:ARG:NH2	2.37	0.55
17:H:58:LYS:HD2	17:H:90:LYS:HD2	1.88	0.55
34:K:837:LEU:HA	34:K:840:LEU:HD12	1.87	0.54
1:2:1260:A:N6	1:2:1617:G:H21	2.03	0.54
8:T:33:TRP:HE1	8:T:102:ARG:NH1	2.04	0.54
16:G:14:LYS:HG3	16:G:124:LEU:HD12	1.89	0.54
34:K:633:PRO:HB2	34:K:636:VAL:HB	1.89	0.54
1:2:527:C:H2'	1:2:528:A:H8	1.72	0.54
1:2:1060:A:O2'	1:2:1062:A:N6	2.40	0.54
1:2:1486:A:N6	1:2:1487:A:N6	2.56	0.54
3:M:32:ALA:HB3	3:M:110:VAL:HB	1.90	0.54
16:G:181:THR:HG22	16:G:183:ARG:H	1.72	0.54
1:2:528:A:H2'	1:2:529:A:H8	1.73	0.54
1:2:561:A:O2'	19:J:134:HIS:NE2	2.41	0.54
1:2:384:U:O4	18:I:5:ARG:NH2	2.37	0.54
2:F:99:ILE:HD13	2:F:171:GLU:HG3	1.90	0.54
1:2:943:U:H2'	1:2:944:A:C8	2.43	0.54
1:2:1228:A:H2'	1:2:1229:G:C8	2.42	0.54
1:2:748:C:H42	1:2:794:A:H61	1.56	0.54
1:2:913:A:H2	17:H:99:ARG:H	1.55	0.54
14:C:199:PRO:HG2	19:J:58:ARG:HD3	1.89	0.54
1:2:982:G:H21	1:2:1045:U:H1'	1.71	0.54
1:2:1144:A:H5'	1:2:1355:C:H41	1.73	0.54
17:H:109:ARG:HD3	17:H:111:LYS:HE3	1.90	0.54
12:A:205:ARG:HD3	12:A:210:ILE:HD11	1.90	0.53
1:2:918:U:H3'	21:N:64:ARG:HH22	1.72	0.53
1:2:1786:U:H2'	1:2:1787:G:H8	1.71	0.53
2:F:195:GLU:HA	2:F:198:ARG:HG2	1.88	0.53
7:S:99:LEU:HD12	7:S:102:GLY:H	1.72	0.53
12:A:29:ASN:HB3	12:A:151:ASP:HB3	1.90	0.53
1:2:69:C:OP2	16:G:167:LYS:NZ	2.41	0.53
1:2:561:A:H5''	19:J:164:PRO:HG2	1.90	0.53
7:S:14:ARG:NH2	7:S:17:ASN:OD1	2.38	0.53
15:E:36:HIS:NE2	15:E:143:ASP:OD1	2.41	0.53
1:2:28:U:H2'	1:2:29:G:H8	1.73	0.53
1:2:67:C:H41	16:G:163:ASN:HA	1.72	0.53
1:2:399:C:O2	20:L:106:HIS:ND1	2.41	0.53
1:2:1598:G:N7	9:Z:85:ARG:NH2	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1616:U:O4	4:P:40:ARG:NH2	2.41	0.53
18:I:3:ILE:O	18:I:30:GLY:N	2.41	0.53
1:2:1478:U:OP1	34:K:874:ARG:NH1	2.41	0.53
20:L:128:VAL:HG12	20:L:142:VAL:HA	1.89	0.53
1:2:913:A:OP2	17:H:99:ARG:NH1	2.42	0.53
1:2:1032:C:H5''	21:N:109:LYS:HD2	1.90	0.53
16:G:57:ASP:OD2	16:G:72:ARG:NH2	2.30	0.53
21:N:84:LEU:HD13	21:N:149:LEU:HD11	1.91	0.53
1:2:1232:U:H2'	1:2:1233:G:H8	1.73	0.53
13:B:121:ILE:HG12	13:B:161:VAL:HG13	1.91	0.53
34:K:386:PRO:O	34:K:390:TRP:HB2	2.09	0.53
3:M:93:LYS:H	3:M:102:LYS:HB3	1.74	0.53
17:H:162:GLN:HE21	17:H:165:ASN:HD22	1.57	0.53
1:2:78:C:OP1	16:G:159:ARG:NH2	2.42	0.52
1:2:948:C:H2'	1:2:949:G:H8	1.73	0.52
16:G:58:LYS:HD2	16:G:107:SER:HB3	1.92	0.52
1:2:1013:U:OP1	1:2:1129:G:O2'	2.25	0.52
1:2:8:U:N3	1:2:1196:A:C6	2.78	0.52
1:2:494:C:N4	1:2:509:G:H21	2.07	0.52
1:2:661:U:OP2	25:X:3:LYS:NZ	2.43	0.52
3:M:94:ILE:HB	3:M:98:GLY:HA2	1.90	0.52
4:P:123:TYR:OH	7:S:124:ARG:NH2	2.35	0.52
34:K:470:LYS:HA	34:K:473:ARG:HG2	1.91	0.52
34:K:810:VAL:HG11	34:K:846:LYS:HE3	1.92	0.52
1:2:1156:U:OP1	24:W:71:LYS:NZ	2.42	0.52
1:2:1456:G:H1'	34:K:711:ARG:HD2	1.91	0.52
16:G:75:LEU:O	16:G:94:ARG:HA	2.08	0.52
26:Y:4:THR:OG1	26:Y:32:LYS:NZ	2.42	0.52
1:2:579:C:O2	26:Y:61:ARG:NH1	2.41	0.52
34:K:112:ARG:HH21	34:K:126:ALA:HB2	1.75	0.52
34:K:315:LEU:HB3	34:K:352:LEU:HD13	1.92	0.52
1:2:106:C:H2'	1:2:107:A:H8	1.73	0.52
13:B:87:ILE:HG12	13:B:101:HIS:HB2	1.92	0.52
1:2:85:A:H5''	26:Y:118:ARG:HE	1.75	0.52
1:2:1302:G:N2	1:2:1308:U:O4	2.43	0.52
12:A:6:ASP:OD1	12:A:6:ASP:N	2.43	0.52
21:N:63:VAL:HG21	21:N:71:ILE:HD11	1.92	0.52
1:2:1144:A:H2'	1:2:1145:A:C8	2.45	0.52
12:A:85:ARG:NH1	12:A:203:PHE:O	2.43	0.51
1:2:1652:G:H1	1:2:1672:U:H3	1.58	0.51
2:F:99:ILE:HD11	9:Z:67:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:3:ARG:HD3	24:W:6:VAL:HG12	1.92	0.51
34:K:421:VAL:HA	34:K:424:LEU:HD12	1.92	0.51
34:K:1024:LEU:HD12	34:K:1032:LEU:HD11	1.91	0.51
3:M:51:VAL:HG22	3:M:77:ILE:HB	1.92	0.51
4:P:83:MET:HB2	4:P:116:LEU:HD13	1.91	0.51
1:2:993:G:OP1	1:2:1131:G:N2	2.36	0.51
2:F:49:LEU:HD13	5:Q:47:LEU:HD12	1.91	0.51
5:Q:105:LYS:HA	5:Q:108:ILE:HG12	1.91	0.51
18:I:151:GLU:HA	18:I:154:LYS:HE2	1.91	0.51
1:2:913:A:H1'	17:H:66:VAL:HB	1.92	0.51
20:L:79:LYS:HE2	20:L:81:LYS:HD2	1.93	0.51
1:2:1158:G:OP1	25:X:5:ARG:NH2	2.44	0.51
1:2:1183:A:H2'	1:2:1184:G:H8	1.75	0.51
4:P:118:GLU:HB2	7:S:120:HIS:H	1.74	0.51
5:Q:9:SER:HB2	5:Q:26:LYS:HD3	1.92	0.51
6:R:57:LEU:HG	6:R:60:ARG:HD2	1.93	0.51
1:2:1260:A:H61	1:2:1617:G:N2	2.07	0.51
1:2:1471:C:N3	34:K:711:ARG:NH1	2.58	0.51
12:A:144:THR:HB	12:A:157:VAL:HA	1.93	0.51
1:2:1531:A:H4'	1:2:1605:G:H4'	1.92	0.51
1:2:1568:C:O2'	1:2:1627:C:O2'	2.29	0.51
1:2:190:G:H5''	18:I:145:ILE:HD13	1.93	0.51
1:2:319:C:H2'	1:2:320:G:H8	1.76	0.51
5:Q:51:LEU:HB2	5:Q:81:ILE:HD11	1.93	0.51
8:T:28:LEU:HD22	8:T:54:TYR:HE1	1.75	0.51
15:E:212:ASP:OD1	15:E:213:ALA:N	2.44	0.51
20:L:104:LYS:O	25:X:11:ARG:NH2	2.44	0.51
23:V:15:ARG:HH21	23:V:24:ILE:HG21	1.76	0.51
34:K:1037:LYS:O	34:K:1041:ARG:N	2.43	0.51
4:P:95:GLY:HA2	4:P:103:ASN:O	2.10	0.51
12:A:33:GLN:HB3	12:A:154:LEU:HD12	1.93	0.51
1:2:685:A:N6	1:2:917:U:N3	2.59	0.50
6:R:106:LEU:HD11	12:A:19:LEU:HD11	1.93	0.50
14:C:200:ARG:O	19:J:54:ARG:NH2	2.39	0.50
16:G:49:VAL:HB	16:G:115:LYS:HB2	1.93	0.50
2:F:128:ILE:HD12	2:F:137:GLN:HB2	1.93	0.50
8:T:28:LEU:HA	8:T:110:LEU:HD21	1.93	0.50
12:A:41:ARG:HE	12:A:45:GLY:HA2	1.76	0.50
34:K:619:GLN:HA	34:K:622:MET:HG3	1.93	0.50
1:2:163:U:H2'	1:2:164:A:H8	1.76	0.50
12:A:17:LYS:HB3	12:A:173:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:52:LEU:HD11	25:X:73:GLN:HB2	1.92	0.50
34:K:780:LEU:HD11	34:K:795:LEU:HD11	1.93	0.50
1:2:988:C:H5'	13:B:116:LYS:HA	1.94	0.50
5:Q:33:LYS:NZ	8:T:8:ASP:OD1	2.37	0.50
34:K:194:PHE:HB3	34:K:217:LEU:HD21	1.92	0.50
34:K:838:LYS:O	34:K:841:LEU:HB3	2.11	0.50
1:2:941:C:H2'	1:2:942:G:C8	2.44	0.50
12:A:77:ILE:HG12	12:A:99:ILE:HB	1.92	0.50
13:B:33:VAL:HG13	13:B:44:ILE:HB	1.93	0.50
14:C:78:LEU:HD12	14:C:81:ILE:HD12	1.94	0.50
18:I:142:SER:HB2	18:I:145:ILE:HD12	1.93	0.50
24:W:69:LEU:HD21	24:W:72:CYS:HB2	1.92	0.50
1:2:1533:A:H5'	1:2:1637:A:H62	1.77	0.50
6:R:91:LEU:HD21	12:A:173:LEU:HD12	1.93	0.50
13:B:82:ARG:HH12	13:B:191:ASP:HB2	1.77	0.50
17:H:98:ARG:NH2	17:H:132:ASP:OD2	2.45	0.50
1:2:382:C:H2'	1:2:383:G:H8	1.77	0.50
1:2:508:A:H3'	1:2:509:G:H8	1.75	0.50
1:2:980:A:H2'	1:2:981:A:C8	2.46	0.50
18:I:165:GLN:NE2	18:I:195:LEU:HD11	2.25	0.50
1:2:1648:G:H5''	5:Q:125:ARG:HD2	1.94	0.50
34:K:730:ASN:ND2	34:K:765:ASP:OD1	2.45	0.50
1:2:983:A:OP1	1:2:1073:U:O2'	2.26	0.49
6:R:97:GLU:OE1	6:R:120:THR:OG1	2.26	0.49
34:K:131:VAL:HG22	34:K:135:ILE:HG13	1.94	0.49
1:2:1748:G:H2'	1:2:1749:G:H8	1.77	0.49
16:G:3:LEU:HD11	16:G:111:LEU:HD22	1.92	0.49
16:G:218:LYS:NZ	16:G:222:GLU:OE1	2.45	0.49
1:2:126:G:OP1	16:G:198:ARG:NH1	2.43	0.49
1:2:145:G:H2'	1:2:146:G:C8	2.47	0.49
1:2:1256:G:H21	1:2:1659:U:H5'	1.76	0.49
24:W:25:VAL:HB	24:W:63:VAL:HG22	1.94	0.49
1:2:434:G:OP2	18:I:25:ARG:NH2	2.46	0.49
1:2:1064:C:H2'	1:2:1065:G:H8	1.75	0.49
2:F:55:ARG:NH2	5:Q:123:ASP:OD1	2.45	0.49
18:I:89:GLU:HA	18:I:92:ARG:HD3	1.94	0.49
34:K:865:CYS:HA	34:K:868:GLU:HB2	1.93	0.49
16:G:7:PHE:O	16:G:11:GLY:N	2.45	0.49
12:A:84:GLN:HE22	12:A:101:GLY:H	1.60	0.49
1:2:561:A:HO2'	19:J:134:HIS:HE2	1.55	0.49
1:2:570:C:H4'	26:Y:36:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:582:U:H5'	19:J:162:ARG:HH22	1.78	0.49
1:2:681:U:O2'	1:2:1160:U:OP1	2.27	0.49
1:2:1845:A:H2'	1:2:1846:G:C8	2.48	0.49
1:2:1320:G:H2'	1:2:1321:G:C8	2.48	0.49
1:2:1338:G:OP1	34:K:1037:LYS:N	2.43	0.49
14:C:134:ASN:HA	14:C:218:GLY:HA3	1.95	0.49
1:2:1337:C:OP1	34:K:1036:ARG:NH2	2.47	0.48
1:2:495:U:O2'	15:E:27:PHE:O	2.30	0.48
1:2:656:G:O2'	14:C:227:ARG:NH1	2.45	0.48
14:C:115:GLN:OE1	14:C:120:GLN:NE2	2.46	0.48
1:2:617:G:H4'	25:X:88:ASP:HB3	1.95	0.48
1:2:1609:C:H3'	7:S:132:ARG:HH12	1.78	0.48
1:2:1726:G:H2'	1:2:1727:G:H8	1.78	0.48
2:F:103:LEU:HD22	2:F:178:ILE:HD13	1.95	0.48
3:M:48:HIS:ND1	3:M:112:LYS:O	2.36	0.48
17:H:103:LYS:HD2	17:H:104:PRO:HD2	1.96	0.48
22:O:46:ASP:OD1	22:O:47:LEU:N	2.45	0.48
34:K:975:VAL:HA	34:K:978:LEU:HD12	1.95	0.48
1:2:160:U:O2'	1:2:162:C:OP2	2.28	0.48
9:Z:73:VAL:HG12	9:Z:79:ILE:HD11	1.96	0.48
24:W:44:HIS:NE2	24:W:112:ASP:OD2	2.47	0.48
1:2:57:U:OP1	1:2:504:G:O2'	2.32	0.48
1:2:919:A:H4'	1:2:920:A:H5''	1.96	0.48
17:H:17:ASP:OD1	17:H:18:GLU:N	2.47	0.48
24:W:106:THR:HG21	24:W:121:THR:HG23	1.96	0.48
1:2:43:U:OP2	1:2:485:A:N6	2.43	0.48
1:2:546:G:H2'	1:2:547:G:H3'	1.95	0.48
1:2:640:A:H2'	1:2:641:A:C8	2.49	0.48
1:2:1534:C:O2	1:2:1598:G:N2	2.47	0.48
1:2:1636:G:H1'	2:F:164:ARG:HH12	1.79	0.48
2:F:179:ASN:HA	2:F:182:LYS:HE3	1.95	0.48
7:S:115:LYS:HE3	7:S:126:PHE:HB2	1.95	0.48
1:2:643:A:OP1	19:J:39:ASN:ND2	2.46	0.48
1:2:1518:C:H5''	1:2:1519:U:H5''	1.96	0.48
2:F:35:LEU:HD11	2:F:146:ARG:HD2	1.96	0.48
1:2:524:U:OP1	1:2:525:A:O2'	2.26	0.48
1:2:1331:C:H2'	1:2:1332:A:H8	1.79	0.48
12:A:157:VAL:O	23:V:65:SER:OG	2.32	0.48
1:2:1122:A:H4'	13:B:205:TYR:CD1	2.49	0.47
1:2:1585:U:O2	5:Q:73:LYS:NZ	2.46	0.47
1:2:1656:G:H2'	1:2:1657:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1726:G:H2'	1:2:1727:G:C8	2.49	0.47
1:2:1781:A:H2'	1:2:1782:G:C8	2.49	0.47
5:Q:85:ARG:NH2	5:Q:116:ASP:OD2	2.46	0.47
1:2:1758:G:C2	1:2:1775:U:O2	2.67	0.47
8:T:115:LYS:HD3	8:T:121:ARG:HH21	1.79	0.47
34:K:535:VAL:HG11	34:K:568:TRP:HZ3	1.79	0.47
1:2:1302:G:C2	1:2:1308:U:O4	2.67	0.47
1:2:1590:C:H5''	1:2:1591:C:H5	1.79	0.47
12:A:176:TRP:NE1	12:A:197:VAL:O	2.47	0.47
1:2:1112:U:O2'	13:B:146:ARG:NH2	2.47	0.47
1:2:1566:G:H5''	8:T:101:ARG:HH22	1.80	0.47
13:B:164:ILE:O	13:B:168:MET:HG3	2.13	0.47
21:N:99:ARG:O	21:N:103:GLU:HG2	2.15	0.47
1:2:1277:C:H2'	1:2:1278:A:H8	1.79	0.47
1:2:1785:C:O2'	1:2:1786:U:O4'	2.33	0.47
19:J:53:ILE:HG23	19:J:77:LEU:HD11	1.97	0.47
1:2:1101:U:H2'	1:2:1102:G:H8	1.79	0.47
1:2:1245:G:C5	1:2:1255:G:N2	2.83	0.47
7:S:39:ARG:HH21	8:T:38:LYS:HG3	1.79	0.47
15:E:192:ILE:HD12	15:E:243:GLY:HA3	1.97	0.47
20:L:93:LEU:HD12	20:L:102:PHE:HB3	1.97	0.47
24:W:87:GLU:OE1	24:W:90:GLN:NE2	2.47	0.47
34:K:389:ALA:O	34:K:393:VAL:HG13	2.15	0.47
2:F:51:HIS:ND1	5:Q:82:TYR:OH	2.45	0.47
13:B:104:ASP:OD1	13:B:105:LEU:N	2.47	0.47
1:2:379:C:O2	18:I:5:ARG:NE	2.48	0.47
25:X:107:ARG:HD3	25:X:112:VAL:HG22	1.96	0.47
18:I:10:LYS:HE2	18:I:10:LYS:HB3	1.76	0.47
1:2:527:C:H4'	19:J:121:LYS:HD2	1.97	0.46
1:2:1677:U:OP1	2:F:71:ARG:NH2	2.48	0.46
17:H:145:ARG:HD3	24:W:51:GLU:HG2	1.97	0.46
1:2:1220:A:N3	1:2:1677:U:O2'	2.43	0.46
1:2:1725:U:H2'	1:2:1726:G:H8	1.81	0.46
15:E:129:ILE:HG12	15:E:139:LEU:HD23	1.96	0.46
1:2:197:U:H3	1:2:202:G:H1	1.64	0.46
1:2:1516:G:H4'	4:P:122:THR:HG21	1.96	0.46
12:A:77:ILE:HD12	12:A:122:LEU:HD11	1.97	0.46
15:E:48:LEU:HD23	15:E:61:VAL:HG13	1.97	0.46
20:L:75:GLY:HA3	20:L:88:ILE:HD12	1.98	0.46
25:X:40:PRO:O	25:X:77:ASN:ND2	2.44	0.46
1:2:106:C:H2'	1:2:107:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1005:G:OP2	13:B:162:ARG:NH2	2.46	0.46
1:2:1195:A:H2'	1:2:1196:A:C8	2.51	0.46
15:E:11:ARG:HA	15:E:28:ALA:HB2	1.96	0.46
16:G:56:ASN:HB2	16:G:108:VAL:HG12	1.98	0.46
17:H:87:PHE:HB3	17:H:90:LYS:HE2	1.97	0.46
18:I:89:GLU:O	18:I:92:ARG:HB2	2.15	0.46
1:2:528:A:H2'	1:2:529:A:C8	2.49	0.46
1:2:1485:U:H2'	1:2:1486:A:H8	1.80	0.46
22:O:61:LYS:NZ	22:O:80:ASP:OD2	2.36	0.46
1:2:1257:G:H4'	1:2:1258:A:H5'	1.97	0.46
15:E:35:PRO:HD2	15:E:83:PRO:HG2	1.98	0.46
1:2:1010:G:H2'	1:2:1011:A:C8	2.51	0.46
1:2:1536:G:H2'	1:2:1537:A:C8	2.51	0.46
4:P:44:ARG:NH1	4:P:82:ASP:OD1	2.49	0.46
6:R:91:LEU:HD23	12:A:17:LYS:HG2	1.98	0.46
1:2:1498:A:H5'	1:2:1499:U:H5'	1.98	0.46
19:J:128:VAL:O	19:J:132:GLN:HG2	2.16	0.46
22:O:39:ASP:HB3	22:O:68:GLU:HG2	1.98	0.46
9:Z:58:LEU:HD12	9:Z:62:VAL:HG21	1.98	0.46
16:G:50:VAL:HG22	16:G:113:ILE:HA	1.98	0.46
25:X:70:VAL:HG12	25:X:72:VAL:HG13	1.98	0.46
34:K:921:ILE:HD11	34:K:950:LEU:HD13	1.98	0.46
34:K:1002:MET:SD	34:K:1002:MET:N	2.87	0.46
34:K:308:LEU:HD23	34:K:311:LEU:HD12	1.97	0.46
1:2:296:U:O2'	15:E:131:VAL:O	2.27	0.45
1:2:1545:A:H2'	1:2:1546:G:C8	2.51	0.45
7:S:66:ARG:O	7:S:70:ILE:HG12	2.15	0.45
7:S:74:PRO:HG2	7:S:97:GLN:HG2	1.97	0.45
15:E:100:ARG:HG2	15:E:102:ILE:HG12	1.98	0.45
18:I:57:ALA:HB2	18:I:183:GLY:HA2	1.99	0.45
21:N:87:ASP:N	21:N:87:ASP:OD1	2.47	0.45
34:K:1024:LEU:HD13	34:K:1028:TYR:HB3	1.98	0.45
9:Z:100:VAL:HB	9:Z:108:ILE:HG23	1.98	0.45
22:O:149:ARG:HE	22:O:150:ARG:H	1.63	0.45
34:K:282:ILE:HG13	34:K:319:PRO:HG3	1.97	0.45
1:2:380:G:OP1	18:I:56:ARG:NH2	2.45	0.45
1:2:1213:C:H2'	1:2:1214:A:C8	2.51	0.45
1:2:1562:C:H2'	1:2:1563:G:H8	1.80	0.45
13:B:30:TRP:HZ2	22:O:88:LEU:HD21	1.81	0.45
15:E:151:ASP:OD1	16:G:216:ARG:NH2	2.47	0.45
15:E:187:ALA:O	15:E:245:ARG:NH1	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:7:PHE:HB2	16:G:124:LEU:HD21	1.97	0.45
15:E:126:VAL:HA	15:E:141:THR:HA	1.98	0.45
1:2:74:G:O6	16:G:168:LYS:NZ	2.40	0.45
1:2:107:A:H2'	1:2:108:G:C8	2.51	0.45
1:2:581:U:H4'	26:Y:66:GLY:HA2	1.98	0.45
1:2:1533:A:N6	1:2:1602:U:H3	2.03	0.45
9:Z:42:ASP:OD1	9:Z:42:ASP:N	2.49	0.45
16:G:7:PHE:O	16:G:11:GLY:CA	2.64	0.45
1:2:1113:A:OP1	1:2:1114:U:O2'	2.32	0.45
34:K:936:GLY:O	34:K:939:THR:OG1	2.24	0.45
1:2:391:C:H2'	1:2:392:A:H8	1.82	0.45
1:2:1228:A:H2'	1:2:1229:G:H8	1.80	0.45
1:2:1240:A:C6	4:P:100:LYS:HB2	2.52	0.45
7:S:39:ARG:NH2	8:T:36:THR:O	2.44	0.45
12:A:108:PHE:HB3	12:A:140:VAL:HG11	1.98	0.45
14:C:108:LYS:HE2	14:C:233:LEU:HD13	1.97	0.45
19:J:111:GLN:HE21	19:J:123:ILE:HG13	1.81	0.45
34:K:585:PHE:HA	34:K:589:PHE:HD2	1.81	0.45
1:2:671:A:H4'	1:2:672:A:H5''	1.99	0.45
1:2:1748:G:H2'	1:2:1749:G:C8	2.52	0.45
12:A:5:LEU:HD21	23:V:41:LYS:HA	1.98	0.45
13:B:35:ALA:HB2	13:B:44:ILE:HD11	1.99	0.45
34:K:113:PHE:HB2	34:K:127:VAL:HG11	1.98	0.45
1:2:115:U:OP1	1:2:382:C:O2'	2.32	0.45
1:2:544:G:H2'	1:2:545:A:H8	1.82	0.45
1:2:552:G:H2'	1:2:553:U:C6	2.52	0.45
2:F:103:LEU:HD12	9:Z:67:LEU:HD13	1.97	0.45
2:F:168:THR:O	2:F:172:CYS:N	2.47	0.45
16:G:102:VAL:HG13	16:G:106:LEU:HD22	1.99	0.45
1:2:920:A:OP1	24:W:57:ARG:NE	2.37	0.45
1:2:1657:G:H1	1:2:1667:U:H3	1.65	0.45
13:B:70:SER:OG	22:O:128:ARG:NH1	2.50	0.45
25:X:68:LYS:HB3	25:X:91:LEU:HD22	1.98	0.45
1:2:352:U:O2	20:L:71:ARG:NE	2.38	0.44
1:2:375:U:H2'	1:2:376:A:C8	2.52	0.44
1:2:1562:C:H2'	1:2:1563:G:C8	2.52	0.44
16:G:58:LYS:HD2	16:G:58:LYS:HA	1.86	0.44
25:X:48:LYS:HB2	25:X:48:LYS:HE3	1.74	0.44
7:S:31:THR:HG23	7:S:37:GLY:HA2	1.99	0.44
15:E:31:PRO:HG2	15:E:38:LEU:HB2	1.99	0.44
1:2:639:C:H2'	1:2:640:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1786:U:H2'	1:2:1787:G:C8	2.50	0.44
3:M:49:LEU:HB2	3:M:111:VAL:HB	1.98	0.44
1:2:1597:C:OP2	9:Z:85:ARG:NH1	2.50	0.44
6:R:62:GLN:O	34:K:621:GLN:NE2	2.51	0.44
12:A:108:PHE:HB2	12:A:136:GLU:HB3	1.98	0.44
18:I:131:PRO:O	18:I:134:GLU:HG2	2.18	0.44
1:2:527:C:H2'	1:2:528:A:C8	2.51	0.44
1:2:1129:G:H3'	1:2:1130:G:H21	1.83	0.44
9:Z:68:ILE:HB	9:Z:109:TYR:HB2	2.00	0.44
13:B:179:ASN:HB3	13:B:183:GLU:HB2	1.99	0.44
14:C:88:ILE:HD13	14:C:94:ILE:HD11	2.00	0.44
34:K:888:PHE:HD2	34:K:902:TYR:HB2	1.82	0.44
1:2:1245:G:C6	1:2:1255:G:C2	3.06	0.44
3:M:85:LEU:HA	3:M:88:TRP:HD1	1.83	0.44
1:2:4:C:H4'	14:C:207:ALA:HB2	1.98	0.44
1:2:297:A:H5'	15:E:132:GLY:HA2	2.00	0.44
8:T:42:HIS:HB3	8:T:93:SER:HB3	1.99	0.44
1:2:1513:C:H2'	1:2:1514:G:H8	1.82	0.44
24:W:11:LEU:HD12	24:W:74:VAL:HB	1.99	0.44
34:K:338:HIS:CE1	34:K:340:LEU:HB2	2.53	0.44
8:T:71:GLY:O	8:T:74:SER:OG	2.30	0.43
34:K:468:VAL:HA	34:K:471:MET:SD	2.58	0.43
1:2:12:U:H2'	1:2:13:C:C6	2.53	0.43
1:2:77:A:H2	16:G:175:LYS:HG3	1.82	0.43
1:2:1037:G:H4'	1:2:1845:A:H4'	2.00	0.43
1:2:1101:U:H2'	1:2:1102:G:C8	2.53	0.43
3:M:21:VAL:HG21	3:M:124:ILE:HD13	1.99	0.43
9:Z:92:LEU:HD13	9:Z:109:TYR:HE2	1.82	0.43
18:I:175:ILE:HD13	18:I:185:ALA:HB1	2.00	0.43
1:2:561:A:OP1	19:J:171:GLY:N	2.37	0.43
1:2:1545:A:N3	1:2:1671:G:O2'	2.40	0.43
1:2:1546:G:H1	1:2:1655:C:H1'	1.84	0.43
17:H:93:VAL:HG11	17:H:133:LEU:HD12	1.99	0.43
18:I:116:HIS:HD2	18:I:152:ARG:HD3	1.84	0.43
34:K:1009:THR:HA	34:K:1035:ILE:HG21	1.99	0.43
1:2:1655:C:H2'	1:2:1656:G:H8	1.83	0.43
2:F:30:ILE:HG21	2:F:36:GLN:HA	2.01	0.43
15:E:60:GLU:OE1	26:Y:20:ARG:NH2	2.52	0.43
15:E:115:THR:HG23	15:E:118:GLU:H	1.84	0.43
12:A:119:PRO:HD2	12:A:142:LEU:HD11	2.01	0.43
25:X:46:HIS:CD2	25:X:103:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:1037:LYS:HA	34:K:1040:ALA:HB3	2.01	0.43
1:2:1725:U:H2'	1:2:1726:G:C8	2.54	0.43
15:E:92:ILE:HD12	15:E:99:PHE:HE2	1.83	0.43
34:K:869:VAL:O	34:K:874:ARG:NH2	2.44	0.43
3:M:92:CYS:HB3	3:M:100:PRO:HB3	2.00	0.43
12:A:89:LYS:HA	12:A:89:LYS:HD3	1.73	0.43
34:K:1029:HIS:HA	34:K:1032:LEU:HD12	2.01	0.43
6:R:19:LYS:HA	6:R:19:LYS:HD2	1.77	0.43
13:B:106:THR:HG22	13:B:108:ASP:H	1.84	0.43
18:I:10:LYS:HZ1	20:L:136:LYS:HD2	1.82	0.43
1:2:1195:A:H2'	1:2:1196:A:H8	1.83	0.43
1:2:1746:U:H4'	16:G:65:GLN:NE2	2.34	0.43
6:R:121:GLN:HE21	6:R:121:GLN:HB2	1.59	0.43
1:2:1743:G:N2	1:2:1791:A:H62	2.14	0.43
6:R:21:TYR:HA	6:R:24:LEU:HD12	2.01	0.43
7:S:111:LEU:O	7:S:115:LYS:HG2	2.19	0.43
15:E:100:ARG:HD3	15:E:102:ILE:HD11	2.01	0.43
12:A:73:ASP:HB3	12:A:120:ARG:HB2	2.01	0.42
22:O:74:ALA:HB1	22:O:115:ALA:HB2	2.01	0.42
34:K:516:LEU:HD23	34:K:516:LEU:HA	1.91	0.42
1:2:885:U:O2	1:2:901:G:N2	2.46	0.42
1:2:1779:G:H2'	1:2:1780:G:C8	2.54	0.42
3:M:52:LEU:HD13	3:M:65:VAL:HG21	2.01	0.42
12:A:208:GLU:OE1	12:A:212:LYS:NZ	2.52	0.42
16:G:24:LEU:HB3	16:G:28:TYR:CZ	2.54	0.42
21:N:115:LEU:O	21:N:119:GLU:HG2	2.19	0.42
1:2:639:C:H2'	1:2:640:A:C8	2.54	0.42
1:2:1613:G:OP2	4:P:39:ALA:N	2.53	0.42
18:I:161:LEU:O	18:I:165:GLN:HG3	2.19	0.42
34:K:221:LEU:HD11	34:K:237:VAL:HG12	2.00	0.42
34:K:456:SER:HA	34:K:504:GLN:HB3	2.01	0.42
34:K:1017:PHE:HZ	34:K:1033:VAL:HG12	1.84	0.42
1:2:28:U:H2'	1:2:29:G:C8	2.53	0.42
1:2:483:C:H5''	25:X:48:LYS:HE3	2.02	0.42
1:2:1279:C:H2'	1:2:1280:G:H8	1.85	0.42
1:2:1329:U:H2'	1:2:1330:G:C8	2.54	0.42
13:B:34:LYS:HE3	13:B:34:LYS:HB3	1.83	0.42
18:I:83:TYR:HB3	18:I:101:ILE:HB	2.01	0.42
34:K:311:LEU:HD23	34:K:311:LEU:HA	1.90	0.42
1:2:674:C:H2'	1:2:675:U:C6	2.55	0.42
14:C:169:TYR:OH	14:C:175:GLY:O	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:170:TRP:CE2	14:C:199:PRO:HG3	2.55	0.42
15:E:173:ILE:HD11	15:E:235:TRP:CE2	2.55	0.42
16:G:186:GLN:HA	16:G:189:ARG:HG2	2.02	0.42
17:H:50:GLU:OE2	17:H:58:LYS:HG3	2.20	0.42
1:2:747:U:H2'	1:2:748:C:C6	2.54	0.42
5:Q:32:ILE:HD12	5:Q:68:ILE:HD12	2.01	0.42
12:A:207:PRO:HA	12:A:210:ILE:HB	2.01	0.42
17:H:19:PHE:HZ	17:H:60:ILE:HD12	1.85	0.42
18:I:42:ARG:HD2	18:I:58:LEU:HD12	2.01	0.42
19:J:60:LEU:HD22	19:J:70:ARG:HA	2.01	0.42
1:2:51:U:H2'	1:2:52:G:C8	2.54	0.42
1:2:220:U:H2'	1:2:221:A:C8	2.54	0.42
1:2:1609:C:H5'	7:S:131:VAL:HB	2.00	0.42
1:2:1821:U:H2'	1:2:1822:A:C8	2.53	0.42
4:P:50:ARG:H	4:P:53:GLN:NE2	2.18	0.42
4:P:57:LEU:HD23	4:P:61:ARG:HD2	2.01	0.42
16:G:7:PHE:O	16:G:11:GLY:HA2	2.19	0.42
1:2:1239:U:H5''	4:P:124:LYS:HD2	2.02	0.42
8:T:75:MET:N	8:T:75:MET:SD	2.92	0.42
15:E:44:LEU:HD11	15:E:70:ILE:HG21	2.01	0.42
22:O:106:LYS:HG2	22:O:135:ILE:HG12	2.02	0.42
34:K:863:ILE:O	34:K:866:THR:OG1	2.24	0.42
1:2:433:A:OP1	18:I:25:ARG:NH1	2.43	0.42
1:2:944:A:N6	1:2:982:G:H1	2.14	0.42
5:Q:42:ILE:HG22	5:Q:44:PRO:HD2	2.01	0.42
12:A:78:SER:HB2	12:A:87:VAL:HG21	2.01	0.42
17:H:43:LEU:HD22	17:H:68:GLN:HB3	2.02	0.42
17:H:51:ILE:HG13	17:H:59:ALA:HB3	2.02	0.42
17:H:144:ILE:HB	24:W:52:ILE:HB	2.01	0.42
18:I:165:GLN:HE22	18:I:195:LEU:HD11	1.85	0.42
34:K:223:LYS:HD3	34:K:223:LYS:HA	1.90	0.42
1:2:1172:U:H2'	1:2:1173:A:H8	1.84	0.42
1:2:1726:G:O6	1:2:1808:U:O4	2.38	0.42
34:K:330:LEU:HA	34:K:333:VAL:HG22	2.02	0.42
1:2:798:G:H4'	17:H:108:SER:HB2	2.02	0.41
1:2:1629:C:H5'	7:S:39:ARG:HG2	2.01	0.41
1:2:1659:U:O4	1:2:1664:A:C6	2.73	0.41
13:B:140:VAL:HB	13:B:213:ARG:HD2	2.02	0.41
18:I:150:ASP:HA	18:I:153:LYS:HG2	2.02	0.41
21:N:132:LYS:HD3	21:N:132:LYS:HA	1.84	0.41
22:O:32:HIS:HB2	22:O:43:HIS:HB3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:142:GLU:HA	34:K:143:THR:HA	1.59	0.41
34:K:901:CYS:HA	34:K:904:VAL:HG22	2.02	0.41
1:2:1605:G:OP1	8:T:84:ARG:NH2	2.53	0.41
15:E:29:PRO:HG2	15:E:46:ILE:HD11	2.01	0.41
34:K:357:PRO:HB2	34:K:361:THR:HB	2.02	0.41
1:2:560:A:H8	19:J:173:VAL:HG11	1.85	0.41
1:2:1245:G:O6	1:2:1255:G:N1	2.53	0.41
1:2:1485:U:H2'	1:2:1486:A:C8	2.55	0.41
5:Q:86:GLN:NE2	5:Q:120:LEU:O	2.52	0.41
15:E:45:ILE:HA	15:E:61:VAL:HG11	2.01	0.41
25:X:60:LYS:HE2	25:X:116:PRO:HB3	2.02	0.41
1:2:428:U:H1'	19:J:2:PRO:HA	2.01	0.41
1:2:560:A:C8	19:J:173:VAL:HG11	2.56	0.41
1:2:1692:U:H2'	1:2:1693:G:C8	2.55	0.41
1:2:1798:C:H2'	1:2:1799:G:O4'	2.21	0.41
4:P:110:GLU:HB2	7:S:117:ILE:HD11	2.02	0.41
13:B:124:HIS:HA	13:B:137:LEU:O	2.20	0.41
7:S:43:VAL:HG21	7:S:83:PHE:HE2	1.86	0.41
13:B:35:ALA:HB3	13:B:42:ARG:HA	2.02	0.41
16:G:72:ARG:HD3	16:G:96:SER:HB3	2.03	0.41
34:K:201:GLN:OE1	34:K:204:SER:OG	2.39	0.41
1:2:747:U:H4'	17:H:109:ARG:HD2	2.02	0.41
6:R:30:THR:HA	6:R:33:ARG:HG2	2.03	0.41
6:R:94:GLU:O	6:R:116:ASN:ND2	2.39	0.41
7:S:36:VAL:HG23	7:S:40:TYR:HB3	2.03	0.41
7:S:116:LYS:HB2	7:S:116:LYS:HE3	1.80	0.41
15:E:20:LEU:HD21	15:E:46:ILE:HD12	2.02	0.41
21:N:99:ARG:NH2	21:N:143:SER:OG	2.54	0.41
23:V:21:ASN:HB3	24:W:67:GLY:HA3	2.01	0.41
34:K:182:VAL:O	34:K:186:LYS:HG3	2.21	0.41
1:2:436:G:N7	1:2:471:G:C2	2.89	0.41
1:2:1375:G:H2'	1:2:1376:A:H8	1.84	0.41
9:Z:50:PHE:HZ	9:Z:87:ALA:HB2	1.85	0.41
15:E:171:ASP:OD1	15:E:171:ASP:N	2.54	0.41
18:I:7:ASN:O	18:I:18:ARG:NH1	2.54	0.41
34:K:407:ASP:N	34:K:407:ASP:OD1	2.54	0.41
1:2:559:G:O2'	1:2:560:A:O5'	2.33	0.41
1:2:570:C:O2'	26:Y:34:THR:O	2.29	0.41
3:M:60:MET:HA	3:M:63:LYS:HB2	2.02	0.41
7:S:81:ASP:HA	7:S:84:LEU:HD13	2.03	0.41
9:Z:65:TYR:O	9:Z:67:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:780:LEU:O	34:K:788:GLN:NE2	2.43	0.41
1:2:561:A:H2'	1:2:562:U:O4'	2.21	0.41
1:2:929:G:H2'	1:2:930:C:O4'	2.21	0.41
1:2:1330:G:H1	1:2:1499:U:H3	1.69	0.41
1:2:1649:U:H2'	1:2:1650:A:H8	1.86	0.41
4:P:53:GLN:HA	4:P:56:LEU:HB3	2.03	0.41
12:A:143:PRO:HG3	23:V:32:ILE:HG23	2.03	0.41
17:H:69:LEU:HD22	17:H:96:ALA:HB2	2.03	0.41
17:H:145:ARG:HE	24:W:49:GLU:HB3	1.85	0.41
18:I:84:ASN:ND2	18:I:90:LEU:HD23	2.36	0.41
22:O:39:ASP:N	22:O:39:ASP:OD1	2.53	0.41
34:K:690:LEU:HA	34:K:690:LEU:HD23	1.84	0.41
34:K:1030:ARG:O	34:K:1033:VAL:HG22	2.21	0.41
1:2:49:C:H2'	1:2:472:C:H41	1.85	0.41
1:2:126:G:H2'	1:2:181:A:H1'	2.03	0.41
15:E:233:LYS:HB3	15:E:233:LYS:HE3	1.78	0.41
20:L:23:VAL:HG23	20:L:26:GLY:H	1.86	0.41
1:2:115:U:H2'	1:2:116:U:C6	2.57	0.40
1:2:448:A:H5''	18:I:25:ARG:HA	2.03	0.40
1:2:1004:U:H2'	1:2:1005:G:C8	2.56	0.40
1:2:1277:C:H2'	1:2:1278:A:C8	2.57	0.40
5:Q:17:LYS:HA	5:Q:126:ARG:HG2	2.03	0.40
7:S:63:GLU:HA	7:S:66:ARG:HG2	2.03	0.40
7:S:79:ILE:HA	7:S:80:PRO:HD3	1.97	0.40
12:A:41:ARG:HD3	12:A:47:TYR:CZ	2.56	0.40
15:E:256:LEU:O	15:E:260:GLN:HG2	2.21	0.40
26:Y:80:ASP:OD1	26:Y:81:TYR:N	2.54	0.40
34:K:394:MET:O	34:K:398:HIS:ND1	2.46	0.40
1:2:909:G:H2'	1:2:910:G:C8	2.56	0.40
1:2:913:A:H62	17:H:119:SER:HB3	1.85	0.40
1:2:1579:A:O2'	1:2:1582:C:N4	2.55	0.40
1:2:1659:U:O4	1:2:1664:A:N6	2.54	0.40
13:B:86:LEU:HB3	13:B:98:THR:HB	2.03	0.40
16:G:164:LYS:HB3	16:G:167:LYS:HD2	2.03	0.40
23:V:70:LEU:HD12	23:V:70:LEU:HA	1.91	0.40
26:Y:27:VAL:HG11	26:Y:35:VAL:HG11	2.03	0.40
34:K:187:PHE:HD1	34:K:220:LEU:HD11	1.86	0.40
1:2:5:U:H2'	1:2:6:G:C8	2.55	0.40
1:2:655:A:H4'	1:2:656:G:H3'	2.04	0.40
18:I:194:GLU:HG2	20:L:10:TYR:CE2	2.57	0.40
34:K:725:ASP:OD1	34:K:725:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:218:U:O2	18:I:184:ARG:NH1	2.48	0.40
1:2:1172:U:H2'	1:2:1173:A:C8	2.56	0.40
1:2:1310:U:P	3:M:40:LYS:HZ3	2.45	0.40
2:F:51:HIS:CE1	5:Q:82:TYR:HH	2.38	0.40
4:P:103:ASN:ND2	4:P:119:PHE:O	2.49	0.40
23:V:1:MET:O	23:V:9:VAL:N	2.54	0.40
34:K:171:LEU:O	34:K:175:LEU:HB2	2.21	0.40
34:K:947:VAL:HG21	34:K:965:PHE:CD2	2.56	0.40
1:2:222:U:H5''	20:L:17:PHE:CG	2.57	0.40
1:2:508:A:H3'	1:2:509:G:C8	2.55	0.40
1:2:792:C:H2'	1:2:793:G:H8	1.87	0.40
4:P:52:LYS:O	4:P:55:SER:OG	2.31	0.40
7:S:13:LEU:HB2	7:S:20:ILE:HB	2.03	0.40
34:K:867:LYS:HB2	34:K:919:CYS:SG	2.61	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	
2	F	187/204 (92%)	180 (96%)	7 (4%)	0	100	100
3	M	121/132 (92%)	115 (95%)	6 (5%)	0	100	100
4	P	118/145 (81%)	117 (99%)	1 (1%)	0	100	100
5	Q	120/146 (82%)	114 (95%)	6 (5%)	0	100	100
6	R	112/135 (83%)	110 (98%)	1 (1%)	1 (1%)	17	48
7	S	128/152 (84%)	123 (96%)	5 (4%)	0	100	100
8	T	142/145 (98%)	134 (94%)	8 (6%)	0	100	100
9	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
10	c	59/69 (86%)	56 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	f	71/156 (46%)	62 (87%)	8 (11%)	1 (1%)	11	38
12	A	214/295 (72%)	207 (97%)	7 (3%)	0	100	100
13	B	211/264 (80%)	205 (97%)	6 (3%)	0	100	100
14	C	216/293 (74%)	208 (96%)	7 (3%)	1 (0%)	29	61
15	E	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
16	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
17	H	184/194 (95%)	177 (96%)	7 (4%)	0	100	100
18	I	203/208 (98%)	191 (94%)	12 (6%)	0	100	100
19	J	178/194 (92%)	173 (97%)	4 (2%)	1 (1%)	25	57
20	L	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
21	N	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
22	O	133/151 (88%)	127 (96%)	6 (4%)	0	100	100
23	V	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
24	W	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
25	X	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
26	Y	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
27	b	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
28	e	53/59 (90%)	51 (96%)	2 (4%)	0	100	100
29	x	176/252 (70%)	173 (98%)	3 (2%)	0	100	100
30	y	319/412 (77%)	304 (95%)	15 (5%)	0	100	100
31	u	619/804 (77%)	592 (96%)	27 (4%)	0	100	100
32	w	247/437 (56%)	242 (98%)	5 (2%)	0	100	100
33	t	119/475 (25%)	107 (90%)	11 (9%)	1 (1%)	19	51
34	K	899/1297 (69%)	856 (95%)	42 (5%)	1 (0%)	51	81
35	v	316/552 (57%)	300 (95%)	16 (5%)	0	100	100
All	All	6547/8690 (75%)	6287 (96%)	254 (4%)	6 (0%)	54	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	f	85	TYR
14	C	135	GLY
34	K	381	GLU

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Mol	Chain	Res	Type
33	t	261	GLU
19	J	138	ARG
6	R	42	PRO

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	
2	F	159/170 (94%)	159 (100%)	0	100	100
3	M	104/108 (96%)	103 (99%)	1 (1%)	76	86
4	P	107/130 (82%)	105 (98%)	2 (2%)	57	77
5	Q	103/121 (85%)	101 (98%)	2 (2%)	57	77
6	R	105/122 (86%)	103 (98%)	2 (2%)	57	77
7	S	114/132 (86%)	114 (100%)	0	100	100
8	T	114/115 (99%)	113 (99%)	1 (1%)	78	87
9	Z	64/103 (62%)	64 (100%)	0	100	100
10	c	52/62 (84%)	51 (98%)	1 (2%)	57	77
11	f	65/140 (46%)	65 (100%)	0	100	100
12	A	180/243 (74%)	180 (100%)	0	100	100
13	B	194/231 (84%)	194 (100%)	0	100	100
14	C	184/225 (82%)	184 (100%)	0	100	100
15	E	224/225 (100%)	224 (100%)	0	100	100
16	G	200/218 (92%)	198 (99%)	2 (1%)	76	86
17	H	167/174 (96%)	167 (100%)	0	100	100
18	I	178/180 (99%)	178 (100%)	0	100	100
19	J	160/168 (95%)	160 (100%)	0	100	100
20	L	135/142 (95%)	133 (98%)	2 (2%)	65	81
21	N	130/131 (99%)	130 (100%)	0	100	100
22	O	105/119 (88%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	66/67 (98%)	66 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	113/115 (98%)	113 (100%)	0	100	100
26	Y	108/115 (94%)	107 (99%)	1 (1%)	78	87
27	b	74/76 (97%)	74 (100%)	0	100	100
28	e	45/48 (94%)	44 (98%)	1 (2%)	52	74
29	x	150/208 (72%)	150 (100%)	0	100	100
30	y	285/367 (78%)	282 (99%)	3 (1%)	73	85
31	u	550/705 (78%)	549 (100%)	1 (0%)	93	97
32	w	217/370 (59%)	217 (100%)	0	100	100
33	t	113/434 (26%)	111 (98%)	2 (2%)	59	78
34	K	778/1094 (71%)	776 (100%)	2 (0%)	92	96
35	v	274/489 (56%)	272 (99%)	2 (1%)	84	90
All	All	5729/7460 (77%)	5704 (100%)	25 (0%)	91	95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	101	ARG
4	P	54	HIS
4	P	64	LYS
5	Q	62	ARG
5	Q	105	LYS
6	R	5	ARG
6	R	121	GLN
8	T	122	LYS
10	c	67	ARG
16	G	92	ARG
16	G	98	ARG
20	L	69	ARG
20	L	144	LYS
26	Y	46	LYS
28	e	58	ASN
30	y	31	ARG
30	y	247	GLN
30	y	397	ARG
31	u	499	ARG

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Mol	Chain	Res	Type
33	t	252	ARG
33	t	442	ARG
34	K	186	LYS
34	K	632	ARG
35	v	126	ARG
35	v	276	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
6	R	121	GLN
8	T	42	HIS
17	H	162	GLN
28	e	58	ASN
32	w	397	GLN
34	K	811	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1609/1873 (85%)	401 (24%)	23 (1%)

All (401) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	5	U
1	2	9	U
1	2	33	G
1	2	41	G
1	2	42	A
1	2	44	U
1	2	46	A
1	2	56	G
1	2	58	C
1	2	59	U
1	2	62	G
1	2	66	G
1	2	67	C
1	2	68	A

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Mol	Chain	Res	Type
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	103	A
1	2	113	G
1	2	115	U
1	2	126	G
1	2	127	C
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	147	A
1	2	155	G
1	2	163	U
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	190	G
1	2	215	G
1	2	291	G
1	2	292	A
1	2	295	C
1	2	306	C
1	2	309	G
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	321	C
1	2	332	G
1	2	333	G
1	2	338	G

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Mol	Chain	Res	Type
1	2	343	A
1	2	347	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	381	C
1	2	384	U
1	2	385	G
1	2	386	C
1	2	387	C
1	2	399	C
1	2	400	C
1	2	408	A
1	2	409	C
1	2	413	G
1	2	418	A
1	2	421	G
1	2	429	C
1	2	441	C
1	2	448	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	482	G
1	2	487	U
1	2	492	C
1	2	496	C
1	2	502	C
1	2	530	U
1	2	531	A
1	2	534	G
1	2	535	G
1	2	537	C
1	2	544	G
1	2	545	A
1	2	547	G

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Mol	Chain	Res	Type
1	2	548	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	594	A
1	2	598	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	608	C
1	2	614	C
1	2	617	G
1	2	628	A
1	2	629	A
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	659	G
1	2	660	C
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	685	A
1	2	686	U
1	2	687	C
1	2	688	U

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Mol	Chain	Res	Type
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	799	U
1	2	809	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	845	G
1	2	847	A
1	2	852	G
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	885	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	898	U
1	2	903	A
1	2	905	C
1	2	908	A
1	2	913	A
1	2	914	U
1	2	919	A
1	2	920	A

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Mol	Chain	Res	Type
1	2	933	G
1	2	934	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	978	G
1	2	981	A
1	2	988	C
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1031	A
1	2	1040	G
1	2	1045	U
1	2	1049	A
1	2	1053	C
1	2	1058	A
1	2	1059	G
1	2	1060	A
1	2	1062	A
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1087	A
1	2	1088	U
1	2	1096	G
1	2	1099	G
1	2	1100	A
1	2	1108	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1121	G
1	2	1126	G
1	2	1138	C

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Mol	Chain	Res	Type
1	2	1139	C
1	2	1148	A
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1170	A
1	2	1171	G
1	2	1195	A
1	2	1199	A
1	2	1200	A
1	2	1201	U
1	2	1204	A
1	2	1205	C
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1248	U
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1253	A
1	2	1254	C
1	2	1255	G
1	2	1256	G
1	2	1257	G
1	2	1258	A
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1264	C
1	2	1269	G
1	2	1274	G

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Mol	Chain	Res	Type
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1296	U
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1304	U
1	2	1305	C
1	2	1306	U
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1315	U
1	2	1316	C
1	2	1317	C
1	2	1321	G
1	2	1322	G
1	2	1324	G
1	2	1325	G
1	2	1327	G
1	2	1335	G
1	2	1337	C
1	2	1338	G
1	2	1339	U
1	2	1348	G
1	2	1358	U
1	2	1372	U
1	2	1378	A
1	2	1382	A
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1445	U
1	2	1446	A
1	2	1454	A

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Mol	Chain	Res	Type
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1476	A
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1509	U
1	2	1512	C
1	2	1519	U
1	2	1523	C
1	2	1526	G
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1544	C
1	2	1548	G
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1567	G
1	2	1569	A
1	2	1571	G
1	2	1574	C
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1590	C

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Mol	Chain	Res	Type
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1611	G
1	2	1617	G
1	2	1618	C
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1632	G
1	2	1637	A
1	2	1639	G
1	2	1647	A
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1683	C
1	2	1686	G
1	2	1699	A
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1751	C
1	2	1756	C
1	2	1775	U
1	2	1776	G
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1805	G
1	2	1816	G
1	2	1819	A
1	2	1826	G
1	2	1839	U

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Mol	Chain	Res	Type
1	2	1841	C
1	2	1859	A
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1870	A
1	2	1872	G
1	2	1873	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	465	A
1	2	547	G
1	2	604	A
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1316	C
1	2	1326	U
1	2	1338	G
1	2	1493	C
1	2	1511	U
1	2	1534	C
1	2	1558	C
1	2	1601	A
1	2	1648	G
1	2	1726	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

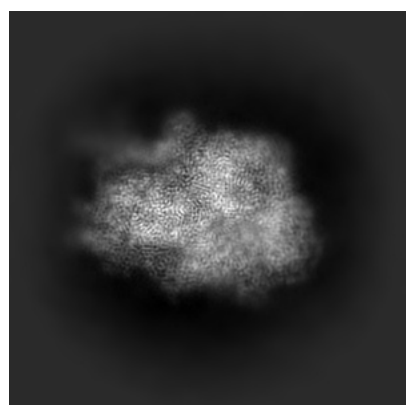
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32807. These allow visual inspection of the internal detail of the map and identification of artifacts.

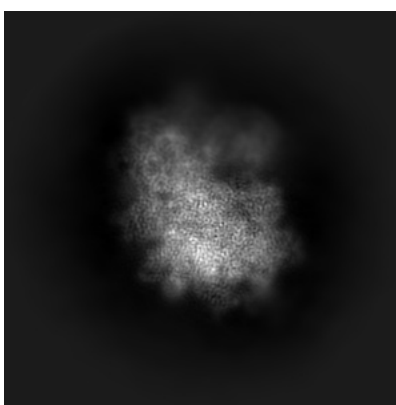
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

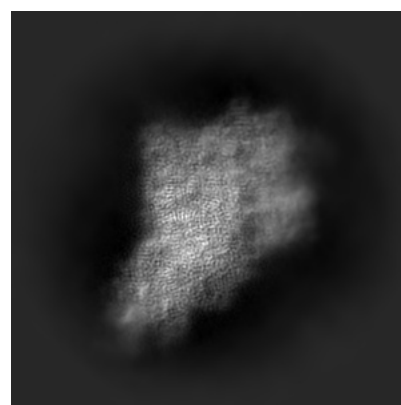
6.1.1 Primary map



X



Y

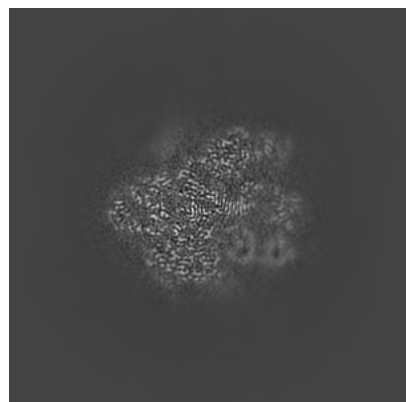


Z

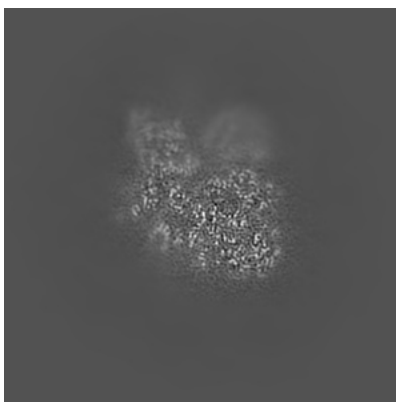
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

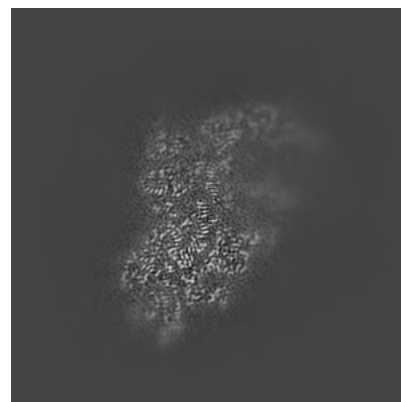
6.2.1 Primary map



X Index: 180



Y Index: 180

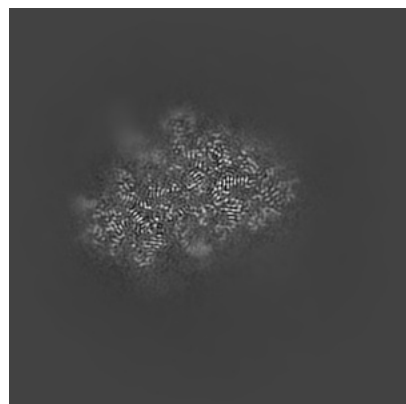


Z Index: 180

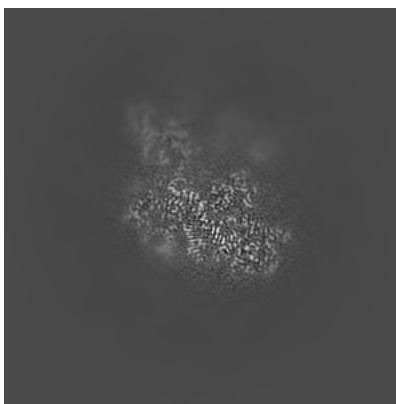
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

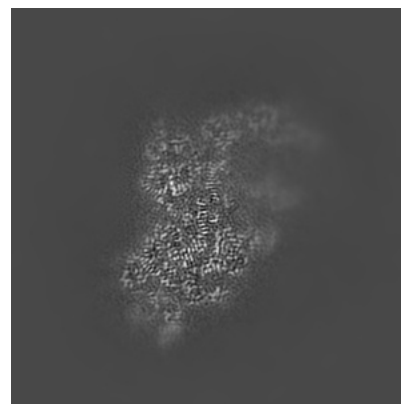
6.3.1 Primary map



X Index: 143



Y Index: 172

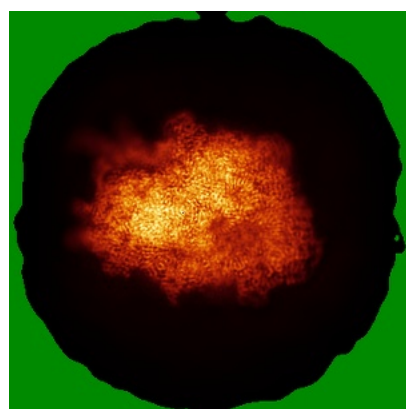


Z Index: 181

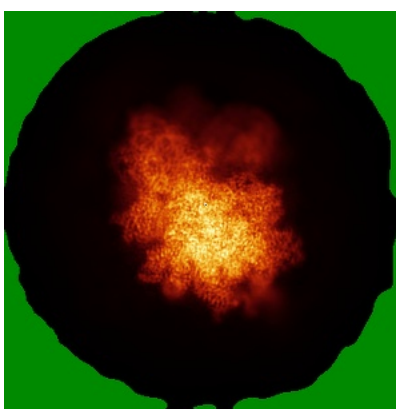
The images above show the largest variance slices of the map in three orthogonal directions.

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

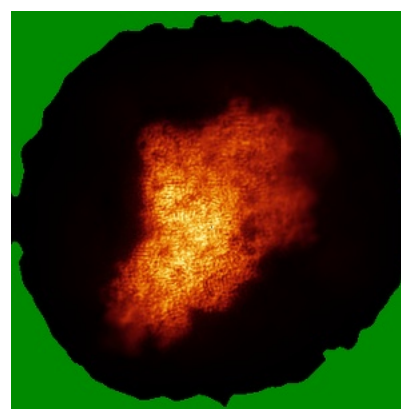
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

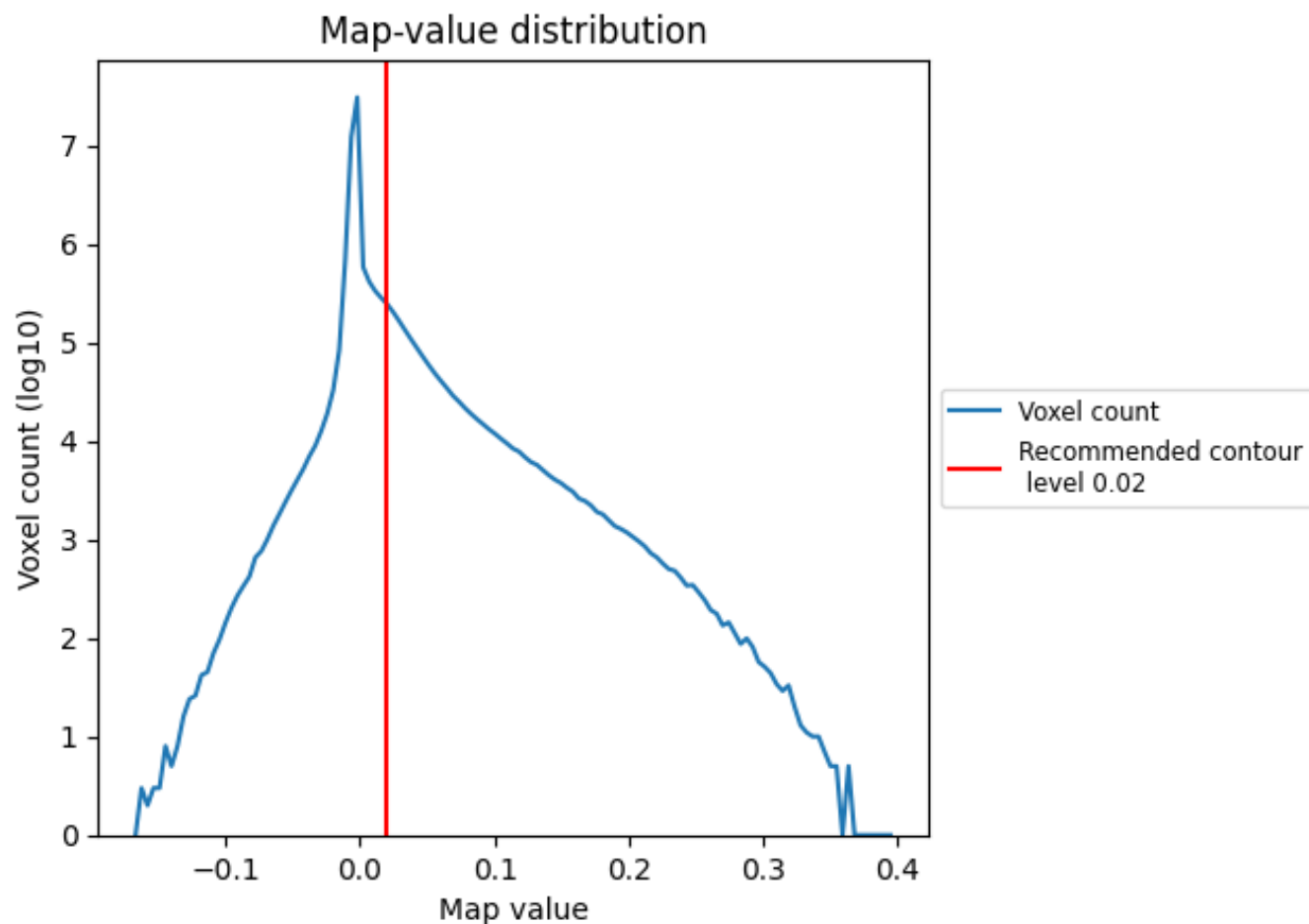
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

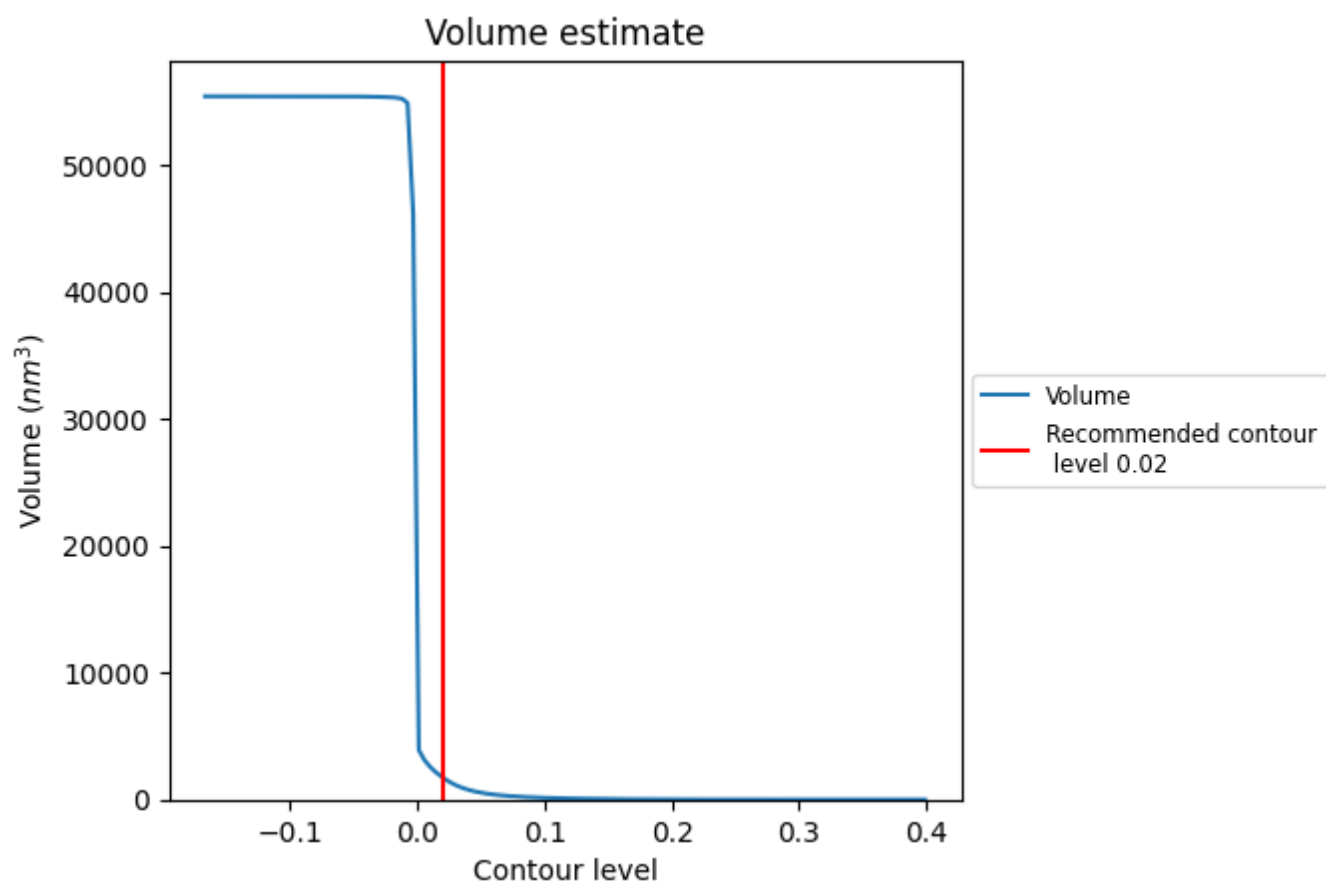
This section contains the results of statistical analysis of the map.

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.

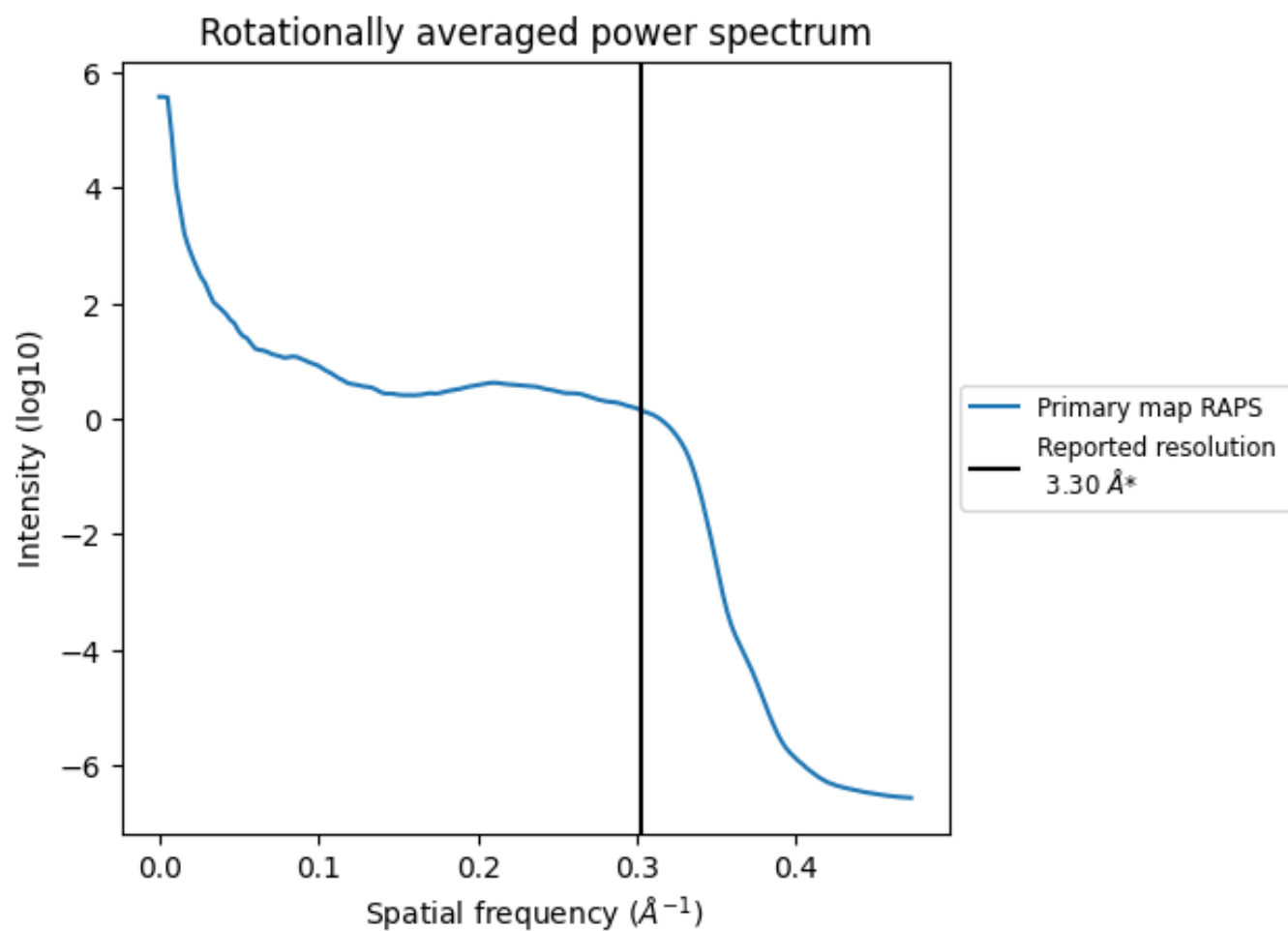
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1731 nm³; this corresponds to an approximate mass of 1563 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 ⓘ

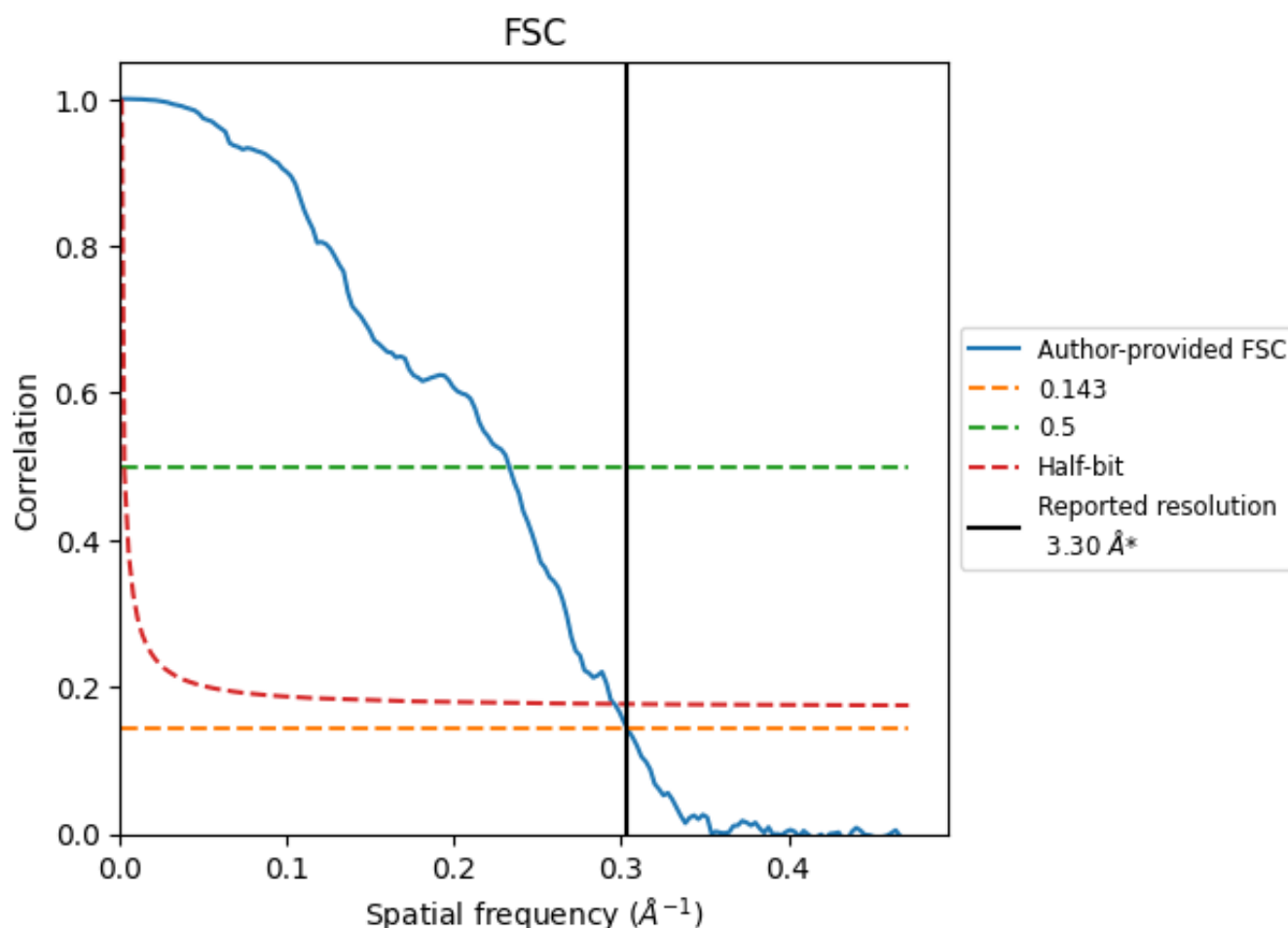


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

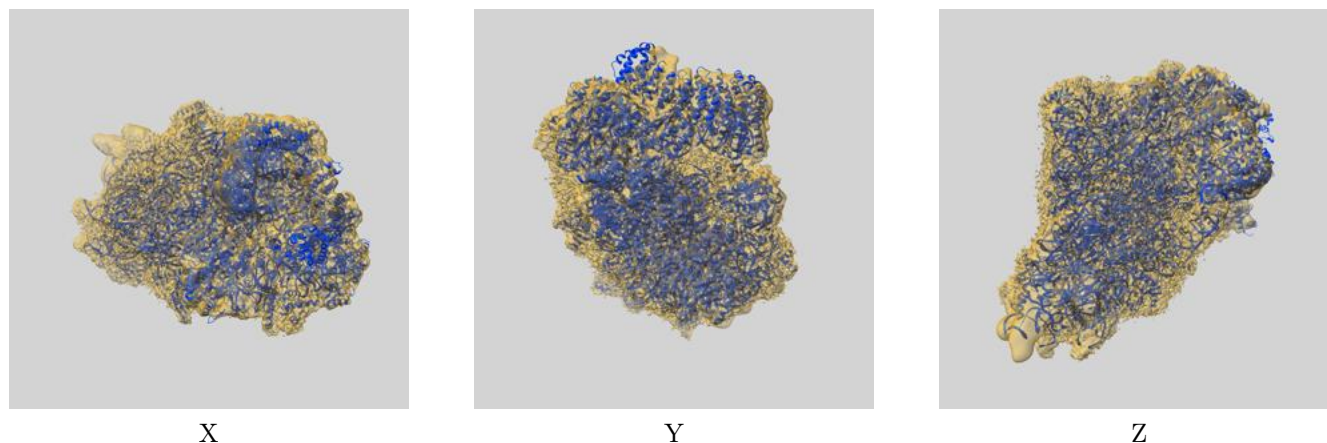
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	4.29	3.38
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

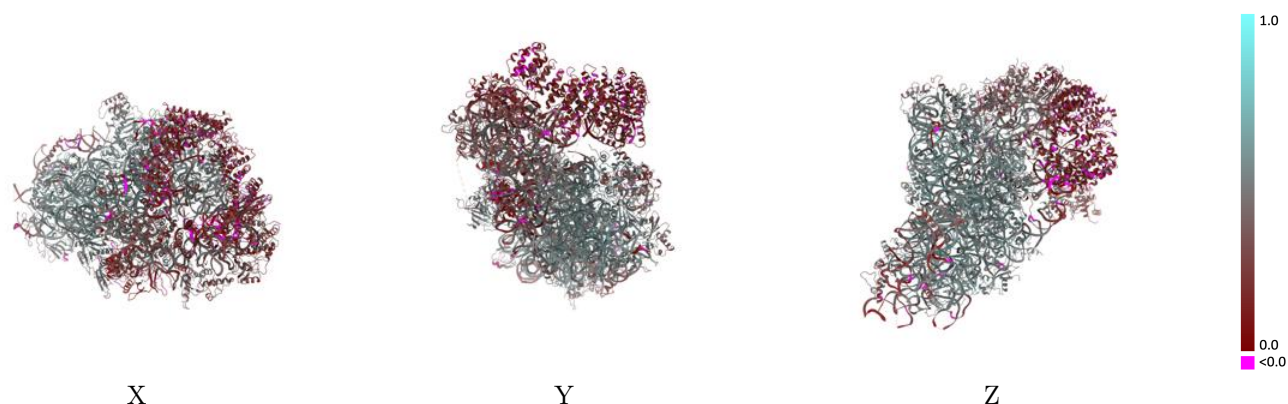
This section contains information regarding the fit between EMDB map EMD-32807 and PDB model 7WU0. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



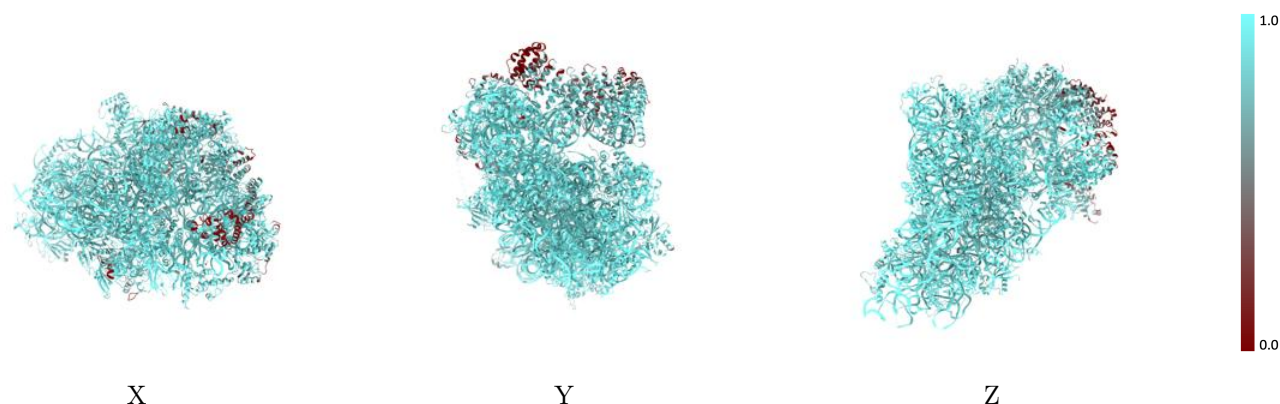
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



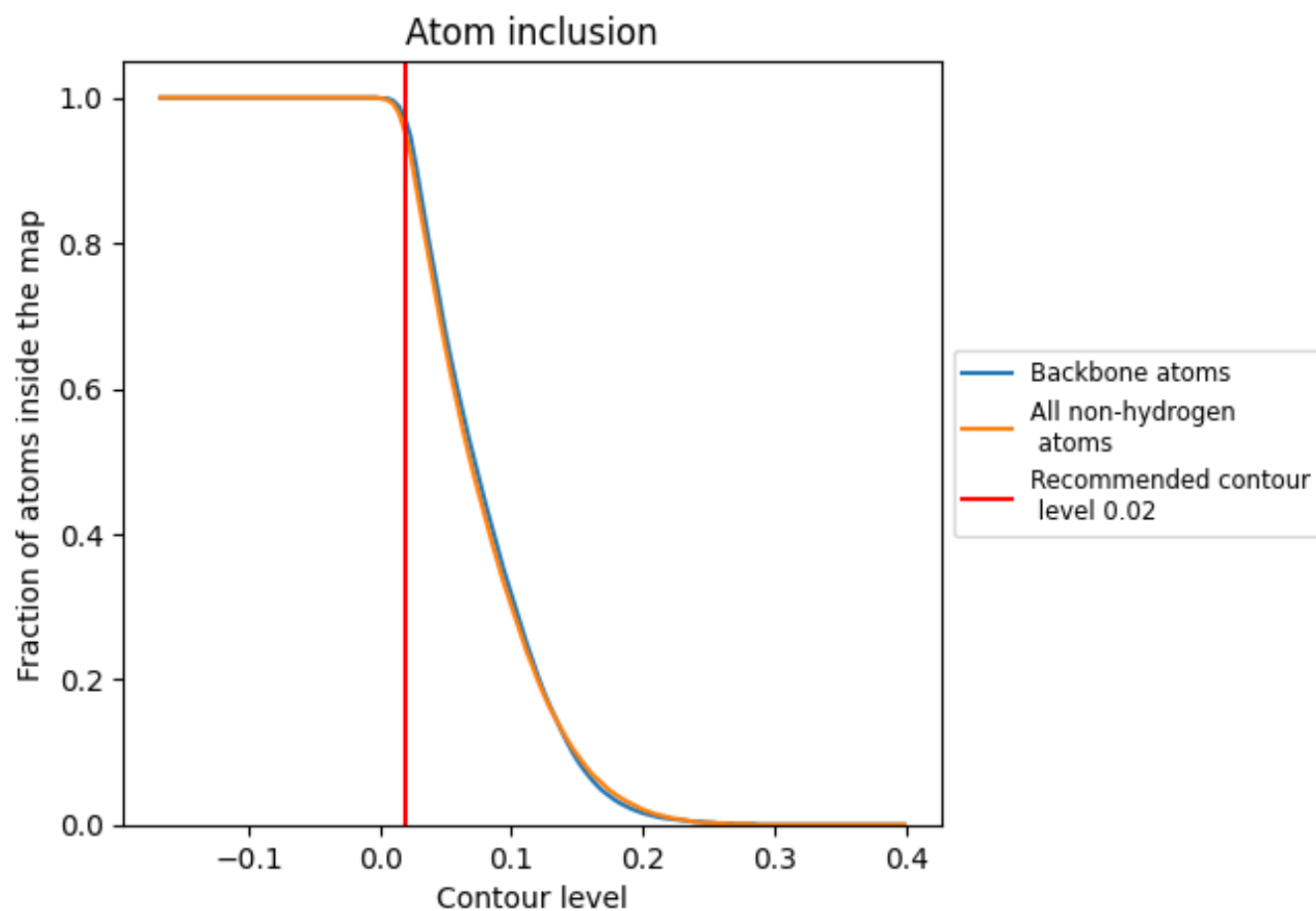
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).









































































9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.4140
2	 0.9890	 0.4500
A	 0.9870	 0.5250
B	 0.9650	 0.4910
C	 0.9900	 0.5260
E	 0.9870	 0.5430
F	 0.9530	 0.3560
G	 0.9360	 0.3940
H	 0.9480	 0.4270
I	 0.9640	 0.4730
J	 0.9970	 0.5470
K	 0.6950	 0.1360
L	 0.9640	 0.5220
M	 0.6720	 0.1650
N	 0.9920	 0.5220
O	 0.9570	 0.4680
P	 0.9340	 0.4020
Q	 0.8940	 0.2670
R	 0.9440	 0.2840
S	 0.8200	 0.3030
T	 0.8930	 0.2880
V	 0.9940	 0.5380
W	 0.9960	 0.5600
X	 0.9920	 0.5620
Y	 0.9920	 0.5290
Z	 0.7610	 0.2710
b	 0.9830	 0.5040
c	 0.9740	 0.4320
e	 0.9790	 0.4940
f	 0.8480	 0.2130
t	 0.9570	 0.3590
u	 0.9820	 0.4910
v	 0.9610	 0.2360
w	 0.9570	 0.3300
x	 0.9840	 0.5170
y	 0.9640	 0.4000

