



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:49 PM UTC

PDB ID : 5OQL / pdb_00005oql
EMDB ID : EMD-3847
Title : Cryo-EM structure of the 90S pre-ribosome from *Chaetomium thermophilum*
Authors : Cheng, J.; Kellner, N.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2017-08-12
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

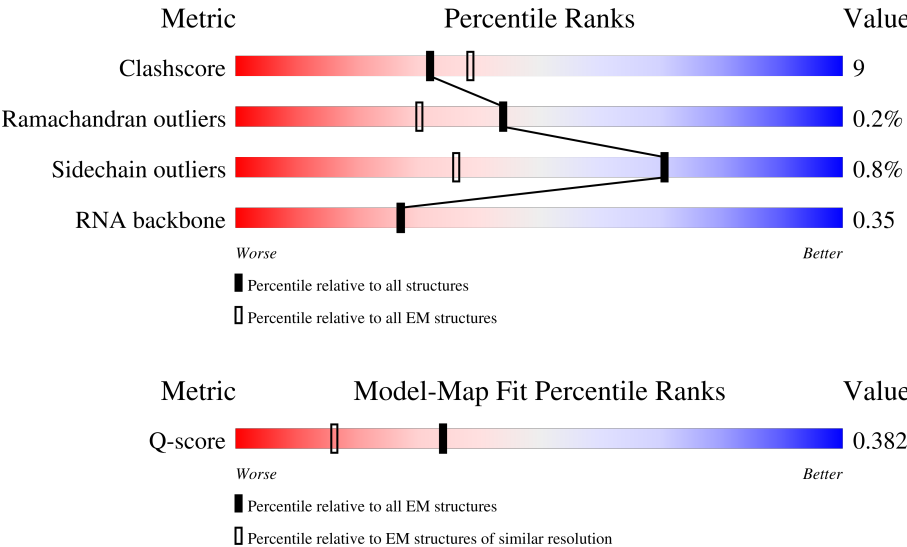
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	904	
2	B	907	
3	C	648	

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Mol	Chain	Length	Quality of chain
4	D	884	
5	E	414	
6	F	558	
7	G	1802	
8	H	270	
9	I	962	
10	J	912	
11	K	938	
12	L	557	
13	M	960	
14	N	618	
15	O	1049	
16	P	194	
17	Q	391	
18	R	313	
18	S	313	
19	T	523	
20	U	582	
21	V	127	
21	W	127	
22	X	630	
23	Y	411	
24	Z	1163	
25	a	183	
26	b	297	

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Mol	Chain	Length	Quality of chain
27	c	785	
28	d	446	
29	e	252	
29	f	252	
30	g	322	
31	h	259	
32	i	1073	
32	j	1073	
33	k	203	
34	l	255	
35	m	264	
36	n	212	
37	o	239	
38	p	203	
39	q	202	
40	r	190	
41	s	151	
42	t	150	
43	u	143	
44	v	161	
45	w	130	
46	x	145	
47	y	136	
48	z	68	
49	0	311	

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Mol	Chain	Length	Quality of chain
50	1	2568	7%26%21%6%47%
51	2	274	18%45%30%9%16%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 135120 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	827	Total	C	N	O	S	0	0
			6242	4029	1114	1077	22		

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	69	Total	C	N	O	0	0
			537	338	121	78		

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	74	Total	C	N	O	0	0
			588	371	120	97		

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	292	Total	C	N	O	S	0	0
			2170	1383	403	373	11		

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	331	Total	C	N	O	S	0	0
			2591	1674	504	399	14		

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	429	Total	C	N	O	S	0	0
			3282	2103	611	557	11		

- Molecule 7 is a protein called Utp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	363	Total	C	N	O	S	0	0
			2772	1784	501	473	14		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1456	915	306	230	5		

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	155	Total	C	N	O	S	0	0
			1230	788	222	214	6		

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	151	Total	C	N	O	S	0	0
			1201	765	214	222			

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	147	Total	C	N	O	S	0	0
			1139	725	215	194	5		

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	280	Total	C	N	O	S	0	0
			2070	1320	379	363	8		

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	284	Total	C	N	O	S	0	0
			2134	1386	364	378	6		

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	443	Total	C	N	O	S	0	0
			3435	2181	646	598	10		

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	864	Total	C	N	O	S	0	0
			6446	4152	1189	1079	26		

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	190	Total	C	N	O	S	0	0
			1460	928	281	241	10		

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	182	Total	C	N	O		0	0
			905	541	182	182			

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	242	Total	C	N	O	S	0	0
			1778	1149	327	293	9		
18	S	237	Total	C	N	O	S	0	0
			1816	1154	318	335	9		

- Molecule 19 is a protein called Putative nucleolar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	387	Total	C	N	O	S	0	0
			2866	1836	527	492	11		

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	405	Total	C	N	O	S	0	0
			3035	1954	539	532	10		

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	W	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	347	Total	C	N	O	S	0	0
			2686	1707	486	481	12		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	345	Total	C	N	O	S	0	0
			2594	1648	465	472	9		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	639	Total	C	N	O	S	0	0
			4848	3145	903	782	18		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	291	Total	C	N	O	S	0	0
			2279	1445	437	389	8		

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	175	Total	C	N	O	S	0	0
			1387	869	269	244	5		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	439	Total	C	N	O	S	0	0
			3436	2158	663	600	15		

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		
29	f	215	Total	C	N	O	S	0	0
			1683	1067	293	313	10		

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	174	Total	C	N	O	S	0	0
			1393	890	250	244	9		

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	167	Total	C	N	O	S	0	0
			1288	817	234	231	6		

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	659	Total	C	N	O		0	0
			3254	1936	659	659			
32	j	677	Total	C	N	O		0	0
			3342	1988	677	677			

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	117	Total	C	N	O	S	0	0
			930	589	179	158	4		

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	214	Total	C	N	O	S	0	0
			1735	1105	322	303	5		

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	258	Total	C	N	O	S	0	0
			2057	1305	386	359	7		

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	192	Total	C	N	O	S	0	0
			1447	918	277	245	7		

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	237	Total	C	N	O	S	0	0
			1911	1192	384	330	5		

- Molecule 38 is a protein called 40S ribosomal protein S7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	159	Total	C	N	O	S	0	0
			1279	810	237	232			

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	201	Total	C	N	O	S	0	0
			1622	1009	330	282	1		

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	159	Total	C	N	O	S	0	0
			1242	801	255	184	2		

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	49	Total	C	N	O	S	0	0
			416	270	82	64			

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	115	Total	C	N	O	S	0	0
			791	492	154	141	4		

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	157	Total	C	N	O	S	0	0
			1286	825	248	208	5		

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	w	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	94	Total	C	N	O	S	0	0
			684	445	129	108	2		

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	93	Total	C	N	O	S	0	0
			752	481	140	129	2		

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	61	Total	C	N	O	0	0
			455	284	97	74		

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	0	92	Total	C	N	O	S	0	0
			694	426	144	120	4		

- Molecule 50 is a RNA chain called 35S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	1350	Total	C	N	O	P	0	0
			28796	12851	5157	9440	1348		

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

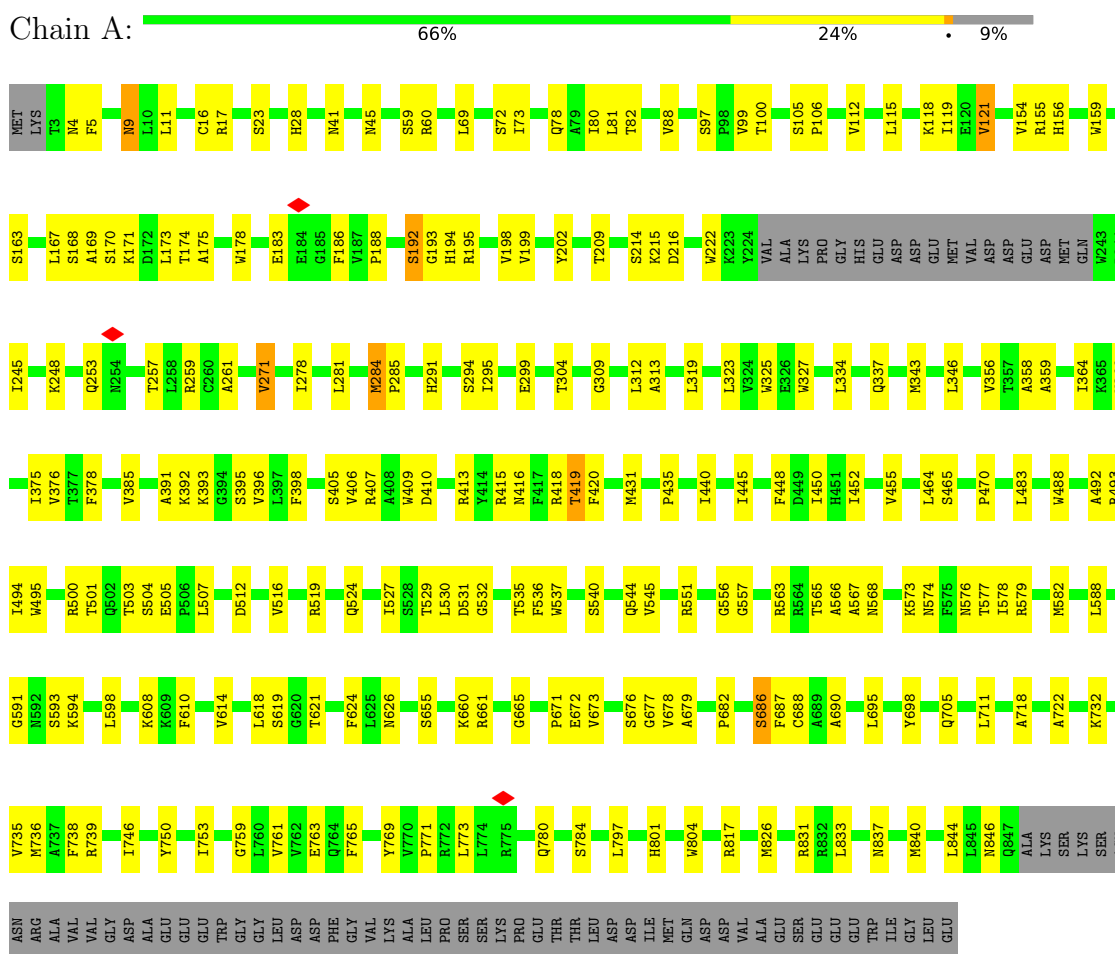
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	P	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: Periodic tryptophan protein 2-like protein



• Molecule 2: Utp2



[illegible]

Chain D: 26% 7% 67%

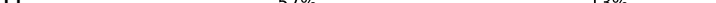


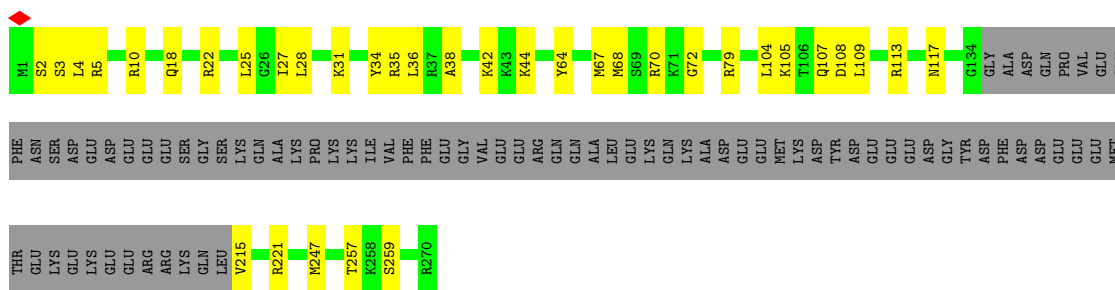




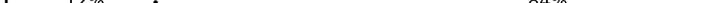
[illegible]

- Molecule 8: U3 small nucleolar RNA-associated protein 11

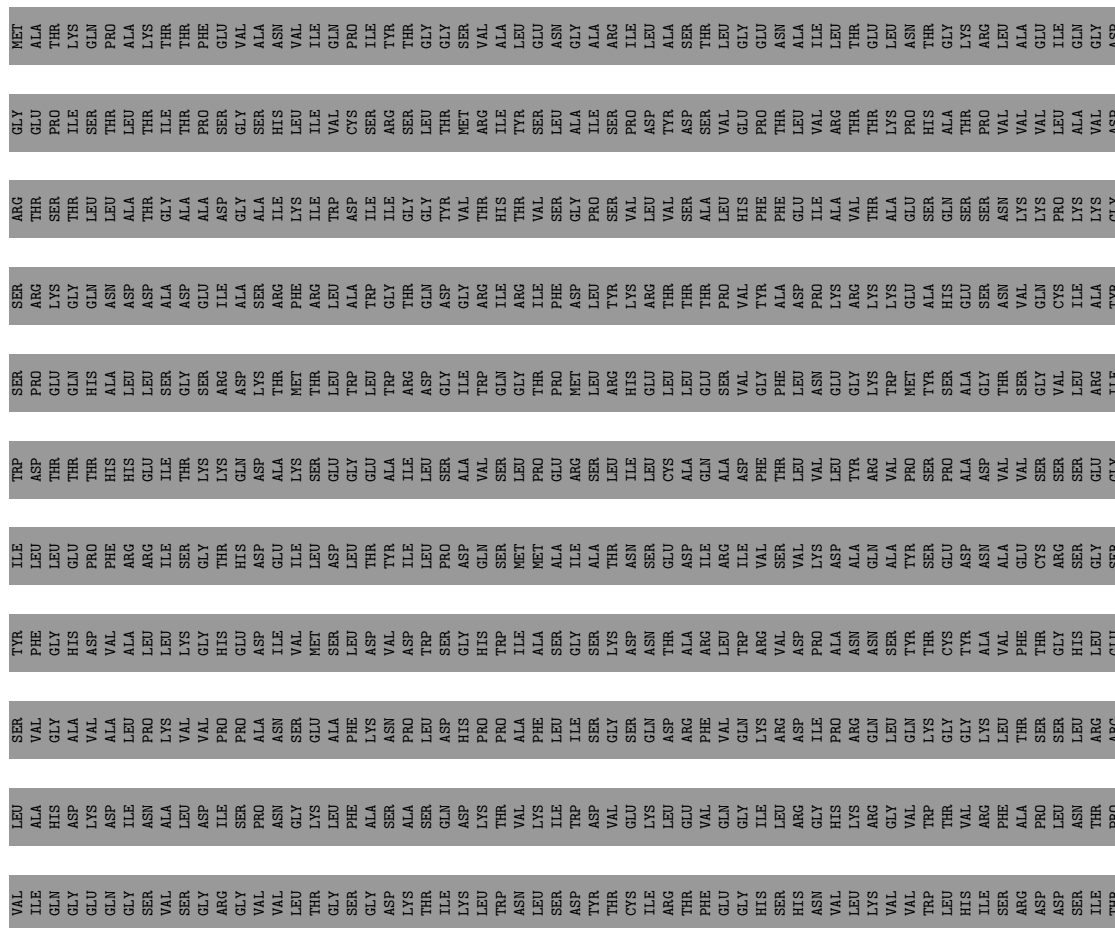
Chain H:  57% 13% 30%



- Molecule 9: Utp12

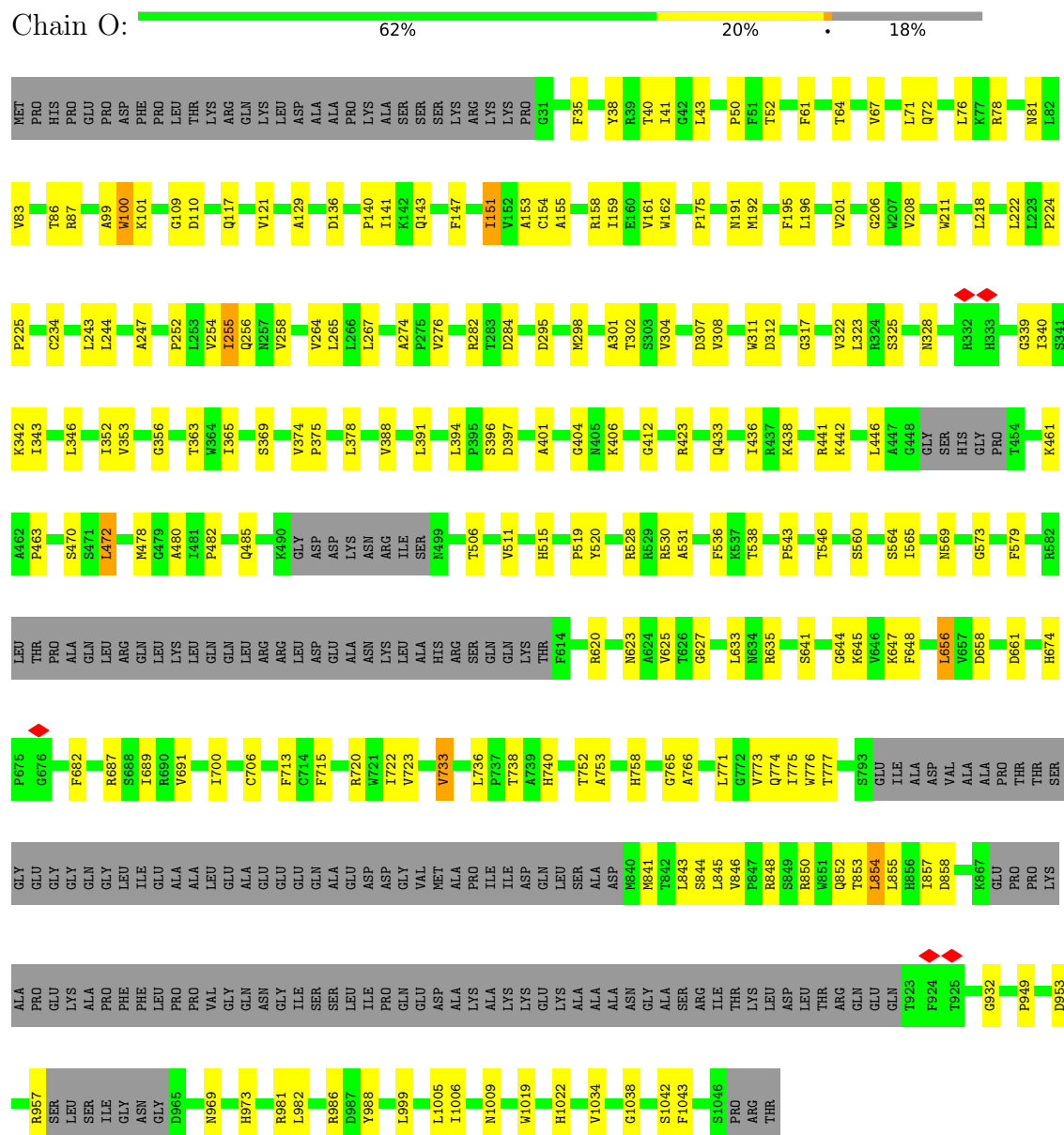
Chain I:  12% 84%

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

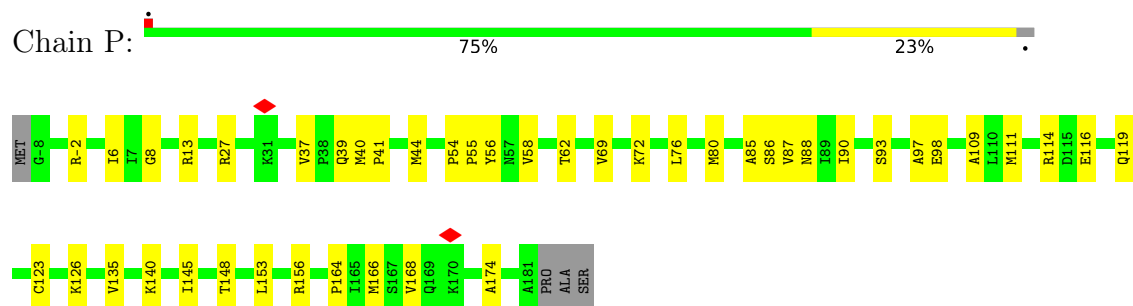




- Molecule 15: Putative U3 snoRNP protein

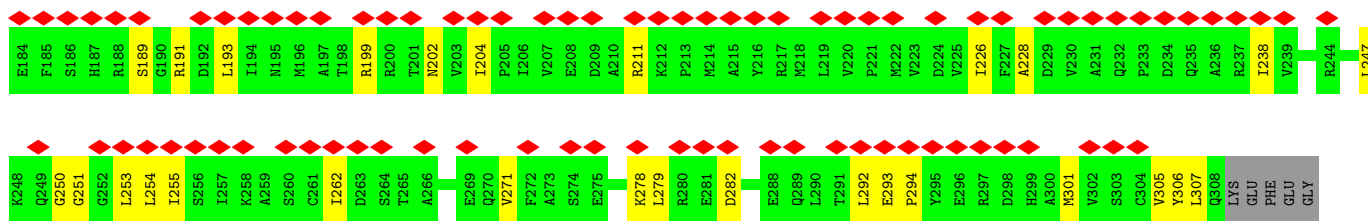


- Molecule 16: Utp24

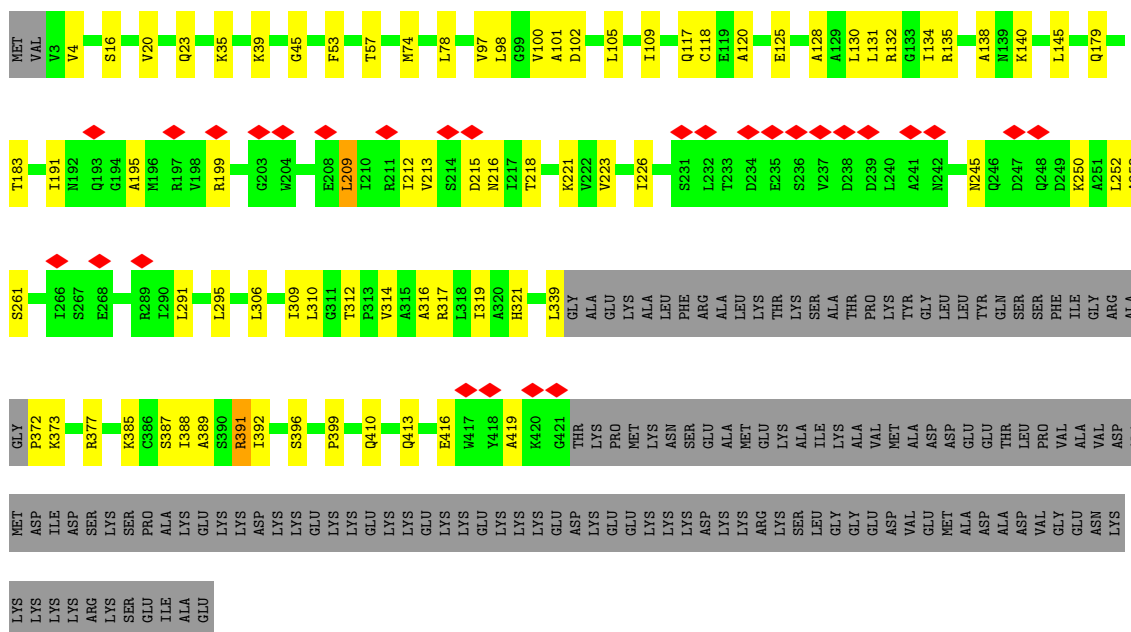


- Molecule 17: Utp30

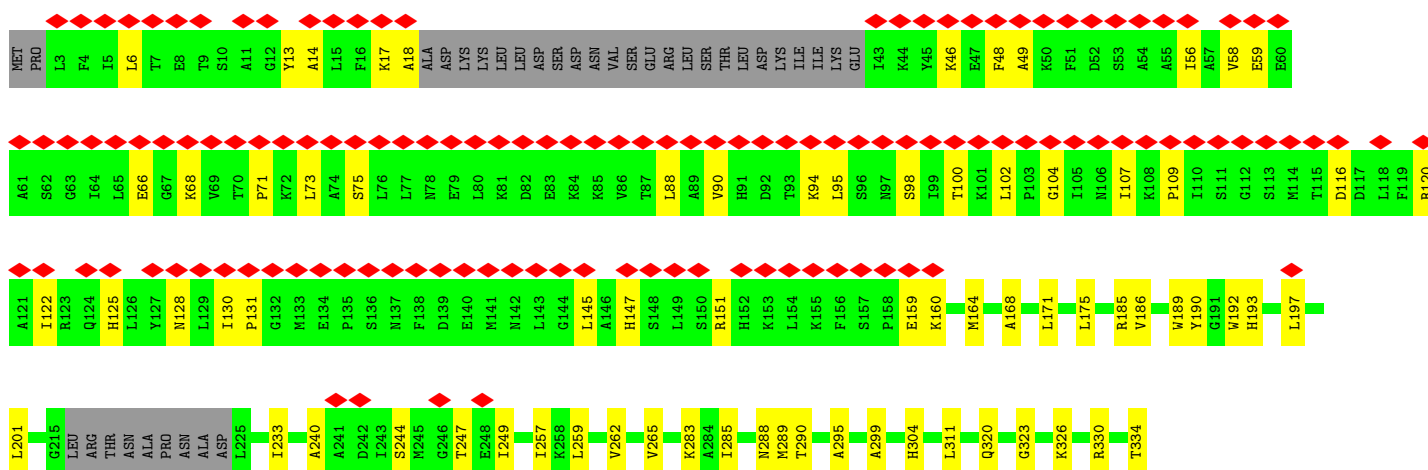




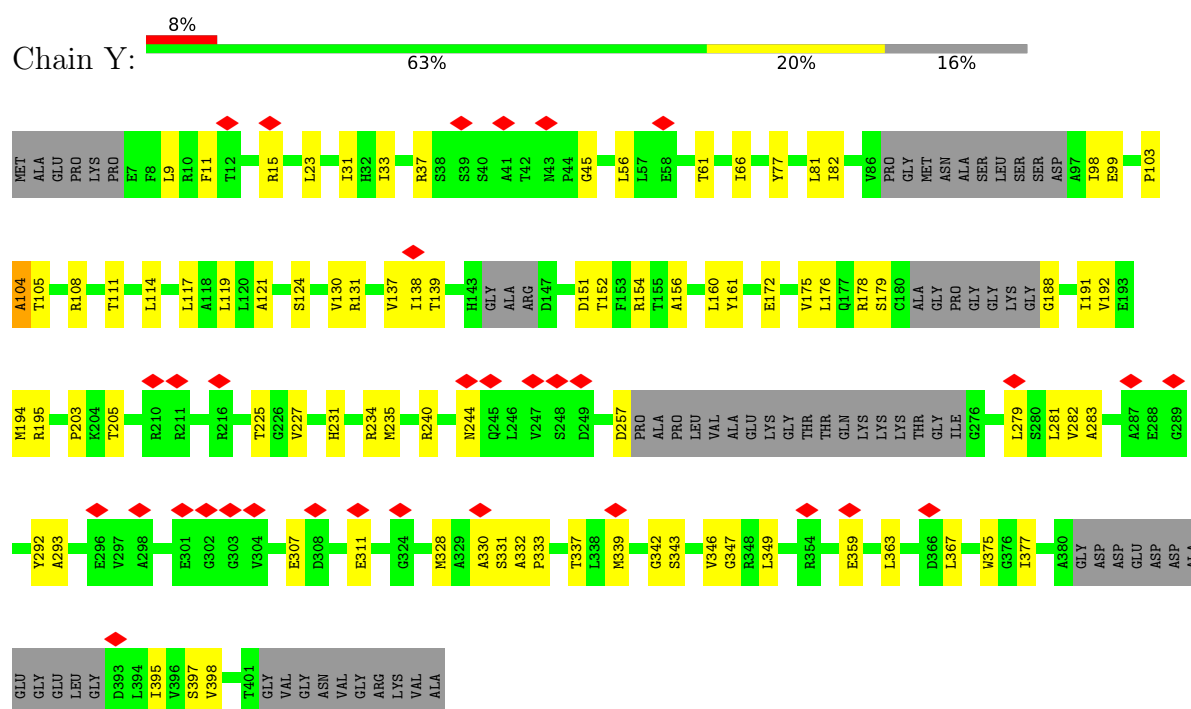
• Molecule 19: Putative nucleolar protein



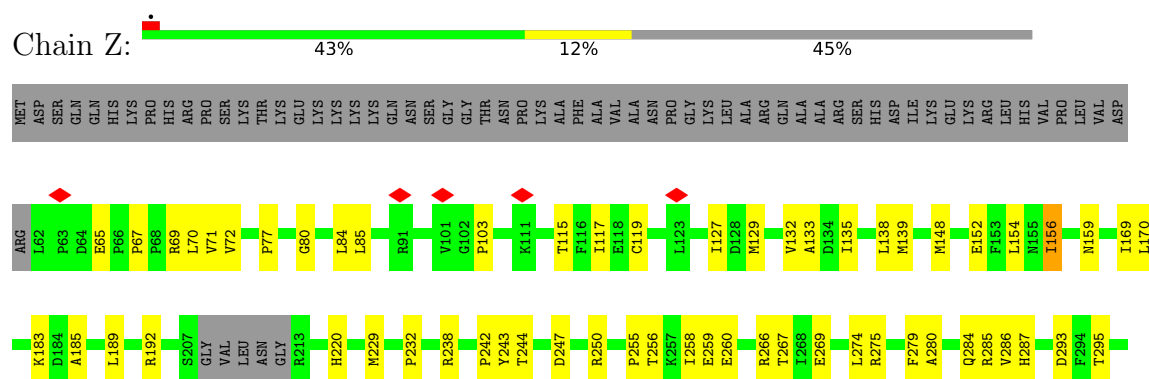
• Molecule 20: Nop58



- Molecule 23: RNA 3'-terminal phosphate cyclase-like protein.

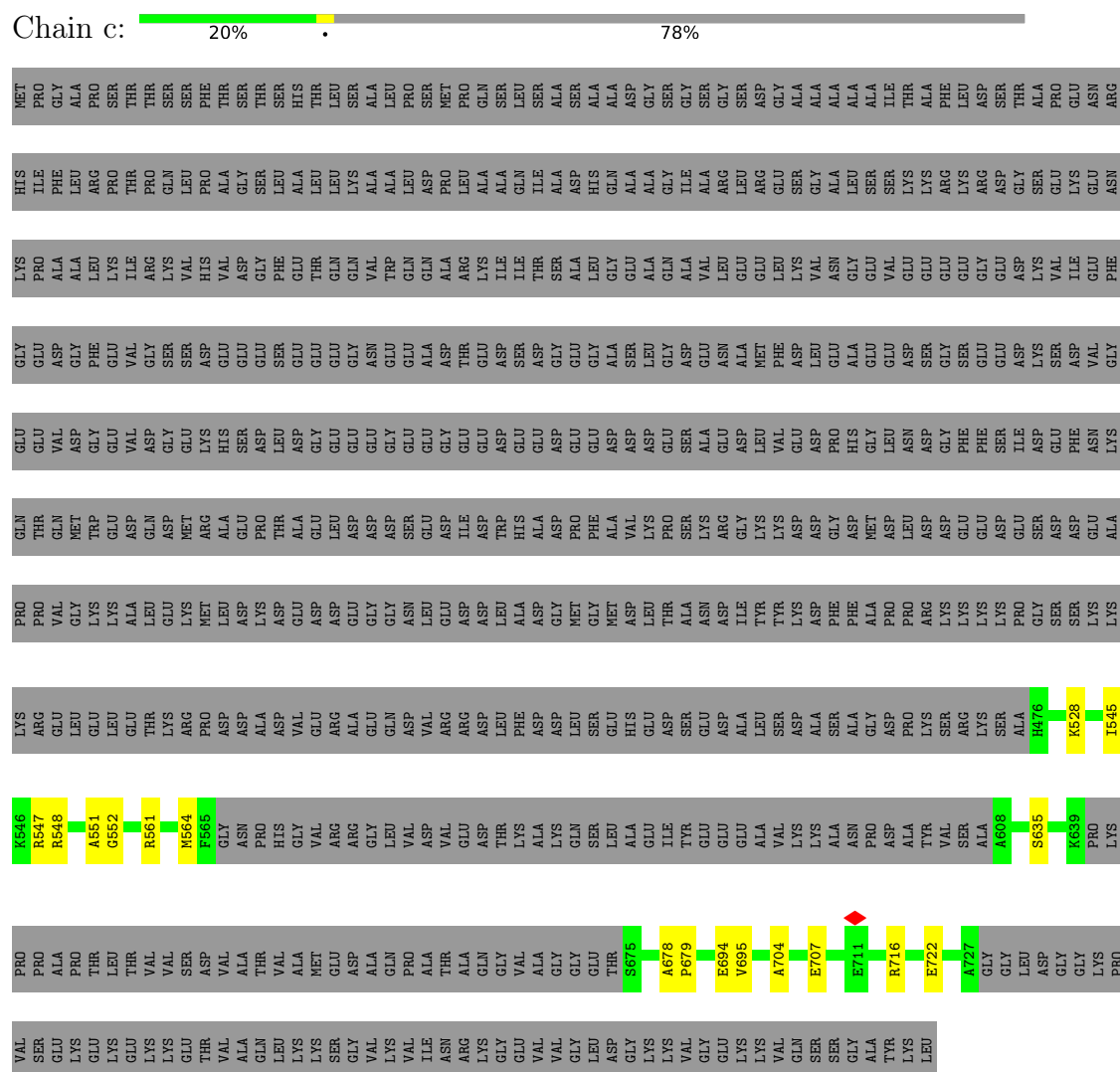


- Molecule 24: Bms1

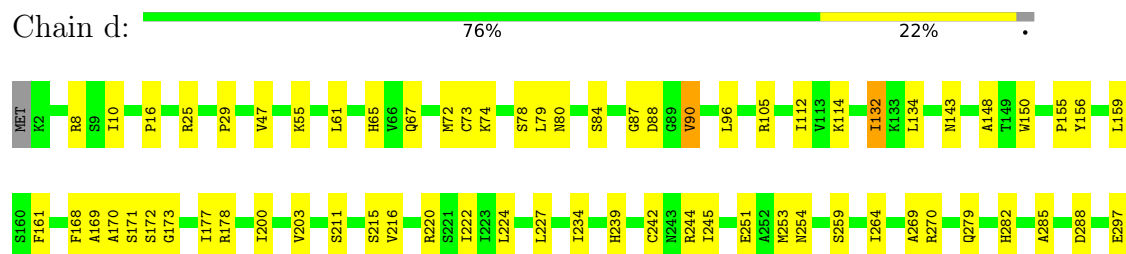


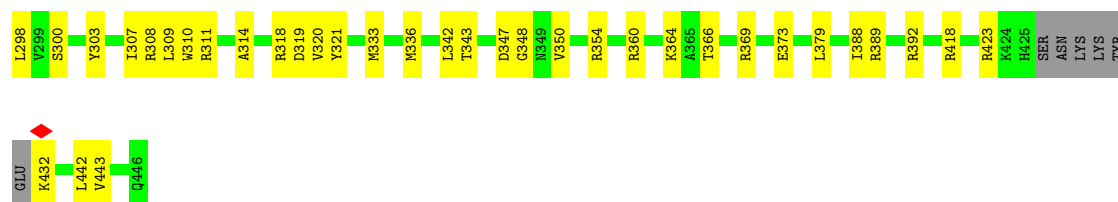


- Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

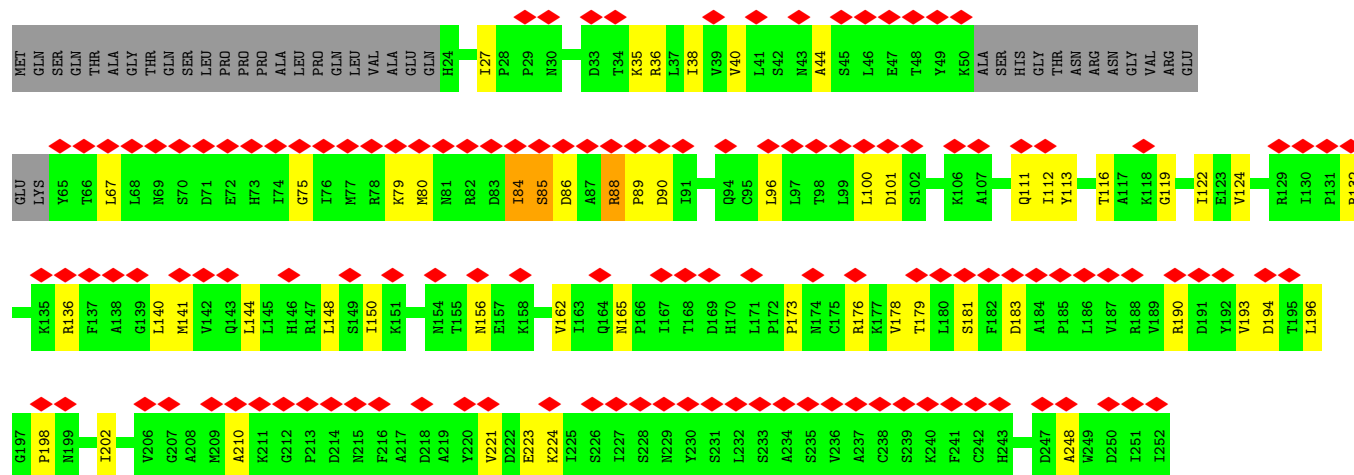


- Molecule 28: Sof1

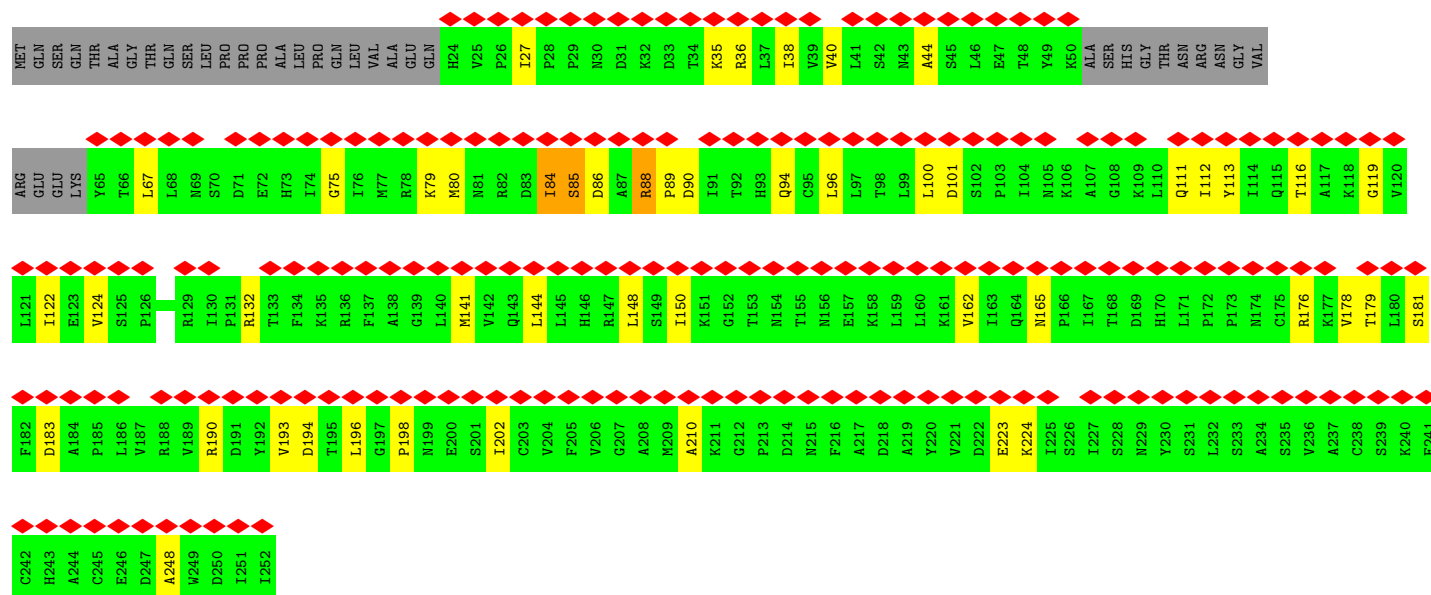
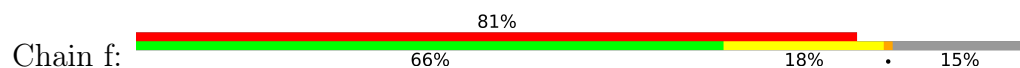




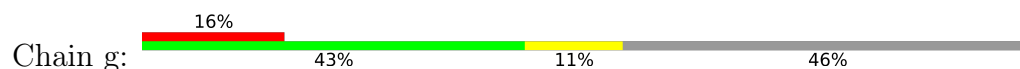
• Molecule 29: Emg1

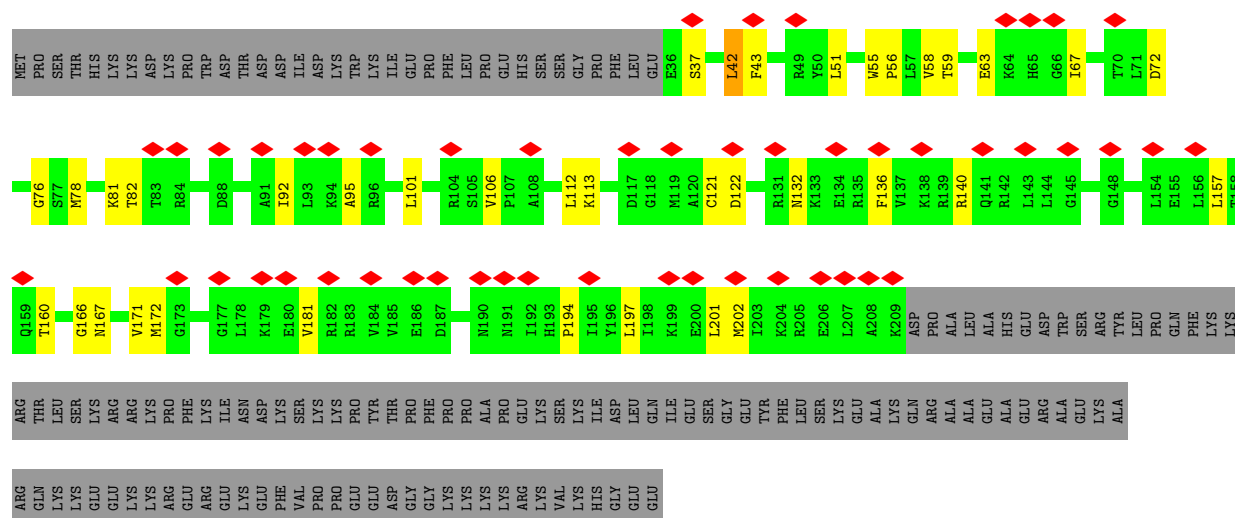


• Molecule 29: Emg1

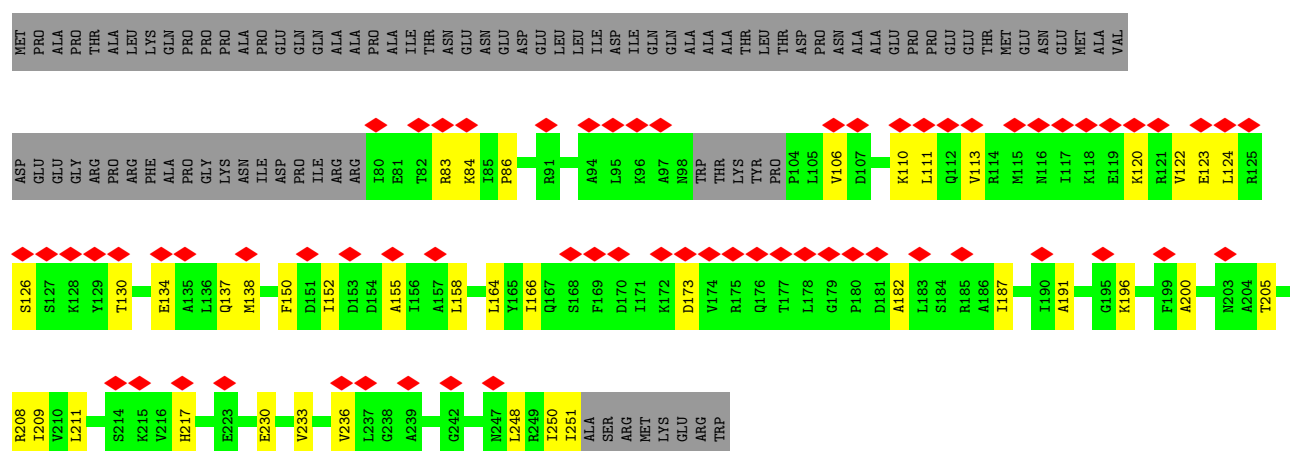


• Molecule 30: KRR1 small subunit processome component

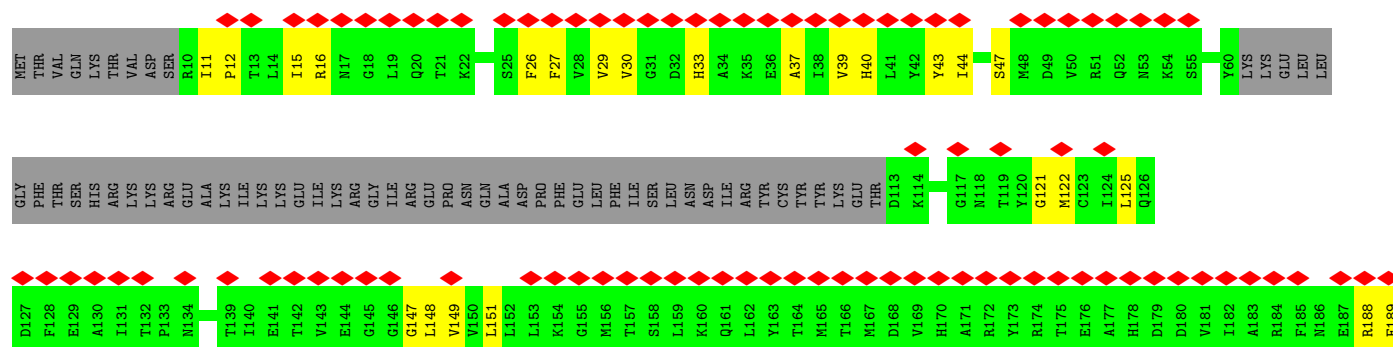




• Molecule 31: Pre-rRNA-processing protein PNO1



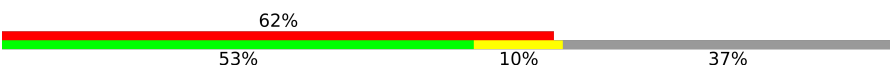
• Molecule 32: RNA cytidine acetyltransferase



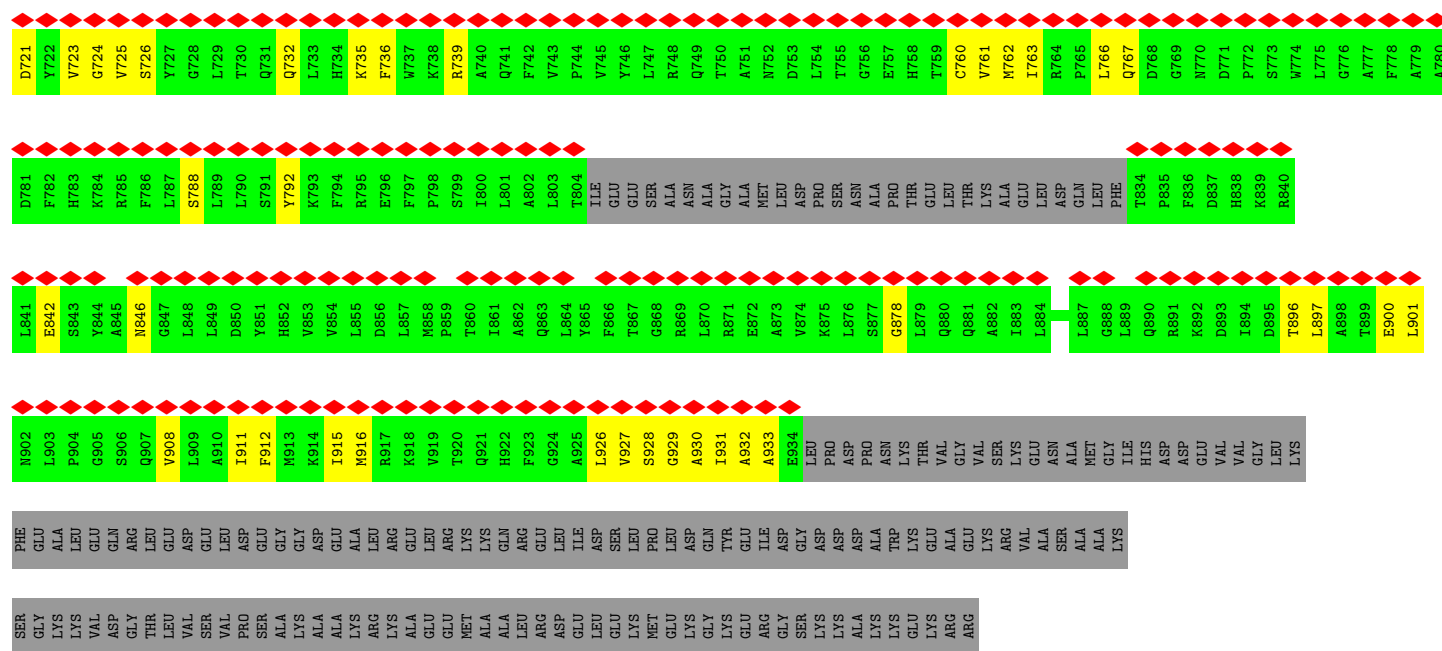


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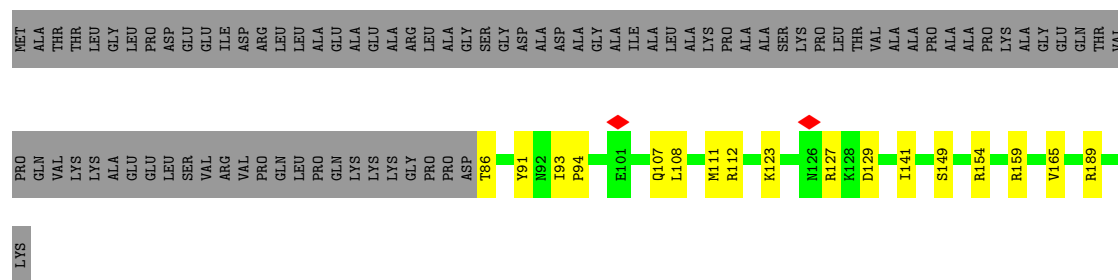
● Molecule 32: RNA cytidine acetyltransferase

Chain j: 

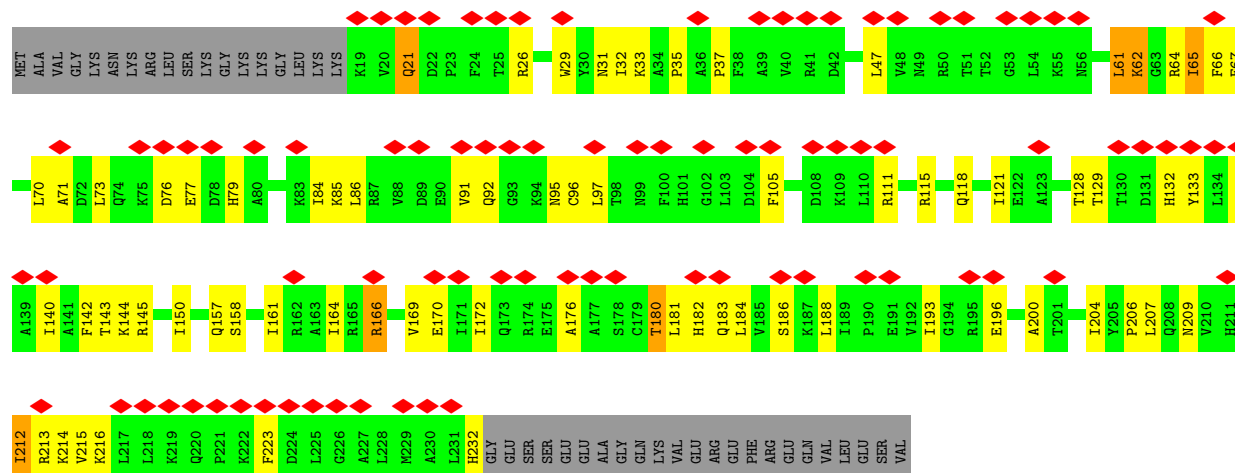
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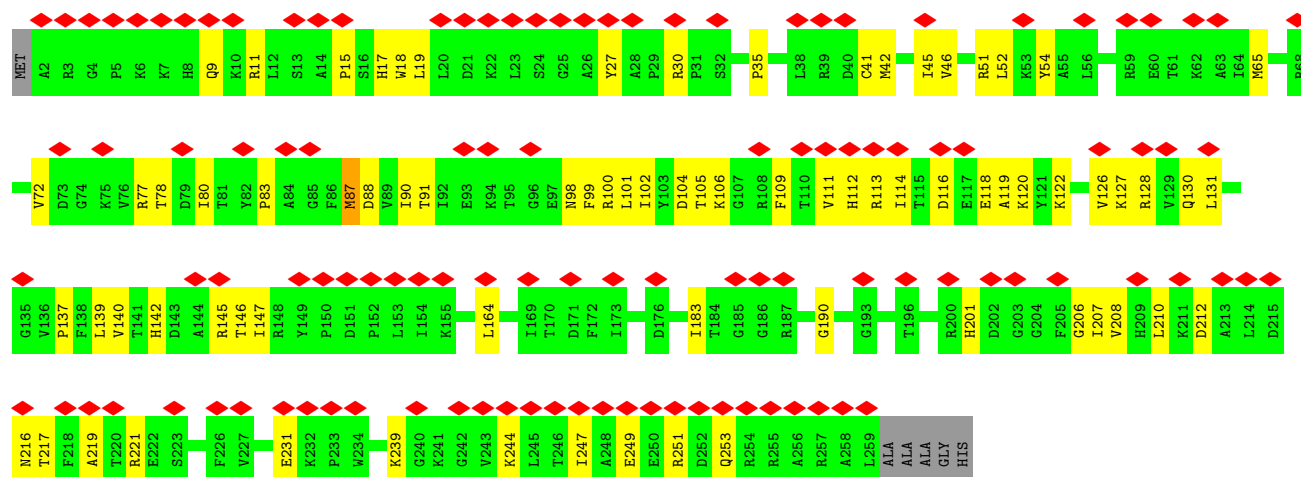
• Molecule 33: Fcf2



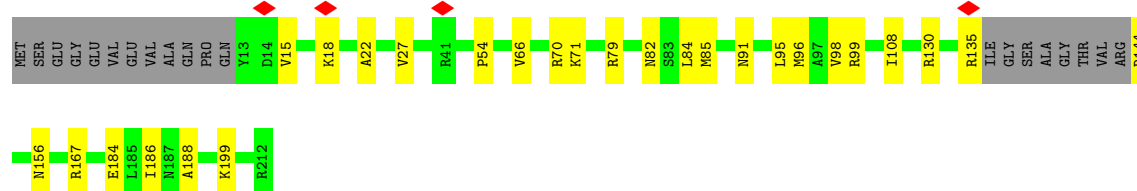
• Molecule 34: 40S ribosomal protein S1



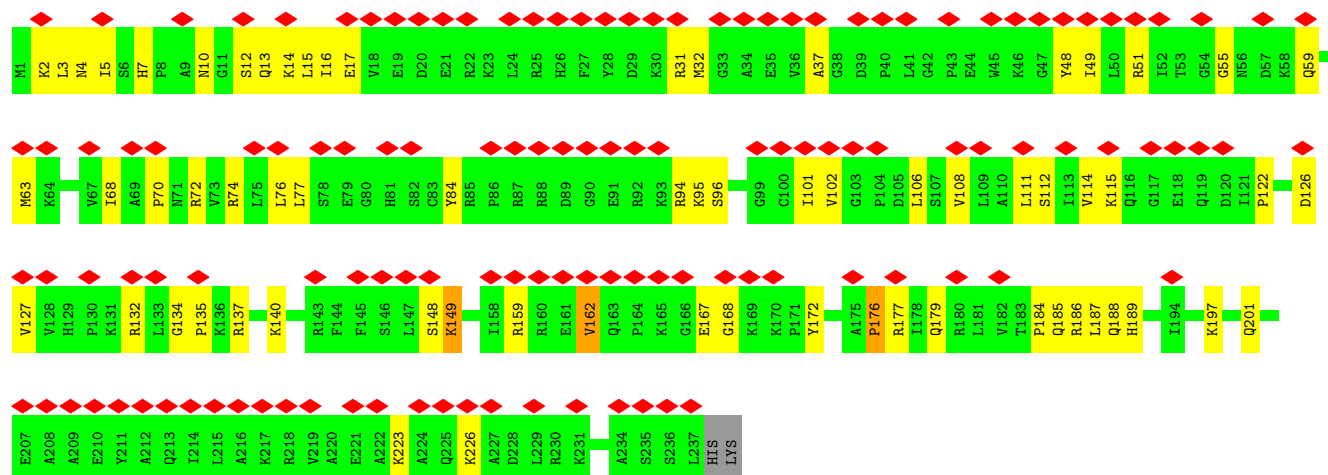
Chain m: 43% 69% 28%

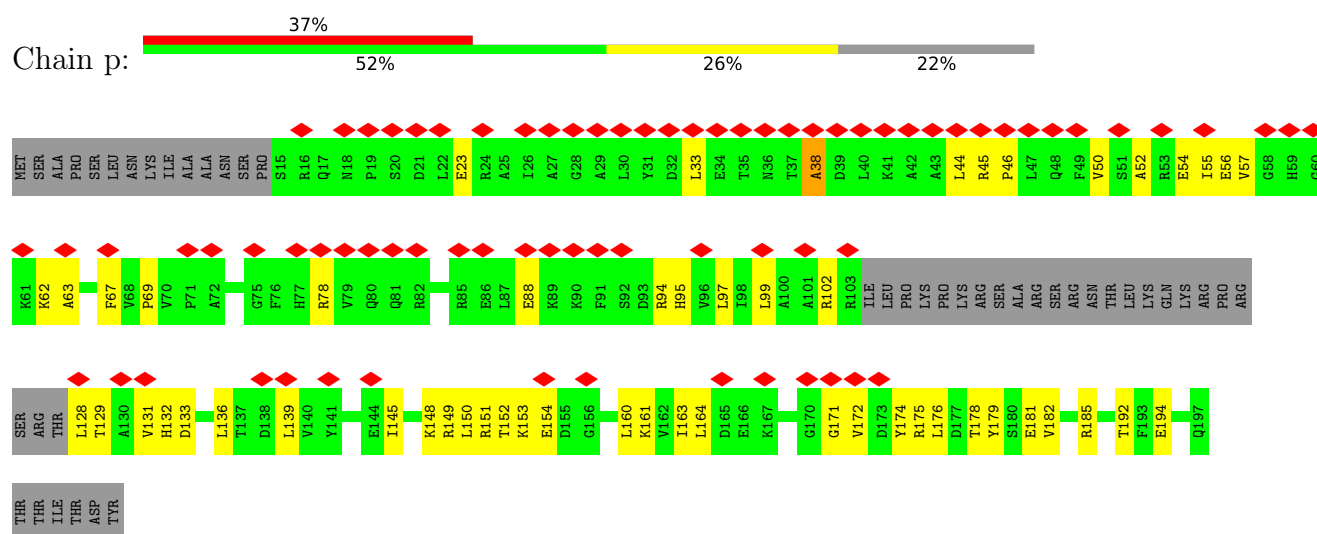


Chain n: 78% 13% 9%

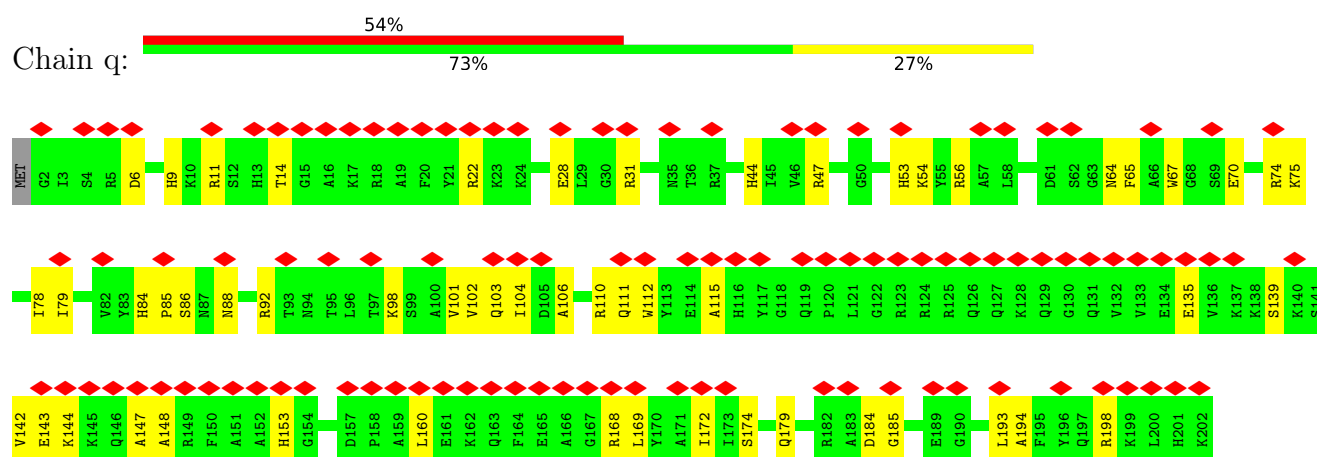


Chain o:

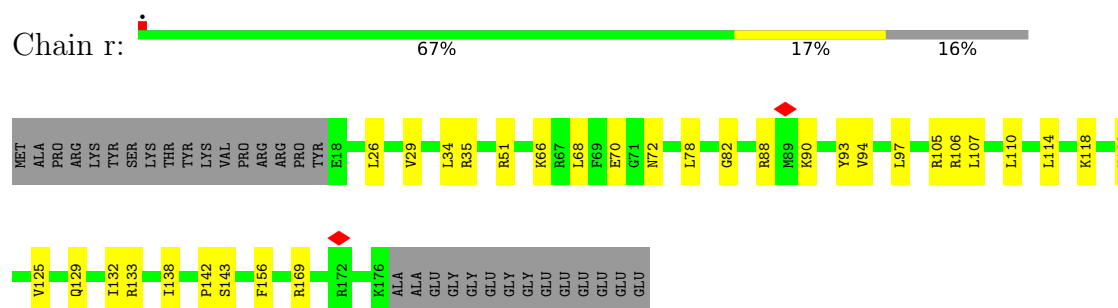




• Molecule 39: 40S ribosomal protein S8

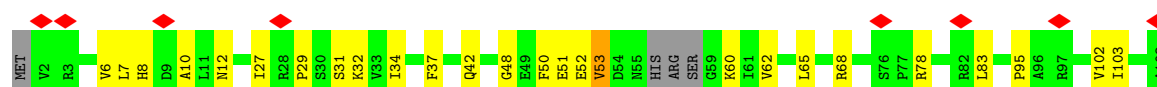


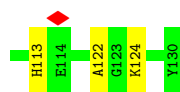
• Molecule 40: 40S ribosomal protein s9-like protein



• Molecule 41: 40S ribosomal protein S13-like protein

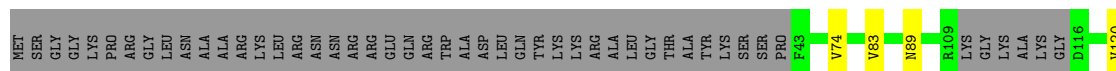






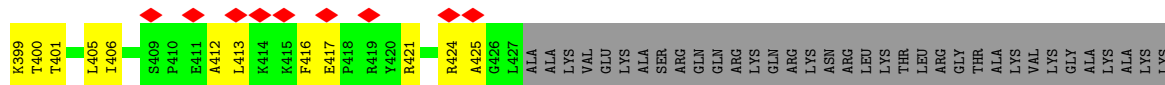
- Molecule 46: 40S ribosomal protein s23-like protein

Chain x: 61% 35%



- Molecule 47: 40S ribosomal protein S24

Chain y: 27% 46% 22% 32%



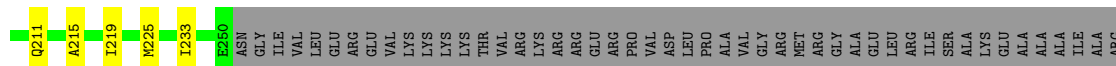
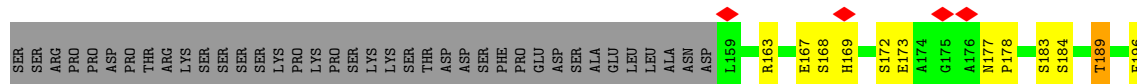
- Molecule 48: 40S ribosomal protein S28-like protein

Chain z: 74% 16% 10%



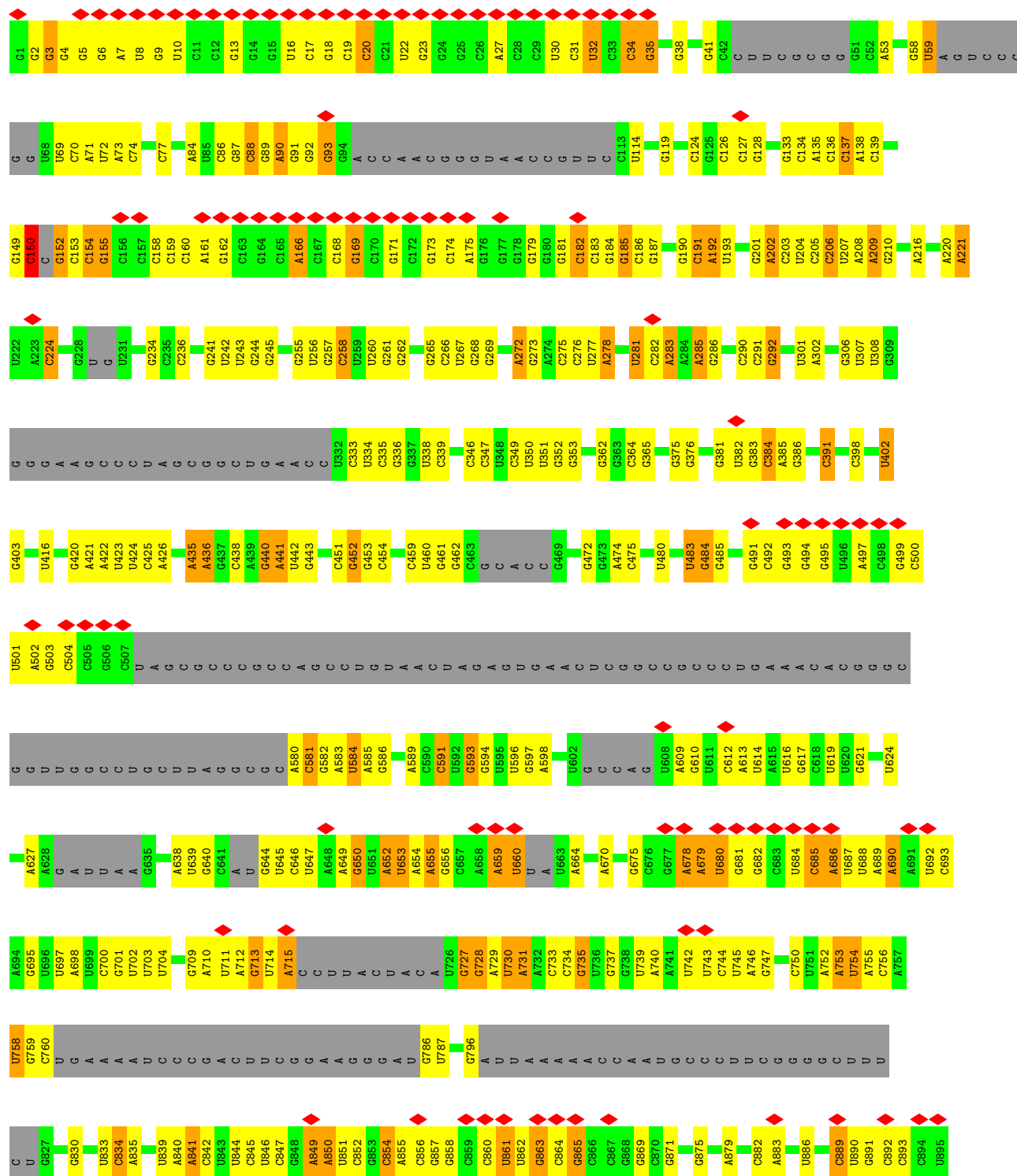
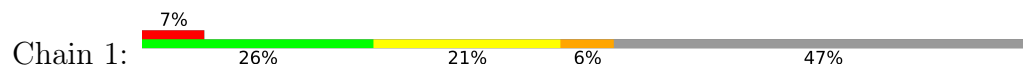
- Molecule 49: Faf1

Chain 0: 24% 5% 70%

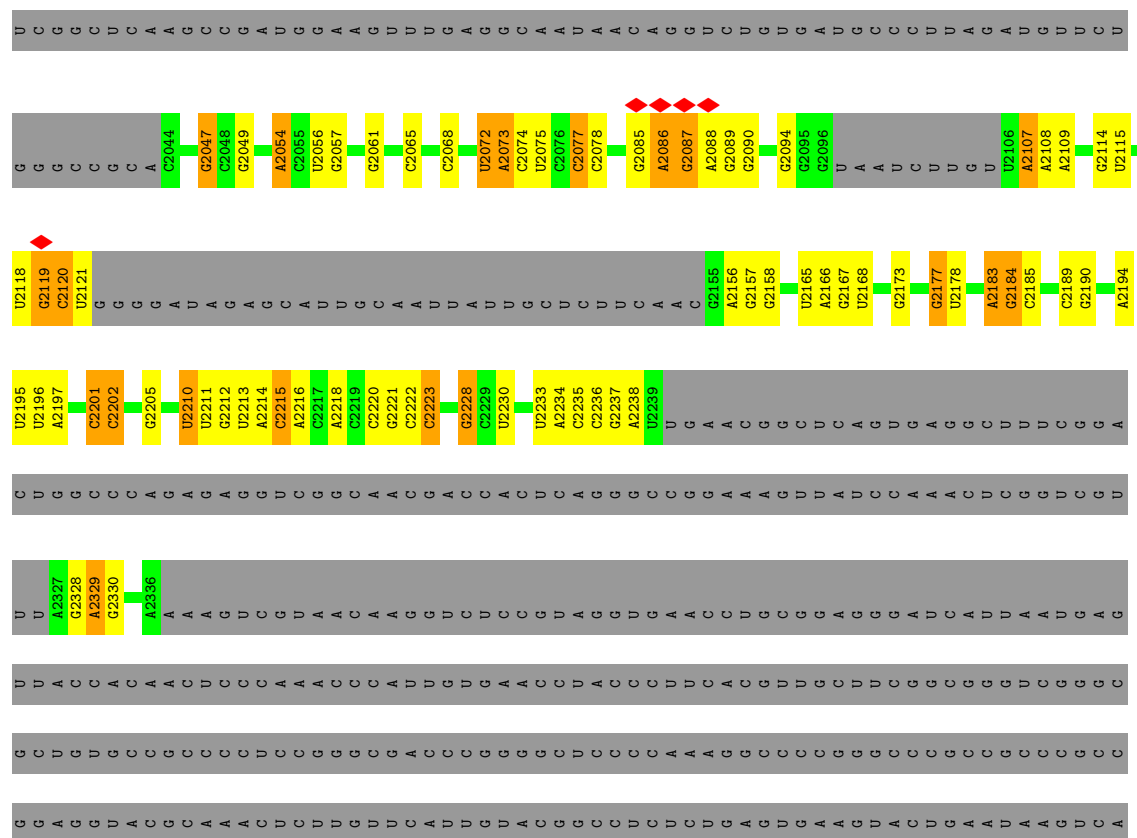


GLU
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ARG
ARG

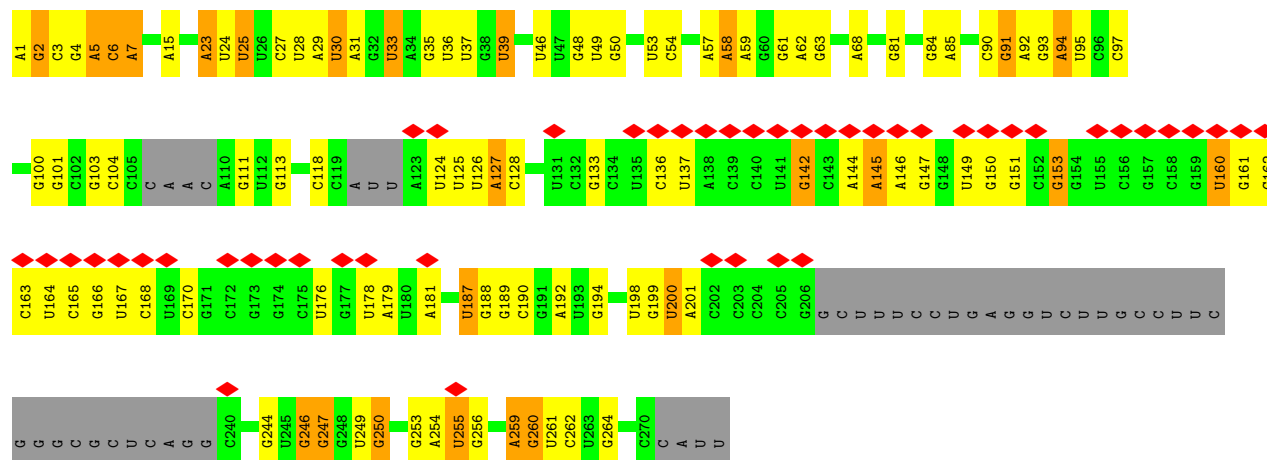
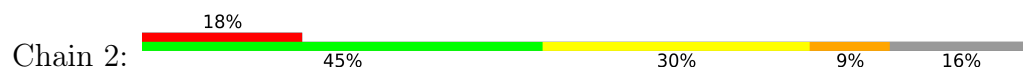
● Molecule 50: 35S rRNA







• Molecule 51: U3 snoRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231121	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.596	Depositor
Minimum map value	-0.325	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	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	A	0.45	0/6395	0.80	4/8703 (0.0%)
2	B	0.26	0/541	0.54	0/713
3	C	0.35	0/595	0.61	0/786
4	D	0.33	0/2209	0.70	1/2986 (0.0%)
5	E	0.33	0/2657	0.61	0/3596
6	F	0.47	0/3353	0.80	3/4544 (0.1%)
7	G	0.38	0/2828	0.69	3/3841 (0.1%)
8	H	0.38	0/1468	0.63	0/1946
9	I	0.31	0/1251	0.68	0/1696
10	J	0.34	0/1221	0.71	0/1662
11	K	0.37	0/1161	0.65	0/1570
12	L	0.29	0/2117	0.70	0/2887
13	M	0.33	0/2179	0.82	4/2972 (0.1%)
14	N	0.38	0/3508	0.65	0/4742
15	O	0.42	0/6604	0.83	7/8981 (0.1%)
16	P	0.38	0/1483	0.73	0/1998
17	Q	0.18	0/900	0.56	0/1249
18	R	0.32	0/1814	0.63	0/2456
18	S	0.33	0/1853	0.62	0/2511
19	T	0.33	0/2911	0.69	0/3937
20	U	0.31	0/3085	0.68	1/4169 (0.0%)
21	V	0.35	0/891	0.71	0/1214
21	W	0.35	0/876	0.71	0/1195
22	X	0.32	0/2739	0.75	4/3699 (0.1%)
23	Y	0.29	0/2638	0.61	0/3580
24	Z	0.35	0/4960	0.69	2/6710 (0.0%)
25	a	0.46	0/1462	0.78	0/1967
26	b	0.42	0/2324	0.77	1/3144 (0.0%)
27	c	0.32	0/1405	0.61	0/1879
28	d	0.44	0/3506	0.76	2/4739 (0.0%)
29	e	0.21	0/1714	0.54	1/2325 (0.0%)
29	f	0.21	0/1714	0.54	1/2325 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	g	0.33	1/1412 (0.1%)	0.64	0/1897
31	h	0.23	0/1304	0.63	0/1751
32	i	0.15	0/3246	0.44	0/4507
32	j	0.15	0/3335	0.44	0/4632
33	k	0.34	0/945	0.62	0/1264
34	l	0.30	0/1764	0.84	0/2377
35	m	0.25	0/2097	0.69	0/2821
36	n	0.35	0/1468	0.69	0/1987
37	o	0.31	0/1942	0.74	2/2595 (0.1%)
38	p	0.34	1/1298 (0.1%)	0.80	4/1750 (0.2%)
39	q	0.24	0/1655	0.64	0/2213
40	r	0.34	0/1259	0.67	0/1687
41	s	0.20	0/422	0.50	0/561
42	t	0.28	0/801	0.65	0/1087
43	u	0.42	0/958	0.80	0/1293
44	v	0.24	0/1315	0.64	0/1760
45	w	0.29	0/1001	0.63	0/1345
46	x	0.35	0/693	0.58	0/928
47	y	0.24	0/766	0.65	0/1027
48	z	0.33	0/458	0.71	0/617
49	0	0.29	0/702	0.60	0/939
50	1	0.28	0/32166	0.51	11/50073 (0.0%)
51	2	0.32	0/5459	0.59	8/8498 (0.1%)
All	All	0.33	2/140828 (0.0%)	0.65	59/198331 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
4	D	0	1
6	F	0	3
12	L	0	1
13	M	0	4
14	N	0	1
15	O	0	5
17	Q	0	3
18	R	0	1
18	S	0	1
21	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	W	0	1
22	X	0	4
23	Y	0	2
24	Z	0	3
26	b	0	1
28	d	0	1
29	e	0	3
29	f	0	3
31	h	0	2
32	i	0	1
32	j	0	1
34	l	0	5
35	m	0	2
37	o	0	2
38	p	0	1
39	q	0	1
42	t	0	1
43	u	0	1
44	v	0	2
46	x	0	1
47	y	0	1
All	All	0	64

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	42	LEU	C-N	6.37	1.44	1.33
38	p	45	ARG	C-N	5.12	1.39	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	222	LEU	CA-C-N	17.52	145.38	120.49
15	O	222	LEU	C-N-CA	17.52	145.38	120.49
51	2	2	G	OP1-P-OP2	-13.34	79.59	119.60
51	2	2	G	O5'-P-OP1	-12.24	71.28	108.00
51	2	1	A	OP2-P-O3'	-9.42	79.73	108.00
51	2	1	A	OP1-P-O3'	9.14	135.41	108.00
38	p	38	ALA	CA-C-N	8.53	137.06	121.70
38	p	38	ALA	C-N-CA	8.53	137.06	121.70
51	2	2	G	O5'-P-OP2	8.51	133.53	108.00
20	U	233	ILE	N-CA-C	-8.14	104.82	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	858	ASP	N-CA-C	-7.92	105.59	114.62
13	M	428	MET	CA-C-N	7.49	139.83	122.31
13	M	428	MET	C-N-CA	7.49	139.83	122.31
50	1	1163	A	P-O3'-C3'	7.06	130.79	120.20
50	1	152	G	C3'-C2'-O2'	6.49	120.43	110.70
38	p	69	PRO	CA-C-N	6.31	126.49	120.43
38	p	69	PRO	C-N-CA	6.31	126.49	120.43
37	o	159	ARG	N-CA-C	6.16	118.24	110.24
28	d	10	ILE	CB-CA-C	6.12	121.33	111.29
50	1	1163	A	C2'-C3'-O3'	5.94	118.41	109.50
29	e	85	SER	N-CA-C	5.80	123.15	110.80
29	f	85	SER	N-CA-C	5.78	123.11	110.80
6	F	56	PRO	CA-C-N	5.77	132.57	121.54
6	F	56	PRO	C-N-CA	5.77	132.57	121.54
13	M	355	ARG	CA-C-N	5.72	132.47	121.54
13	M	355	ARG	C-N-CA	5.72	132.47	121.54
50	1	150	C	C1'-C2'-O2'	-5.71	103.23	111.80
50	1	152	G	C2'-C3'-O3'	-5.69	105.16	113.70
7	G	305	LEU	CA-C-N	5.62	127.12	120.09
7	G	305	LEU	C-N-CA	5.62	127.12	120.09
28	d	10	ILE	N-CA-CB	-5.46	102.23	111.23
22	X	322	TYR	CA-C-N	-5.36	117.71	122.97
22	X	322	TYR	C-N-CA	-5.36	117.71	122.97
50	1	281	U	P-O3'-C3'	5.35	128.22	120.20
50	1	209	A	P-O3'-C3'	5.28	128.12	120.20
6	F	176	LEU	N-CA-CB	-5.27	108.16	114.17
51	2	255	U	P-O3'-C3'	5.26	128.09	120.20
1	A	529	THR	CA-C-N	5.25	129.01	120.60
1	A	529	THR	C-N-CA	5.25	129.01	120.60
15	O	100	TRP	CA-C-N	5.23	129.51	121.19
15	O	100	TRP	C-N-CA	5.23	129.51	121.19
37	o	149	LYS	N-CA-C	5.22	121.91	110.80
1	A	769	TYR	CA-C-N	5.19	124.48	120.33
1	A	769	TYR	C-N-CA	5.19	124.48	120.33
24	Z	819	ARG	CA-C-N	-5.17	112.80	121.39
24	Z	819	ARG	C-N-CA	-5.17	112.80	121.39
51	2	1	A	O3'-P-O5'	-5.15	96.28	104.00
15	O	623	ASN	CA-C-N	5.14	129.58	121.56
15	O	623	ASN	C-N-CA	5.14	129.58	121.56
7	G	273	MET	CB-CG-SD	-5.13	97.30	112.70
26	b	40	LYS	N-CA-C	5.12	121.13	109.81
50	1	34	C	P-O3'-C3'	5.11	127.86	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	23	A	P-O3'-C3'	5.11	127.86	120.20
50	1	593	G	P-O3'-C3'	5.09	127.84	120.20
4	D	129	HIS	N-CA-C	5.07	116.50	110.97
22	X	307	SER	CA-C-N	5.07	130.42	120.99
22	X	307	SER	C-N-CA	5.07	130.42	120.99
50	1	1001	A	C2'-C3'-O3'	5.03	117.04	109.50
50	1	152	G	N9-C1'-C2'	-5.02	104.47	112.00

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	SER	Peptide
1	A	284	MET	Peptide
1	A	556	GLY	Peptide
1	A	686	SER	Peptide
4	D	169	GLU	Peptide
6	F	229	PHE	Peptide
6	F	321	ASP	Peptide
6	F	56	PRO	Peptide
12	L	266	LEU	Peptide
13	M	218	ILE	Peptide
13	M	248	ALA	Peptide
13	M	250	GLY	Peptide
13	M	386	THR	Peptide
14	N	363	ILE	Peptide
15	O	369	SER	Peptide
15	O	397	ASP	Peptide
15	O	472	LEU	Peptide
15	O	644	GLY	Peptide
15	O	758	HIS	Peptide
17	Q	103	ASP	Peptide
17	Q	104	PRO	Peptide
17	Q	236	SER	Peptide
18	R	293	GLU	Peptide
18	S	293	GLU	Peptide
21	V	60	GLN	Peptide
21	W	60	GLN	Peptide
22	X	179	CYS	Peptide
22	X	197	LEU	Peptide
22	X	266	ALA	Peptide
22	X	502	VAL	Peptide

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Mol	Chain	Res	Type	Group
23	Y	104	ALA	Peptide
23	Y	161	TYR	Peptide
24	Z	132	VAL	Peptide
24	Z	65	GLU	Peptide
24	Z	909	ASP	Peptide
26	b	287	TYR	Peptide
28	d	336	MET	Peptide
29	e	80	MET	Peptide
29	e	84	ILE	Peptide
29	e	88	ARG	Peptide
29	f	80	MET	Peptide
29	f	84	ILE	Peptide
29	f	88	ARG	Peptide
31	h	173	ASP	Peptide
31	h	182	ALA	Peptide
32	i	531	PRO	Peptide
32	j	531	PRO	Peptide
34	l	180	THR	Peptide
34	l	21	GLN	Peptide
34	l	212	ILE	Peptide
34	l	61	LEU	Peptide
34	l	65	ILE	Peptide
35	m	231	GLU	Peptide
35	m	87	MET	Peptide
37	o	148	SER	Peptide
37	o	59	GLN	Peptide
38	p	38	ALA	Peptide
39	q	135	GLU	Peptide
42	t	137	ASP	Peptide
43	u	41	PRO	Peptide
44	v	12	ALA	Peptide
44	v	37	ARG	Peptide
46	x	120	VAL	Peptide
47	y	365	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6242	0	6135	148	0
2	B	537	0	569	3	0
3	C	588	0	647	10	0
4	D	2170	0	2191	34	0
5	E	2591	0	2642	33	0
6	F	3282	0	3289	72	0
7	G	2772	0	2847	30	0
8	H	1456	0	1571	31	0
9	I	1230	0	1297	30	0
10	J	1201	0	1218	35	0
11	K	1139	0	1151	21	0
12	L	2070	0	2073	53	0
13	M	2134	0	2117	48	0
14	N	3435	0	3455	46	0
15	O	6446	0	6453	128	0
16	P	1460	0	1522	31	0
17	Q	905	0	400	10	0
18	R	1778	0	1830	38	0
18	S	1816	0	1847	34	0
19	T	2866	0	2960	56	0
20	U	3035	0	3159	71	0
21	V	879	0	918	14	0
21	W	864	0	900	20	0
22	X	2686	0	2676	78	0
23	Y	2594	0	2660	51	0
24	Z	4848	0	4850	89	0
25	a	1434	0	1482	26	0
26	b	2279	0	2314	57	0
27	c	1387	0	1424	17	0
28	d	3436	0	3437	67	0
29	e	1683	0	1726	32	0
29	f	1683	0	1726	28	0
30	g	1393	0	1499	28	0
31	h	1288	0	1357	25	0
32	i	3254	0	1481	57	0
32	j	3342	0	1522	59	0
33	k	930	0	957	16	0
34	l	1735	0	1825	58	0
35	m	2057	0	2140	50	0
36	n	1447	0	1483	18	0
37	o	1911	0	2022	51	0
38	p	1279	0	1322	34	0
39	q	1622	0	1645	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	r	1242	0	1354	21	0
41	s	416	0	451	9	0
42	t	791	0	795	24	0
43	u	943	0	1002	18	0
44	v	1286	0	1366	27	0
45	w	985	0	1021	18	0
46	x	684	0	730	3	0
47	y	752	0	797	24	0
48	z	455	0	482	10	0
49	0	694	0	717	12	0
50	1	28796	0	14588	317	0
51	2	4891	0	2476	58	0
52	P	1	0	0	0	0
All	All	135120	0	116518	2140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (2140) 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)
50:1:152:G:O2'	50:1:153:C:H6	1.28	1.17
4:D:83:VAL:O	4:D:100:SER:HA	1.57	1.03
10:J:748:TYR:CD2	10:J:757:ALA:HB2	1.93	1.03
50:1:2237:G:H1	50:1:2329:A:N6	1.56	1.02
50:1:149:G:O2'	50:1:150:C:H5'	1.65	0.97
3:C:644:LYS:HA	16:P:37:VAL:O	1.65	0.96
35:m:88:ASP:O	35:m:100:ARG:HA	1.64	0.96
50:1:1702:G:H1	51:2:7:A:H61	1.05	0.95
51:2:103:G:O6	51:2:250:G:C6	2.18	0.95
13:M:381:LEU:HB2	13:M:390:ASP:O	1.67	0.95
50:1:2054:A:N6	50:1:2119:G:C2	2.35	0.95
26:b:128:VAL:O	26:b:132:GLN:HB2	1.64	0.95
37:o:3:LEU:O	37:o:15:LEU:HA	1.67	0.95
15:O:648:PHE:HB2	15:O:658:ASP:O	1.67	0.94
51:2:137:U:H3	51:2:150:G:H1	0.99	0.94
10:J:748:TYR:CE2	10:J:757:ALA:HB2	2.01	0.94
5:E:2:ALA:N	51:2:39:U:HO2'	1.66	0.94
7:G:136:LEU:O	7:G:140:LEU:HB2	1.69	0.93
39:q:104:ILE:O	39:q:168:ARG:HA	1.68	0.93
31:h:86:PRO:HA	31:h:120:LYS:O	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:q:103:GLN:HA	39:q:169:LEU:O	1.70	0.92
24:Z:152:GLU:O	24:Z:156:ILE:HB	1.69	0.92
50:1:2238:A:H62	50:1:2328:G:H21	1.16	0.92
50:1:2238:A:H62	50:1:2328:G:N2	1.66	0.91
32:i:281:VAL:O	32:i:409:PHE:HA	1.71	0.91
32:j:281:VAL:O	32:j:409:PHE:HA	1.71	0.91
26:b:229:THR:O	26:b:239:VAL:HA	1.70	0.90
50:1:1702:G:H1	51:2:7:A:N6	1.69	0.90
20:U:147:HIS:O	20:U:151:ARG:HB2	1.71	0.90
42:t:30:ALA:O	42:t:94:ILE:HA	1.70	0.90
44:v:92:ARG:HA	44:v:110:LYS:O	1.71	0.89
47:y:341:ARG:O	47:y:355:VAL:HB	1.74	0.88
13:M:146:SER:HA	13:M:157:TRP:O	1.74	0.88
44:v:91:ILE:O	44:v:111:ASN:HA	1.74	0.88
50:1:381:G:H21	50:1:385:A:H62	1.22	0.88
37:o:48:TYR:HA	37:o:115:LYS:O	1.74	0.88
50:1:152:G:O2'	50:1:153:C:C6	2.10	0.88
1:A:11:LEU:O	1:A:695:LEU:HB3	1.75	0.87
47:y:391:LEU:HA	47:y:401:THR:O	1.74	0.86
32:j:928:SER:O	32:j:932:ALA:HB3	1.75	0.86
13:M:405:SER:HB3	13:M:410:ALA:O	1.73	0.85
50:1:1460:G:H1	50:1:1537:A:H61	1.19	0.85
32:i:928:SER:O	32:i:932:ALA:HB3	1.75	0.85
24:Z:833:LEU:O	24:Z:843:GLN:HA	1.76	0.85
26:b:230:PHE:HA	26:b:238:GLU:O	1.76	0.84
32:j:284:THR:HA	32:j:412:SER:O	1.77	0.84
10:J:748:TYR:CE2	10:J:757:ALA:N	2.46	0.84
32:i:284:THR:HA	32:i:412:SER:O	1.77	0.84
27:c:548:ARG:O	27:c:552:GLY:HA2	1.79	0.83
32:i:726:SER:HA	32:i:760:CYS:O	1.78	0.83
19:T:317:ARG:O	19:T:321:HIS:HB2	1.79	0.83
32:j:726:SER:HA	32:j:760:CYS:O	1.78	0.83
50:1:149:G:C2'	50:1:150:C:H5'	2.08	0.83
50:1:2238:A:N6	50:1:2328:G:H21	1.76	0.83
12:L:245:THR:O	12:L:260:LEU:HB3	1.77	0.82
10:J:748:TYR:CE2	10:J:757:ALA:CB	2.62	0.82
31:h:106:VAL:O	31:h:110:LYS:HA	1.77	0.82
50:1:1448:A:N6	50:1:1549:U:C4	2.47	0.82
24:Z:269:GLU:HA	24:Z:779:LEU:O	1.79	0.81
50:1:712:A:H62	50:1:875:G:H21	1.27	0.81
15:O:244:LEU:O	15:O:255:ILE:HA	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:835:PHE:O	24:Z:841:ARG:HA	1.80	0.81
12:L:71:ASP:HA	12:L:84:PHE:O	1.80	0.81
24:Z:80:GLY:O	24:Z:84:LEU:HB2	1.80	0.81
22:X:470:ARG:O	22:X:479:PHE:HB2	1.81	0.80
31:h:84:LYS:HA	31:h:122:VAL:O	1.81	0.80
38:p:67:PHE:HA	38:p:99:LEU:O	1.81	0.80
21:W:19:GLN:HE22	22:X:396:GLY:HA2	1.47	0.80
13:M:415:LEU:HB2	13:M:419:SER:O	1.82	0.80
32:i:725:VAL:O	32:i:761:VAL:HA	1.81	0.80
19:T:134:ILE:O	19:T:138:ALA:HB2	1.81	0.80
10:J:748:TYR:HE2	10:J:757:ALA:CB	1.94	0.80
32:j:725:VAL:O	32:j:761:VAL:HA	1.81	0.80
39:q:44:HIS:O	39:q:56:ARG:HB3	1.82	0.79
32:i:313:THR:O	32:i:388:ILE:HA	1.83	0.79
9:I:895:MET:O	9:I:899:LEU:HB2	1.83	0.79
13:M:419:SER:HA	13:M:434:VAL:O	1.82	0.78
1:A:9:ASN:HD22	1:A:9:ASN:N	1.79	0.78
32:j:313:THR:O	32:j:388:ILE:HA	1.83	0.78
37:o:4:ASN:HA	37:o:14:LYS:O	1.83	0.78
39:q:172:ILE:O	39:q:185:GLY:HA3	1.83	0.78
1:A:732:LYS:O	1:A:736:MET:HB2	1.82	0.78
22:X:271:VAL:HA	22:X:282:LYS:O	1.83	0.78
29:f:190:ARG:O	29:f:194:ASP:HB2	1.84	0.78
32:i:125:LEU:O	32:i:151:LEU:HA	1.84	0.78
12:L:205:LEU:O	12:L:216:VAL:HA	1.84	0.78
24:Z:886:CYS:HB3	24:Z:901:ALA:O	1.83	0.77
29:e:190:ARG:O	29:e:194:ASP:HB2	1.84	0.77
42:t:33:PHE:HA	42:t:97:ARG:O	1.84	0.77
39:q:88:ASN:O	39:q:92:ARG:HB2	1.85	0.77
28:d:169:ALA:HA	28:d:178:ARG:O	1.85	0.77
24:Z:1084:GLY:O	24:Z:1088:ARG:HB2	1.83	0.77
39:q:139:SER:O	39:q:143:GLU:HB2	1.86	0.76
37:o:162:VAL:O	37:o:172:TYR:HB2	1.85	0.76
32:j:125:LEU:O	32:j:151:LEU:HA	1.84	0.75
50:1:2054:A:N6	50:1:2119:G:N2	2.35	0.75
10:J:748:TYR:HD2	10:J:757:ALA:HB2	1.47	0.75
26:b:88:VAL:HA	26:b:138:ASP:O	1.87	0.75
24:Z:834:ILE:HA	24:Z:842:PHE:O	1.86	0.74
13:M:321:GLY:O	13:M:352:HIS:HA	1.87	0.74
15:O:312:ASP:O	15:O:317:GLY:HA2	1.88	0.74
32:i:282:THR:O	32:i:471:GLU:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:p:163:ILE:HA	38:p:194:GLU:O	1.86	0.74
35:m:99:PHE:HA	35:m:112:HIS:O	1.88	0.74
15:O:243:LEU:HA	15:O:256:GLN:O	1.88	0.74
19:T:100:VAL:O	19:T:120:ALA:HA	1.87	0.74
48:z:31:VAL:HB	48:z:41:ILE:O	1.86	0.74
15:O:323:LEU:HD11	15:O:375:PRO:HD2	1.69	0.73
32:j:282:THR:O	32:j:471:GLU:HA	1.88	0.73
34:l:67:GLU:HA	34:l:84:ILE:O	1.88	0.73
49:0:189:THR:HG23	50:1:338:U:H5''	1.71	0.73
35:m:98:ASN:O	35:m:113:ARG:HA	1.87	0.73
44:v:97:HIS:O	44:v:105:TYR:HA	1.88	0.73
23:Y:347:GLY:O	23:Y:397:SER:HA	1.88	0.73
50:1:93:G:H1	50:1:114:U:H3	1.37	0.72
50:1:1665:A:N3	50:1:1666:C:N4	2.35	0.72
23:Y:152:THR:O	23:Y:156:ALA:HB3	1.88	0.72
25:a:96:ALA:O	25:a:100:ASN:HB3	1.89	0.72
50:1:152:G:O2'	50:1:153:C:O5'	2.08	0.72
6:F:51:LYS:HE2	28:d:29:PRO:HD2	1.72	0.71
32:i:29:VAL:HA	32:i:202:ILE:O	1.90	0.71
10:J:766:HIS:HB2	27:c:707:GLU:HG3	1.72	0.71
40:r:68:LEU:O	40:r:72:ASN:HB2	1.91	0.71
4:D:44:LEU:O	4:D:55:ILE:HA	1.91	0.71
11:K:895:GLN:O	11:K:899:ARG:HB3	1.91	0.71
1:A:198:VAL:HA	1:A:214:SER:HA	1.73	0.71
15:O:234:CYS:O	15:O:247:ALA:HB3	1.91	0.71
32:j:29:VAL:HA	32:j:202:ILE:O	1.90	0.71
50:1:1448:A:N6	50:1:1549:U:N3	2.40	0.70
24:Z:250:ARG:HB3	24:Z:269:GLU:O	1.89	0.70
38:p:161:LYS:HA	38:p:192:THR:O	1.91	0.70
50:1:35:G:N1	50:1:59:U:N3	2.39	0.70
15:O:298:MET:HB3	15:O:311:TRP:HB2	1.73	0.70
14:N:397:MET:HG3	14:N:411:GLN:HE21	1.56	0.70
32:i:30:VAL:O	32:i:203:ASP:HA	1.92	0.70
32:j:926:LEU:O	32:j:930:ALA:HB3	1.92	0.70
10:J:766:HIS:C	27:c:707:GLU:OE2	2.34	0.70
32:i:585:VAL:O	32:i:638:ILE:HA	1.92	0.70
15:O:302:THR:HG22	15:O:304:VAL:H	1.56	0.70
24:Z:787:GLU:O	24:Z:791:ASN:HB2	1.92	0.70
50:1:1029:A:H61	50:1:1046:G:H1'	1.56	0.70
12:L:282:ALA:HB3	12:L:287:ARG:O	1.92	0.69
22:X:332:GLU:O	22:X:349:ALA:HB2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:243:GLN:HG3	22:X:280:PRO:HD2	1.73	0.69
1:A:493:ARG:HD2	1:A:504:SER:HB3	1.74	0.69
22:X:264:GLY:HA2	22:X:269:ARG:O	1.91	0.69
1:A:170:SER:HB2	1:A:174:THR:O	1.92	0.69
32:i:926:LEU:O	32:i:930:ALA:HB3	1.92	0.69
32:j:30:VAL:O	32:j:203:ASP:HA	1.92	0.69
8:H:38:ALA:O	8:H:42:LYS:HG2	1.93	0.69
31:h:83:ARG:O	31:h:124:LEU:HB2	1.92	0.69
32:j:585:VAL:O	32:j:638:ILE:HA	1.92	0.69
51:2:127:A:N7	51:2:187:U:O4	2.26	0.69
39:q:139:SER:H	39:q:142:VAL:HB	1.58	0.68
50:1:1759:U:O4	50:1:2047:G:O6	2.11	0.68
24:Z:1085:ARG:HD2	50:1:391:C:H5''	1.75	0.68
50:1:1488:U:O2	50:1:1491:A:N7	2.27	0.68
15:O:52:THR:HG21	15:O:99:ALA:H	1.58	0.68
24:Z:786:ALA:O	24:Z:790:LYS:HB2	1.93	0.68
39:q:143:GLU:O	39:q:147:ALA:HB3	1.93	0.68
50:1:1460:G:H1	50:1:1537:A:N6	1.91	0.68
50:1:152:G:HO2'	50:1:153:C:H6	0.74	0.68
1:A:565:THR:HG23	51:2:61:G:H5'	1.74	0.68
22:X:164:THR:O	22:X:602:VAL:HA	1.93	0.68
18:S:111:VAL:O	18:S:125:THR:HB	1.94	0.68
23:Y:282:VAL:HA	23:Y:292:TYR:O	1.93	0.68
12:L:122:ARG:HA	12:L:140:TRP:O	1.93	0.68
37:o:7:HIS:HB3	37:o:12:SER:O	1.94	0.68
18:R:111:VAL:O	18:R:125:THR:HB	1.94	0.67
34:l:135:LEU:HA	34:l:216:LYS:O	1.94	0.67
1:A:41:ASN:O	1:A:45:ASN:HA	1.93	0.67
50:1:2237:G:H1	50:1:2329:A:H61	0.78	0.67
6:F:270:ASN:ND2	6:F:461:LEU:O	2.27	0.67
15:O:141:ILE:HA	15:O:155:ALA:HA	1.77	0.67
47:y:405:LEU:HD12	47:y:421:ARG:HH22	1.59	0.67
22:X:306:CYS:HB2	22:X:333:ILE:HD13	1.77	0.67
41:s:127:ARG:HH12	50:1:1213:U:H5''	1.59	0.67
30:g:113:LYS:NZ	49:O:184:SER:OG	2.28	0.67
1:A:844:LEU:HD13	15:O:1006:ILE:HD11	1.77	0.67
12:L:70:ASN:O	12:L:85:SER:HA	1.95	0.67
20:U:375:THR:HG21	20:U:393:VAL:HG21	1.76	0.67
24:Z:845:LEU:HD11	24:Z:998:LYS:HB2	1.77	0.67
4:D:204:CYS:HB2	4:D:208:THR:O	1.94	0.67
13:M:189:ASP:HB2	13:M:208:LEU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:11:PHE:HB2	23:Y:33:ILE:HG12	1.77	0.67
50:1:1472:A:N1	50:1:1510:G:O6	2.28	0.67
35:m:90:ILE:HB	35:m:99:PHE:HB2	1.77	0.66
47:y:351:ARG:HH21	47:y:416:PHE:HB3	1.60	0.66
24:Z:1101:ARG:HD2	33:k:111:MET:HG2	1.77	0.66
35:m:87:MET:HA	35:m:101:LEU:O	1.95	0.66
35:m:116:ASP:O	35:m:120:LYS:HB3	1.95	0.66
26:b:88:VAL:O	26:b:114:ALA:HA	1.96	0.66
15:O:423:ARG:NH1	50:1:258:C:N3	2.44	0.66
20:U:171:LEU:O	20:U:175:LEU:HB2	1.96	0.66
19:T:388:ILE:HD12	19:T:391:ARG:HE	1.61	0.66
28:d:309:LEU:HD12	28:d:319:ASP:HB3	1.78	0.66
37:o:223:LYS:HA	37:o:226:LYS:HB3	1.76	0.66
22:X:561:ASN:O	22:X:587:ARG:NH2	2.29	0.66
1:A:346:LEU:HD23	1:A:690:ALA:HB2	1.77	0.65
16:P:90:ILE:HG22	16:P:119:GLN:HB2	1.79	0.65
26:b:94:ARG:NH2	50:1:2189:C:OP2	2.29	0.65
36:n:79:ARG:NH2	36:n:156:ASN:OD1	2.29	0.65
51:2:103:G:C6	51:2:250:G:C6	2.83	0.65
7:G:297:VAL:HG21	7:G:328:VAL:HA	1.77	0.65
12:L:72:LEU:O	12:L:84:PHE:HB2	1.95	0.65
22:X:262:VAL:HA	22:X:271:VAL:O	1.97	0.65
23:Y:61:THR:HG22	23:Y:82:ILE:HG22	1.78	0.65
23:Y:377:ILE:HA	23:Y:395:ILE:O	1.97	0.65
12:L:160:LEU:HB2	12:L:172:TRP:HB2	1.78	0.65
28:d:297:GLU:OE2	28:d:318:ARG:NH2	2.29	0.65
9:I:843:HIS:O	9:I:847:LEU:HB2	1.96	0.65
10:J:748:TYR:OH	10:J:756:ASP:N	2.30	0.65
15:O:406:LYS:HB3	15:O:423:ARG:HE	1.61	0.65
20:U:13:TYR:HB2	20:U:49:ALA:HB3	1.77	0.65
32:i:724:GLY:HA2	32:i:762:MET:O	1.97	0.65
34:l:92:GLN:HB2	34:l:95:ASN:HB3	1.79	0.65
1:A:687:PHE:HB3	1:A:698:TYR:O	1.96	0.65
4:D:291:ILE:HB	4:D:303:TYR:HB2	1.79	0.65
16:P:55:PRO:HA	16:P:86:SER:O	1.96	0.65
25:a:168:GLN:O	25:a:172:LYS:HB2	1.97	0.65
34:l:64:ARG:NH2	42:t:47:SER:OG	2.29	0.65
37:o:184:PRO:HA	37:o:187:LEU:HB2	1.79	0.65
9:I:871:VAL:HA	9:I:874:THR:HG22	1.78	0.65
20:U:197:LEU:O	20:U:201:LEU:HB2	1.97	0.65
29:e:178:VAL:HA	29:e:223:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:474:PRO:HB2	14:N:477:LEU:HB2	1.79	0.65
39:q:194:ALA:O	39:q:198:ARG:HB2	1.97	0.65
50:1:1213:U:O2	50:1:1555:A:N7	2.29	0.65
24:Z:127:ILE:HD13	24:Z:156:ILE:HG12	1.79	0.64
32:j:724:GLY:HA2	32:j:762:MET:O	1.97	0.64
49:0:168:SER:O	49:0:172:SER:HB3	1.97	0.64
6:F:284:LEU:HB3	6:F:294:VAL:O	1.98	0.64
6:F:442:ARG:NH2	50:1:426:A:OP1	2.29	0.64
11:K:916:GLN:HE22	50:1:441:A:H62	1.45	0.64
1:A:445:ILE:HA	1:A:470:PRO:HB3	1.80	0.64
18:R:106:GLU:OE2	18:R:128:ARG:NH1	2.31	0.64
4:D:80:LEU:HA	4:D:103:PHE:O	1.98	0.64
29:f:178:VAL:HA	29:f:223:GLU:O	1.96	0.64
28:d:288:ASP:O	28:d:300:SER:HA	1.97	0.63
12:L:150:THR:HA	12:L:161:MET:O	1.98	0.63
28:d:343:THR:O	28:d:350:VAL:HA	1.98	0.63
28:d:242:CYS:HA	28:d:259:SER:HA	1.80	0.63
7:G:52:CYS:O	7:G:55:GLY:N	2.30	0.63
8:H:70:ARG:NH1	24:Z:1063:GLN:OE1	2.31	0.63
13:M:421:MET:HA	13:M:432:MET:O	1.97	0.63
40:r:51:ARG:NH2	40:r:97:LEU:O	2.31	0.63
47:y:344:ILE:HB	47:y:353:GLN:HB2	1.80	0.63
22:X:176:VAL:HB	22:X:581:VAL:HG21	1.78	0.63
13:M:324:TYR:HA	13:M:349:ARG:O	1.98	0.63
18:S:106:GLU:OE2	18:S:128:ARG:NH1	2.31	0.63
40:r:125:VAL:O	40:r:129:GLN:HB2	1.98	0.63
50:1:1759:U:H3	50:1:2047:G:H1	1.45	0.63
20:U:288:ASN:HB3	20:U:372:SER:HB2	1.81	0.63
34:l:32:ILE:HA	34:l:96:CYS:HB3	1.80	0.63
1:A:259:ARG:NH1	1:A:299:GLU:OE1	2.32	0.62
23:Y:117:LEU:O	23:Y:121:ALA:HB3	1.99	0.62
38:p:56:GLU:HA	38:p:62:LYS:HA	1.81	0.62
20:U:122:ILE:HA	20:U:125:HIS:HB3	1.80	0.62
45:w:52:GLU:HA	45:w:60:LYS:O	1.99	0.62
4:D:279:VAL:HA	4:D:295:GLY:HA2	1.81	0.62
35:m:100:ARG:HH22	35:m:118:GLU:HG2	1.63	0.62
9:I:782:ILE:O	9:I:786:LEU:HB2	1.99	0.62
37:o:76:LEU:HA	37:o:94:ARG:HA	1.81	0.62
1:A:418:ARG:NH2	1:A:455:VAL:O	2.32	0.62
1:A:735:VAL:O	1:A:739:ARG:HB2	2.00	0.62
21:V:53:VAL:O	21:V:79:TYR:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:53:VAL:O	21:W:79:TYR:HA	2.00	0.62
22:X:270:LEU:O	22:X:283:ALA:HA	1.98	0.62
30:g:72:ASP:O	30:g:76:GLY:HA2	1.99	0.62
20:U:335:LYS:NZ	24:Z:1079:ARG:O	2.33	0.62
20:U:397:ALA:O	20:U:401:LEU:HB2	2.00	0.62
50:1:902:U:H3	50:1:930:G:H1	1.45	0.62
1:A:440:ILE:O	1:A:452:ILE:HA	2.00	0.62
4:D:198:ASN:HD22	4:D:215:ARG:HE	1.47	0.62
37:o:51:ARG:HB3	37:o:112:SER:HB2	1.81	0.62
45:w:7:LEU:HA	45:w:34:ILE:HD11	1.81	0.62
15:O:201:VAL:O	15:O:208:VAL:HA	1.98	0.62
10:J:748:TYR:HE2	10:J:757:ALA:N	1.97	0.62
23:Y:160:LEU:HD11	23:Y:331:SER:HB2	1.82	0.62
26:b:164:MET:HB2	26:b:267:SER:HB3	1.82	0.62
11:K:335:ARG:NH2	50:1:581:C:N3	2.47	0.62
22:X:263:THR:O	22:X:270:LEU:HA	1.98	0.62
38:p:148:LYS:O	45:w:53:VAL:HA	2.00	0.62
48:z:42:ILE:HD11	48:z:65:ARG:HH21	1.65	0.62
1:A:826:MET:HG3	1:A:831:ARG:HH12	1.65	0.61
28:d:73:CYS:SG	28:d:74:LYS:N	2.72	0.61
28:d:298:LEU:HB2	28:d:310:TRP:HB2	1.82	0.61
15:O:391:LEU:HD21	15:O:773:VAL:HG11	1.82	0.61
15:O:436:ILE:HD13	15:O:461:LYS:HG2	1.82	0.61
6:F:219:VAL:HA	6:F:235:SER:HA	1.81	0.61
6:F:233:THR:HG23	6:F:241:LYS:HB2	1.81	0.61
31:h:187:ILE:O	31:h:191:ALA:HB3	2.01	0.61
6:F:230:LEU:HA	6:F:243:GLN:O	1.99	0.61
26:b:188:TYR:O	26:b:215:ARG:NH2	2.33	0.61
4:D:243:CYS:SG	4:D:244:LEU:N	2.72	0.61
6:F:323:LYS:HG2	50:1:278:A:H61	1.65	0.61
25:a:82:LEU:HD22	25:a:88:LEU:HG	1.82	0.61
28:d:88:ASP:HB2	28:d:90:VAL:HG12	1.83	0.61
35:m:9:GLN:HB2	35:m:30:ARG:HB2	1.81	0.61
26:b:15:ARG:NH2	26:b:74:ASP:OD2	2.33	0.61
30:g:101:LEU:HD11	30:g:121:CYS:HB3	1.82	0.61
31:h:134:GLU:O	31:h:138:MET:HB2	2.00	0.61
6:F:315:MET:HB2	6:F:329:ILE:HD12	1.83	0.61
28:d:253:MET:SD	28:d:270:ARG:NH1	2.72	0.61
38:p:181:GLU:OE1	38:p:185:ARG:NH2	2.31	0.61
40:r:122:HIS:ND1	50:1:1062:C:O2'	2.34	0.61
50:1:18:G:H1	50:1:20:C:N4	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ILE:HG23	1:A:464:LEU:HB2	1.82	0.61
9:I:831:LEU:HD22	9:I:869:LEU:HB3	1.83	0.61
15:O:143:GLN:O	15:O:153:ALA:HA	2.01	0.61
18:S:102:SER:OG	18:S:108:ARG:NH1	2.34	0.61
24:Z:938:PHE:HD2	24:Z:944:ILE:HD13	1.65	0.61
39:q:47:ARG:HA	39:q:53:HIS:HA	1.83	0.61
50:1:381:G:N2	50:1:385:A:H62	1.95	0.61
4:D:261:TRP:HA	4:D:268:GLN:HA	1.83	0.60
22:X:235:ARG:HH11	22:X:240:LYS:HZ2	1.49	0.60
9:I:816:PRO:HA	9:I:819:VAL:HG22	1.82	0.60
9:I:883:LYS:HG3	15:O:1043:PHE:HE1	1.67	0.60
14:N:402:ASN:O	14:N:406:MET:N	2.34	0.60
29:f:179:THR:HB	29:f:224:LYS:HG2	1.84	0.60
30:g:42:LEU:HD11	34:l:115:ARG:HH21	1.65	0.60
3:C:619:LYS:HB3	16:P:40:MET:HE2	1.83	0.60
42:t:70:PRO:HD3	42:t:109:PRO:HB2	1.83	0.60
17:Q:97:VAL:O	17:Q:125:GLY:HA3	2.02	0.60
34:l:166:ARG:O	34:l:170:GLU:HB2	2.01	0.60
34:l:121:ILE:O	34:l:140:ILE:HA	2.02	0.60
37:o:179:GLN:HE22	50:1:753:A:H4'	1.66	0.60
10:J:808:GLN:OE1	10:J:812:ARG:NH2	2.34	0.60
20:U:240:ALA:O	20:U:244:SER:HB2	2.02	0.60
22:X:303:LEU:HB3	22:X:315:TRP:HB2	1.82	0.60
26:b:117:LEU:HD11	43:u:126:PRO:HA	1.84	0.60
38:p:54:GLU:OE2	38:p:94:ARG:NH1	2.34	0.60
1:A:78:GLN:NE2	50:1:258:C:O2'	2.34	0.60
1:A:216:ASP:O	50:1:285:A:N6	2.33	0.60
8:H:221:ARG:NH2	50:1:376:G:OP1	2.33	0.60
50:1:2177:G:O2'	50:1:2183:A:N6	2.34	0.60
1:A:392:LYS:HE3	1:A:435:PRO:HB2	1.82	0.60
24:Z:156:ILE:HD11	24:Z:887:PHE:HZ	1.66	0.60
50:1:787:U:O2	50:1:847:C:N3	2.35	0.60
11:K:907:PRO:O	28:d:25:ARG:NH2	2.35	0.60
13:M:295:ILE:HD11	13:M:312:ILE:HD11	1.83	0.60
14:N:273:HIS:ND1	14:N:293:SER:OG	2.28	0.60
15:O:159:ILE:HD12	15:O:211:TRP:HZ3	1.66	0.60
15:O:982:LEU:HD22	15:O:1022:HIS:HB3	1.84	0.60
22:X:265:GLY:O	22:X:268:LYS:N	2.35	0.60
23:Y:339:MET:HE1	23:Y:349:LEU:HB2	1.83	0.60
4:D:135:PHE:HA	4:D:155:VAL:O	2.01	0.59
18:R:181:TYR:HA	18:R:204:ILE:HG22	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:181:TYR:HA	18:S:204:ILE:HG22	1.82	0.59
24:Z:243:TYR:HA	24:Z:800:VAL:O	2.02	0.59
24:Z:793:GLN:OE1	24:Z:795:ARG:NH2	2.35	0.59
51:2:103:G:C5	51:2:250:G:N1	2.70	0.59
1:A:531:ASP:O	1:A:551:ARG:NH2	2.35	0.59
29:f:27:ILE:HD13	29:f:36:ARG:HE	1.66	0.59
1:A:544:GLN:OE1	43:u:114:ARG:NH2	2.34	0.59
1:A:545:VAL:O	43:u:111:GLN:NE2	2.35	0.59
4:D:298:ARG:NH1	4:D:323:GLN:O	2.35	0.59
22:X:177:ALA:HB3	22:X:184:TYR:HB2	1.83	0.59
28:d:360:ARG:O	28:d:364:LYS:NZ	2.35	0.59
16:P:72:LYS:HE3	45:w:95:PRO:HA	1.84	0.59
21:W:96:ARG:NH1	22:X:590:ARG:O	2.36	0.59
34:l:111:ARG:NH2	42:t:134:THR:OG1	2.35	0.59
15:O:753:ALA:O	15:O:765:GLY:HA2	2.03	0.59
32:i:929:GLY:O	32:i:933:ALA:HB2	2.03	0.59
32:j:929:GLY:O	32:j:933:ALA:HB2	2.03	0.59
47:y:351:ARG:NH2	47:y:416:PHE:O	2.34	0.59
1:A:192:SER:OG	1:A:193:GLY:N	2.35	0.59
30:g:194:PRO:HA	30:g:197:LEU:HB2	1.84	0.59
12:L:276:VAL:HA	12:L:292:SER:HA	1.84	0.59
19:T:74:MET:HB2	19:T:78:LEU:HD23	1.85	0.59
50:1:204:U:OP1	50:1:206:C:N4	2.35	0.59
18:R:102:SER:OG	18:R:108:ARG:NH1	2.34	0.59
26:b:111:PHE:HB2	26:b:114:ALA:HB2	1.85	0.59
30:g:140:ARG:NH1	30:g:166:GLY:O	2.36	0.59
6:F:450:LEU:HB3	25:a:13:LEU:HD21	1.85	0.59
9:I:814:ARG:NH1	9:I:823:ASN:OD1	2.34	0.59
12:L:147:VAL:HA	12:L:164:SER:HA	1.84	0.59
14:N:398:LEU:HB2	14:N:412:ALA:HB3	1.85	0.59
26:b:232:ASN:HB3	26:b:237:ILE:HG22	1.84	0.59
5:E:275:SER:O	5:E:315:ARG:NH2	2.36	0.59
13:M:158:VAL:HB	13:M:166:TRP:HB2	1.84	0.59
13:M:255:ALA:HB3	13:M:262:HIS:HB2	1.82	0.59
17:Q:68:THR:HA	17:Q:278:VAL:HA	1.85	0.59
28:d:132:ILE:HG23	28:d:150:TRP:HB2	1.85	0.59
6:F:300:ARG:NH2	50:1:283:A:OP2	2.33	0.58
10:J:766:HIS:HB2	27:c:707:GLU:CG	2.33	0.58
12:L:50:PRO:HB3	12:L:109:PRO:HA	1.85	0.58
29:e:179:THR:HB	29:e:224:LYS:HG2	1.83	0.58
1:A:846:ASN:HD21	10:J:835:LYS:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:137:VAL:HG12	23:Y:138:ILE:HG13	1.85	0.58
24:Z:920:LEU:HD12	24:Z:989:LEU:HD23	1.85	0.58
26:b:244:TYR:HB3	26:b:254:LEU:HD23	1.84	0.58
29:e:75:GLY:O	29:e:79:LYS:HB2	2.03	0.58
37:o:177:ARG:NH2	50:1:752:A:O2'	2.35	0.58
38:p:128:LEU:O	38:p:132:HIS:ND1	2.36	0.58
50:1:712:A:H62	50:1:875:G:N2	1.99	0.58
24:Z:69:ARG:HD3	24:Z:229:MET:HE2	1.86	0.58
40:r:35:ARG:NH2	50:1:1060:U:O4	2.35	0.58
42:t:85:LYS:NZ	42:t:121:SER:O	2.35	0.58
43:u:65:ILE:HD11	43:u:89:ILE:HD11	1.85	0.58
16:P:8:GLY:HA3	25:a:34:ARG:HH11	1.68	0.58
19:T:179:GLN:HE21	20:U:185:ARG:HH22	1.51	0.58
28:d:155:PRO:HG2	28:d:173:GLY:HA3	1.84	0.58
28:d:161:PHE:HD1	28:d:168:PHE:HB3	1.67	0.58
35:m:100:ARG:NH2	35:m:118:GLU:O	2.37	0.58
35:m:122:LYS:HB2	35:m:164:LEU:HD12	1.85	0.58
5:E:104:PRO:HB2	5:E:136:LEU:HD22	1.85	0.58
29:e:38:ILE:HA	29:e:111:GLN:O	2.03	0.58
37:o:37:ALA:HA	37:o:49:ILE:HA	1.84	0.58
25:a:104:SER:OG	25:a:108:ARG:NH1	2.28	0.58
5:E:169:ARG:NH2	11:K:370:GLU:OE1	2.36	0.58
15:O:647:LYS:HG2	15:O:656:LEU:HD21	1.84	0.58
14:N:422:ASP:O	14:N:435:ALA:HB3	2.04	0.58
15:O:264:VAL:HG12	15:O:265:LEU:HD12	1.86	0.58
28:d:72:MET:HE2	28:d:333:MET:HE2	1.84	0.58
41:s:124:ARG:NH2	50:1:1212:G:OP1	2.37	0.58
5:E:337:VAL:O	5:E:341:GLN:HB2	2.04	0.58
22:X:560:VAL:HG22	22:X:582:THR:HG22	1.86	0.58
35:m:104:ASP:HB2	35:m:239:LYS:HE2	1.86	0.57
50:1:652:A:N6	50:1:670:A:OP2	2.37	0.57
50:1:758:U:N3	50:1:850:A:C6	2.72	0.57
15:O:953:ASP:O	15:O:957:ARG:HB2	2.05	0.57
29:e:27:ILE:HD13	29:e:36:ARG:HE	1.66	0.57
29:f:38:ILE:HA	29:f:111:GLN:O	2.03	0.57
38:p:149:ARG:HB2	38:p:161:LYS:O	2.05	0.57
21:V:94:VAL:HG12	21:V:96:ARG:H	1.69	0.57
21:W:94:VAL:HG12	21:W:96:ARG:H	1.69	0.57
37:o:5:ILE:HD12	37:o:16:ILE:HD12	1.86	0.57
1:A:9:ASN:ND2	1:A:9:ASN:H	2.02	0.57
1:A:626:ASN:HB3	50:1:256:U:H2'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:682:PHE:O	15:O:689:ILE:HA	2.05	0.57
21:V:41:THR:HG23	21:V:102:SER:HB2	1.85	0.57
21:W:41:THR:HG23	21:W:102:SER:HB2	1.85	0.57
29:f:75:GLY:O	29:f:79:LYS:HB2	2.03	0.57
37:o:188:GLN:OE1	50:1:855:A:N6	2.36	0.57
49:O:225:MET:HE1	49:O:233:ILE:HD12	1.86	0.57
6:F:406:ILE:HG22	6:F:419:ILE:HG22	1.84	0.57
13:M:145:SER:O	13:M:158:VAL:HA	2.04	0.57
19:T:100:VAL:HG12	19:T:102:ASP:H	1.69	0.57
28:d:253:MET:O	28:d:269:ALA:HB2	2.04	0.57
39:q:47:ARG:NH2	50:1:981:A:OP2	2.37	0.57
40:r:142:PRO:HD2	50:1:1058:A:H5''	1.86	0.57
22:X:301:ASN:O	22:X:317:LEU:HB3	2.05	0.57
26:b:52:LEU:O	26:b:56:PHE:HB2	2.04	0.57
32:j:121:GLY:HA3	32:j:147:GLY:HA3	1.86	0.57
37:o:184:PRO:O	37:o:188:GLN:HB2	2.04	0.57
50:1:1514:A:OP2	50:1:1516:C:N4	2.38	0.57
51:2:103:G:C6	51:2:250:G:N1	2.73	0.57
51:2:144:A:OP2	51:2:145:A:N6	2.38	0.57
3:C:602:VAL:HG21	50:1:1061:A:H5'	1.86	0.57
12:L:70:ASN:HA	12:L:86:ILE:HG12	1.86	0.57
18:R:250:GLY:HA2	18:R:306:TYR:O	2.04	0.57
20:U:164:MET:O	20:U:168:ALA:HB2	2.05	0.57
30:g:37:SER:O	30:g:81:LYS:HA	2.04	0.57
10:J:745:LEU:HD13	10:J:764:LEU:HD12	1.85	0.57
16:P:145:ILE:HG23	16:P:164:PRO:HB2	1.85	0.57
20:U:441:ASN:ND2	50:1:272:A:OP1	2.37	0.57
39:q:103:GLN:HB2	39:q:168:ARG:HG2	1.86	0.57
1:A:281:LEU:HD21	1:A:327:TRP:HB2	1.86	0.57
20:U:363:ARG:NH1	51:2:85:A:OP2	2.38	0.57
29:e:122:ILE:HG12	29:e:162:VAL:HG22	1.87	0.57
29:f:122:ILE:HG12	29:f:162:VAL:HG22	1.86	0.57
50:1:902:U:O2	50:1:930:G:N2	2.35	0.57
4:D:338:SER:HB3	4:D:354:LEU:HD12	1.86	0.57
5:E:173:ARG:NH2	19:T:57:THR:O	2.38	0.57
14:N:307:ALA:HB3	14:N:311:PRO:HA	1.87	0.57
23:Y:281:LEU:O	23:Y:293:ALA:HA	2.05	0.57
32:i:121:GLY:HA3	32:i:147:GLY:HA3	1.86	0.57
37:o:2:LYS:O	37:o:108:VAL:HA	2.05	0.57
9:I:879:PHE:O	9:I:883:LYS:HB2	2.05	0.56
10:J:766:HIS:O	27:c:707:GLU:OE2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:251:ARG:HB2	13:M:266:LEU:HD21	1.87	0.56
1:A:718:ALA:O	1:A:722:ALA:HB2	2.04	0.56
15:O:340:ILE:HA	15:O:356:GLY:HA2	1.88	0.56
34:l:169:VAL:HA	34:l:172:ILE:HG22	1.87	0.56
40:r:90:LYS:HB3	40:r:93:TYR:HD2	1.69	0.56
47:y:413:LEU:O	47:y:417:GLU:CB	2.53	0.56
50:1:460:U:H3	50:1:472:G:H1	1.53	0.56
50:1:1487:G:N2	50:1:1493:U:O4	2.37	0.56
1:A:281:LEU:HD23	1:A:291:HIS:HB3	1.87	0.56
3:C:587:LYS:NZ	50:1:1130:U:OP1	2.35	0.56
5:E:360:SER:O	5:E:364:LEU:HB2	2.05	0.56
16:P:76:LEU:O	16:P:80:MET:HB2	2.05	0.56
18:S:250:GLY:HA2	18:S:306:TYR:O	2.04	0.56
34:l:71:ALA:HB1	34:l:77:GLU:HA	1.87	0.56
36:n:184:GLU:O	36:n:188:ALA:HB2	2.06	0.56
37:o:132:ARG:NH1	50:1:733:C:O2'	2.38	0.56
49:0:177:ASN:O	49:0:183:SER:OG	2.23	0.56
50:1:1747:A:N3	50:1:2196:U:O2'	2.31	0.56
14:N:583:GLU:O	50:1:241:G:N2	2.36	0.56
18:R:85:ARG:HB3	33:k:112:ARG:HH22	1.71	0.56
23:Y:328:MET:O	23:Y:332:ALA:HB2	2.05	0.56
29:f:119:GLY:O	29:f:165:ASN:ND2	2.35	0.56
33:k:107:GLN:NE2	50:1:402:U:OP2	2.38	0.56
34:l:31:ASN:O	34:l:96:CYS:HB3	2.05	0.56
35:m:18:TRP:HD1	35:m:46:VAL:HG21	1.71	0.56
1:A:115:LEU:HB2	1:A:118:LYS:HB3	1.87	0.56
15:O:546:THR:HG21	15:O:627:GLY:HA2	1.88	0.56
15:O:853:THR:O	15:O:857:ILE:HB	2.05	0.56
18:R:66:LYS:NZ	33:k:149:SER:O	2.39	0.56
22:X:575:GLY:HA2	22:X:606:VAL:O	2.05	0.56
32:j:122:MET:H	32:j:148:LEU:H	1.53	0.56
48:z:9:LYS:HB3	48:z:33:PHE:HE1	1.71	0.56
10:J:748:TYR:OH	10:J:755:ARG:N	2.39	0.56
6:F:114:GLN:HE22	6:F:418:ILE:HB	1.71	0.56
15:O:136:ASP:O	15:O:158:ARG:NH1	2.37	0.56
15:O:433:GLN:HB2	15:O:436:ILE:HD11	1.88	0.56
35:m:102:ILE:O	35:m:109:PHE:HA	2.06	0.56
40:r:110:LEU:O	40:r:114:LEU:HB2	2.05	0.56
42:t:30:ALA:HB2	42:t:92:LEU:HD13	1.88	0.56
50:1:727:G:N2	50:1:728:G:O6	2.39	0.56
1:A:619:SER:HB3	1:A:672:GLU:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:868:GLU:OE1	9:I:912:ARG:NH2	2.38	0.56
14:N:170:GLU:OE2	14:N:174:ARG:NH2	2.39	0.56
25:a:30:HIS:HA	25:a:33:ILE:HB	1.88	0.56
30:g:67:ILE:HG12	30:g:82:THR:HG22	1.86	0.56
32:i:122:MET:H	32:i:148:LEU:H	1.53	0.56
1:A:676:SER:N	1:A:690:ALA:O	2.30	0.56
11:K:895:GLN:O	11:K:899:ARG:CB	2.54	0.56
22:X:401:VAL:HG23	22:X:411:THR:HG22	1.87	0.56
28:d:220:ARG:NH1	28:d:239:HIS:O	2.39	0.56
28:d:311:ARG:HB2	28:d:314:ALA:HB2	1.88	0.56
36:n:82:ASN:HA	36:n:85:MET:HE3	1.88	0.56
45:w:83:LEU:HB2	45:w:122:ALA:HB2	1.88	0.56
35:m:17:HIS:O	35:m:51:ARG:NH2	2.40	0.55
1:A:465:SER:HB2	26:b:134:GLU:HA	1.87	0.55
6:F:164:ASP:HB3	6:F:169:LYS:HB2	1.87	0.55
11:K:308:ASP:O	11:K:312:ARG:HB2	2.07	0.55
15:O:151:ILE:HG23	15:O:162:TRP:HB2	1.87	0.55
20:U:349:LEU:HD23	20:U:365:LEU:HD12	1.87	0.55
22:X:356:TYR:HB3	22:X:365:LEU:HB3	1.88	0.55
26:b:100:LEU:HD11	26:b:142:LEU:HG	1.88	0.55
28:d:270:ARG:NH2	50:1:580:A:N7	2.53	0.55
50:1:1664:U:C2	50:1:1675:A:N6	2.74	0.55
5:E:320:VAL:HG12	5:E:324:MET:HE2	1.89	0.55
22:X:261:VAL:O	22:X:272:VAL:HA	2.05	0.55
29:f:178:VAL:HG12	29:f:223:GLU:HB3	1.88	0.55
31:h:208:ARG:NH1	31:h:209:ILE:O	2.39	0.55
35:m:11:ARG:NH2	35:m:27:TYR:O	2.39	0.55
40:r:88:ARG:HD3	40:r:93:TYR:HB3	1.88	0.55
44:v:30:THR:O	44:v:33:GLY:C	2.48	0.55
15:O:147:PHE:HB3	15:O:191:ASN:HD22	1.71	0.55
17:Q:99:LEU:O	17:Q:127:VAL:HA	2.06	0.55
22:X:172:THR:N	22:X:599:CYS:SG	2.77	0.55
26:b:144:GLU:HA	26:b:149:PRO:HA	1.87	0.55
36:n:108:ILE:HA	36:n:186:ILE:HD11	1.88	0.55
42:t:30:ALA:HB3	42:t:94:ILE:HG12	1.89	0.55
50:1:1648:G:H2'	50:1:1649:A:H8	1.71	0.55
51:2:160:U:H2'	51:2:161:G:H8	1.72	0.55
4:D:101:ARG:HH21	4:D:168:ILE:HG13	1.71	0.55
18:S:128:ARG:NH2	18:S:172:ASP:OD2	2.37	0.55
28:d:307:ILE:HB	28:d:321:TYR:HB2	1.89	0.55
32:i:583:LEU:O	32:i:640:THR:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:31:ARG:NH2	50:1:1503:U:O3'	2.39	0.55
6:F:45:TYR:OH	6:F:57:ARG:NH1	2.40	0.55
24:Z:72:VAL:HG12	24:Z:117:ILE:HD11	1.88	0.55
30:g:56:PRO:HA	30:g:59:THR:HG22	1.87	0.55
31:h:196:LYS:O	31:h:200:ALA:HB2	2.06	0.55
34:l:204:ILE:O	50:1:1648:G:O2'	2.24	0.55
50:1:686:A:N6	50:1:969:A:N3	2.52	0.55
1:A:660:LYS:HE3	25:a:143:VAL:HG22	1.89	0.55
19:T:4:VAL:O	19:T:23:GLN:NE2	2.39	0.55
34:l:150:ILE:HG12	50:1:1651:C:H5''	1.88	0.55
47:y:360:HIS:HB3	47:y:366:ILE:HD13	1.88	0.55
50:1:1122:A:H5'	50:1:1127:C:H41	1.70	0.55
50:1:1753:G:N1	50:1:2158:G:OP2	2.36	0.55
1:A:170:SER:CB	1:A:174:THR:O	2.55	0.55
14:N:426:TRP:HB3	14:N:478:GLY:HA3	1.89	0.55
22:X:344:CYS:HB2	22:X:357:TRP:HB2	1.87	0.55
23:Y:328:MET:HG3	23:Y:330:ALA:H	1.72	0.55
32:j:583:LEU:O	32:j:640:THR:HA	2.06	0.55
35:m:105:THR:HG22	35:m:239:LYS:HE3	1.89	0.55
37:o:197:LYS:NZ	50:1:849:A:OP2	2.38	0.55
51:2:5:A:O2'	51:2:6:C:O5'	2.24	0.55
5:E:282:VAL:O	5:E:286:ALA:HB2	2.07	0.55
6:F:245:THR:O	25:a:21:TYR:OH	2.23	0.55
26:b:16:ARG:NH1	26:b:281:GLU:OE2	2.38	0.55
42:t:26:VAL:O	42:t:91:ALA:HB3	2.07	0.55
51:2:103:G:O6	51:2:250:G:C5	2.58	0.55
1:A:195:ARG:NH1	50:1:285:A:OP1	2.40	0.55
1:A:415:ARG:NH1	50:1:2215:C:O2	2.40	0.55
12:L:302:THR:HG23	12:L:303:THR:HG23	1.88	0.55
23:Y:98:ILE:O	23:Y:130:VAL:HA	2.06	0.55
35:m:72:VAL:HB	35:m:77:ARG:HG3	1.88	0.55
37:o:122:PRO:HA	37:o:126:ASP:HB3	1.89	0.55
6:F:100:LEU:HD23	6:F:421:PRO:HG2	1.90	0.54
6:F:304:ARG:N	6:F:318:THR:O	2.41	0.54
16:P:166:MET:HA	16:P:174:ALA:O	2.07	0.54
18:R:189:SER:O	18:R:193:LEU:HB2	2.07	0.54
26:b:112:PRO:HG3	26:b:226:ARG:HH22	1.72	0.54
29:e:119:GLY:O	29:e:165:ASN:ND2	2.35	0.54
37:o:135:PRO:HB3	37:o:140:LYS:HG3	1.89	0.54
50:1:746:A:H3'	50:1:747:G:H21	1.72	0.54
1:A:837:ASN:HB3	15:O:1019:TRP:HH2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:579:ILE:HA	24:Z:148:MET:HE2	1.89	0.54
13:M:111:ILE:HG23	13:M:125:ILE:HB	1.88	0.54
18:S:145:LEU:HD23	18:S:148:ILE:HG22	1.90	0.54
1:A:678:VAL:HA	1:A:688:CYS:O	2.07	0.54
16:P:56:TYR:HB2	16:P:87:VAL:HG12	1.90	0.54
13:M:156:LEU:CB	13:M:168:ILE:O	2.55	0.54
15:O:932:GLY:HA3	15:O:973:HIS:HD2	1.72	0.54
29:e:178:VAL:HG12	29:e:223:GLU:HB3	1.88	0.54
31:h:196:LYS:O	31:h:200:ALA:CB	2.56	0.54
35:m:183:ILE:O	35:m:190:GLY:N	2.39	0.54
44:v:77:THR:HG22	44:v:129:VAL:HG22	1.89	0.54
50:1:1056:U:H2'	50:1:1057:A:H8	1.71	0.54
51:2:103:G:C5	51:2:250:G:C2	2.96	0.54
51:2:153:G:O6	51:2:176:U:O2	2.26	0.54
1:A:4:ASN:ND2	1:A:705:GLN:OE1	2.38	0.54
13:M:243:SER:O	13:M:256:ALA:HB3	2.08	0.54
18:S:175:GLY:O	18:S:202:ASN:ND2	2.38	0.54
24:Z:80:GLY:O	24:Z:84:LEU:CB	2.53	0.54
30:g:160:THR:OG1	30:g:172:MET:O	2.21	0.54
18:S:189:SER:O	18:S:193:LEU:HB2	2.07	0.54
19:T:191:ILE:O	19:T:195:ALA:HB3	2.08	0.54
36:n:84:LEU:O	36:n:167:ARG:NH2	2.40	0.54
50:1:152:G:O2'	50:1:153:C:P	2.65	0.54
50:1:796:G:N2	50:1:834:C:OP2	2.36	0.54
1:A:579:ARG:HG3	1:A:679:ALA:HA	1.90	0.54
18:R:65:ALA:O	18:R:107:LYS:NZ	2.33	0.54
25:a:10:GLN:O	25:a:13:LEU:C	2.50	0.54
32:i:281:VAL:HA	32:i:470:LYS:O	2.08	0.54
33:k:189:ARG:O	50:1:2072:U:N3	2.41	0.54
50:1:1625:G:H2'	50:1:1626:G:C8	2.42	0.54
50:1:2054:A:H62	50:1:2119:G:N2	2.04	0.54
10:J:813:LEU:O	10:J:817:ASN:HB2	2.08	0.54
18:R:77:ARG:NH2	18:R:145:LEU:O	2.41	0.54
21:V:68:ILE:HG22	21:V:71:ILE:HD11	1.90	0.54
21:W:68:ILE:HG22	21:W:71:ILE:HD11	1.90	0.54
22:X:398:MET:HA	22:X:413:SER:HA	1.89	0.54
50:1:1213:U:OP2	50:1:1554:C:N4	2.40	0.54
14:N:408:TRP:NE1	14:N:410:ALA:O	2.41	0.54
14:N:418:HIS:HB2	14:N:437:ARG:HE	1.73	0.54
15:O:463:PRO:HB2	15:O:515:HIS:HB3	1.90	0.54
17:Q:103:ASP:O	17:Q:105:GLN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:43:LYS:NZ	51:2:113:G:O6	2.41	0.54
47:y:413:LEU:O	47:y:417:GLU:HB2	2.08	0.54
1:A:761:VAL:O	1:A:765:PHE:HB2	2.08	0.54
13:M:421:MET:HE2	13:M:423:LEU:HD21	1.90	0.54
13:M:427:GLU:OE2	14:N:359:LYS:N	2.41	0.54
15:O:252:PRO:HA	15:O:267:LEU:O	2.08	0.54
20:U:66:GLU:OE1	20:U:68:LYS:NZ	2.40	0.54
28:d:251:GLU:OE1	28:d:254:ASN:ND2	2.36	0.54
29:f:112:ILE:HG23	29:f:124:VAL:HB	1.90	0.54
35:m:128:ARG:HH22	50:1:879:A:H4'	1.72	0.54
38:p:133:ASP:OD1	38:p:148:LYS:NZ	2.40	0.54
50:1:221:A:O2'	50:1:224:C:N4	2.33	0.54
26:b:103:PHE:HD2	26:b:142:LEU:HD21	1.73	0.53
32:j:281:VAL:HA	32:j:470:LYS:O	2.08	0.53
42:t:37:ASN:ND2	50:1:1487:G:OP2	2.41	0.53
49:0:163:ARG:O	49:0:167:GLU:HB2	2.08	0.53
50:1:685:C:O2	50:1:686:A:N6	2.41	0.53
50:1:1735:A:N1	50:1:2210:U:O4	2.40	0.53
1:A:73:ILE:HG21	1:A:99:VAL:HB	1.89	0.53
1:A:568:ASN:ND2	51:2:61:G:OP1	2.39	0.53
8:H:107:GLN:OE1	24:Z:1079:ARG:NH2	2.40	0.53
18:S:77:ARG:NH2	18:S:145:LEU:O	2.41	0.53
20:U:102:LEU:HD23	20:U:104:GLY:H	1.72	0.53
28:d:389:ARG:NH2	50:1:591:C:N3	2.52	0.53
1:A:112:VAL:HG22	1:A:121:VAL:HB	1.91	0.53
6:F:267:ASN:ND2	6:F:270:ASN:OD1	2.41	0.53
9:I:862:ASN:OD1	9:I:905:ASN:ND2	2.40	0.53
9:I:895:MET:O	9:I:899:LEU:CB	2.54	0.53
15:O:307:ASP:HA	15:O:323:LEU:O	2.08	0.53
18:R:145:LEU:HD23	18:R:148:ILE:HG22	1.90	0.53
19:T:252:LEU:O	19:T:256:GLN:CB	2.56	0.53
24:Z:70:LEU:HB2	24:Z:275:ARG:HH12	1.73	0.53
47:y:385:GLN:O	47:y:406:ILE:HA	2.08	0.53
7:G:86:MET:HE3	7:G:90:GLU:HB3	1.91	0.53
22:X:272:VAL:HG21	22:X:317:LEU:HD11	1.90	0.53
50:1:1515:A:N7	50:1:1516:C:N4	2.56	0.53
51:2:91:G:OP1	51:2:91:G:N2	2.41	0.53
1:A:492:ALA:HB3	1:A:507:LEU:HB2	1.90	0.53
5:E:130:MET:HE2	5:E:147:ALA:HB2	1.90	0.53
9:I:879:PHE:O	9:I:883:LYS:CB	2.56	0.53
15:O:175:PRO:HG3	15:O:211:TRP:HH2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:27:ARG:NH1	51:2:46:U:O2'	2.40	0.53
24:Z:931:THR:HG22	24:Z:976:THR:HG22	1.90	0.53
29:f:35:LYS:HD2	29:f:198:PRO:HA	1.90	0.53
30:g:72:ASP:O	30:g:76:GLY:CA	2.55	0.53
31:h:158:LEU:HG	31:h:164:LEU:HD23	1.89	0.53
46:x:74:VAL:HB	46:x:83:VAL:O	2.09	0.53
18:S:307:LEU:HD22	20:U:120:ARG:HH22	1.73	0.53
21:V:59:THR:HG23	21:V:99:ILE:HD11	1.90	0.53
50:1:1729:U:O2	50:1:2228:G:N2	2.40	0.53
6:F:214:ARG:NH2	50:1:292:G:OP2	2.41	0.53
6:F:355:LEU:HD12	6:F:423:ALA:HB2	1.91	0.53
7:G:220:ILE:O	7:G:224:ALA:CB	2.56	0.53
10:J:756:ASP:O	10:J:760:LEU:CB	2.56	0.53
14:N:155:ARG:O	14:N:158:ARG:NE	2.42	0.53
15:O:50:PRO:HB2	15:O:342:LYS:HD2	1.91	0.53
25:a:82:LEU:HD23	25:a:87:ILE:HB	1.91	0.53
1:A:97:SER:HB2	1:A:115:LEU:HD22	1.91	0.53
6:F:82:ALA:HA	11:K:914:THR:HG21	1.91	0.53
19:T:252:LEU:O	19:T:256:GLN:HB3	2.09	0.53
20:U:361:ILE:HG12	20:U:364:GLN:HE21	1.73	0.53
22:X:243:GLN:HA	22:X:280:PRO:HB2	1.90	0.53
28:d:244:ARG:HD3	28:d:288:ASP:HA	1.91	0.53
35:m:128:ARG:HB3	35:m:140:VAL:HB	1.90	0.53
1:A:155:ARG:HH11	1:A:199:VAL:HG23	1.74	0.53
8:H:117:ASN:HB3	51:2:260:G:H4'	1.89	0.53
15:O:482:PRO:HA	15:O:528:ARG:HH12	1.74	0.53
18:R:222:MET:HG2	19:T:135:ARG:HG2	1.90	0.53
19:T:140:LYS:HE2	50:1:436:A:H62	1.72	0.53
19:T:291:LEU:O	19:T:295:LEU:HB2	2.09	0.53
50:1:704:U:H3	50:1:882:C:H42	1.56	0.53
50:1:1735:A:N1	50:1:2210:U:C4	2.77	0.53
1:A:312:LEU:HD12	1:A:325:TRP:HD1	1.74	0.52
24:Z:1142:TRP:O	24:Z:1146:GLY:HA3	2.09	0.52
30:g:43:PHE:HB3	30:g:78:MET:HE2	1.90	0.52
36:n:71:LYS:O	36:n:79:ARG:NH1	2.42	0.52
36:n:95:LEU:HA	36:n:98:VAL:HG22	1.92	0.52
37:o:185:GLN:HE22	50:1:854:C:H41	1.57	0.52
1:A:501:THR:HG22	1:A:503:THR:HB	1.91	0.52
1:A:577:THR:HG21	1:A:677:GLY:HA2	1.90	0.52
3:C:583:ILE:O	24:Z:192:ARG:NH1	2.38	0.52
6:F:270:ASN:HB2	6:F:272:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:342:PRO:HD2	11:K:926:LYS:HB2	1.91	0.52
22:X:415:ASN:ND2	22:X:417:ASP:OD2	2.42	0.52
28:d:308:ARG:HD3	28:d:320:VAL:HG12	1.91	0.52
29:e:35:LYS:HD2	29:e:198:PRO:HA	1.90	0.52
29:e:112:ILE:HG23	29:e:124:VAL:HB	1.90	0.52
34:l:129:THR:O	34:l:132:HIS:N	2.43	0.52
40:r:29:VAL:HG23	40:r:34:LEU:HB2	1.91	0.52
1:A:106:PRO:HG2	1:A:163:SER:HB2	1.92	0.52
16:P:54:PRO:HB3	16:P:85:ALA:HB1	1.91	0.52
22:X:185:THR:HG23	22:X:195:TRP:HE1	1.73	0.52
26:b:125:PRO:HA	26:b:128:VAL:HG22	1.90	0.52
1:A:500:ARG:NH2	50:1:2201:C:OP2	2.43	0.52
6:F:304:ARG:H	6:F:319:GLY:HA2	1.74	0.52
12:L:248:LEU:HD23	12:L:255:ILE:HD11	1.91	0.52
28:d:369:ARG:NH1	28:d:373:GLU:OE2	2.43	0.52
34:l:128:THR:HA	34:l:133:TYR:O	2.10	0.52
38:p:54:GLU:HG2	38:p:62:LYS:HE2	1.91	0.52
50:1:619:U:C2	50:1:1179:G:N1	2.78	0.52
50:1:924:A:H2'	50:1:925:G:H8	1.74	0.52
7:G:232:MET:HB3	7:G:243:ASN:HB3	1.91	0.52
16:P:126:LYS:HE3	51:2:33:U:H4'	1.92	0.52
22:X:264:GLY:CA	22:X:269:ARG:O	2.58	0.52
23:Y:15:ARG:NH1	23:Y:359:GLU:OE2	2.43	0.52
24:Z:115:THR:HG21	24:Z:275:ARG:HH22	1.74	0.52
24:Z:298:LYS:HB3	24:Z:780:VAL:HB	1.91	0.52
50:1:35:G:O6	50:1:59:U:O4	2.27	0.52
4:D:251:SER:OG	4:D:259:CYS:SG	2.67	0.52
6:F:215:LYS:O	6:F:241:LYS:NZ	2.42	0.52
13:M:156:LEU:HB3	13:M:168:ILE:O	2.09	0.52
15:O:325:SER:HB3	15:O:446:LEU:HG	1.92	0.52
16:P:93:SER:OG	16:P:123:CYS:SG	2.68	0.52
21:W:59:THR:HG23	21:W:99:ILE:HD11	1.90	0.52
24:Z:935:LYS:NZ	50:1:2077:C:OP1	2.43	0.52
26:b:229:THR:HG21	27:c:545:ILE:HD11	1.92	0.52
28:d:224:LEU:HD12	28:d:234:ILE:HD11	1.92	0.52
35:m:247:ILE:O	35:m:251:ARG:HB2	2.09	0.52
37:o:2:LYS:HG2	37:o:17:GLU:HA	1.90	0.52
44:v:98:TYR:HA	44:v:104:ARG:O	2.09	0.52
5:E:324:MET:HB3	5:E:334:THR:HG22	1.92	0.52
6:F:297:LEU:HB2	11:K:868:ASP:O	2.10	0.52
20:U:107:ILE:HG12	20:U:109:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:304:HIS:ND1	51:2:93:G:O6	2.29	0.52
31:h:230:GLU:HA	31:h:233:VAL:HG12	1.92	0.52
34:l:136:ARG:NH2	50:1:1469:A:OP1	2.43	0.52
38:p:102:ARG:NH2	38:p:131:VAL:O	2.42	0.52
44:v:91:ILE:HB	44:v:112:LEU:HB2	1.91	0.52
44:v:108:ARG:NH1	50:1:891:G:OP1	2.42	0.52
6:F:313:ARG:HD3	6:F:330:ARG:HE	1.75	0.52
8:H:18:GLN:HG3	8:H:28:LEU:HB2	1.91	0.52
8:H:27:ILE:HD11	24:Z:1041:PRO:HD2	1.92	0.52
13:M:194:ALA:O	13:M:251:ARG:NH1	2.43	0.52
15:O:76:LEU:HD11	15:O:346:LEU:HD13	1.92	0.52
19:T:373:LYS:O	19:T:377:ARG:HB2	2.10	0.52
23:Y:119:LEU:HD13	23:Y:337:THR:HG21	1.90	0.52
23:Y:346:VAL:HB	23:Y:397:SER:HB2	1.91	0.52
28:d:87:GLY:HA2	28:d:112:ILE:HG22	1.92	0.52
30:g:51:LEU:O	30:g:55:TRP:HB2	2.10	0.52
34:l:157:GLN:NE2	50:1:1632:G:OP2	2.43	0.52
34:l:172:ILE:O	34:l:176:ALA:CB	2.57	0.52
50:1:1744:A:H2'	50:1:1745:C:H6	1.74	0.52
51:2:137:U:O4	51:2:150:G:O6	2.28	0.52
4:D:104:SER:OG	4:D:114:TRP:NE1	2.37	0.52
11:K:896:GLN:O	11:K:900:SER:OG	2.28	0.52
12:L:72:LEU:HD22	12:L:333:HIS:HE1	1.74	0.52
12:L:93:LYS:HZ1	12:L:134:ALA:HB2	1.74	0.52
12:L:292:SER:O	12:L:319:SER:OG	2.27	0.52
26:b:133:ARG:O	26:b:135:ARG:NH2	2.42	0.52
35:m:41:CYS:SG	35:m:42:MET:N	2.82	0.52
47:y:344:ILE:HG22	47:y:346:ASN:H	1.74	0.52
49:O:178:PRO:HA	49:O:184:SER:HB3	1.93	0.52
50:1:2:G:O6	50:1:32:U:O4	2.28	0.52
50:1:186:C:H2'	50:1:187:G:H8	1.75	0.52
50:1:494:G:H3'	50:1:495:G:H21	1.74	0.52
50:1:903:U:O2'	50:1:907:A:N7	2.39	0.52
50:1:1748:G:O2'	50:1:2195:U:O2	2.27	0.52
8:H:2:SER:OG	8:H:10:ARG:NH2	2.43	0.51
35:m:52:LEU:HD21	35:m:111:VAL:HG11	1.92	0.51
35:m:139:LEU:HD22	35:m:147:ILE:HD12	1.91	0.51
50:1:1047:U:O2'	50:1:1111:A:N6	2.43	0.51
50:1:1759:U:O4	50:1:2047:G:C6	2.63	0.51
15:O:846:VAL:HG13	15:O:850:ARG:HD2	1.91	0.51
20:U:71:PRO:O	20:U:75:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:314:VAL:O	22:X:323:VAL:HB	2.10	0.51
50:1:1472:A:N1	50:1:1510:G:C6	2.78	0.51
14:N:327:ARG:NH1	14:N:376:PHE:O	2.40	0.51
23:Y:203:PRO:HD2	23:Y:342:GLY:HA2	1.92	0.51
50:1:202:A:H2	50:1:206:C:H5	1.58	0.51
16:P:114:ARG:NH1	28:d:347:ASP:O	2.43	0.51
22:X:419:ALA:HA	22:X:430:HIS:O	2.11	0.51
22:X:560:VAL:HA	22:X:582:THR:HA	1.92	0.51
31:h:166:ILE:HB	31:h:217:HIS:CE1	2.46	0.51
37:o:132:ARG:NH2	50:1:655:A:N7	2.58	0.51
50:1:18:G:N1	50:1:20:C:C4	2.79	0.51
50:1:166:A:N6	50:1:171:G:O6	2.44	0.51
24:Z:929:LYS:H	50:1:2177:G:H3'	1.76	0.51
26:b:123:ILE:HG23	26:b:126:ASP:HB2	1.92	0.51
41:s:122:ILE:O	41:s:126:ALA:HB3	2.11	0.51
42:t:32:ILE:HA	42:t:40:PHE:O	2.09	0.51
42:t:73:ALA:O	42:t:77:ALA:CB	2.58	0.51
50:1:730:U:H2'	50:1:731:A:H8	1.75	0.51
6:F:246:SER:HB2	25:a:16:HIS:HD2	1.75	0.51
6:F:318:THR:HG21	6:F:345:ALA:HB3	1.93	0.51
13:M:370:LEU:HB3	13:M:382:TRP:HB2	1.93	0.51
17:Q:134:LYS:O	17:Q:138:LYS:CB	2.58	0.51
17:Q:252:PRO:O	17:Q:256:ALA:HB2	2.10	0.51
32:i:285:ALA:O	32:i:413:THR:HA	2.11	0.51
34:l:21:GLN:O	34:l:26:ARG:NH1	2.39	0.51
38:p:151:ARG:HA	45:w:51:GLU:HA	1.93	0.51
1:A:398:PHE:HB3	1:A:431:MET:HE2	1.93	0.51
14:N:278:SER:OG	14:N:325:LEU:O	2.26	0.51
14:N:461:ILE:HD11	21:V:91:ALA:HA	1.92	0.51
15:O:394:LEU:HD21	15:O:472:LEU:HD21	1.91	0.51
15:O:396:SER:HA	15:O:404:GLY:H	1.76	0.51
24:Z:285:ARG:HG2	24:Z:295:THR:HG22	1.91	0.51
32:j:723:VAL:O	32:j:763:ILE:HA	2.10	0.51
47:y:393:THR:OG1	50:1:1115:C:O2	2.28	0.51
1:A:406:VAL:HG23	1:A:420:PHE:HB2	1.93	0.51
1:A:407:ARG:HG2	1:A:419:THR:HB	1.93	0.51
4:D:128:GLN:HE22	18:S:271:VAL:HA	1.76	0.51
18:R:175:GLY:O	18:R:202:ASN:ND2	2.38	0.51
19:T:20:VAL:HG21	19:T:130:LEU:HD21	1.93	0.51
32:i:12:PRO:O	32:i:16:ARG:CB	2.59	0.51
40:r:133:ARG:NH2	40:r:156:PHE:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:145:A:H2'	51:2:146:A:C8	2.46	0.51
1:A:156:HIS:HB3	1:A:169:ALA:HB3	1.92	0.51
15:O:633:LEU:HD23	15:O:635:ARG:HE	1.76	0.51
17:Q:97:VAL:O	17:Q:125:GLY:CA	2.59	0.51
19:T:253:ALA:O	19:T:257:ALA:HB2	2.11	0.51
32:j:911:ILE:O	32:j:915:ILE:CB	2.59	0.51
42:t:51:THR:N	50:1:1480:G:O2'	2.44	0.51
32:i:723:VAL:O	32:i:763:ILE:HA	2.10	0.50
32:j:12:PRO:O	32:j:16:ARG:CB	2.59	0.50
34:l:144:LYS:NZ	34:l:145:ARG:O	2.36	0.50
36:n:18:LYS:O	36:n:22:ALA:HB2	2.11	0.50
1:A:494:ILE:HB	1:A:505:GLU:HB3	1.93	0.50
4:D:118:LYS:HE2	4:D:120:ARG:HD2	1.93	0.50
6:F:200:VAL:O	6:F:213:LEU:HB2	2.10	0.50
15:O:100:TRP:CG	15:O:101:LYS:H	2.29	0.50
24:Z:67:PRO:HB3	24:Z:774:GLY:HA2	1.93	0.50
24:Z:170:LEU:HD11	24:Z:189:LEU:HD23	1.92	0.50
29:f:101:ASP:OD2	29:f:132:ARG:NH1	2.44	0.50
37:o:70:PRO:HB3	37:o:101:ILE:HB	1.93	0.50
38:p:150:LEU:HD12	38:p:160:LEU:HD12	1.93	0.50
5:E:92:THR:HA	5:E:95:ILE:HD12	1.93	0.50
10:J:827:GLN:NE2	10:J:867:THR:OG1	2.42	0.50
12:L:206:VAL:HA	12:L:215:ARG:O	2.11	0.50
14:N:584:GLN:HE22	50:1:245:G:H5'	1.75	0.50
15:O:720:ARG:O	15:O:736:LEU:HB2	2.10	0.50
28:d:211:SER:HB2	28:d:227:LEU:HB3	1.94	0.50
34:l:62:LYS:HE2	34:l:223:PHE:HZ	1.75	0.50
34:l:76:ASP:HB3	34:l:79:HIS:HD2	1.76	0.50
42:t:98:ALA:HB2	42:t:107:PRO:HA	1.92	0.50
50:1:1448:A:C6	50:1:1549:U:O4	2.64	0.50
1:A:759:GLY:O	1:A:763:GLU:CB	2.59	0.50
5:E:161:ARG:HH12	5:E:278:ILE:HG21	1.76	0.50
13:M:369:TYR:OH	14:N:408:TRP:O	2.25	0.50
20:U:58:VAL:HG23	20:U:145:LEU:HG	1.93	0.50
20:U:94:LYS:O	20:U:98:SER:HB3	2.12	0.50
20:U:370:ALA:O	20:U:374:ARG:HB2	2.10	0.50
35:m:126:VAL:HG22	35:m:139:LEU:HD21	1.94	0.50
37:o:10:ASN:ND2	37:o:127:VAL:O	2.44	0.50
38:p:95:HIS:HD2	38:p:175:ARG:HE	1.58	0.50
44:v:15:LYS:HB3	44:v:59:ILE:HB	1.93	0.50
50:1:645:U:H4'	50:1:1035:G:H21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HB2	1:A:186:PHE:HB3	1.94	0.50
1:A:278:ILE:HA	1:A:294:SER:HA	1.92	0.50
1:A:431:MET:HE1	1:A:440:ILE:HD12	1.94	0.50
4:D:318:HIS:NE2	50:1:70:C:OP1	2.35	0.50
8:H:28:LEU:HD11	24:Z:986:ILE:HG22	1.93	0.50
9:I:887:LYS:HA	9:I:890:VAL:HG22	1.92	0.50
15:O:1038:GLY:O	15:O:1042:SER:HB3	2.11	0.50
29:e:190:ARG:HG3	29:e:248:ALA:HB2	1.94	0.50
32:i:635:ILE:H	32:i:725:VAL:HA	1.77	0.50
37:o:137:ARG:HE	50:1:752:A:H5'	1.76	0.50
50:1:2089:G:H2'	50:1:2090:G:C8	2.47	0.50
51:2:246:G:H2'	51:2:247:G:C8	2.46	0.50
9:I:815:ASN:HB3	9:I:818:PHE:HD2	1.75	0.50
12:L:280:SER:HB2	12:L:323:ILE:HG12	1.93	0.50
28:d:442:LEU:HD13	28:d:443:VAL:HG13	1.92	0.50
35:m:207:ILE:HD12	35:m:219:ALA:HB1	1.93	0.50
35:m:210:LEU:O	35:m:217:THR:HA	2.12	0.50
38:p:171:GLY:HA2	38:p:174:TYR:HD2	1.76	0.50
46:x:126:LYS:HG2	46:x:131:GLY:HA2	1.94	0.50
50:1:191:C:O2'	50:1:192:A:N7	2.42	0.50
1:A:594:LYS:HD3	1:A:621:THR:HA	1.93	0.50
15:O:64:THR:HA	15:O:72:GLN:O	2.11	0.50
15:O:565:ILE:HB	15:O:579:PHE:HB2	1.94	0.50
17:Q:105:GLN:O	17:Q:109:LYS:CB	2.59	0.50
19:T:291:LEU:O	19:T:295:LEU:CB	2.60	0.50
23:Y:205:THR:HG1	23:Y:343:SER:HG	1.58	0.50
24:Z:103:PRO:HG2	24:Z:247:ASP:HA	1.93	0.50
29:e:101:ASP:OD2	29:e:132:ARG:NH1	2.44	0.50
32:i:911:ILE:O	32:i:915:ILE:CB	2.59	0.50
37:o:176:PRO:HA	50:1:653:U:H5'	1.93	0.50
44:v:96:LEU:HA	44:v:106:GLU:O	2.12	0.50
18:R:94:THR:O	18:R:127:TYR:HA	2.11	0.50
19:T:101:ALA:HB2	19:T:131:LEU:HD21	1.94	0.50
29:e:75:GLY:O	29:e:79:LYS:CB	2.59	0.50
29:f:75:GLY:O	29:f:79:LYS:CB	2.59	0.50
32:j:285:ALA:O	32:j:413:THR:HA	2.11	0.50
39:q:106:ALA:O	39:q:110:ARG:HB2	2.12	0.50
50:1:644:G:N2	50:1:1035:G:O2'	2.45	0.50
1:A:563:ARG:HH12	16:P:-2:ARG:HB2	1.76	0.50
4:D:179:LEU:HD13	4:D:217:GLY:HA2	1.94	0.50
9:I:843:HIS:O	9:I:847:LEU:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:931:LEU:HD21	10:J:856:LEU:HD23	1.94	0.50
12:L:326:GLY:HA2	12:L:331:ASP:HA	1.93	0.50
13:M:354:HIS:NE2	13:M:373:GLY:O	2.45	0.50
13:M:380:VAL:HA	13:M:391:PHE:HB3	1.94	0.50
15:O:353:VAL:HG22	15:O:363:THR:HB	1.94	0.50
15:O:738:THR:HG22	15:O:740:HIS:HD2	1.76	0.50
20:U:311:LEU:HD23	20:U:373:VAL:HG21	1.93	0.50
34:l:142:PHE:HB2	34:l:209:ASN:HB2	1.93	0.50
36:n:184:GLU:O	36:n:188:ALA:CB	2.60	0.50
37:o:49:ILE:HG12	37:o:115:LYS:HB2	1.94	0.50
38:p:153:LYS:O	45:w:42:GLN:NE2	2.45	0.50
40:r:66:LYS:O	40:r:70:GLU:CB	2.60	0.50
50:1:483:U:H4'	50:1:484:G:H5''	1.92	0.50
1:A:115:LEU:HD12	1:A:118:LYS:HD2	1.94	0.49
1:A:738:PHE:HZ	1:A:773:LEU:HD13	1.76	0.49
3:C:598:ARG:NH2	50:1:1129:A:OP1	2.40	0.49
7:G:48:ILE:HD13	7:G:123:ARG:HE	1.77	0.49
8:H:5:ARG:HD2	8:H:10:ARG:HE	1.76	0.49
23:Y:152:THR:O	23:Y:156:ALA:CB	2.59	0.49
32:i:614:ILE:O	32:i:618:VAL:CB	2.60	0.49
35:m:54:TYR:OH	35:m:113:ARG:NH2	2.45	0.49
36:n:135:ARG:O	48:z:23:ARG:NH1	2.35	0.49
51:2:149:U:H2'	51:2:150:G:H8	1.77	0.49
18:S:116:SER:HB3	18:S:119:ASP:HB2	1.94	0.49
19:T:223:VAL:HA	19:T:226:ILE:HG22	1.94	0.49
20:U:56:ILE:HA	20:U:59:GLU:HB2	1.92	0.49
20:U:262:VAL:HA	20:U:265:VAL:HG12	1.94	0.49
22:X:301:ASN:HB2	22:X:317:LEU:HB3	1.93	0.49
32:j:635:ILE:H	32:j:725:VAL:HA	1.77	0.49
34:l:172:ILE:O	34:l:176:ALA:HB2	2.12	0.49
50:1:695:G:O6	50:1:890:U:O4	2.29	0.49
5:E:312:CYS:HB2	5:E:315:ARG:HE	1.77	0.49
9:I:861:LEU:HD21	9:I:877:ILE:HD11	1.94	0.49
13:M:429:LYS:HD2	13:M:430:PRO:HD2	1.94	0.49
15:O:109:GLY:HA3	15:O:117:GLN:HA	1.93	0.49
15:O:191:ASN:OD1	15:O:191:ASN:N	2.45	0.49
18:S:94:THR:O	18:S:127:TYR:HA	2.11	0.49
19:T:309:ILE:HG13	19:T:310:LEU:HG	1.94	0.49
23:Y:117:LEU:O	23:Y:121:ALA:CB	2.60	0.49
24:Z:976:THR:OG1	26:b:287:TYR:OH	2.25	0.49
26:b:90:VAL:HG11	26:b:108:ARG:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:92:THR:HA	26:b:142:LEU:HB3	1.94	0.49
50:1:681:G:H3'	50:1:682:G:H8	1.78	0.49
50:1:2054:A:C6	50:1:2119:G:N2	2.80	0.49
6:F:468:ASN:O	11:K:884:ALA:N	2.45	0.49
19:T:45:GLY:HA3	50:1:435:A:N1	2.28	0.49
19:T:385:LYS:HA	19:T:388:ILE:HG22	1.93	0.49
28:d:156:TYR:HA	28:d:172:SER:HA	1.93	0.49
50:1:675:G:N2	50:1:1036:A:OP2	2.43	0.49
50:1:712:A:N6	50:1:875:G:H21	2.05	0.49
20:U:18:ALA:HB3	20:U:46:LYS:HD3	1.95	0.49
23:Y:151:ASP:OD2	23:Y:178:ARG:NH1	2.46	0.49
23:Y:346:VAL:HA	23:Y:398:VAL:O	2.13	0.49
28:d:80:ASN:HB2	28:d:96:LEU:H	1.77	0.49
28:d:134:LEU:HB3	28:d:148:ALA:HB3	1.94	0.49
35:m:65:MET:HG2	35:m:78:THR:HA	1.95	0.49
37:o:94:ARG:NE	50:1:991:A:OP1	2.46	0.49
38:p:152:THR:HG23	45:w:42:GLN:HE22	1.76	0.49
39:q:111:GLN:O	39:q:115:ALA:CB	2.61	0.49
1:A:532:GLY:HA2	1:A:574:ASN:HA	1.94	0.49
16:P:148:THR:HG21	16:P:153:LEU:HD23	1.95	0.49
19:T:16:SER:HB3	19:T:53:PHE:HD1	1.77	0.49
20:U:190:TYR:HD1	20:U:257:ILE:HD12	1.77	0.49
28:d:285:ALA:O	28:d:303:TYR:N	2.42	0.49
47:y:341:ARG:O	47:y:342:LYS:C	2.54	0.49
50:1:1509:A:H2'	50:1:1510:G:C8	2.48	0.49
6:F:356:THR:HG21	6:F:370:LEU:HD12	1.95	0.49
20:U:116:ASP:O	20:U:120:ARG:HB3	2.11	0.49
26:b:204:VAL:HA	26:b:207:ILE:HG12	1.94	0.49
30:g:160:THR:HG21	30:g:181:VAL:HG21	1.94	0.49
34:l:164:ILE:HG12	34:l:207:LEU:HD11	1.95	0.49
39:q:144:LYS:O	39:q:148:ALA:CB	2.60	0.49
47:y:412:ALA:O	47:y:416:PHE:HB2	2.12	0.49
1:A:557:GLY:HA3	1:A:566:ALA:HB1	1.93	0.49
3:C:639:LYS:HE2	33:k:123:LYS:HB3	1.95	0.49
8:H:22:ARG:HG3	8:H:25:LEU:HD12	1.94	0.49
8:H:64:TYR:H	8:H:67:MET:HE2	1.77	0.49
15:O:211:TRP:HD1	15:O:218:LEU:HA	1.77	0.49
38:p:54:GLU:HA	38:p:63:ALA:O	2.13	0.49
41:s:105:ASN:ND2	50:1:1464:G:O2'	2.46	0.49
1:A:364:ILE:HG23	1:A:378:PHE:HB2	1.95	0.49
1:A:593:SER:OG	1:A:594:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:301:PHE:O	5:E:305:ALA:HB2	2.11	0.49
7:G:214:ILE:HG12	7:G:267:ILE:HG13	1.94	0.49
13:M:205:LEU:O	13:M:221:TYR:C	2.56	0.49
14:N:155:ARG:NH1	50:1:275:C:OP1	2.46	0.49
14:N:376:PHE:HB3	14:N:387:LEU:HD23	1.95	0.49
16:P:39:GLN:NE2	18:R:291:THR:OG1	2.45	0.49
18:S:109:ILE:HB	18:S:127:TYR:HB2	1.95	0.49
20:U:361:ILE:HA	20:U:364:GLN:HG2	1.95	0.49
29:e:156:ASN:ND2	50:1:2120:C:O4'	2.46	0.49
29:f:190:ARG:HG3	29:f:248:ALA:HB2	1.94	0.49
32:i:616:TRP:O	32:i:620:GLN:CB	2.61	0.49
34:l:136:ARG:HH22	50:1:1469:A:H5'	1.78	0.49
35:m:91:THR:HA	35:m:98:ASN:HD22	1.78	0.49
35:m:127:LYS:HB2	35:m:142:HIS:HA	1.95	0.49
38:p:145:ILE:HA	38:p:164:LEU:HD23	1.95	0.49
41:s:108:ASP:OD1	50:1:1463:G:O2'	2.30	0.49
50:1:649:A:O2'	50:1:852:C:O2	2.31	0.49
51:2:200:U:O2	51:2:246:G:N2	2.46	0.49
15:O:565:ILE:HD11	15:O:625:VAL:HG11	1.94	0.49
15:O:691:VAL:O	15:O:700:ILE:N	2.45	0.49
15:O:957:ARG:HD3	31:h:250:ILE:HD12	1.94	0.49
19:T:209:LEU:HA	19:T:212:ILE:HG22	1.94	0.49
21:W:21:LEU:HD23	21:W:118:LEU:HD21	1.95	0.49
24:Z:220:HIS:HE1	50:1:639:U:H4'	1.78	0.49
32:j:614:ILE:O	32:j:618:VAL:CB	2.60	0.49
33:k:154:ARG:NH1	51:2:97:C:OP2	2.38	0.49
37:o:137:ARG:NH2	50:1:753:A:OP2	2.46	0.49
49:0:169:HIS:O	49:0:173:GLU:CB	2.61	0.49
50:1:1218:G:N2	50:1:1550:U:OP2	2.36	0.49
51:2:144:A:H3'	51:2:145:A:C8	2.48	0.49
5:E:7:LYS:HG3	5:E:48:LEU:HD13	1.94	0.48
6:F:139:PRO:HA	6:F:412:ASN:HA	1.94	0.48
6:F:264:LEU:HD13	6:F:275:ILE:HG22	1.94	0.48
8:H:215:VAL:HG21	18:S:88:LYS:HB3	1.95	0.48
24:Z:255:PRO:O	24:Z:259:GLU:CB	2.61	0.48
24:Z:944:ILE:HD12	24:Z:973:PHE:HB3	1.94	0.48
32:i:189:PHE:O	32:i:193:LEU:CB	2.61	0.48
45:w:102:VAL:H	45:w:113:HIS:HD2	1.61	0.48
1:A:309:GLY:O	1:A:327:TRP:NE1	2.45	0.48
6:F:332:PHE:HB3	11:K:869:VAL:HG21	1.95	0.48
7:G:285:ASN:H	7:G:288:ILE:HD12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:GLN:O	24:Z:1036:ARG:NH2	2.46	0.48
13:M:113:VAL:HG23	13:M:122:VAL:HB	1.94	0.48
16:P:116:GLU:OE1	28:d:105:ARG:NH1	2.38	0.48
21:V:96:ARG:HD3	51:2:81:G:C5	2.48	0.48
23:Y:151:ASP:HA	23:Y:154:ARG:HG2	1.95	0.48
29:f:144:LEU:HD13	29:f:150:ILE:HG12	1.95	0.48
30:g:58:VAL:HA	30:g:112:LEU:HD11	1.95	0.48
36:n:27:VAL:HG11	36:n:54:PRO:HB2	1.95	0.48
47:y:359:LEU:HG	47:y:399:LYS:HA	1.95	0.48
1:A:483:LEU:HB3	1:A:495:TRP:HB2	1.95	0.48
12:L:51:ALA:H	12:L:109:PRO:HB3	1.78	0.48
14:N:494:VAL:O	14:N:533:THR:N	2.45	0.48
15:O:441:ARG:NE	51:2:68:A:OP1	2.47	0.48
18:R:226:ILE:HG13	18:R:247:LEU:HD13	1.95	0.48
22:X:467:THR:O	22:X:587:ARG:NH2	2.46	0.48
32:i:788:SER:O	32:i:792:TYR:CB	2.61	0.48
32:j:616:TRP:O	32:j:620:GLN:CB	2.61	0.48
32:j:908:VAL:O	32:j:912:PHE:CB	2.62	0.48
39:q:153:HIS:HD2	44:v:28:LYS:HE3	1.78	0.48
50:1:861:U:H3'	50:1:863:G:H21	1.78	0.48
50:1:1044:A:H3'	50:1:1045:G:H8	1.79	0.48
1:A:516:VAL:HG22	1:A:527:ILE:HG22	1.95	0.48
6:F:70:ARG:NH1	11:K:335:ARG:O	2.47	0.48
24:Z:133:ALA:O	24:Z:238:ARG:NH1	2.45	0.48
28:d:65:HIS:HE2	28:d:84:SER:HG	1.57	0.48
28:d:114:LYS:HE3	38:p:154:GLU:HG3	1.95	0.48
29:e:144:LEU:HD13	29:e:150:ILE:HG12	1.95	0.48
38:p:178:THR:O	38:p:182:VAL:HB	2.13	0.48
40:r:118:LYS:H	40:r:122:HIS:HD2	1.60	0.48
50:1:13:G:O6	50:1:22:U:O2	2.32	0.48
8:H:22:ARG:O	8:H:25:LEU:N	2.47	0.48
12:L:153:SER:OG	12:L:156:GLU:O	2.30	0.48
15:O:78:ARG:NH2	50:1:262:G:OP1	2.44	0.48
15:O:723:VAL:HG22	15:O:733:VAL:HB	1.95	0.48
18:R:91:LEU:HD22	18:R:129:ILE:HD13	1.95	0.48
18:S:228:ALA:HB3	18:S:255:ILE:HG12	1.94	0.48
20:U:193:HIS:ND1	20:U:247:THR:O	2.45	0.48
32:i:11:ILE:O	32:i:15:ILE:CB	2.62	0.48
32:i:264:ALA:O	32:i:268:PHE:CB	2.62	0.48
32:i:908:VAL:O	32:i:912:PHE:CB	2.62	0.48
50:1:659:A:O2'	50:1:660:U:O4'	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2107:A:H2'	50:1:2108:A:C8	2.49	0.48
1:A:202:TYR:OH	1:A:261:ALA:O	2.20	0.48
14:N:232:SER:HA	14:N:235:ARG:HG2	1.94	0.48
15:O:244:LEU:HD13	15:O:258:VAL:HG11	1.95	0.48
18:S:226:ILE:HG13	18:S:247:LEU:HD13	1.95	0.48
20:U:186:VAL:HA	20:U:189:TRP:HB3	1.95	0.48
32:i:878:GLY:HA3	32:i:912:PHE:HA	1.96	0.48
32:j:189:PHE:O	32:j:193:LEU:CB	2.61	0.48
49:0:168:SER:O	49:0:172:SER:CB	2.62	0.48
50:1:1705:C:N4	51:2:5:A:H61	2.12	0.48
1:A:194:HIS:ND1	1:A:214:SER:HB3	2.29	0.48
15:O:687:ARG:HB3	15:O:706:CYS:HB2	1.96	0.48
16:P:114:ARG:NH1	28:d:348:GLY:O	2.45	0.48
18:R:70:LYS:NZ	33:k:159:ARG:O	2.44	0.48
18:S:91:LEU:HD22	18:S:129:ILE:HD13	1.95	0.48
24:Z:829:THR:HG22	24:Z:848:TYR:H	1.78	0.48
37:o:55:GLY:HA3	37:o:108:VAL:O	2.14	0.48
39:q:143:GLU:O	39:q:147:ALA:CB	2.59	0.48
50:1:154:C:H2'	50:1:155:G:H8	1.79	0.48
50:1:690:A:H62	50:1:891:G:H2'	1.78	0.48
50:1:1644:U:O2'	50:1:1645:U:O2	2.24	0.48
1:A:524:GLN:HE21	1:A:536:PHE:HB3	1.79	0.48
12:L:168:THR:HG22	12:L:184:THR:HG22	1.95	0.48
14:N:139:SER:O	14:N:143:ARG:NE	2.47	0.48
22:X:566:PHE:HB2	22:X:577:CYS:O	2.13	0.48
28:d:47:VAL:HG21	28:d:388:ILE:HG23	1.96	0.48
29:f:96:LEU:O	29:f:100:LEU:HB2	2.14	0.48
34:l:29:TRP:CD1	34:l:47:LEU:HG	2.49	0.48
34:l:144:LYS:HB3	34:l:206:PRO:HB2	1.96	0.48
44:v:38:ARG:NE	44:v:56:GLY:O	2.47	0.48
51:2:27:C:O2'	51:2:30:U:O4	2.29	0.48
4:D:267:THR:HG21	14:N:451:THR:HB	1.96	0.48
6:F:117:ILE:O	6:F:121:VAL:HB	2.13	0.48
6:F:274:HIS:CE1	6:F:329:ILE:HD11	2.49	0.48
9:I:839:PRO:HA	9:I:842:LEU:HB2	1.95	0.48
15:O:519:PRO:HA	15:O:543:PRO:HA	1.95	0.48
18:R:82:PHE:HE2	18:R:95:ALA:HB2	1.78	0.48
18:R:228:ALA:HB3	18:R:255:ILE:HG12	1.94	0.48
21:V:21:LEU:HD23	21:V:118:LEU:HD21	1.95	0.48
25:a:75:GLU:OE2	26:b:61:SER:OG	2.31	0.48
26:b:89:LEU:HB2	26:b:136:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:101:LEU:HD13	30:g:172:MET:HE2	1.96	0.48
32:j:264:ALA:O	32:j:268:PHE:CB	2.62	0.48
5:E:40:ARG:HD2	5:E:63:TRP:CZ3	2.49	0.48
6:F:225:LEU:HD12	6:F:230:LEU:HD22	1.95	0.48
6:F:293:LEU:O	11:K:872:ASN:HB3	2.14	0.48
8:H:44:LYS:NZ	50:1:2072:U:OP1	2.47	0.48
20:U:330:ARG:O	20:U:334:THR:OG1	2.27	0.48
29:e:96:LEU:O	29:e:100:LEU:HB2	2.14	0.48
43:u:59:LYS:HD2	43:u:93:TYR:HE2	1.79	0.48
44:v:89:ILE:O	44:v:113:ALA:HA	2.13	0.48
50:1:166:A:H2	50:1:169:G:H3'	1.79	0.48
11:K:364:THR:OG1	11:K:370:GLU:OE2	2.32	0.47
14:N:408:TRP:HZ2	14:N:411:GLN:HB2	1.78	0.47
23:Y:283:ALA:HB3	23:Y:292:TYR:HB2	1.95	0.47
25:a:139:GLY:N	25:a:157:PHE:O	2.46	0.47
31:h:150:PHE:HE2	31:h:217:HIS:HD2	1.61	0.47
32:j:11:ILE:O	32:j:15:ILE:CB	2.62	0.47
43:u:40:ALA:HB3	43:u:48:LEU:HD11	1.96	0.47
44:v:99:ILE:HG22	44:v:102:TYR:H	1.79	0.47
50:1:715:A:N6	50:1:786:G:O6	2.47	0.47
1:A:512:ASP:HB2	1:A:530:LEU:HD13	1.96	0.47
6:F:315:MET:O	6:F:326:ILE:HA	2.14	0.47
16:P:41:PRO:HG2	16:P:44:MET:HG3	1.96	0.47
18:S:191:ARG:NE	20:U:159:GLU:OE2	2.46	0.47
20:U:374:ARG:HD3	21:V:67:HIS:CD2	2.49	0.47
24:Z:119:CYS:HA	24:Z:129:MET:HE1	1.97	0.47
24:Z:828:LYS:NZ	50:1:1162:U:OP2	2.31	0.47
24:Z:950:ALA:HB3	24:Z:962:ILE:HD12	1.95	0.47
26:b:256:GLU:OE1	26:b:260:ARG:NH2	2.47	0.47
32:j:878:GLY:HA3	32:j:912:PHE:HA	1.95	0.47
32:j:927:VAL:O	32:j:931:ILE:CB	2.63	0.47
34:l:70:LEU:HD23	34:l:73:LEU:HD12	1.96	0.47
38:p:57:VAL:HG22	38:p:185:ARG:HH22	1.79	0.47
50:1:493:G:H2'	50:1:494:G:C8	2.49	0.47
4:D:213:ASP:O	4:D:217:GLY:CA	2.62	0.47
5:E:4:VAL:O	5:E:8:ALA:CB	2.62	0.47
12:L:83:ILE:O	12:L:92:LEU:N	2.45	0.47
38:p:97:LEU:HD21	38:p:139:LEU:HD23	1.95	0.47
47:y:382:GLN:H	47:y:385:GLN:HE21	1.62	0.47
50:1:174:C:H2'	50:1:175:A:H8	1.79	0.47
50:1:923:C:H2'	50:1:924:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1472:A:H2	50:1:1510:G:H1	1.58	0.47
5:E:54:PRO:HB3	5:E:109:LEU:HG	1.96	0.47
15:O:43:LEU:HD22	15:O:67:VAL:HG13	1.97	0.47
15:O:192:MET:HB2	15:O:195:PHE:HB2	1.96	0.47
15:O:722:ILE:O	15:O:733:VAL:HA	2.15	0.47
18:R:247:LEU:O	19:T:132:ARG:NH2	2.35	0.47
18:S:82:PHE:HE2	18:S:95:ALA:HB2	1.78	0.47
20:U:164:MET:O	20:U:168:ALA:CB	2.62	0.47
23:Y:234:ARG:NE	23:Y:307:GLU:OE2	2.42	0.47
29:f:88:ARG:O	29:f:90:ASP:N	2.47	0.47
32:j:788:SER:O	32:j:792:TYR:CB	2.62	0.47
34:l:166:ARG:HA	34:l:169:VAL:HG12	1.96	0.47
39:q:64:ASN:ND2	50:1:841:A:N3	2.62	0.47
50:1:1669:U:H5'	50:1:1680:G:H2'	1.95	0.47
1:A:170:SER:OG	1:A:171:LYS:N	2.47	0.47
1:A:253:GLN:O	50:1:286:G:N2	2.48	0.47
1:A:448:PHE:O	26:b:135:ARG:NH1	2.47	0.47
6:F:205:HIS:CE1	16:P:13:ARG:HH22	2.32	0.47
26:b:163:LEU:HD12	26:b:268:ILE:HG12	1.95	0.47
26:b:272:THR:H	26:b:275:ASN:HD22	1.63	0.47
31:h:187:ILE:HB	31:h:211:LEU:HD21	1.95	0.47
45:w:6:VAL:HG13	45:w:29:PRO:HB2	1.96	0.47
50:1:90:A:H3'	50:1:91:G:H8	1.79	0.47
50:1:1097:U:H2'	50:1:1098:G:C8	2.49	0.47
50:1:1507:G:H2'	50:1:1508:A:H8	1.79	0.47
1:A:9:ASN:N	1:A:9:ASN:ND2	2.46	0.47
1:A:470:PRO:HD2	1:A:488:TRP:HB2	1.95	0.47
12:L:46:HIS:HB3	12:L:75:VAL:HB	1.96	0.47
13:M:364:SER:O	13:M:364:SER:OG	2.32	0.47
15:O:35:PHE:HB3	15:O:776:TRP:HB3	1.95	0.47
15:O:506:THR:O	15:O:506:THR:OG1	2.31	0.47
25:a:27:HIS:HB3	25:a:30:HIS:CE1	2.50	0.47
25:a:49:ARG:NH2	50:1:292:G:OP2	2.47	0.47
28:d:171:SER:HB3	28:d:203:VAL:HB	1.95	0.47
31:h:152:ILE:HA	31:h:155:ALA:HB3	1.96	0.47
36:n:130:ARG:HD2	48:z:56:VAL:HG11	1.96	0.47
37:o:134:GLY:N	50:1:653:U:O4	2.47	0.47
51:2:2:G:H2'	51:2:3:C:C6	2.50	0.47
1:A:540:SER:O	36:n:70:ARG:NH2	2.48	0.47
4:D:192:ILE:HG22	4:D:202:VAL:HG22	1.97	0.47
7:G:256:SER:HA	7:G:295:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:249:ALA:O	12:L:256:SER:OG	2.25	0.47
18:R:109:ILE:HB	18:R:127:TYR:HB2	1.95	0.47
21:W:95:SER:HA	22:X:591:TRP:CE2	2.50	0.47
29:e:40:VAL:HG22	29:e:113:TYR:HB2	1.97	0.47
29:f:40:VAL:HG22	29:f:113:TYR:HB2	1.97	0.47
32:i:927:VAL:O	32:i:931:ILE:CB	2.63	0.47
35:m:201:HIS:HB2	35:m:206:GLY:HA2	1.96	0.47
42:t:84:CYS:HB3	42:t:89:ILE:HG12	1.96	0.47
43:u:53:LEU:H	43:u:53:LEU:HG	1.60	0.47
50:1:1129:A:H4'	50:1:1130:U:H5'	1.96	0.47
50:1:1538:G:H2'	50:1:1539:G:H8	1.79	0.47
7:G:205:ARG:NH2	7:G:257:GLU:OE1	2.47	0.47
9:I:896:ARG:HA	9:I:899:LEU:HB3	1.95	0.47
10:J:756:ASP:O	10:J:760:LEU:HB3	2.14	0.47
12:L:107:ILE:HG22	12:L:114:LEU:HB2	1.97	0.47
15:O:520:TYR:HA	15:O:536:PHE:O	2.15	0.47
22:X:476:ASP:HB2	22:X:492:LEU:HB3	1.97	0.47
24:Z:267:THR:HA	24:Z:781:ILE:O	2.14	0.47
28:d:379:LEU:HB3	28:d:392:ARG:NH2	2.30	0.47
37:o:31:ARG:HE	37:o:68:ILE:HG12	1.80	0.47
38:p:172:VAL:O	38:p:176:LEU:HB2	2.15	0.47
1:A:409:TRP:HA	1:A:416:ASN:HA	1.97	0.47
4:D:238:VAL:HA	4:D:253:ASP:HA	1.97	0.47
5:E:282:VAL:O	5:E:286:ALA:CB	2.62	0.47
6:F:313:ARG:HG3	6:F:373:LYS:HE2	1.97	0.47
14:N:370:GLN:HG2	14:N:389:ALA:HA	1.97	0.47
16:P:62:THR:HG21	16:P:98:GLU:HB2	1.96	0.47
19:T:191:ILE:O	19:T:195:ALA:CB	2.63	0.47
20:U:283:LYS:HG2	20:U:290:THR:HG21	1.96	0.47
38:p:56:GLU:HG3	38:p:62:LYS:HG2	1.97	0.47
44:v:30:THR:O	44:v:33:GLY:O	2.32	0.47
50:1:137:C:H2'	50:1:138:A:H8	1.80	0.47
50:1:2233:U:H2'	50:1:2234:A:C8	2.50	0.47
4:D:129:HIS:CE1	4:D:164:VAL:HG21	2.50	0.47
6:F:323:LYS:HA	6:F:339:TYR:O	2.14	0.47
15:O:932:GLY:HA3	15:O:973:HIS:CD2	2.49	0.47
22:X:166:PHE:O	22:X:600:GLY:HA2	2.15	0.47
23:Y:82:ILE:HG13	23:Y:124:SER:HA	1.96	0.47
26:b:101:MET:HB2	26:b:116:ARG:HH22	1.78	0.47
39:q:106:ALA:HB2	39:q:169:LEU:HG	1.97	0.47
51:2:2:G:H2'	51:2:3:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:HB3	1:A:222:TRP:HH2	1.80	0.46
1:A:431:MET:HE1	1:A:440:ILE:HG23	1.97	0.46
7:G:220:ILE:O	7:G:224:ALA:HB3	2.14	0.46
12:L:324:THR:HG22	12:L:334:LEU:HG	1.96	0.46
15:O:844:SER:OG	15:O:845:LEU:N	2.48	0.46
18:R:292:LEU:HD11	18:R:301:MET:HE2	1.97	0.46
20:U:240:ALA:O	20:U:244:SER:CB	2.63	0.46
23:Y:81:LEU:HD11	24:Z:877:LEU:HD21	1.97	0.46
34:l:180:THR:O	34:l:183:GLN:N	2.47	0.46
39:q:11:ARG:HB2	50:1:907:A:H5"	1.97	0.46
1:A:535:THR:OG1	1:A:544:GLN:NE2	2.48	0.46
1:A:618:LEU:HD23	1:A:671:PRO:HG2	1.97	0.46
18:S:292:LEU:HD11	18:S:301:MET:HE2	1.97	0.46
22:X:491:ARG:NH1	22:X:500:GLU:OE2	2.48	0.46
25:a:168:GLN:O	25:a:172:LYS:CB	2.63	0.46
28:d:432:LYS:NZ	50:1:584:U:O2'	2.47	0.46
30:g:132:ASN:O	30:g:136:PHE:CB	2.62	0.46
32:j:39:VAL:O	32:j:43:TYR:CB	2.64	0.46
34:l:136:ARG:HB2	34:l:216:LYS:HB2	1.97	0.46
35:m:183:ILE:O	35:m:190:GLY:CA	2.64	0.46
4:D:186:LYS:NZ	50:1:191:C:OP2	2.43	0.46
9:I:830:VAL:HA	9:I:833:THR:HG22	1.97	0.46
12:L:164:SER:OG	12:L:165:ASP:N	2.48	0.46
15:O:206:GLY:HA3	15:O:224:PRO:HG3	1.98	0.46
22:X:312:VAL:HG13	22:X:326:LEU:HB2	1.97	0.46
24:Z:159:ASN:ND2	24:Z:885:CYS:SG	2.88	0.46
25:a:47:TYR:HB3	25:a:106:PHE:HD2	1.79	0.46
29:e:88:ARG:O	29:e:90:ASP:N	2.48	0.46
32:i:39:VAL:O	32:i:43:TYR:CB	2.64	0.46
5:E:394:LEU:HD23	5:E:399:ARG:HE	1.80	0.46
8:H:4:LEU:HB3	46:x:89:ASN:HD21	1.80	0.46
9:I:899:LEU:HA	9:I:902:VAL:HG12	1.98	0.46
13:M:426:ALA:HB1	14:N:360:VAL:HG13	1.96	0.46
15:O:438:LYS:O	15:O:442:LYS:HB2	2.15	0.46
15:O:625:VAL:HA	15:O:641:SER:HA	1.97	0.46
22:X:301:ASN:O	22:X:317:LEU:CB	2.63	0.46
24:Z:966:LEU:HG	24:Z:969:PRO:HD2	1.97	0.46
25:a:96:ALA:O	25:a:100:ASN:CB	2.61	0.46
34:l:196:GLU:O	34:l:200:ALA:CB	2.64	0.46
35:m:208:VAL:O	35:m:219:ALA:HA	2.15	0.46
35:m:249:GLU:OE2	35:m:253:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:q:106:ALA:O	39:q:110:ARG:CB	2.64	0.46
50:1:899:A:N6	50:1:934:A:O4'	2.49	0.46
50:1:1626:G:H2'	50:1:1627:G:C8	2.50	0.46
9:I:842:LEU:O	9:I:846:LEU:HB2	2.15	0.46
10:J:869:ARG:HE	27:c:679:PRO:HG3	1.81	0.46
12:L:266:LEU:HD13	12:L:268:LEU:HB2	1.98	0.46
12:L:322:VAL:HG12	12:L:336:VAL:HA	1.97	0.46
20:U:185:ARG:O	20:U:189:TRP:CB	2.63	0.46
22:X:253:LYS:HD2	22:X:295:ALA:HA	1.98	0.46
22:X:478:ILE:HB	22:X:490:TRP:HB2	1.97	0.46
28:d:161:PHE:CD1	28:d:168:PHE:HB3	2.49	0.46
31:h:111:LEU:HD12	31:h:130:THR:HG21	1.96	0.46
37:o:77:LEU:HD13	37:o:84:TYR:HB2	1.98	0.46
45:w:78:ARG:HG2	45:w:124:LYS:HE2	1.98	0.46
50:1:1705:C:H42	51:2:5:A:N6	2.12	0.46
1:A:598:LEU:HD23	1:A:608:LYS:HB3	1.97	0.46
6:F:403:PHE:O	28:d:8:ARG:NH2	2.41	0.46
7:G:323:GLN:HB3	7:G:360:LEU:HD23	1.98	0.46
8:H:105:LYS:HD2	8:H:247:MET:HE1	1.98	0.46
11:K:307:GLN:HA	11:K:310:LEU:HB2	1.98	0.46
15:O:78:ARG:HH12	15:O:83:VAL:HG22	1.80	0.46
15:O:438:LYS:O	15:O:442:LYS:CB	2.64	0.46
15:O:1005:LEU:O	15:O:1009:ASN:CB	2.64	0.46
19:T:317:ARG:O	19:T:321:HIS:CB	2.59	0.46
20:U:259:LEU:HA	20:U:262:VAL:HG12	1.96	0.46
22:X:171:GLY:N	22:X:599:CYS:SG	2.89	0.46
26:b:190:HIS:HB2	26:b:227:VAL:HA	1.97	0.46
29:e:88:ARG:HH21	29:e:210:ALA:HA	1.81	0.46
34:l:181:LEU:HA	34:l:184:LEU:HB3	1.97	0.46
50:1:3:G:H2'	50:1:4:G:H4'	1.96	0.46
50:1:972:A:OP1	50:1:986:C:N4	2.46	0.46
1:A:746:ILE:O	1:A:750:TYR:HB2	2.15	0.46
6:F:140:TYR:HA	6:F:154:ALA:O	2.16	0.46
7:G:24:ALA:O	7:G:28:SER:CB	2.64	0.46
8:H:108:ASP:HA	20:U:335:LYS:HE2	1.96	0.46
9:I:838:LYS:HA	9:I:839:PRO:HD3	1.73	0.46
9:I:907:ARG:O	9:I:911:ARG:HB2	2.16	0.46
15:O:569:ASN:O	15:O:573:GLY:CA	2.64	0.46
19:T:98:LEU:O	19:T:118:CYS:HA	2.16	0.46
20:U:71:PRO:O	20:U:75:SER:CB	2.63	0.46
20:U:185:ARG:O	20:U:189:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:1:MET:HE2	26:b:132:GLN:HG2	1.98	0.46
28:d:264:ILE:HB	28:d:279:GLN:HB2	1.97	0.46
33:k:111:MET:HE2	33:k:111:MET:HB3	1.74	0.46
1:A:119:ILE:HD11	1:A:154:VAL:HG21	1.96	0.46
8:H:109:LEU:HG	8:H:113:ARG:HE	1.81	0.46
10:J:756:ASP:O	10:J:760:LEU:HB2	2.16	0.46
12:L:89:ARG:HH11	12:L:345:ILE:HG13	1.80	0.46
15:O:71:LEU:H	15:O:86:THR:HB	1.81	0.46
32:j:912:PHE:O	32:j:916:MET:CB	2.64	0.46
44:v:74:ARG:NH1	50:1:889:C:O4'	2.44	0.46
44:v:128:VAL:HG22	44:v:147:VAL:HG22	1.98	0.46
1:A:576:ASN:H	1:A:591:GLY:HA2	1.80	0.46
4:D:200:VAL:O	4:D:211:ALA:HA	2.16	0.46
6:F:230:LEU:HD11	6:F:456:PRO:HB3	1.96	0.46
7:G:240:GLN:OE1	14:N:257:ARG:NH1	2.49	0.46
8:H:34:TYR:CZ	24:Z:958:ILE:HD11	2.51	0.46
16:P:135:VAL:HG21	16:P:156:ARG:HE	1.81	0.46
27:c:561:ARG:NH2	27:c:564:MET:SD	2.88	0.46
34:l:214:LYS:HD2	34:l:216:LYS:HE2	1.98	0.46
39:q:179:GLN:HE21	50:1:915:G:H3'	1.80	0.46
42:t:27:PHE:HA	42:t:91:ALA:HB3	1.97	0.46
50:1:1213:U:H2'	50:1:1214:A:H8	1.80	0.46
50:1:1664:U:N3	50:1:1675:A:C6	2.84	0.46
50:1:1664:U:O2	50:1:1675:A:N6	2.49	0.46
1:A:682:PRO:O	1:A:817:ARG:NH2	2.40	0.46
5:E:87:ALA:O	5:E:91:ARG:HB2	2.16	0.46
7:G:127:ILE:HG13	7:G:131:ASN:HB2	1.98	0.46
12:L:75:VAL:HG21	12:L:105:GLY:H	1.81	0.46
15:O:569:ASN:O	15:O:573:GLY:HA2	2.16	0.46
15:O:569:ASN:O	15:O:573:GLY:N	2.49	0.46
16:P:93:SER:O	16:P:97:ALA:HB2	2.15	0.46
24:Z:183:LYS:NZ	50:1:1049:G:O2'	2.45	0.46
32:i:912:PHE:O	32:i:916:MET:CB	2.64	0.46
33:k:127:ARG:NH2	33:k:129:ASP:O	2.49	0.46
34:l:97:LEU:HB3	34:l:232:HIS:CE1	2.51	0.46
35:m:15:PRO:HB2	35:m:18:TRP:HZ3	1.80	0.46
37:o:167:GLU:HA	37:o:168:GLY:HA3	1.66	0.46
14:N:277:ILE:HG13	14:N:609:GLY:HA2	1.98	0.45
15:O:41:ILE:HD12	15:O:775:ILE:HG13	1.98	0.45
19:T:253:ALA:O	19:T:257:ALA:CB	2.63	0.45
22:X:469:LEU:HA	22:X:479:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:580:VAL:HG22	22:X:602:VAL:HB	1.97	0.45
34:l:188:LEU:HD23	34:l:193:ILE:HD13	1.98	0.45
35:m:114:ILE:HG23	35:m:119:ALA:HB2	1.98	0.45
50:1:1509:A:H2'	50:1:1510:G:H8	1.80	0.45
1:A:9:ASN:HD22	1:A:9:ASN:H	1.54	0.45
4:D:244:LEU:HD11	4:D:313:TRP:HH2	1.81	0.45
6:F:282:VAL:HG23	6:F:296:LEU:HB2	1.97	0.45
19:T:97:VAL:HA	19:T:117:GLN:O	2.16	0.45
20:U:90:VAL:HG11	20:U:95:LEU:HD22	1.99	0.45
34:l:129:THR:HB	34:l:133:TYR:HB2	1.97	0.45
1:A:304:THR:HG22	1:A:313:ALA:HB3	1.99	0.45
13:M:370:LEU:HB2	13:M:384:LEU:HD22	1.98	0.45
14:N:593:ILE:HG22	14:N:604:VAL:HG22	1.98	0.45
19:T:416:GLU:HA	19:T:419:ALA:HB3	1.97	0.45
20:U:192:TRP:HD1	20:U:249:ILE:HD11	1.81	0.45
21:W:83:PRO:HB2	22:X:462:GLN:HE21	1.81	0.45
23:Y:56:LEU:HD21	23:Y:117:LEU:HD11	1.97	0.45
23:Y:139:THR:HG23	23:Y:188:GLY:HA2	1.98	0.45
29:f:88:ARG:HH21	29:f:210:ALA:HA	1.81	0.45
30:g:132:ASN:O	30:g:136:PHE:HB2	2.16	0.45
30:g:167:ASN:ND2	50:1:1518:A:OP2	2.49	0.45
31:h:233:VAL:HA	31:h:236:VAL:HG12	1.98	0.45
39:q:139:SER:O	39:q:143:GLU:CB	2.62	0.45
39:q:194:ALA:O	39:q:198:ARG:CB	2.65	0.45
42:t:33:PHE:HD1	42:t:97:ARG:HG3	1.82	0.45
13:M:95:ILE:O	13:M:104:ILE:HB	2.16	0.45
13:M:161:SER:O	13:M:187:LEU:N	2.50	0.45
15:O:480:ALA:O	15:O:506:THR:OG1	2.31	0.45
19:T:35:LYS:O	19:T:39:LYS:HB2	2.16	0.45
21:V:78:PRO:HG2	21:V:119:ARG:HB2	1.97	0.45
22:X:165:GLN:HG2	22:X:602:VAL:HG22	1.98	0.45
22:X:598:ARG:NH2	51:2:188:G:N7	2.59	0.45
32:i:26:PHE:O	32:i:200:LEU:CB	2.65	0.45
50:1:861:U:H5	50:1:865:G:H21	1.64	0.45
2:B:857:GLN:HB3	2:B:861:ARG:HH12	1.80	0.45
5:E:122:ALA:O	5:E:126:TRP:HB2	2.17	0.45
9:I:884:THR:HB	48:z:30:ARG:HH22	1.82	0.45
10:J:774:PHE:HA	10:J:777:VAL:HG12	1.98	0.45
21:W:78:PRO:HG2	21:W:119:ARG:HB2	1.97	0.45
23:Y:175:VAL:HG12	23:Y:192:VAL:HG12	1.99	0.45
24:Z:605:GLU:O	24:Z:609:LYS:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:105:LYS:O	26:b:109:LEU:HB2	2.16	0.45
32:j:26:PHE:O	32:j:200:LEU:CB	2.65	0.45
41:s:122:ILE:O	41:s:126:ALA:CB	2.65	0.45
45:w:8:HIS:CE1	45:w:12:ASN:HD21	2.35	0.45
50:1:1447:A:H61	50:1:1548:A:H2'	1.82	0.45
50:1:1453:G:H2'	50:1:1454:A:H8	1.81	0.45
50:1:1459:C:H2'	50:1:1460:G:C8	2.51	0.45
10:J:810:LEU:HD13	10:J:860:LEU:HD11	1.99	0.45
12:L:142:ILE:HD12	12:L:172:TRP:HH2	1.81	0.45
24:Z:69:ARG:HH12	24:Z:232:PRO:HD3	1.82	0.45
32:j:312:ILE:HA	32:j:387:VAL:O	2.17	0.45
35:m:146:THR:HG21	50:1:709:G:H21	1.80	0.45
40:r:26:LEU:HA	40:r:29:VAL:HG12	1.97	0.45
50:1:639:U:H2'	50:1:640:G:C8	2.52	0.45
1:A:82:THR:OG1	1:A:88:VAL:O	2.30	0.45
8:H:3:SER:OG	50:1:1133:G:OP2	2.25	0.45
11:K:360:ILE:HD12	11:K:370:GLU:HG3	1.98	0.45
18:R:251:GLY:O	18:R:305:VAL:HA	2.17	0.45
23:Y:333:PRO:HB3	23:Y:363:LEU:HD22	1.99	0.45
32:i:538:GLN:O	32:i:542:ALA:CB	2.65	0.45
42:t:73:ALA:O	42:t:77:ALA:HB2	2.16	0.45
43:u:24:GLN:OE1	43:u:92:TYR:OH	2.35	0.45
50:1:86:C:H2'	50:1:87:G:H8	1.82	0.45
1:A:346:LEU:HA	1:A:356:VAL:O	2.17	0.45
1:A:519:ARG:HD2	1:A:524:GLN:HB3	1.97	0.45
8:H:104:LEU:HD22	24:Z:1079:ARG:HH12	1.81	0.45
14:N:441:VAL:HG21	14:N:485:ILE:HD13	1.98	0.45
15:O:538:THR:HB	15:O:560:SER:HB3	1.98	0.45
22:X:173:VAL:HG23	22:X:187:THR:HG22	1.99	0.45
32:i:732:GLN:O	32:i:736:PHE:CB	2.65	0.45
32:j:538:GLN:O	32:j:542:ALA:CB	2.65	0.45
34:l:31:ASN:O	34:l:96:CYS:CB	2.64	0.45
35:m:131:LEU:O	50:1:835:A:O2'	2.34	0.45
35:m:145:ARG:HG2	50:1:709:G:H4'	1.99	0.45
42:t:115:LEU:O	42:t:119:ALA:HB2	2.16	0.45
50:1:1532:C:H2'	50:1:1533:G:H8	1.82	0.45
51:2:259:A:H1'	51:2:260:G:C2	2.51	0.45
1:A:168:SER:O	1:A:175:ALA:HA	2.17	0.45
1:A:780:GLN:O	1:A:784:SER:OG	2.30	0.45
5:E:314:GLU:O	5:E:318:SER:OG	2.29	0.45
12:L:126:PHE:HB3	12:L:136:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:251:GLY:O	18:S:305:VAL:HA	2.17	0.45
19:T:258:ALA:HA	19:T:261:SER:HB2	1.97	0.45
22:X:332:GLU:O	22:X:349:ALA:CB	2.61	0.45
24:Z:933:PHE:HA	24:Z:973:PHE:O	2.15	0.45
24:Z:966:LEU:H	24:Z:973:PHE:HA	1.82	0.45
38:p:46:PRO:HG3	38:p:78:ARG:HH12	1.81	0.45
38:p:176:LEU:HA	38:p:179:TYR:HD2	1.82	0.45
44:v:11:ARG:NH1	50:1:927:C:O2'	2.50	0.45
50:1:730:U:H2'	50:1:731:A:C8	2.51	0.45
50:1:1623:U:O2'	50:1:1675:A:N7	2.47	0.45
51:2:103:G:C6	51:2:250:G:C2	3.05	0.45
1:A:59:SER:N	1:A:73:ILE:O	2.41	0.45
1:A:271:VAL:HG11	1:A:312:LEU:HD13	1.98	0.45
8:H:109:LEU:HD21	8:H:113:ARG:HH21	1.81	0.45
10:J:748:TYR:CE2	10:J:757:ALA:CA	3.00	0.45
10:J:766:HIS:ND1	27:c:707:GLU:HG2	2.32	0.45
15:O:40:THR:HA	15:O:774:GLN:HA	1.98	0.45
26:b:18:LEU:HD23	26:b:21:ARG:HD2	1.99	0.45
32:j:27:PHE:CB	32:j:149:VAL:O	2.65	0.45
38:p:88:GLU:OE2	38:p:175:ARG:NH2	2.50	0.45
47:y:413:LEU:O	47:y:417:GLU:HB3	2.17	0.45
1:A:405:SER:OG	1:A:407:ARG:NH1	2.50	0.44
1:A:578:ILE:HA	1:A:588:LEU:O	2.16	0.44
5:E:126:TRP:CZ2	5:E:150:ARG:HD3	2.52	0.44
6:F:267:ASN:HA	6:F:308:VAL:HG21	1.98	0.44
6:F:340:PHE:HB3	50:1:278:A:C6	2.52	0.44
7:G:188:ASN:OD1	7:G:231:LYS:NZ	2.50	0.44
7:G:236:ARG:HD2	7:G:239:ILE:HD12	1.99	0.44
12:L:250:ALA:HB2	12:L:255:ILE:HG13	1.99	0.44
13:M:110:SER:OG	13:M:125:ILE:O	2.33	0.44
14:N:402:ASN:O	14:N:406:MET:CA	2.65	0.44
15:O:211:TRP:CD1	15:O:218:LEU:HA	2.52	0.44
15:O:478:MET:SD	50:1:255:G:N2	2.91	0.44
22:X:196:LYS:HG3	22:X:198:GLN:HE22	1.81	0.44
24:Z:85:LEU:HD11	24:Z:169:ILE:HD13	1.99	0.44
24:Z:185:ALA:O	24:Z:189:LEU:HB2	2.17	0.44
35:m:45:ILE:HD11	35:m:80:ILE:HB	1.99	0.44
39:q:160:LEU:HG	39:q:193:LEU:HD22	1.99	0.44
50:1:597:G:H2'	50:1:598:A:H8	1.82	0.44
50:1:1448:A:C6	50:1:1549:U:C4	3.04	0.44
13:M:422:VAL:HB	13:M:432:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:183:THR:HB	20:U:185:ARG:HD3	1.98	0.44
21:W:19:GLN:OE1	22:X:350:ARG:NH2	2.50	0.44
21:W:35:LYS:HB3	21:W:40:GLU:HG2	1.98	0.44
22:X:186:THR:HA	22:X:191:TYR:O	2.18	0.44
31:h:110:LYS:O	31:h:130:THR:OG1	2.35	0.44
35:m:201:HIS:CD2	35:m:207:ILE:HG12	2.52	0.44
36:n:96:MET:SD	36:n:99:ARG:NH1	2.90	0.44
39:q:79:ILE:HG21	39:q:168:ARG:HD2	1.99	0.44
44:v:92:ARG:HH12	44:v:155:VAL:HG13	1.81	0.44
50:1:597:G:H2'	50:1:598:A:C8	2.52	0.44
50:1:1707:C:H2'	50:1:1708:A:C4	2.53	0.44
5:E:4:VAL:O	5:E:8:ALA:HB3	2.17	0.44
7:G:18:SER:OG	7:G:19:SER:N	2.50	0.44
15:O:78:ARG:O	15:O:81:ASN:ND2	2.50	0.44
18:R:255:ILE:HD12	18:R:279:LEU:HD21	1.99	0.44
21:V:35:LYS:HB3	21:V:40:GLU:HG2	1.99	0.44
22:X:179:CYS:HB3	22:X:182:TYR:HB2	2.00	0.44
27:c:722:GLU:OE2	50:1:2223:C:N4	2.45	0.44
28:d:55:LYS:O	28:d:354:ARG:NH2	2.45	0.44
30:g:157:LEU:HD21	30:g:202:MET:HE2	1.98	0.44
32:i:896:THR:O	32:i:900:GLU:CB	2.64	0.44
43:u:22:CYS:HA	43:u:64:ASP:O	2.17	0.44
43:u:31:VAL:HG22	43:u:67:ILE:HD12	1.99	0.44
48:z:23:ARG:H	50:1:2202:C:H1'	1.81	0.44
50:1:650:G:O2'	50:1:754:U:OP1	2.33	0.44
6:F:274:HIS:HE1	6:F:329:ILE:HD11	1.83	0.44
17:Q:267:VAL:O	17:Q:271:VAL:HA	2.18	0.44
19:T:396:SER:HB3	19:T:399:PRO:HB3	1.98	0.44
24:Z:958:ILE:HD13	24:Z:958:ILE:HA	1.76	0.44
27:c:694:GLU:HA	27:c:704:ALA:HA	1.98	0.44
32:j:929:GLY:O	32:j:933:ALA:CB	2.65	0.44
34:l:166:ARG:O	34:l:170:GLU:CB	2.64	0.44
35:m:139:LEU:HB3	35:m:147:ILE:HB	1.98	0.44
50:1:184:G:H2'	50:1:185:G:C8	2.52	0.44
1:A:624:PHE:HB3	15:O:478:MET:HE2	1.98	0.44
4:D:134:CYS:O	4:D:156:ALA:HA	2.18	0.44
8:H:257:THR:HG23	8:H:259:SER:H	1.82	0.44
18:R:75:PRO:HG3	33:k:93:ILE:HD12	1.99	0.44
28:d:418:ARG:NH2	50:1:1653:G:O3'	2.47	0.44
32:j:896:THR:O	32:j:900:GLU:CB	2.64	0.44
39:q:65:PHE:HE1	39:q:184:ASP:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:35:SER:OG	42:t:36:PHE:N	2.49	0.44
44:v:110:LYS:NZ	50:l:890:U:OP1	2.39	0.44
50:l:2237:G:N2	50:l:2329:A:N1	2.51	0.44
1:A:173:LEU:HD13	6:F:320:GLN:HG3	1.99	0.44
1:A:413:ARG:HH12	27:c:678:ALA:HA	1.81	0.44
6:F:398:VAL:HG23	6:F:409:ILE:HG23	1.99	0.44
8:H:68:MET:HG3	51:2:58:A:H4'	2.00	0.44
12:L:185:GLY:HA3	12:L:215:ARG:HH12	1.83	0.44
19:T:179:GLN:HB3	20:U:185:ARG:CZ	2.47	0.44
22:X:598:ARG:NH1	51:2:188:G:O6	2.51	0.44
24:Z:280:ALA:HB3	24:Z:284:GLN:HB2	2.00	0.44
26:b:73:ILE:HD12	26:b:75:ASP:HB2	2.00	0.44
32:j:732:GLN:O	32:j:736:PHE:CB	2.65	0.44
39:q:84:HIS:HD2	39:q:85:PRO:HD2	1.82	0.44
43:u:13:LYS:HD2	43:u:13:LYS:HA	1.90	0.44
43:u:13:LYS:HG3	43:u:14:LYS:H	1.83	0.44
47:y:381:ALA:HA	47:y:385:GLN:HE21	1.83	0.44
51:2:3:C:H2'	51:2:4:G:C8	2.52	0.44
1:A:72:SER:HB2	1:A:80:ILE:HG22	2.00	0.44
2:B:887:ASN:O	2:B:891:ARG:HB2	2.17	0.44
7:G:3:SER:HB2	7:G:6:ALA:HB3	1.99	0.44
8:H:2:SER:O	8:H:10:ARG:NH2	2.50	0.44
10:J:826:ALA:O	10:J:830:LEU:HB2	2.18	0.44
15:O:121:VAL:HB	15:O:129:ALA:HB3	1.99	0.44
15:O:282:ARG:HG2	15:O:284:ASP:H	1.82	0.44
18:S:255:ILE:HD12	18:S:279:LEU:HD21	1.99	0.44
20:U:295:ALA:O	20:U:299:ALA:HB2	2.17	0.44
23:Y:235:MET:HE2	23:Y:279:LEU:HB2	1.98	0.44
37:o:63:MET:HE2	37:o:106:LEU:HD22	1.99	0.44
39:q:144:LYS:O	39:q:148:ALA:HB2	2.18	0.44
50:l:1648:G:H2'	50:l:1649:A:C8	2.52	0.44
1:A:535:THR:HG23	1:A:537:TRP:HE1	1.83	0.44
1:A:687:PHE:CB	1:A:698:TYR:O	2.64	0.44
15:O:564:SER:HB3	15:O:620:ARG:HH12	1.83	0.44
18:S:131:ASN:HD22	18:S:132:PRO:HD2	1.83	0.44
19:T:245:ASN:HB2	19:T:250:LYS:HD3	2.00	0.44
21:W:52:LEU:HD12	21:W:119:ARG:HB3	2.00	0.44
24:Z:138:LEU:HD11	24:Z:154:LEU:HD12	1.99	0.44
26:b:52:LEU:O	26:b:56:PHE:CB	2.66	0.44
28:d:61:LEU:HB2	28:d:350:VAL:HG13	1.99	0.44
38:p:55:ILE:O	38:p:185:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:37:PHE:CE1	45:w:103:ILE:HG13	2.53	0.44
15:O:87:ARG:HA	15:O:87:ARG:HD3	1.75	0.44
15:O:848:ARG:O	15:O:852:GLN:HB2	2.18	0.44
20:U:326:LYS:H	51:2:91:G:H22	1.66	0.44
22:X:195:TRP:HA	22:X:226:ARG:HA	2.00	0.44
22:X:468:ALA:O	22:X:480:SER:HA	2.18	0.44
23:Y:9:LEU:HB2	23:Y:31:ILE:HG22	2.00	0.44
23:Y:99:GLU:OE1	23:Y:131:ARG:NH2	2.51	0.44
32:i:929:GLY:O	32:i:933:ALA:CB	2.65	0.44
34:l:115:ARG:HD2	34:l:118:GLN:HE22	1.83	0.44
50:1:461:G:H2'	50:1:462:G:C8	2.53	0.44
50:1:495:G:O6	50:1:503:G:O6	2.35	0.44
51:2:149:U:H2'	51:2:150:G:C8	2.52	0.44
1:A:358:ALA:HB1	1:A:385:VAL:HB	1.99	0.43
1:A:410:ASP:CB	1:A:415:ARG:O	2.66	0.43
6:F:200:VAL:HG13	6:F:213:LEU:HB2	2.00	0.43
7:G:83:ARG:NH1	7:G:125:PHE:O	2.51	0.43
15:O:328:ASN:O	15:O:339:GLY:N	2.48	0.43
20:U:14:ALA:HA	20:U:48:PHE:HA	2.00	0.43
21:V:52:LEU:HD12	21:V:119:ARG:HB3	2.00	0.43
28:d:366:THR:HG21	50:1:438:C:H3'	2.00	0.43
29:e:181:SER:OG	29:e:183:ASP:OD1	2.34	0.43
32:i:897:LEU:O	32:i:901:LEU:CB	2.66	0.43
32:j:570:LEU:O	32:j:583:LEU:N	2.50	0.43
35:m:88:ASP:HB2	35:m:101:LEU:HB2	2.00	0.43
50:1:18:G:N1	50:1:20:C:N4	2.65	0.43
50:1:1491:A:H2'	50:1:1492:A:C8	2.52	0.43
1:A:393:LYS:HD2	1:A:396:VAL:HG23	1.99	0.43
1:A:505:GLU:HG3	36:n:66:VAL:HG11	1.99	0.43
4:D:83:VAL:HG11	4:D:168:ILE:HD11	2.00	0.43
5:E:382:VAL:HG22	5:E:406:LYS:HG3	2.00	0.43
12:L:319:SER:HA	12:L:338:MET:HG2	2.00	0.43
12:L:334:LEU:O	12:L:345:ILE:HA	2.19	0.43
13:M:119:SER:OG	13:M:120:LEU:N	2.49	0.43
15:O:645:LYS:HB2	15:O:661:ASP:HA	2.00	0.43
18:R:250:GLY:CA	18:R:306:TYR:O	2.66	0.43
19:T:199:ARG:HH21	19:T:216:ASN:HA	1.83	0.43
23:Y:349:LEU:O	23:Y:395:ILE:HA	2.18	0.43
24:Z:244:THR:O	24:Z:800:VAL:HB	2.18	0.43
24:Z:287:HIS:HA	24:Z:293:ASP:HA	2.01	0.43
25:a:63:LEU:HD22	49:0:196:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:216:VAL:HG12	28:d:222:ILE:HG22	2.01	0.43
28:d:423:ARG:HG3	50:1:1637:C:H42	1.82	0.43
29:e:176:ARG:HB2	29:e:202:ILE:HA	1.99	0.43
29:f:176:ARG:HB2	29:f:202:ILE:HA	2.00	0.43
30:g:72:ASP:O	30:g:76:GLY:N	2.51	0.43
31:h:113:VAL:HA	31:h:123:GLU:O	2.18	0.43
31:h:250:ILE:HG13	31:h:251:ILE:HG23	2.00	0.43
32:i:312:ILE:HA	32:i:387:VAL:O	2.17	0.43
34:l:35:PRO:HB2	34:l:37:PRO:HD2	1.99	0.43
35:m:130:GLN:O	35:m:137:PRO:HA	2.18	0.43
39:q:6:ASP:OD1	39:q:9:HIS:ND1	2.51	0.43
51:2:49:U:H2'	51:2:50:G:H8	1.82	0.43
1:A:295:ILE:HB	1:A:323:LEU:HD21	2.00	0.43
1:A:391:ALA:HB3	1:A:393:LYS:HG2	2.00	0.43
6:F:453:LYS:NZ	51:2:25:U:O4	2.47	0.43
12:L:45:SER:C	12:L:321:SER:HG	2.24	0.43
13:M:187:LEU:HD22	13:M:207:THR:HG21	1.99	0.43
15:O:225:PRO:HG2	15:O:254:VAL:HG11	1.99	0.43
16:P:69:VAL:HG11	16:P:109:ALA:HB2	2.01	0.43
20:U:6:LEU:HB2	20:U:88:LEU:HD21	2.00	0.43
24:Z:813:VAL:HG12	24:Z:815:VAL:HG23	2.00	0.43
29:e:44:ALA:HB3	29:e:116:THR:HG22	2.01	0.43
29:e:84:ILE:O	29:e:86:ASP:N	2.46	0.43
32:j:897:LEU:O	32:j:901:LEU:CB	2.66	0.43
37:o:201:GLN:NE2	50:1:713:G:O4'	2.51	0.43
40:r:169:ARG:NH2	50:1:1121:G:O6	2.41	0.43
50:1:1740:C:H2'	50:1:1741:A:H8	1.82	0.43
1:A:366:VAL:O	1:A:375:ILE:N	2.48	0.43
6:F:372:ASN:H	6:F:378:GLN:HE22	1.65	0.43
17:Q:236:SER:O	17:Q:238:SER:N	2.51	0.43
20:U:130:ILE:HG13	20:U:131:PRO:HD3	2.00	0.43
20:U:160:LYS:HB2	20:U:285:ILE:HG12	2.00	0.43
22:X:575:GLY:CA	22:X:606:VAL:O	2.66	0.43
29:e:173:PRO:HB2	36:n:199:LYS:HD3	2.01	0.43
30:g:122:ASP:HB3	30:g:171:VAL:HG13	1.99	0.43
32:i:27:PHE:CB	32:i:149:VAL:O	2.65	0.43
37:o:74:ARG:HA	37:o:96:SER:HA	2.00	0.43
39:q:139:SER:HB2	39:q:142:VAL:H	1.83	0.43
40:r:107:LEU:HD21	40:r:132:ILE:HD11	2.00	0.43
44:v:21:LEU:HD23	44:v:24:LYS:HZ1	1.84	0.43
44:v:135:PRO:HB3	44:v:141:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:w:50:PHE:HA	45:w:62:VAL:O	2.18	0.43
6:F:137:LEU:HD22	6:F:159:HIS:HB2	2.00	0.43
15:O:143:GLN:HB3	15:O:154:CYS:HB2	1.99	0.43
18:S:109:ILE:O	18:S:126:GLU:HA	2.19	0.43
26:b:272:THR:OG1	26:b:273:LEU:N	2.38	0.43
28:d:78:SER:OG	28:d:79:LEU:N	2.52	0.43
32:i:188:ARG:O	32:i:192:SER:CB	2.67	0.43
39:q:22:ARG:NH2	39:q:28:GLU:OE2	2.51	0.43
39:q:74:ARG:HH21	39:q:112:TRP:CD1	2.36	0.43
44:v:72:ARG:HA	50:1:830:G:H1	1.83	0.43
50:1:335:C:H2'	50:1:336:G:H8	1.84	0.43
14:N:322:ARG:NH2	50:1:133:G:H22	2.17	0.43
15:O:274:ALA:HB1	15:O:302:THR:HG21	2.00	0.43
15:O:981:ARG:HD2	15:O:986:ARG:HB2	2.01	0.43
18:R:109:ILE:O	18:R:126:GLU:HA	2.19	0.43
22:X:478:ILE:O	22:X:489:VAL:HA	2.18	0.43
32:j:386:VAL:CB	32:j:407:LEU:O	2.67	0.43
34:l:182:HIS:O	34:l:186:SER:OG	2.33	0.43
47:y:421:ARG:O	47:y:425:ALA:CB	2.67	0.43
50:1:440:G:H4'	50:1:441:A:H5''	2.00	0.43
50:1:752:A:H2'	50:1:753:A:C8	2.54	0.43
1:A:343:MET:HA	1:A:359:ALA:HA	2.01	0.43
7:G:277:ILE:HG12	13:M:952:PHE:HE2	1.83	0.43
20:U:88:LEU:HB3	20:U:109:PRO:HB3	2.01	0.43
20:U:288:ASN:ND2	20:U:375:THR:OG1	2.52	0.43
22:X:167:ARG:HD2	22:X:598:ARG:HD2	1.99	0.43
24:Z:258:ILE:HG13	24:Z:266:ARG:HH21	1.83	0.43
26:b:100:LEU:HD13	26:b:144:GLU:HB3	2.01	0.43
26:b:143:HIS:HB2	26:b:151:ALA:HB3	2.00	0.43
29:f:44:ALA:HB3	29:f:116:THR:HG22	2.01	0.43
37:o:2:LYS:HA	37:o:16:ILE:O	2.18	0.43
49:0:211:GLN:HA	49:0:215:ALA:HB3	2.00	0.43
50:1:181:G:N7	50:1:182:C:O2'	2.52	0.43
50:1:452:G:H1	50:1:480:U:H3	1.66	0.43
50:1:639:U:H2'	50:1:640:G:H8	1.84	0.43
50:1:923:C:H2'	50:1:924:A:H8	1.83	0.43
50:1:1448:A:C5	50:1:1549:U:O4	2.72	0.43
1:A:618:LEU:HD13	1:A:673:VAL:HG22	2.00	0.43
6:F:386:MET:HB2	6:F:386:MET:HE2	1.80	0.43
15:O:38:TYR:HB2	15:O:777:THR:HG23	2.00	0.43
15:O:308:VAL:HG22	15:O:323:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:87:ALA:O	21:W:91:ALA:HB2	2.19	0.43
24:Z:242:PRO:HG2	24:Z:802:GLY:HA3	2.01	0.43
32:i:40:HIS:O	32:i:44:ILE:CB	2.67	0.43
34:l:66:PHE:HB3	34:l:86:LEU:HB2	1.99	0.43
37:o:74:ARG:HG2	37:o:94:ARG:HG2	2.00	0.43
39:q:14:THR:O	50:1:931:G:N2	2.50	0.43
39:q:64:ASN:HA	39:q:75:LYS:HA	2.01	0.43
50:1:58:G:H2'	50:1:59:U:H5	1.84	0.43
50:1:186:C:H2'	50:1:187:G:C8	2.54	0.43
1:A:840:MET:HG2	15:O:999:LEU:HB3	2.01	0.43
4:D:213:ASP:O	4:D:217:GLY:N	2.52	0.43
6:F:429:ASP:HA	28:d:25:ARG:HA	1.99	0.43
8:H:72:GLY:O	8:H:79:ARG:NH1	2.51	0.43
14:N:434:ILE:O	14:N:441:VAL:HA	2.19	0.43
15:O:854:LEU:HD22	15:O:949:PRO:HB3	2.00	0.43
20:U:100:THR:HA	20:U:109:PRO:HD2	2.01	0.43
20:U:185:ARG:HE	20:U:189:TRP:HB2	1.84	0.43
32:j:188:ARG:O	32:j:192:SER:CB	2.67	0.43
37:o:77:LEU:HD12	37:o:95:LYS:HD3	2.00	0.43
38:p:136:LEU:HA	38:p:139:LEU:HD12	2.01	0.43
39:q:54:LYS:HD3	39:q:179:GLN:HG2	2.00	0.43
39:q:84:HIS:CE1	39:q:86:SER:HB2	2.53	0.43
6:F:45:TYR:HE1	6:F:80:LYS:HG3	1.84	0.43
10:J:757:ALA:O	10:J:761:ALA:CB	2.67	0.43
12:L:336:VAL:HB	12:L:344:SER:HB2	2.01	0.43
13:M:110:SER:OG	13:M:111:ILE:N	2.52	0.43
18:R:108:ARG:HG3	33:k:141:ILE:HD12	2.01	0.43
19:T:212:ILE:HG23	19:T:213:VAL:HG23	2.01	0.43
22:X:163:TYR:HA	22:X:604:PHE:HA	2.00	0.43
25:a:108:ARG:NH1	50:1:350:U:OP1	2.34	0.43
30:g:92:ILE:HD12	30:g:95:ALA:HB3	2.01	0.43
1:A:23:SER:HB3	1:A:28:HIS:HB2	2.01	0.42
7:G:136:LEU:HD11	7:G:155:LEU:HD21	2.00	0.42
15:O:312:ASP:O	15:O:317:GLY:CA	2.65	0.42
15:O:343:ILE:HG23	15:O:352:ILE:HD11	2.00	0.42
18:R:131:ASN:HD22	18:R:132:PRO:HD2	1.83	0.42
26:b:89:LEU:HD11	26:b:117:LEU:HB2	2.01	0.42
28:d:170:ALA:O	28:d:177:ILE:HA	2.19	0.42
28:d:379:LEU:HB3	28:d:392:ARG:HH22	1.84	0.42
30:g:101:LEU:HD22	30:g:172:MET:HE2	2.00	0.42
32:i:721:ASP:O	32:i:766:LEU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:n:82:ASN:O	50:l:2194:A:O2'	2.36	0.42
39:q:86:SER:OG	50:l:912:U:O2	2.29	0.42
40:r:82:GLY:O	40:r:105:ARG:NH1	2.48	0.42
1:A:771:PRO:HD3	1:A:804:TRP:HH2	1.84	0.42
7:G:45:PHE:HE2	28:d:16:PRO:HG2	1.83	0.42
7:G:90:GLU:OE2	14:N:67:ARG:NH1	2.34	0.42
13:M:386:THR:O	13:M:386:THR:OG1	2.36	0.42
15:O:674:HIS:HB2	15:O:715:PHE:CD2	2.54	0.42
22:X:180:PRO:HA	22:X:181:PRO:HA	1.71	0.42
22:X:420:LEU:HB3	22:X:429:LEU:HD23	2.00	0.42
22:X:561:ASN:HD21	22:X:586:MET:HA	1.84	0.42
23:Y:225:THR:HA	23:Y:257:ASP:HB2	2.01	0.42
24:Z:815:VAL:HG21	24:Z:873:PHE:HE1	1.83	0.42
32:i:311:PHE:CB	32:i:385:LEU:O	2.67	0.42
32:i:570:LEU:O	32:i:583:LEU:N	2.50	0.42
37:o:177:ARG:NH2	37:o:179:GLN:OE1	2.52	0.42
51:2:53:U:H2'	51:2:54:C:C6	2.55	0.42
51:2:142:G:H2'	51:2:145:A:H61	1.84	0.42
1:A:614:VAL:HG13	15:O:401:ALA:HA	2.00	0.42
7:G:32:SER:HB3	7:G:123:ARG:HH11	1.84	0.42
8:H:22:ARG:NH2	24:Z:923:THR:OG1	2.51	0.42
13:M:401:ASN:O	13:M:414:HIS:HB3	2.18	0.42
14:N:459:GLY:HA2	21:V:87:ALA:HB2	2.00	0.42
18:S:95:ALA:HA	18:S:127:TYR:HD1	1.85	0.42
18:S:278:LYS:O	18:S:282:ASP:HB2	2.20	0.42
21:W:83:PRO:HB2	22:X:462:GLN:NE2	2.33	0.42
24:Z:139:MET:HE2	24:Z:139:MET:HB3	1.81	0.42
26:b:215:ARG:HG2	26:b:220:ASN:HB3	2.01	0.42
32:i:422:ARG:N	32:i:546:ALA:O	2.52	0.42
32:j:311:PHE:CB	32:j:385:LEU:O	2.67	0.42
34:l:33:LYS:HB2	34:l:97:LEU:HD23	2.01	0.42
37:o:114:VAL:HG12	37:o:115:LYS:HG3	2.02	0.42
42:t:115:LEU:O	42:t:119:ALA:CB	2.67	0.42
50:l:1213:U:C2	50:l:1555:A:N7	2.87	0.42
1:A:567:ALA:O	1:A:573:LYS:NZ	2.34	0.42
6:F:342:ARG:HB2	6:F:360:TRP:CZ3	2.54	0.42
7:G:195:ALA:HA	7:G:198:ARG:HE	1.85	0.42
10:J:771:LEU:HB2	10:J:816:TRP:CZ2	2.54	0.42
14:N:325:LEU:HD13	14:N:325:LEU:HA	1.86	0.42
19:T:105:LEU:O	19:T:109:ILE:HB	2.19	0.42
21:W:96:ARG:HH11	22:X:590:ARG:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:163:TYR:HA	22:X:603:ILE:O	2.19	0.42
23:Y:307:GLU:O	23:Y:311:GLU:HB2	2.19	0.42
28:d:418:ARG:HB2	50:1:1653:G:H5''	2.01	0.42
30:g:59:THR:O	30:g:63:GLU:HB2	2.19	0.42
32:i:265:LEU:O	32:i:269:VAL:CB	2.68	0.42
32:i:386:VAL:CB	32:i:407:LEU:O	2.67	0.42
34:l:158:SER:HA	34:l:161:ILE:HB	2.01	0.42
38:p:23:GLU:HG2	38:p:52:ALA:HB3	2.00	0.42
44:v:72:ARG:NE	50:1:698:A:O2'	2.52	0.42
50:1:1652:C:H2'	50:1:1653:G:C8	2.55	0.42
50:1:1701:U:H2'	50:1:1702:G:C8	2.53	0.42
6:F:351:SER:OG	6:F:352:ASP:N	2.52	0.42
12:L:93:LYS:HE3	12:L:132:THR:HG23	2.00	0.42
14:N:402:ASN:O	14:N:406:MET:HA	2.20	0.42
15:O:752:THR:N	15:O:766:ALA:O	2.44	0.42
19:T:218:THR:HA	19:T:221:LYS:HG2	2.00	0.42
20:U:6:LEU:HD11	20:U:73:LEU:HG	2.02	0.42
24:Z:256:THR:O	24:Z:260:GLU:CB	2.67	0.42
24:Z:799:LEU:HA	24:Z:799:LEU:HD23	1.85	0.42
32:j:554:ASN:O	32:j:558:LEU:CB	2.67	0.42
33:k:189:ARG:NH2	50:1:2072:U:O4	2.52	0.42
41:s:88:LEU:HD23	41:s:91:LEU:HD12	2.01	0.42
41:s:102:LEU:HD11	41:s:112:LYS:HA	2.01	0.42
50:1:906:G:O2'	50:1:921:G:O2'	2.36	0.42
1:A:215:LYS:O	1:A:257:THR:OG1	2.37	0.42
1:A:375:ILE:HG23	1:A:376:VAL:HG23	2.00	0.42
1:A:833:LEU:HD21	15:O:855:LEU:HD21	2.02	0.42
5:E:314:GLU:O	5:E:318:SER:CB	2.67	0.42
20:U:17:LYS:HG2	20:U:46:LYS:HG2	2.00	0.42
22:X:329:HIS:CE1	22:X:355:ARG:HD2	2.55	0.42
23:Y:111:THR:HA	23:Y:114:LEU:HB3	2.02	0.42
23:Y:240:ARG:O	23:Y:244:ASN:HB3	2.19	0.42
26:b:44:PRO:O	26:b:48:ASN:HB2	2.18	0.42
27:c:547:ARG:O	27:c:551:ALA:HB3	2.19	0.42
27:c:695:VAL:HG21	27:c:716:ARG:NH2	2.34	0.42
28:d:112:ILE:HG21	45:w:68:ARG:HH22	1.83	0.42
32:i:554:ASN:O	32:i:558:LEU:CB	2.68	0.42
32:i:842:GLU:O	32:i:846:ASN:CB	2.68	0.42
32:j:40:HIS:O	32:j:44:ILE:CB	2.67	0.42
32:j:265:LEU:O	32:j:269:VAL:CB	2.68	0.42
32:j:735:LYS:O	32:j:739:ARG:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:106:ARG:HD2	40:r:143:SER:HA	2.02	0.42
40:r:118:LYS:H	40:r:122:HIS:CD2	2.37	0.42
47:y:360:HIS:HB2	47:y:363:ARG:HB2	2.02	0.42
50:1:364:C:H2'	50:1:365:G:H8	1.85	0.42
51:2:94:A:H61	51:2:260:G:H22	1.68	0.42
1:A:60:ARG:NH2	1:A:100:THR:O	2.52	0.42
7:G:109:LEU:HD21	7:G:139:PHE:CD1	2.54	0.42
12:L:148:TRP:CD1	12:L:149:VAL:HG13	2.54	0.42
12:L:335:ALA:HA	12:L:345:ILE:HG22	2.01	0.42
19:T:387:SER:O	19:T:391:ARG:HD3	2.20	0.42
24:Z:862:TYR:OH	50:1:1162:U:OP2	2.36	0.42
26:b:198:THR:HG21	26:b:296:TYR:HB2	2.00	0.42
29:e:144:LEU:O	29:e:148:LEU:HA	2.20	0.42
29:e:193:VAL:HG12	29:e:196:LEU:HD12	2.02	0.42
31:h:187:ILE:O	31:h:191:ALA:CB	2.68	0.42
32:j:721:ASP:O	32:j:766:LEU:CB	2.67	0.42
37:o:132:ARG:HE	50:1:655:A:H62	1.67	0.42
43:u:49:TYR:HA	43:u:52:ILE:HD12	2.02	0.42
50:1:1499:G:H21	50:1:1500:A:H62	1.67	0.42
50:1:2168:U:N3	50:1:2194:A:C2	2.82	0.42
51:2:160:U:H2'	51:2:161:G:C8	2.53	0.42
1:A:393:LYS:HG3	1:A:395:SER:H	1.84	0.42
1:A:582:MET:HE3	1:A:682:PRO:HA	2.01	0.42
14:N:324:ASP:OD1	14:N:344:ARG:NH1	2.52	0.42
18:S:130:TRP:CE2	18:S:138:ALA:HB2	2.55	0.42
18:S:250:GLY:CA	18:S:306:TYR:O	2.66	0.42
24:Z:71:VAL:HA	24:Z:135:ILE:O	2.20	0.42
26:b:42:LEU:HD22	26:b:47:ALA:HB2	2.02	0.42
28:d:143:ASN:OD1	28:d:143:ASN:N	2.52	0.42
29:f:84:ILE:O	29:f:86:ASP:N	2.46	0.42
29:f:193:VAL:HG12	29:f:196:LEU:HD12	2.02	0.42
31:h:83:ARG:HH12	31:h:137:GLN:HE22	1.66	0.42
32:i:724:GLY:HA2	32:i:763:ILE:HA	2.01	0.42
43:u:82:ARG:HE	43:u:116:LEU:HD21	1.84	0.42
44:v:90:ILE:HA	44:v:112:LEU:O	2.20	0.42
45:w:31:SER:OG	45:w:32:LYS:N	2.53	0.42
1:A:16:CYS:SG	1:A:17:ARG:N	2.93	0.42
5:E:61:VAL:HG11	5:E:96:PHE:CZ	2.54	0.42
10:J:748:TYR:HE2	10:J:757:ALA:H	1.56	0.42
12:L:181:ARG:HE	12:L:183:PHE:HZ	1.67	0.42
14:N:490:GLY:HA2	14:N:543:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:301:ALA:HB2	15:O:308:VAL:HG12	2.01	0.42
15:O:433:GLN:HA	15:O:531:ALA:HB2	2.02	0.42
16:P:88:ASN:OD1	16:P:88:ASN:N	2.51	0.42
18:R:95:ALA:HA	18:R:127:TYR:HD1	1.85	0.42
19:T:125:GLU:HA	19:T:128:ALA:HB3	2.01	0.42
25:a:159:THR:OG1	25:a:160:TRP:N	2.52	0.42
34:l:118:GLN:HB2	34:l:143:THR:HB	2.01	0.42
34:l:196:GLU:O	34:l:200:ALA:HB3	2.20	0.42
35:m:19:LEU:HB3	35:m:51:ARG:HH12	1.84	0.42
35:m:35:PRO:HD2	35:m:83:PRO:HG2	2.01	0.42
45:w:48:GLY:H	45:w:65:LEU:HA	1.84	0.42
50:1:1071:G:H2'	50:1:1072:G:C8	2.54	0.42
1:A:797:LEU:O	1:A:801:HIS:HB2	2.20	0.42
4:D:123:LYS:HE2	4:D:172:ASP:HA	2.02	0.42
6:F:222:MET:HE2	6:F:231:LEU:HD11	2.02	0.42
11:K:935:LYS:NZ	50:1:451:C:O2'	2.40	0.42
14:N:417:ARG:NH2	50:1:139:C:O2'	2.52	0.42
19:T:389:ALA:HA	19:T:392:ILE:HG22	2.02	0.42
20:U:400:LYS:O	20:U:404:ASN:HB2	2.20	0.42
21:W:77:VAL:HA	21:W:78:PRO:HD3	1.94	0.42
23:Y:37:ARG:HB2	23:Y:45:GLY:H	1.84	0.42
26:b:103:PHE:HZ	26:b:261:PHE:HE2	1.67	0.42
26:b:146:ARG:NH1	50:1:2184:G:O2'	2.52	0.42
26:b:202:GLN:HA	26:b:205:VAL:HG12	2.00	0.42
35:m:212:ASP:OD1	35:m:216:ASN:N	2.49	0.42
37:o:186:ARG:HA	37:o:189:HIS:HD2	1.85	0.42
50:1:150:C:OP2	50:1:150:C:H6	2.03	0.42
50:1:301:U:H2'	50:1:302:A:H8	1.85	0.42
50:1:2086:A:H5''	50:1:2087:G:C8	2.55	0.42
1:A:284:MET:HE2	1:A:284:MET:HB3	1.91	0.41
3:C:648:LEU:HD12	16:P:140:LYS:HD3	2.02	0.41
6:F:278:GLN:HA	6:F:302:PRO:HA	2.02	0.41
9:I:884:THR:HB	48:z:30:ARG:HH12	1.85	0.41
15:O:388:VAL:HA	15:O:412:GLY:HA2	2.01	0.41
18:R:253:LEU:HD21	18:R:255:ILE:HD11	2.02	0.41
18:S:253:LEU:HD21	18:S:255:ILE:HD11	2.02	0.41
19:T:312:THR:O	19:T:316:ALA:HB2	2.20	0.41
20:U:125:HIS:CE1	20:U:128:ASN:HB3	2.55	0.41
22:X:273:TYR:CG	22:X:280:PRO:HA	2.55	0.41
23:Y:139:THR:OG1	23:Y:179:SER:OG	2.37	0.41
24:Z:274:LEU:HB3	24:Z:773:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:735:LYS:O	32:i:739:ARG:CB	2.67	0.41
32:j:724:GLY:HA2	32:j:763:ILE:HA	2.01	0.41
37:o:32:MET:HE1	37:o:63:MET:HB3	2.01	0.41
50:1:87:G:H2'	50:1:88:C:H6	1.85	0.41
50:1:678:A:HO2'	50:1:680:U:H3	1.64	0.41
50:1:1448:A:C6	50:1:1549:U:N3	2.88	0.41
50:1:2165:U:H6	50:1:2165:U:H2'	1.68	0.41
1:A:209:THR:HA	1:A:222:TRP:O	2.20	0.41
1:A:319:LEU:HB3	1:A:337:GLN:HE21	1.84	0.41
15:O:110:ASP:HA	15:O:140:PRO:HG3	2.02	0.41
18:S:101:GLU:HG3	18:S:199:ARG:HH12	1.85	0.41
19:T:392:ILE:HD12	21:W:63:SER:HB3	2.02	0.41
25:a:87:ILE:HD13	25:a:106:PHE:CE1	2.55	0.41
29:f:144:LEU:O	29:f:148:LEU:HA	2.20	0.41
30:g:106:VAL:HG11	30:g:172:MET:HE3	2.01	0.41
32:j:422:ARG:N	32:j:546:ALA:O	2.52	0.41
33:k:86:THR:HG22	33:k:94:PRO:HA	2.02	0.41
34:l:66:PHE:HD1	42:t:47:SER:HB3	1.85	0.41
34:l:136:ARG:O	34:l:215:VAL:HA	2.19	0.41
35:m:106:LYS:HA	35:m:244:LYS:HE2	2.02	0.41
38:p:129:THR:HA	38:p:132:HIS:CE1	2.55	0.41
39:q:78:ILE:HG23	39:q:102:VAL:HG11	2.01	0.41
47:y:336:VAL:HB	47:y:366:ILE:HD11	2.01	0.41
6:F:209:GLU:HB3	16:P:6:ILE:HG23	2.02	0.41
11:K:308:ASP:O	11:K:312:ARG:CB	2.67	0.41
12:L:126:PHE:HA	12:L:137:LEU:H	1.85	0.41
12:L:289:VAL:HB	12:L:299:VAL:HG12	2.02	0.41
19:T:306:LEU:O	19:T:310:LEU:HB2	2.20	0.41
22:X:343:ARG:NH1	22:X:406:ASP:O	2.53	0.41
23:Y:66:ILE:HG12	23:Y:77:TYR:HD1	1.85	0.41
24:Z:279:PHE:HB2	24:Z:771:TYR:HB2	2.02	0.41
32:j:43:TYR:O	32:j:47:SER:CB	2.68	0.41
34:l:61:LEU:HD13	34:l:91:VAL:HG11	2.02	0.41
40:r:78:LEU:HD23	40:r:78:LEU:HA	1.90	0.41
41:s:125:LEU:HD22	41:s:129:TYR:HE2	1.85	0.41
43:u:19:VAL:HG22	43:u:68:ARG:HB2	2.02	0.41
1:A:112:VAL:HG23	1:A:159:TRP:CZ2	2.55	0.41
1:A:661:ARG:H	27:c:635:SER:HB2	1.86	0.41
3:C:648:LEU:HD22	18:R:289:GLN:HB2	2.03	0.41
6:F:337:ASN:HB3	6:F:380:LYS:HD2	2.02	0.41
9:I:800:GLU:HA	9:I:803:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:209:SER:OG	12:L:210:TYR:N	2.52	0.41
18:R:173:ILE:O	33:k:91:TYR:OH	2.29	0.41
19:T:209:LEU:HD23	19:T:213:VAL:HB	2.02	0.41
19:T:215:ASP:O	19:T:218:THR:OG1	2.32	0.41
19:T:321:HIS:CD2	19:T:339:LEU:HD22	2.55	0.41
23:Y:307:GLU:O	23:Y:311:GLU:CB	2.68	0.41
24:Z:72:VAL:HA	24:Z:117:ILE:HD11	2.02	0.41
24:Z:917:LYS:NZ	50:1:1141:G:O3'	2.50	0.41
28:d:319:ASP:OD1	28:d:320:VAL:N	2.54	0.41
30:g:157:LEU:HD13	30:g:201:LEU:HB2	2.02	0.41
37:o:13:GLN:NE2	50:1:735:G:H21	2.18	0.41
39:q:31:ARG:NH1	50:1:917:A:OP2	2.53	0.41
40:r:133:ARG:HA	40:r:138:ILE:HA	2.02	0.41
43:u:52:ILE:HG12	43:u:60:PHE:HE2	1.84	0.41
50:1:1502:U:H2'	50:1:1503:U:H6	1.84	0.41
51:2:3:C:H2'	51:2:4:G:H8	1.86	0.41
4:D:260:ILE:HG23	4:D:270:GLN:HB3	2.01	0.41
12:L:50:PRO:HG3	12:L:107:ILE:HG13	2.03	0.41
14:N:463:GLY:HA2	14:N:487:SER:HA	2.02	0.41
15:O:61:PHE:HD2	15:O:346:LEU:HD22	1.86	0.41
15:O:485:GLN:O	15:O:530:ARG:NH2	2.38	0.41
18:R:157:LEU:HB3	18:R:226:ILE:HG12	2.02	0.41
22:X:402:ALA:HB1	22:X:471:THR:HG22	2.02	0.41
29:e:67:LEU:HD11	29:e:141:MET:HB2	2.02	0.41
32:i:43:TYR:O	32:i:47:SER:CB	2.68	0.41
33:k:108:LEU:HD21	33:k:165:VAL:HG21	2.02	0.41
34:l:65:ILE:HD12	34:l:85:LYS:HD3	2.02	0.41
44:v:116:VAL:HG22	44:v:144:VAL:HG21	2.02	0.41
50:1:384:C:H3'	50:1:385:A:H8	1.86	0.41
50:1:1508:A:H2'	50:1:1509:A:C8	2.56	0.41
1:A:686:SER:HA	1:A:698:TYR:O	2.20	0.41
5:E:9:ARG:HE	28:d:25:ARG:HH11	1.68	0.41
14:N:144:LEU:HD12	15:O:196:LEU:HD21	2.02	0.41
16:P:8:GLY:HA3	25:a:34:ARG:NH1	2.33	0.41
18:S:211:ARG:HG2	18:S:238:ILE:HG12	2.02	0.41
20:U:295:ALA:O	20:U:299:ALA:CB	2.69	0.41
20:U:419:LEU:HD23	20:U:423:GLY:HA2	2.02	0.41
21:V:87:ALA:O	21:V:91:ALA:HB2	2.19	0.41
28:d:216:VAL:HG13	28:d:245:ILE:HB	2.03	0.41
29:e:38:ILE:HG13	29:e:111:GLN:HB3	2.03	0.41
32:j:398:LEU:O	32:j:402:LEU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:n:135:ARG:HA	36:n:144:ARG:HD2	2.03	0.41
45:w:10:ALA:HB1	45:w:27:ILE:HD13	2.01	0.41
51:2:84:G:N2	51:2:264:G:O2'	2.53	0.41
1:A:69:LEU:HD21	1:A:81:LEU:HD22	2.01	0.41
1:A:105:SER:OG	1:A:163:SER:OG	2.28	0.41
1:A:655:SER:HA	1:A:665:GLY:HA3	2.03	0.41
4:D:237:ILE:O	4:D:254:SER:OG	2.30	0.41
7:G:181:ALA:HB2	20:U:412:PRO:HB3	2.02	0.41
11:K:920:LYS:NZ	50:1:440:G:O2'	2.54	0.41
13:M:405:SER:OG	13:M:407:LYS:O	2.38	0.41
15:O:648:PHE:CB	15:O:658:ASP:O	2.54	0.41
15:O:1005:LEU:O	15:O:1009:ASN:HB2	2.21	0.41
19:T:316:ALA:HA	19:T:319:ILE:HG22	2.02	0.41
20:U:116:ASP:O	20:U:120:ARG:CB	2.68	0.41
25:a:133:GLN:OE1	51:2:59:A:O2'	2.27	0.41
26:b:53:ARG:HB2	49:0:219:ILE:HD11	2.02	0.41
29:f:181:SER:OG	29:f:183:ASP:OD1	2.34	0.41
31:h:111:LEU:HG	31:h:126:SER:HA	2.01	0.41
32:i:33:HIS:HA	32:i:37:ALA:HB3	2.03	0.41
32:j:721:ASP:O	32:j:767:GLN:N	2.53	0.41
34:l:35:PRO:HG3	34:l:232:HIS:CE1	2.56	0.41
37:o:72:ARG:NH2	50:1:1003:G:O5'	2.54	0.41
38:p:33:LEU:HB3	38:p:44:LEU:HD13	2.01	0.41
50:1:484:G:H2'	50:1:485:G:C8	2.56	0.41
50:1:1740:C:H2'	50:1:1741:A:C8	2.55	0.41
51:2:93:G:H2'	51:2:94:A:H4'	2.02	0.41
6:F:243:GLN:HE21	6:F:250:ILE:HG22	1.86	0.41
15:O:295:ASP:OD1	15:O:295:ASP:N	2.52	0.41
18:R:130:TRP:CE2	18:R:138:ALA:HB2	2.55	0.41
18:R:211:ARG:HG2	18:R:238:ILE:HG12	2.02	0.41
19:T:372:PRO:HB2	19:T:373:LYS:H	1.65	0.41
19:T:410:GLN:HA	19:T:413:GLN:HG2	2.03	0.41
22:X:273:TYR:HB3	22:X:281:ILE:H	1.84	0.41
23:Y:23:LEU:HD13	23:Y:367:LEU:HD13	2.03	0.41
23:Y:367:LEU:HD23	23:Y:375:TRP:HZ2	1.85	0.41
29:e:221:VAL:HG11	29:e:224:LYS:HE3	2.02	0.41
31:h:205:THR:HB	31:h:248:LEU:HD22	2.03	0.41
32:i:721:ASP:O	32:i:767:GLN:N	2.53	0.41
37:o:68:ILE:HG23	37:o:101:ILE:HD11	2.03	0.41
50:1:1146:G:N2	50:1:1149:C:OP2	2.49	0.41
50:1:1532:C:H2'	50:1:1533:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:2072:U:H4'	50:1:2073:A:H5'	2.03	0.41
2:B:883:ALA:O	2:B:887:ASN:HB2	2.21	0.41
8:H:31:LYS:NZ	8:H:35:ARG:HH21	2.19	0.41
8:H:36:LEU:HD12	24:Z:1043:ARG:HD3	2.03	0.41
9:I:924:LEU:HD13	10:J:864:LYS:HA	2.03	0.41
12:L:333:HIS:HB3	12:L:347:THR:HG22	2.03	0.41
14:N:443:GLU:O	14:N:452:VAL:HB	2.21	0.41
15:O:470:SER:HB2	15:O:511:VAL:HG22	2.03	0.41
16:P:111:MET:HE3	28:d:67:GLN:HG2	2.02	0.41
18:R:255:ILE:HD13	18:R:255:ILE:HG21	1.89	0.41
19:T:310:LEU:HB3	19:T:314:VAL:HG23	2.03	0.41
20:U:341:TYR:CD1	20:U:345:TYR:HB2	2.56	0.41
22:X:168:TRP:CE2	22:X:599:CYS:HB3	2.56	0.41
22:X:270:LEU:HD12	22:X:291:VAL:HG21	2.02	0.41
23:Y:130:VAL:HG22	23:Y:194:MET:HB2	2.03	0.41
23:Y:172:GLU:OE2	23:Y:195:ARG:NH1	2.53	0.41
24:Z:836:SER:HB3	24:Z:885:CYS:HB2	2.03	0.41
25:a:88:LEU:HD11	25:a:97:VAL:HG22	2.03	0.41
29:e:132:ARG:HH21	29:f:94:GLN:HE22	1.67	0.41
32:j:842:GLU:O	32:j:846:ASN:CB	2.68	0.41
34:l:33:LYS:HB2	34:l:96:CYS:O	2.19	0.41
34:l:115:ARG:HB3	34:l:118:GLN:NE2	2.36	0.41
35:m:207:ILE:HG22	35:m:221:ARG:HG2	2.02	0.41
37:o:102:VAL:HG13	37:o:106:LEU:HD12	2.02	0.41
39:q:67:TRP:HD1	39:q:70:GLU:HB2	1.86	0.41
50:1:420:G:H2'	50:1:421:A:H8	1.86	0.41
50:1:679:A:H61	50:1:980:G:H1'	1.85	0.41
50:1:863:G:H8	50:1:865:G:OP2	2.04	0.41
1:A:245:ILE:HD11	1:A:248:LYS:HB3	2.02	0.41
6:F:265:THR:HB	6:F:266:GLN:H	1.71	0.41
6:F:275:ILE:HD13	6:F:275:ILE:HG21	1.89	0.41
10:J:771:LEU:HD13	10:J:816:TRP:CE3	2.56	0.41
10:J:788:LEU:HD23	10:J:832:ALA:HA	2.03	0.41
10:J:814:ARG:HD3	10:J:859:VAL:HG13	2.03	0.41
13:M:324:TYR:HE1	13:M:350:LYS:HG2	1.86	0.41
13:M:360:SER:HB3	13:M:402:ILE:HG12	2.03	0.41
15:O:365:ILE:HB	15:O:378:LEU:HD23	2.03	0.41
15:O:969:ASN:O	15:O:973:HIS:ND1	2.48	0.41
20:U:323:GLY:HA3	20:U:343:ILE:HG13	2.03	0.41
50:1:678:A:O2'	50:1:680:U:N3	2.53	0.41
50:1:1219:A:N7	50:1:1448:A:N6	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1:1705:C:N4	51:2:5:A:N6	2.68	0.41
5:E:40:ARG:HD2	5:E:63:TRP:HZ3	1.84	0.40
23:Y:176:LEU:HB2	23:Y:191:ILE:O	2.21	0.40
24:Z:837:LEU:HD23	24:Z:878:ILE:HD13	2.02	0.40
24:Z:919:LYS:HA	24:Z:989:LEU:O	2.20	0.40
26:b:105:LYS:NZ	50:1:1743:C:O4'	2.45	0.40
26:b:109:LEU:HD11	50:1:1743:C:C4	2.56	0.40
27:c:695:VAL:HG21	27:c:716:ARG:HH22	1.86	0.40
28:d:200:ILE:HD11	28:d:215:SER:HB3	2.03	0.40
29:e:136:ARG:O	29:e:140:LEU:HB2	2.21	0.40
30:g:56:PRO:HG3	50:1:307:U:H5''	2.03	0.40
37:o:5:ILE:HG12	37:o:111:LEU:HD12	2.02	0.40
43:u:77:GLN:NE2	50:1:2065:C:O2'	2.54	0.40
47:y:391:LEU:CA	47:y:401:THR:O	2.59	0.40
47:y:424:ARG:NH1	50:1:1110:A:OP1	2.49	0.40
48:z:31:VAL:O	48:z:40:SER:HA	2.21	0.40
50:1:421:A:H2'	50:1:422:A:H8	1.86	0.40
50:1:728:G:H2'	50:1:729:A:O4'	2.21	0.40
50:1:1056:U:H2'	50:1:1057:A:C8	2.55	0.40
50:1:2328:G:H2'	50:1:2329:A:C8	2.56	0.40
1:A:334:LEU:HA	1:A:334:LEU:HD12	1.87	0.40
5:E:332:PRO:HB3	5:E:377:LEU:HB2	2.03	0.40
6:F:304:ARG:NH1	6:F:346:THR:HG22	2.36	0.40
13:M:217:GLN:HB3	13:M:218:ILE:H	1.79	0.40
20:U:289:MET:HE3	20:U:289:MET:HB3	1.94	0.40
26:b:294:LYS:O	27:c:528:LYS:NZ	2.54	0.40
34:l:61:LEU:HD23	34:l:61:LEU:HA	1.87	0.40
39:q:75:LYS:HD2	50:1:842:C:H5''	2.03	0.40
50:1:3:G:C2	50:1:4:G:H1'	2.56	0.40
50:1:839:U:H2'	50:1:840:A:C8	2.57	0.40
1:A:5:PHE:HB2	1:A:610:PHE:HZ	1.86	0.40
1:A:711:LEU:HB3	15:O:700:ILE:HD11	2.04	0.40
5:E:272:PRO:HB2	5:E:273:ALA:H	1.63	0.40
9:I:874:THR:O	9:I:878:LEU:CB	2.70	0.40
13:M:127:LEU:HD21	13:M:158:VAL:HG11	2.03	0.40
18:S:157:LEU:HB3	18:S:226:ILE:HG12	2.03	0.40
20:U:320:GLN:NE2	20:U:340:LYS:O	2.55	0.40
24:Z:883:SER:HA	24:Z:903:GLY:O	2.21	0.40
26:b:163:LEU:HD13	26:b:207:ILE:HD11	2.03	0.40
28:d:282:HIS:NE2	28:d:300:SER:OG	2.38	0.40
39:q:98:LYS:HG3	39:q:174:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:t:31:ARG:O	42:t:41:VAL:HA	2.21	0.40
48:z:30:ARG:HA	48:z:42:ILE:HG22	2.04	0.40
50:1:364:C:H2'	50:1:365:G:C8	2.57	0.40
6:F:114:GLN:HE22	6:F:418:ILE:HD12	1.86	0.40
6:F:225:LEU:HB2	6:F:230:LEU:HB3	2.02	0.40
7:G:72:THR:HG22	14:N:69:GLN:HB3	2.04	0.40
13:M:378:VAL:HG13	13:M:393:PRO:HA	2.03	0.40
15:O:841:MET:HE2	15:O:988:TYR:CD1	2.57	0.40
23:Y:375:TRP:CD1	23:Y:398:VAL:HG22	2.57	0.40
24:Z:954:THR:HB	24:Z:958:ILE:HB	2.04	0.40
29:f:38:ILE:HG13	29:f:111:GLN:HB3	2.03	0.40
29:f:67:LEU:HD11	29:f:141:MET:HB2	2.02	0.40
32:j:137:ALA:O	32:j:141:GLU:CB	2.69	0.40
32:j:538:GLN:O	32:j:542:ALA:HB2	2.22	0.40
34:l:105:PHE:HB2	34:l:213:ARG:HA	2.02	0.40
44:v:138:LYS:HE2	44:v:138:LYS:HB2	1.91	0.40
50:1:758:U:N3	50:1:850:A:N6	2.69	0.40
50:1:1647:U:H2'	50:1:1648:G:C8	2.57	0.40
1:A:178:TRP:HD1	1:A:188:PRO:HB3	1.87	0.40
4:D:78:ASP:HB3	4:D:105:ILE:HD12	2.03	0.40
12:L:171:LEU:HB3	12:L:181:ARG:HB2	2.02	0.40
12:L:336:VAL:HB	12:L:344:SER:O	2.22	0.40
13:M:165:ILE:H	13:M:180:SER:H	1.70	0.40
15:O:713:PHE:HA	15:O:723:VAL:O	2.20	0.40
23:Y:227:VAL:HB	23:Y:231:HIS:CE1	2.56	0.40
43:u:20:ALA:HA	43:u:66:ARG:O	2.21	0.40
47:y:393:THR:HA	47:y:400:THR:HA	2.03	0.40
50:1:616:U:H2'	50:1:617:G:H8	1.86	0.40
50:1:1702:G:N2	51:2:7:A:N1	2.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	823/904 (91%)	739 (90%)	83 (10%)	1 (0%)	48	79
2	B	67/907 (7%)	66 (98%)	1 (2%)	0	100	100
3	C	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	D	280/884 (32%)	256 (91%)	23 (8%)	1 (0%)	30	62
5	E	325/414 (78%)	312 (96%)	13 (4%)	0	100	100
6	F	425/558 (76%)	390 (92%)	34 (8%)	1 (0%)	43	73
7	G	361/1802 (20%)	340 (94%)	21 (6%)	0	100	100
8	H	186/270 (69%)	178 (96%)	8 (4%)	0	100	100
9	I	153/962 (16%)	141 (92%)	12 (8%)	0	100	100
10	J	147/912 (16%)	139 (95%)	8 (5%)	0	100	100
11	K	9/938 (1%)	8 (89%)	1 (11%)	0	100	100
14	N	210/618 (34%)	197 (94%)	13 (6%)	0	100	100
15	O	850/1049 (81%)	768 (90%)	82 (10%)	0	100	100
16	P	188/194 (97%)	173 (92%)	15 (8%)	0	100	100
17	Q	172/391 (44%)	146 (85%)	23 (13%)	3 (2%)	7	35
18	R	238/313 (76%)	222 (93%)	15 (6%)	1 (0%)	30	62
18	S	235/313 (75%)	221 (94%)	13 (6%)	1 (0%)	30	62
19	T	383/523 (73%)	352 (92%)	31 (8%)	0	100	100
20	U	397/582 (68%)	375 (94%)	22 (6%)	0	100	100
21	V	119/127 (94%)	105 (88%)	13 (11%)	1 (1%)	16	50
21	W	118/127 (93%)	104 (88%)	13 (11%)	1 (1%)	16	50
22	X	337/630 (54%)	294 (87%)	42 (12%)	1 (0%)	36	68
23	Y	333/411 (81%)	300 (90%)	30 (9%)	3 (1%)	14	47
24	Z	627/1163 (54%)	582 (93%)	44 (7%)	1 (0%)	43	73
25	a	177/183 (97%)	162 (92%)	15 (8%)	0	100	100
26	b	287/297 (97%)	263 (92%)	24 (8%)	0	100	100
27	c	169/785 (22%)	160 (95%)	9 (5%)	0	100	100
28	d	435/446 (98%)	390 (90%)	45 (10%)	0	100	100
29	e	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	14	47
29	f	211/252 (84%)	199 (94%)	10 (5%)	2 (1%)	14	47
30	g	172/322 (53%)	164 (95%)	8 (5%)	0	100	100
31	h	163/259 (63%)	154 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	643/1073 (60%)	569 (88%)	74 (12%)	0	100	100
32	j	663/1073 (62%)	588 (89%)	75 (11%)	0	100	100
33	k	115/203 (57%)	101 (88%)	14 (12%)	0	100	100
34	l	212/255 (83%)	184 (87%)	27 (13%)	1 (0%)	24	59
35	m	256/264 (97%)	219 (86%)	37 (14%)	0	100	100
36	n	188/212 (89%)	170 (90%)	17 (9%)	1 (0%)	24	59
37	o	235/239 (98%)	202 (86%)	31 (13%)	2 (1%)	14	47
38	p	155/203 (76%)	137 (88%)	18 (12%)	0	100	100
39	q	199/202 (98%)	187 (94%)	12 (6%)	0	100	100
40	r	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
41	s	47/151 (31%)	45 (96%)	2 (4%)	0	100	100
42	t	113/150 (75%)	95 (84%)	16 (14%)	2 (2%)	6	34
43	u	124/143 (87%)	113 (91%)	11 (9%)	0	100	100
44	v	155/161 (96%)	134 (86%)	21 (14%)	0	100	100
45	w	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
46	x	90/145 (62%)	79 (88%)	11 (12%)	0	100	100
47	y	91/136 (67%)	82 (90%)	9 (10%)	0	100	100
48	z	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
49	0	90/311 (29%)	82 (91%)	8 (9%)	0	100	100
All	All	12594/23745 (53%)	11466 (91%)	1103 (9%)	25 (0%)	44	73

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	e	85	SER
29	f	85	SER
34	l	62	LYS
23	Y	105	THR
36	n	91	ASN
6	F	56	PRO
37	o	176	PRO
42	t	61	VAL
4	D	170	ASP
17	Q	103	ASP
17	Q	104	PRO

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Mol	Chain	Res	Type
21	V	61	PRO
21	W	61	PRO
22	X	582	THR
37	o	149	LYS
42	t	60	LYS
23	Y	104	ALA
24	Z	77	PRO
18	R	294	PRO
18	S	294	PRO
1	A	285	PRO
23	Y	103	PRO
29	e	89	PRO
29	f	89	PRO
17	Q	237	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	633/775 (82%)	627 (99%)	6 (1%)	70	81
2	B	43/788 (6%)	43 (100%)	0	100	100
3	C	61/536 (11%)	60 (98%)	1 (2%)	55	75
4	D	222/738 (30%)	220 (99%)	2 (1%)	70	81
5	E	248/341 (73%)	248 (100%)	0	100	100
6	F	326/474 (69%)	314 (96%)	12 (4%)	30	63
7	G	289/1526 (19%)	287 (99%)	2 (1%)	76	83
8	H	135/227 (60%)	135 (100%)	0	100	100
9	I	134/821 (16%)	134 (100%)	0	100	100
10	J	129/770 (17%)	128 (99%)	1 (1%)	73	82
11	K	115/765 (15%)	115 (100%)	0	100	100
12	L	218/456 (48%)	218 (100%)	0	100	100
13	M	219/817 (27%)	218 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	351/524 (67%)	349 (99%)	2 (1%)	78	84
15	O	638/863 (74%)	626 (98%)	12 (2%)	50	73
16	P	147/168 (88%)	145 (99%)	2 (1%)	59	77
18	R	175/228 (77%)	172 (98%)	3 (2%)	53	75
18	S	195/228 (86%)	193 (99%)	2 (1%)	68	80
19	T	287/435 (66%)	284 (99%)	3 (1%)	68	80
20	U	307/489 (63%)	307 (100%)	0	100	100
21	V	91/108 (84%)	90 (99%)	1 (1%)	65	79
21	W	88/108 (82%)	87 (99%)	1 (1%)	65	79
22	X	273/525 (52%)	272 (100%)	1 (0%)	84	86
23	Y	275/320 (86%)	274 (100%)	1 (0%)	84	86
24	Z	466/1009 (46%)	462 (99%)	4 (1%)	70	81
25	a	147/169 (87%)	144 (98%)	3 (2%)	48	72
26	b	238/266 (90%)	236 (99%)	2 (1%)	73	82
27	c	138/642 (22%)	138 (100%)	0	100	100
28	d	354/383 (92%)	350 (99%)	4 (1%)	65	79
29	e	193/223 (86%)	193 (100%)	0	100	100
29	f	193/223 (86%)	193 (100%)	0	100	100
30	g	153/287 (53%)	153 (100%)	0	100	100
31	h	138/215 (64%)	138 (100%)	0	100	100
33	k	95/167 (57%)	95 (100%)	0	100	100
34	l	189/223 (85%)	187 (99%)	2 (1%)	65	79
35	m	219/221 (99%)	219 (100%)	0	100	100
36	n	144/178 (81%)	143 (99%)	1 (1%)	76	83
37	o	202/204 (99%)	201 (100%)	1 (0%)	81	85
38	p	137/177 (77%)	136 (99%)	1 (1%)	76	83
39	q	163/164 (99%)	162 (99%)	1 (1%)	78	84
40	r	122/162 (75%)	121 (99%)	1 (1%)	73	82
41	s	43/130 (33%)	43 (100%)	0	100	100
42	t	74/117 (63%)	74 (100%)	0	100	100
43	u	92/115 (80%)	90 (98%)	2 (2%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	v	140/143 (98%)	140 (100%)	0	100	100
45	w	103/113 (91%)	102 (99%)	1 (1%)	68	80
46	x	68/116 (59%)	68 (100%)	0	100	100
47	y	81/115 (70%)	81 (100%)	0	100	100
48	z	46/61 (75%)	45 (98%)	1 (2%)	45	71
49	0	68/260 (26%)	67 (98%)	1 (2%)	57	76
All	All	9605/19113 (50%)	9527 (99%)	78 (1%)	70	82

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	121	VAL
1	A	167	LEU
1	A	271	VAL
1	A	419	THR
1	A	753	ILE
3	C	579	ILE
4	D	46	ILE
4	D	199	ILE
6	F	200	VAL
6	F	219	VAL
6	F	230	LEU
6	F	233	THR
6	F	250	ILE
6	F	294	VAL
6	F	303	VAL
6	F	358	VAL
6	F	394	VAL
6	F	395	VAL
6	F	409	ILE
6	F	420	VAL
7	G	140	LEU
7	G	297	VAL
10	J	765	ASN
13	M	171	THR
14	N	144	LEU
14	N	158	ARG
15	O	151	ILE
15	O	161	VAL

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Mol	Chain	Res	Type
15	O	255	ILE
15	O	276	VAL
15	O	322	VAL
15	O	374	VAL
15	O	656	LEU
15	O	733	VAL
15	O	771	LEU
15	O	843	LEU
15	O	854	LEU
15	O	1034	VAL
16	P	58	VAL
16	P	168	VAL
18	R	71	VAL
18	R	254	LEU
18	R	262	ILE
18	S	254	LEU
18	S	262	ILE
19	T	145	LEU
19	T	209	LEU
19	T	391	ARG
21	V	53	VAL
21	W	53	VAL
22	X	578	VAL
23	Y	108	ARG
24	Z	156	ILE
24	Z	286	VAL
24	Z	815	VAL
24	Z	972	TYR
25	a	82	LEU
25	a	136	VAL
25	a	158	VAL
26	b	122	LEU
26	b	231	VAL
28	d	90	VAL
28	d	132	ILE
28	d	159	LEU
28	d	342	LEU
34	l	166	ARG
34	l	212	ILE
36	n	15	VAL
37	o	162	VAL
38	p	50	VAL

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Mol	Chain	Res	Type
39	q	101	VAL
40	r	94	VAL
43	u	9	VAL
43	u	53	LEU
45	w	53	VAL
48	z	11	VAL
49	0	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	78	GLN
1	A	145	HIS
1	A	147	HIS
1	A	196	GLN
1	A	253	GLN
1	A	337	GLN
1	A	451	HIS
1	A	524	GLN
1	A	846	ASN
4	D	124	HIS
5	E	140	ASN
6	F	95	ASN
6	F	96	GLN
6	F	159	HIS
6	F	205	HIS
6	F	206	ASN
6	F	243	GLN
6	F	267	ASN
6	F	270	ASN
6	F	274	HIS
6	F	378	GLN
6	F	427	ASN
6	F	434	ASN
7	G	226	ASN
7	G	295	GLN
7	G	317	GLN
7	G	318	HIS
7	G	349	HIS
8	H	6	HIS
8	H	13	HIS

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Mol	Chain	Res	Type
8	H	23	GLN
9	I	832	ASN
9	I	835	GLN
10	J	765	ASN
10	J	772	ASN
10	J	776	ASN
10	J	805	GLN
11	K	338	HIS
11	K	371	GLN
11	K	916	GLN
11	K	927	GLN
12	L	103	HIS
12	L	296	HIS
12	L	333	HIS
13	M	98	GLN
13	M	108	ASN
13	M	112	GLN
13	M	167	HIS
14	N	319	HIS
14	N	351	ASN
14	N	399	ASN
14	N	411	GLN
14	N	488	ASN
14	N	498	ASN
14	N	553	GLN
14	N	584	GLN
15	O	197	ASN
15	O	334	ASN
15	O	349	GLN
15	O	392	HIS
15	O	621	HIS
15	O	634	ASN
15	O	636	HIS
15	O	740	HIS
15	O	784	HIS
16	P	149	ASN
18	R	78	HIS
18	R	96	ASN
18	R	249	GLN
18	R	308	GLN
18	S	78	HIS
18	S	96	ASN

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Mol	Chain	Res	Type
19	T	5	ASN
19	T	54	ASN
19	T	179	GLN
19	T	321	HIS
19	T	327	ASN
20	U	147	HIS
20	U	167	HIS
20	U	256	ASN
20	U	288	ASN
20	U	364	GLN
20	U	404	ASN
20	U	422	ASN
21	V	19	GLN
21	V	33	GLN
21	V	67	HIS
21	W	67	HIS
22	X	330	GLN
22	X	561	ASN
23	Y	100	HIS
23	Y	209	ASN
23	Y	316	GLN
24	Z	159	ASN
24	Z	172	HIS
24	Z	202	HIS
24	Z	881	ASN
25	a	16	HIS
25	a	59	HIS
26	b	159	HIS
26	b	210	HIS
26	b	275	ASN
28	d	13	GLN
28	d	21	GLN
28	d	32	HIS
28	d	206	ASN
28	d	207	GLN
28	d	263	ASN
28	d	327	GLN
29	e	93	HIS
29	e	111	GLN
29	e	156	ASN
29	e	170	HIS
29	e	243	HIS

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Mol	Chain	Res	Type
29	f	93	HIS
29	f	94	GLN
29	f	111	GLN
30	g	146	GLN
30	g	165	HIS
31	h	137	GLN
34	l	21	GLN
34	l	56	ASN
34	l	99	ASN
34	l	101	HIS
34	l	118	GLN
34	l	124	ASN
34	l	220	GLN
34	l	232	HIS
35	m	9	GLN
35	m	17	HIS
35	m	36	HIS
35	m	98	ASN
35	m	253	GLN
36	n	50	GLN
36	n	82	ASN
36	n	91	ASN
36	n	126	ASN
37	o	13	GLN
37	o	119	GLN
37	o	179	GLN
37	o	185	GLN
37	o	189	HIS
37	o	201	GLN
38	p	80	GLN
38	p	95	HIS
39	q	13	HIS
39	q	52	ASN
39	q	84	HIS
39	q	153	HIS
39	q	163	GLN
39	q	179	GLN
42	t	102	ASN
43	u	77	GLN
44	v	111	ASN
45	w	12	ASN
45	w	16	ASN

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Mol	Chain	Res	Type
45	w	42	GLN
45	w	113	HIS
46	x	89	ASN
47	y	385	GLN
48	z	44	ASN
49	0	185	HIS
49	0	211	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	1	1319/2568 (51%)	479 (36%)	27 (2%)
51	2	226/274 (82%)	76 (33%)	5 (2%)
All	All	1545/2842 (54%)	555 (35%)	32 (2%)

All (555) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	1	3	G
50	1	5	G
50	1	6	G
50	1	7	A
50	1	8	U
50	1	9	G
50	1	10	U
50	1	16	U
50	1	17	C
50	1	19	C
50	1	20	C
50	1	23	G
50	1	27	A
50	1	30	U
50	1	31	C
50	1	32	U
50	1	35	G
50	1	38	G
50	1	41	G
50	1	53	A
50	1	59	U
50	1	69	U
50	1	71	A

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Mol	Chain	Res	Type
50	1	72	U
50	1	73	A
50	1	74	C
50	1	77	C
50	1	84	A
50	1	89	G
50	1	90	A
50	1	92	G
50	1	93	G
50	1	119	G
50	1	124	C
50	1	126	C
50	1	127	C
50	1	128	G
50	1	134	C
50	1	136	C
50	1	137	C
50	1	150	C
50	1	154	C
50	1	155	G
50	1	158	C
50	1	159	C
50	1	160	C
50	1	161	A
50	1	162	G
50	1	166	A
50	1	168	C
50	1	169	G
50	1	173	G
50	1	179	G
50	1	182	C
50	1	183	C
50	1	185	G
50	1	190	G
50	1	191	C
50	1	192	A
50	1	193	U
50	1	201	G
50	1	202	A
50	1	203	C
50	1	205	C
50	1	206	C

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Mol	Chain	Res	Type
50	1	207	U
50	1	208	A
50	1	209	A
50	1	210	G
50	1	216	A
50	1	220	A
50	1	221	A
50	1	224	C
50	1	234	G
50	1	236	C
50	1	242	U
50	1	243	U
50	1	244	G
50	1	257	G
50	1	258	C
50	1	260	U
50	1	261	G
50	1	265	G
50	1	266	C
50	1	267	U
50	1	268	G
50	1	269	G
50	1	272	A
50	1	273	G
50	1	276	C
50	1	277	U
50	1	278	A
50	1	281	U
50	1	282	C
50	1	283	A
50	1	285	A
50	1	290	C
50	1	291	C
50	1	292	G
50	1	306	G
50	1	308	U
50	1	333	C
50	1	334	U
50	1	339	C
50	1	346	C
50	1	347	C
50	1	349	C

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Mol	Chain	Res	Type
50	1	351	U
50	1	352	G
50	1	353	G
50	1	362	G
50	1	375	G
50	1	382	U
50	1	383	G
50	1	384	C
50	1	386	G
50	1	391	C
50	1	398	C
50	1	402	U
50	1	403	G
50	1	416	U
50	1	423	U
50	1	424	U
50	1	425	C
50	1	435	A
50	1	436	A
50	1	440	G
50	1	441	A
50	1	442	U
50	1	443	G
50	1	452	G
50	1	453	G
50	1	454	C
50	1	459	C
50	1	474	A
50	1	475	C
50	1	483	U
50	1	484	G
50	1	491	G
50	1	492	C
50	1	497	A
50	1	499	G
50	1	500	C
50	1	501	U
50	1	502	A
50	1	504	C
50	1	581	C
50	1	582	G
50	1	583	A

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Mol	Chain	Res	Type
50	1	584	U
50	1	585	A
50	1	586	G
50	1	589	A
50	1	591	C
50	1	594	G
50	1	596	U
50	1	609	A
50	1	610	G
50	1	612	C
50	1	613	A
50	1	614	U
50	1	621	G
50	1	624	U
50	1	627	A
50	1	638	A
50	1	646	C
50	1	647	U
50	1	650	G
50	1	652	A
50	1	653	U
50	1	654	A
50	1	655	A
50	1	656	G
50	1	659	A
50	1	660	U
50	1	664	A
50	1	678	A
50	1	679	A
50	1	680	U
50	1	684	U
50	1	685	C
50	1	686	A
50	1	687	U
50	1	688	U
50	1	689	A
50	1	690	A
50	1	692	U
50	1	693	C
50	1	697	U
50	1	700	C
50	1	701	G

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Mol	Chain	Res	Type
50	1	702	U
50	1	703	U
50	1	710	A
50	1	711	U
50	1	713	G
50	1	714	U
50	1	715	A
50	1	727	G
50	1	728	G
50	1	730	U
50	1	731	A
50	1	734	C
50	1	735	G
50	1	737	G
50	1	739	U
50	1	740	A
50	1	742	U
50	1	743	U
50	1	744	C
50	1	745	U
50	1	750	C
50	1	753	A
50	1	754	U
50	1	755	A
50	1	756	C
50	1	758	U
50	1	759	G
50	1	760	C
50	1	833	U
50	1	834	C
50	1	841	A
50	1	844	U
50	1	845	C
50	1	846	U
50	1	849	A
50	1	850	A
50	1	851	U
50	1	854	C
50	1	856	C
50	1	857	G
50	1	858	G
50	1	860	C

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Mol	Chain	Res	Type
50	1	861	U
50	1	862	U
50	1	863	G
50	1	864	C
50	1	865	G
50	1	869	G
50	1	871	G
50	1	883	A
50	1	886	U
50	1	889	C
50	1	892	C
50	1	893	C
50	1	897	U
50	1	898	C
50	1	904	U
50	1	905	C
50	1	906	G
50	1	907	A
50	1	910	G
50	1	913	G
50	1	921	G
50	1	922	C
50	1	927	C
50	1	930	G
50	1	931	G
50	1	935	C
50	1	936	A
50	1	943	A
50	1	944	A
50	1	984	A
50	1	985	A
50	1	986	C
50	1	987	G
50	1	988	G
50	1	989	C
50	1	991	A
50	1	998	C
50	1	1000	A
50	1	1001	A
50	1	1002	G
50	1	1005	A
50	1	1007	G

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Mol	Chain	Res	Type
50	1	1012	A
50	1	1020	A
50	1	1021	A
50	1	1023	U
50	1	1024	U
50	1	1025	A
50	1	1028	C
50	1	1029	A
50	1	1030	A
50	1	1031	U
50	1	1035	G
50	1	1036	A
50	1	1037	C
50	1	1038	A
50	1	1039	C
50	1	1043	G
50	1	1044	A
50	1	1048	A
50	1	1054	A
50	1	1059	A
50	1	1061	A
50	1	1064	G
50	1	1069	A
50	1	1070	G
50	1	1083	U
50	1	1084	C
50	1	1085	U
50	1	1086	U
50	1	1087	G
50	1	1088	U
50	1	1089	A
50	1	1094	G
50	1	1095	A
50	1	1097	U
50	1	1098	G
50	1	1102	A
50	1	1103	C
50	1	1104	A
50	1	1120	C
50	1	1122	A
50	1	1123	G
50	1	1124	G

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Mol	Chain	Res	Type
50	1	1125	A
50	1	1126	A
50	1	1127	C
50	1	1128	A
50	1	1129	A
50	1	1132	G
50	1	1141	G
50	1	1147	U
50	1	1148	G
50	1	1149	C
50	1	1154	A
50	1	1156	C
50	1	1158	G
50	1	1162	U
50	1	1163	A
50	1	1164	A
50	1	1166	U
50	1	1167	C
50	1	1168	C
50	1	1177	U
50	1	1178	A
50	1	1179	G
50	1	1186	U
50	1	1213	U
50	1	1219	A
50	1	1220	A
50	1	1221	C
50	1	1222	C
50	1	1223	U
50	1	1444	A
50	1	1445	U
50	1	1447	A
50	1	1448	A
50	1	1449	U
50	1	1450	A
50	1	1452	G
50	1	1458	U
50	1	1469	A
50	1	1481	U
50	1	1482	C
50	1	1483	A
50	1	1484	G

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Mol	Chain	Res	Type
50	1	1486	G
50	1	1487	G
50	1	1488	U
50	1	1491	A
50	1	1494	U
50	1	1497	U
50	1	1498	G
50	1	1499	G
50	1	1515	A
50	1	1517	A
50	1	1518	A
50	1	1519	C
50	1	1520	U
50	1	1525	A
50	1	1527	G
50	1	1529	A
50	1	1536	A
50	1	1545	U
50	1	1547	C
50	1	1549	U
50	1	1551	A
50	1	1552	A
50	1	1556	G
50	1	1624	A
50	1	1625	G
50	1	1630	C
50	1	1631	G
50	1	1637	C
50	1	1638	G
50	1	1639	U
50	1	1642	A
50	1	1643	U
50	1	1644	U
50	1	1645	U
50	1	1646	U
50	1	1656	C
50	1	1658	G
50	1	1659	C
50	1	1665	A
50	1	1666	C
50	1	1667	G
50	1	1668	A

Continued on next page...

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Mol	Chain	Res	Type
50	1	1670	A
50	1	1673	U
50	1	1674	C
50	1	1675	A
50	1	1676	A
50	1	1678	A
50	1	1679	U
50	1	1680	G
50	1	1681	U
50	1	1683	U
50	1	1684	G
50	1	1698	G
50	1	1699	U
50	1	1701	U
50	1	1735	A
50	1	1742	C
50	1	1744	A
50	1	1751	G
50	1	1758	C
50	1	2047	G
50	1	2049	G
50	1	2054	A
50	1	2056	U
50	1	2057	G
50	1	2061	G
50	1	2068	C
50	1	2072	U
50	1	2073	A
50	1	2074	C
50	1	2075	U
50	1	2077	C
50	1	2078	C
50	1	2085	G
50	1	2086	A
50	1	2087	G
50	1	2088	A
50	1	2094	G
50	1	2107	A
50	1	2109	A
50	1	2114	G
50	1	2115	U
50	1	2118	U

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Mol	Chain	Res	Type
50	1	2119	G
50	1	2120	C
50	1	2121	U
50	1	2156	A
50	1	2157	G
50	1	2166	A
50	1	2167	G
50	1	2173	G
50	1	2177	G
50	1	2178	U
50	1	2183	A
50	1	2184	G
50	1	2185	C
50	1	2190	G
50	1	2197	A
50	1	2201	C
50	1	2202	C
50	1	2205	G
50	1	2210	U
50	1	2211	U
50	1	2212	G
50	1	2213	U
50	1	2214	A
50	1	2215	C
50	1	2216	A
50	1	2218	A
50	1	2220	C
50	1	2221	G
50	1	2222	C
50	1	2223	C
50	1	2228	G
50	1	2230	U
50	1	2235	C
50	1	2236	C
50	1	2329	A
50	1	2330	G
51	2	5	A
51	2	6	C
51	2	7	A
51	2	15	A
51	2	23	A
51	2	24	U

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Mol	Chain	Res	Type
51	2	25	U
51	2	28	U
51	2	29	A
51	2	30	U
51	2	31	A
51	2	33	U
51	2	36	U
51	2	37	U
51	2	39	U
51	2	48	G
51	2	57	A
51	2	58	A
51	2	62	A
51	2	63	G
51	2	90	C
51	2	91	G
51	2	92	A
51	2	94	A
51	2	95	U
51	2	100	G
51	2	101	G
51	2	104	C
51	2	111	G
51	2	118	C
51	2	124	U
51	2	125	U
51	2	126	U
51	2	127	A
51	2	128	C
51	2	133	G
51	2	136	C
51	2	142	G
51	2	145	A
51	2	147	G
51	2	151	G
51	2	153	G
51	2	160	U
51	2	162	C
51	2	163	C
51	2	164	U
51	2	165	C
51	2	166	G

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Mol	Chain	Res	Type
51	2	167	U
51	2	168	C
51	2	170	C
51	2	178	U
51	2	179	A
51	2	181	A
51	2	187	U
51	2	189	G
51	2	190	C
51	2	192	A
51	2	194	G
51	2	198	U
51	2	199	G
51	2	200	U
51	2	201	A
51	2	244	G
51	2	246	G
51	2	247	G
51	2	249	U
51	2	250	G
51	2	253	G
51	2	254	A
51	2	255	U
51	2	256	G
51	2	259	A
51	2	260	G
51	2	261	U
51	2	262	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	1	34	C
50	1	88	C
50	1	89	G
50	1	135	A
50	1	205	C
50	1	209	A
50	1	277	U
50	1	281	U
50	1	424	U
50	1	582	G

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Mol	Chain	Res	Type
50	1	585	A
50	1	593	G
50	1	612	C
50	1	684	U
50	1	742	U
50	1	1001	A
50	1	1068	C
50	1	1085	U
50	1	1087	G
50	1	1128	A
50	1	1163	A
50	1	1481	U
50	1	1485	A
50	1	1638	G
50	1	1734	G
50	1	2156	A
50	1	2177	G
51	2	6	C
51	2	23	A
51	2	35	G
51	2	246	G
51	2	255	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

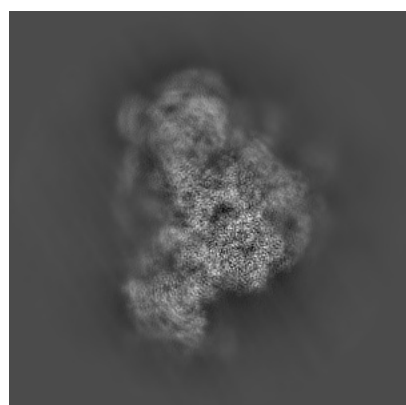
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3847. These allow visual inspection of the internal detail of the map and identification of artifacts.

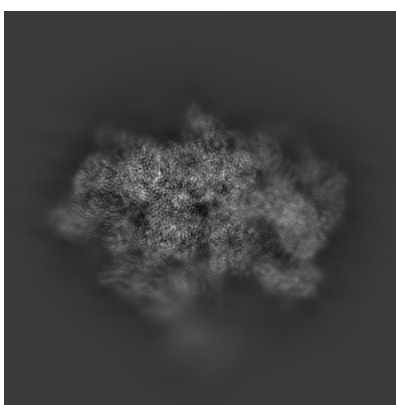
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

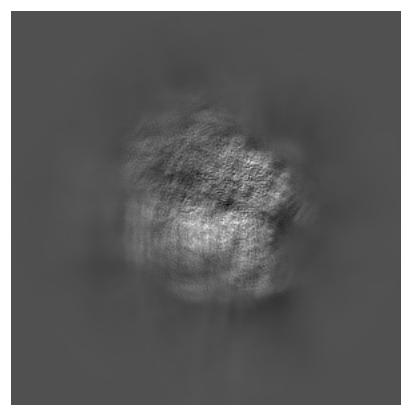
6.1.1 Primary map



X



Y

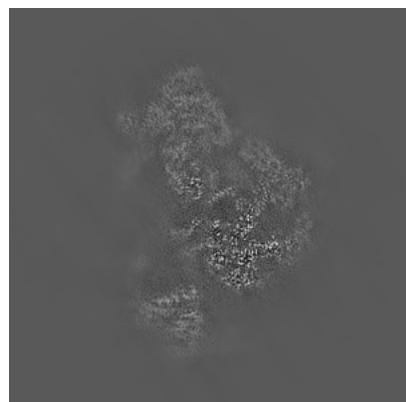


Z

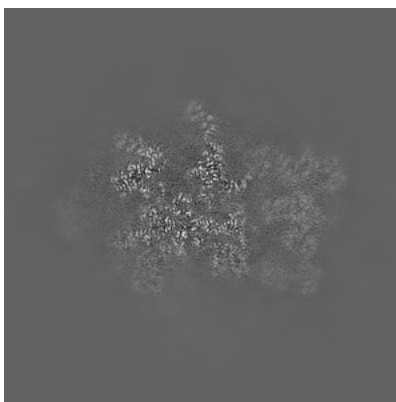
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

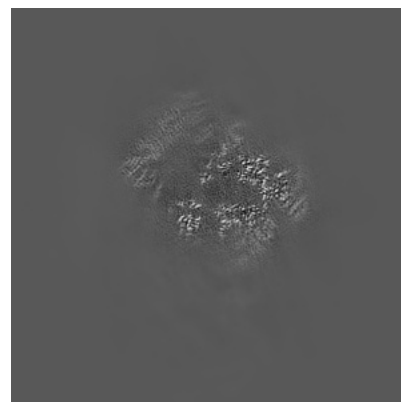
6.2.1 Primary map



X Index: 240



Y Index: 240

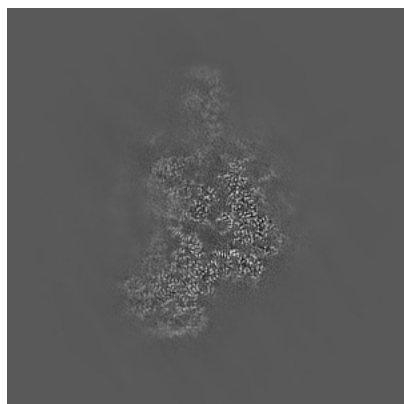


Z Index: 240

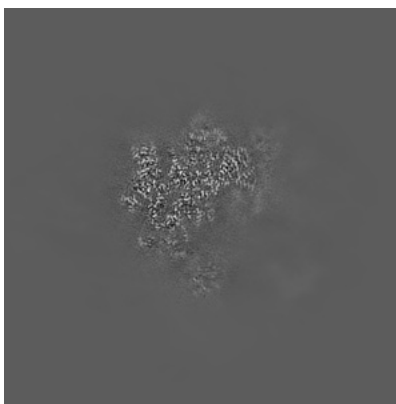
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

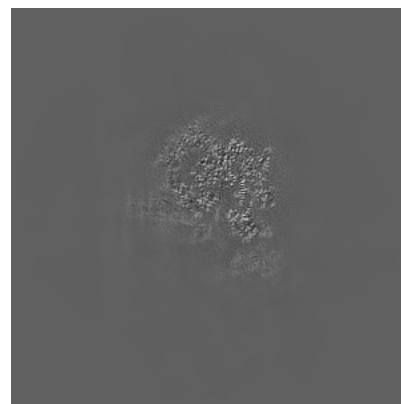
6.3.1 Primary map



X Index: 279



Y Index: 281

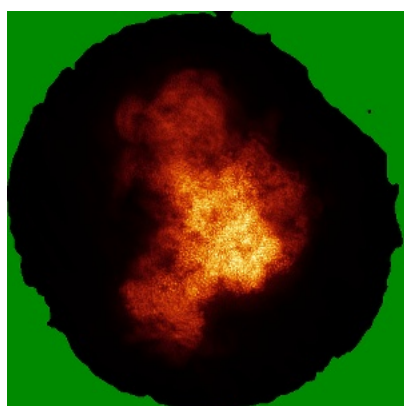


Z Index: 183

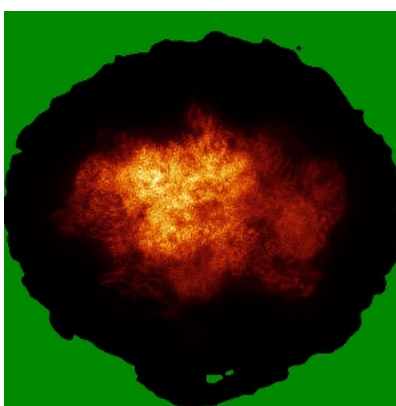
The images above show the largest variance slices of the map in three orthogonal directions.

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

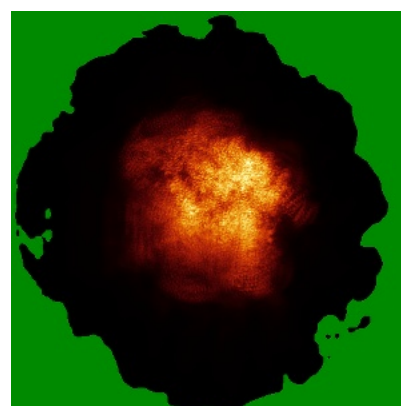
6.4.1 Primary map



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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

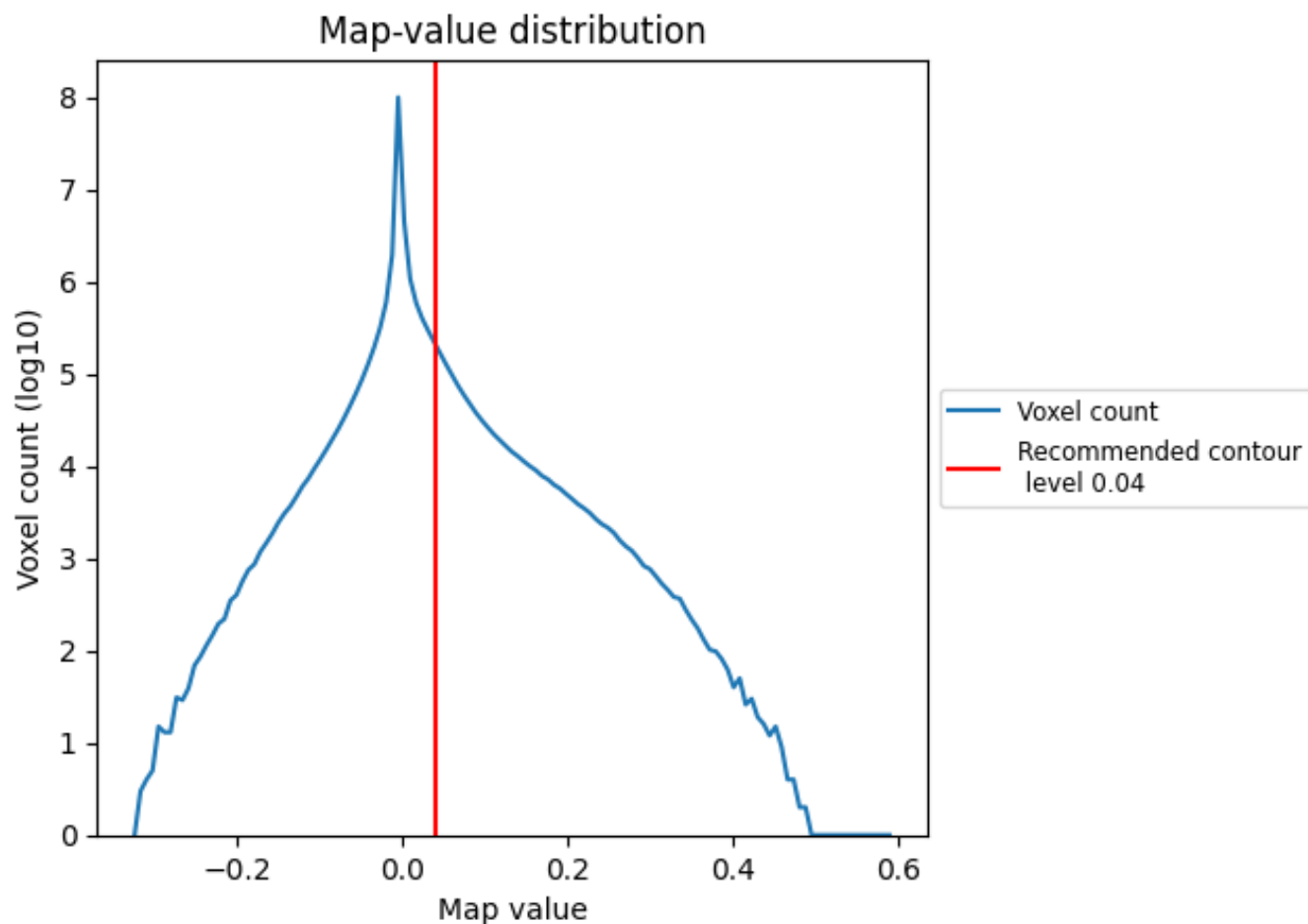
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

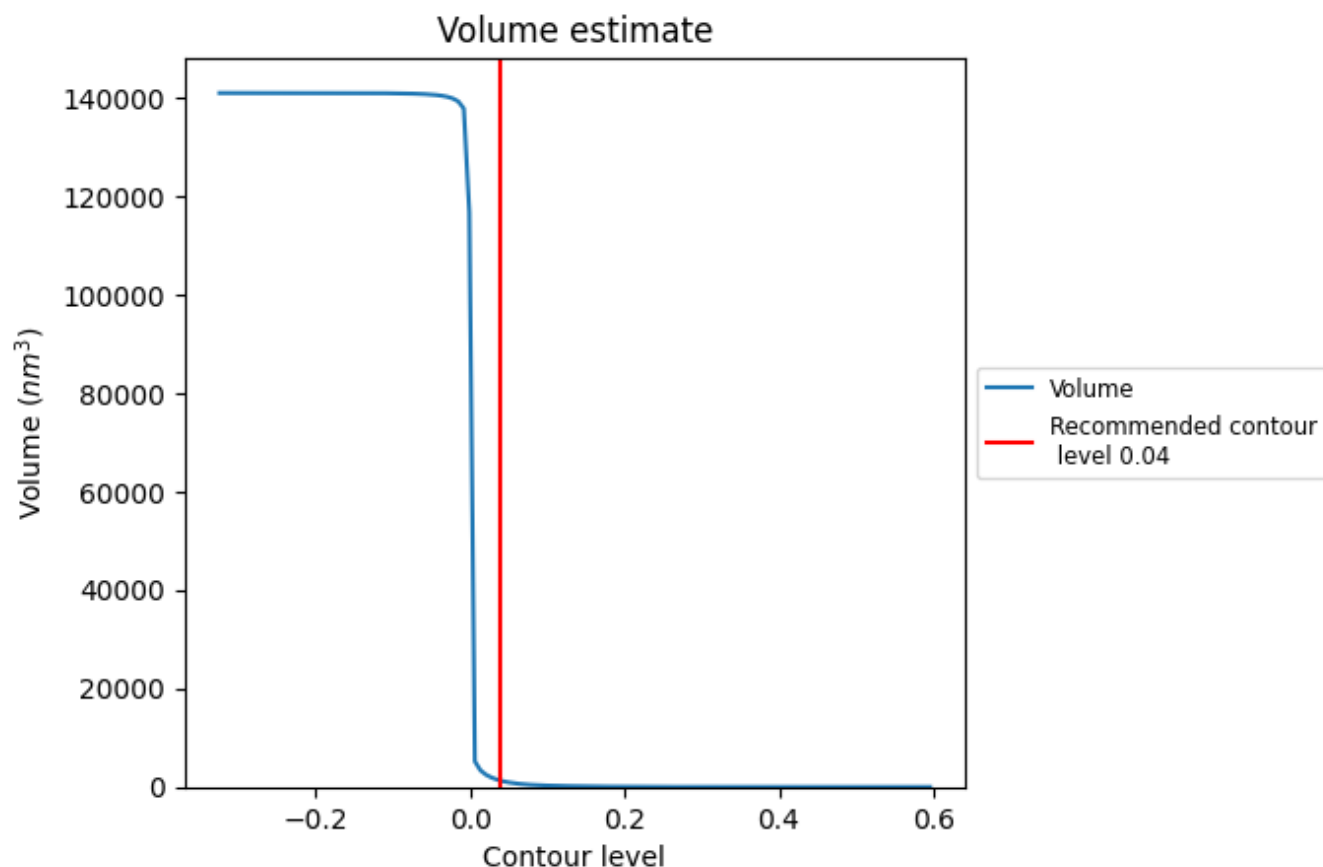
This section contains the results of statistical analysis of the map.

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.

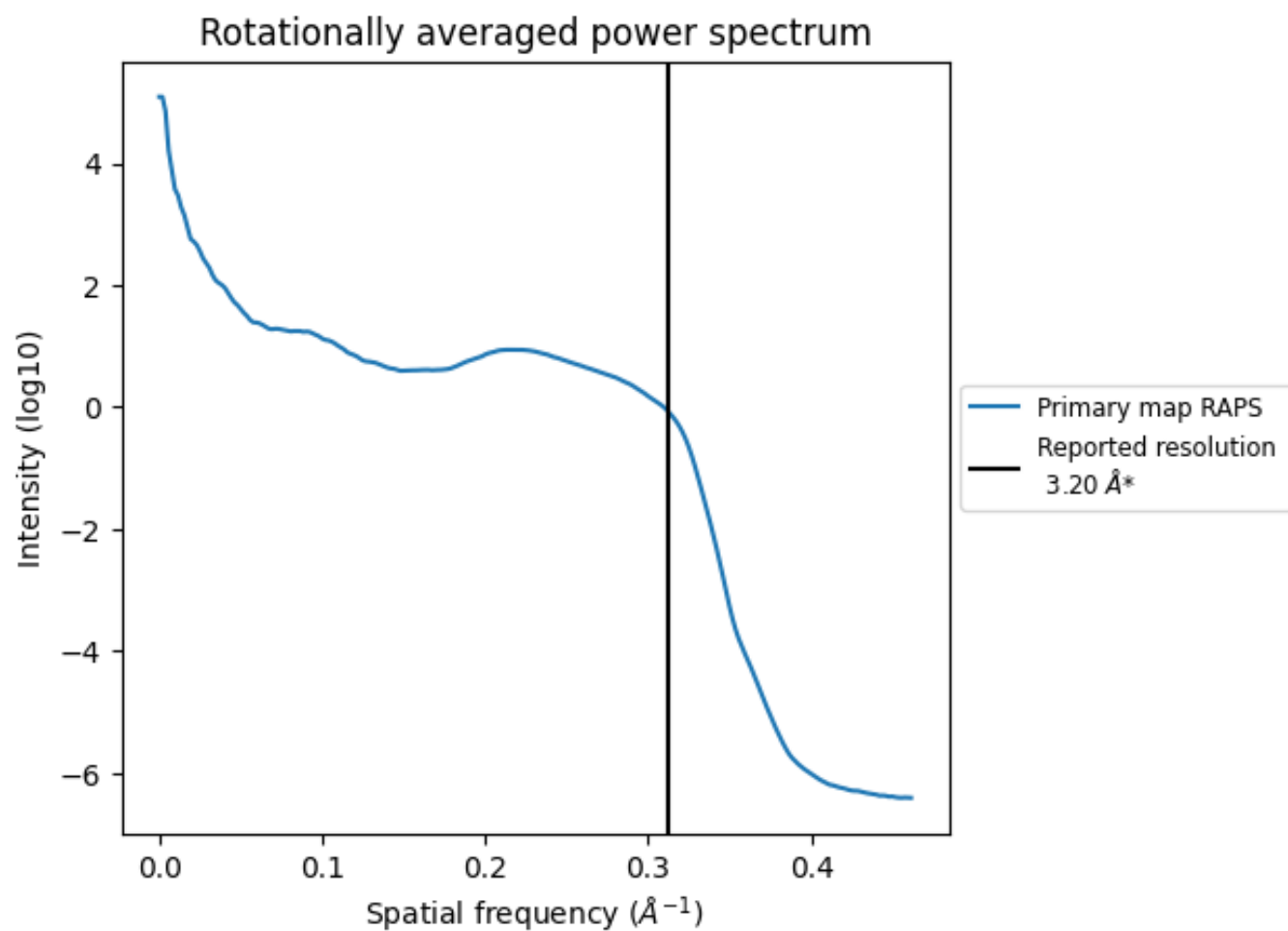
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1269 nm^3 ; this corresponds to an approximate mass of 1146 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 ⓘ

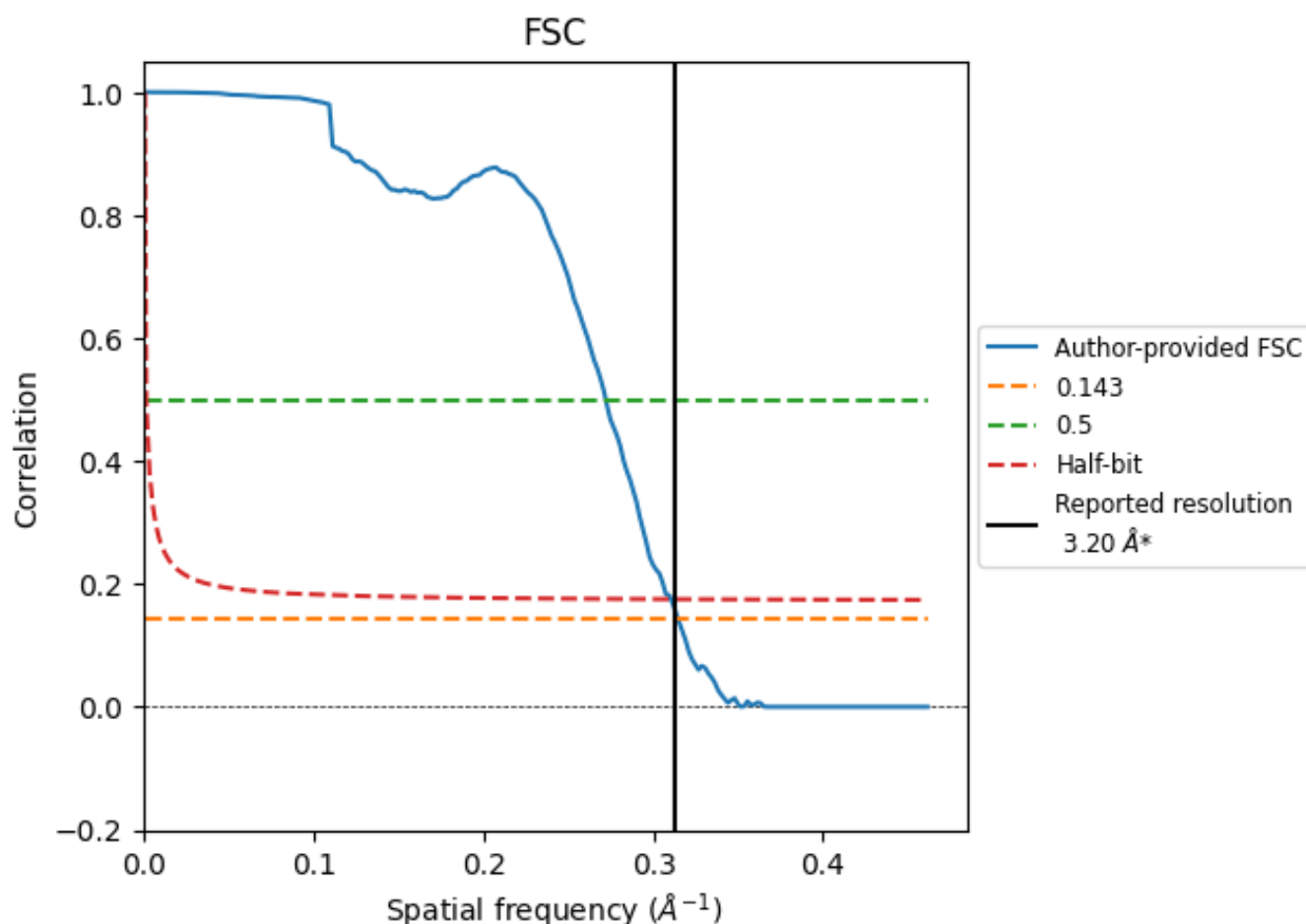


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

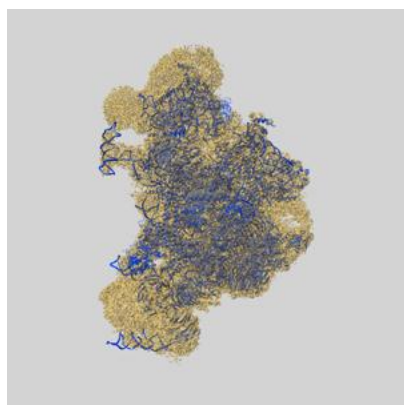
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.68	3.22
Unmasked-calculated*	-	-	-

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

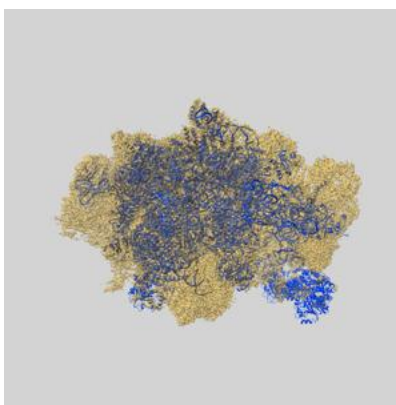
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3847 and PDB model 5OQL. Per-residue inclusion information can be found in section 3 on page 14.

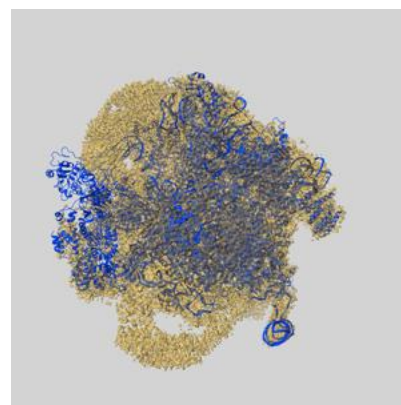
9.1 Map-model overlay [i](#)



X



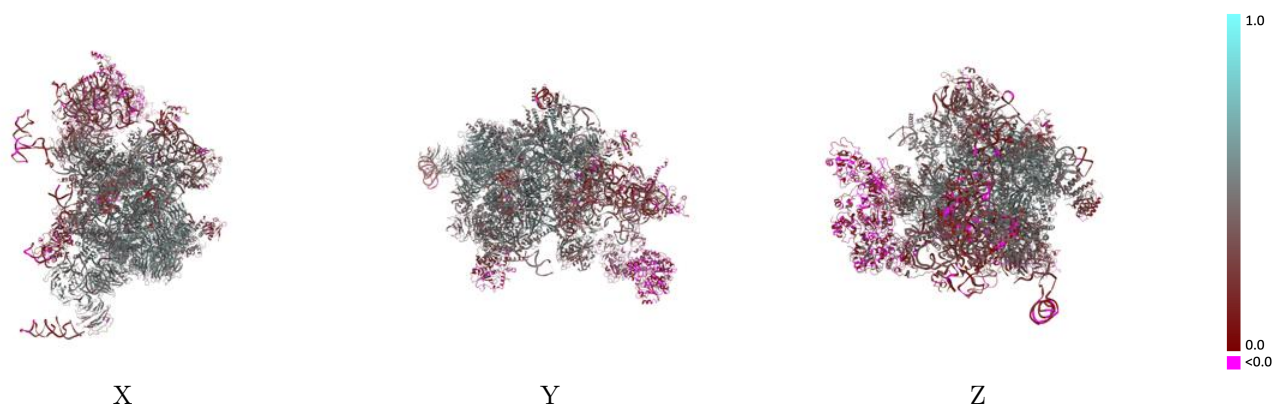
Y



Z

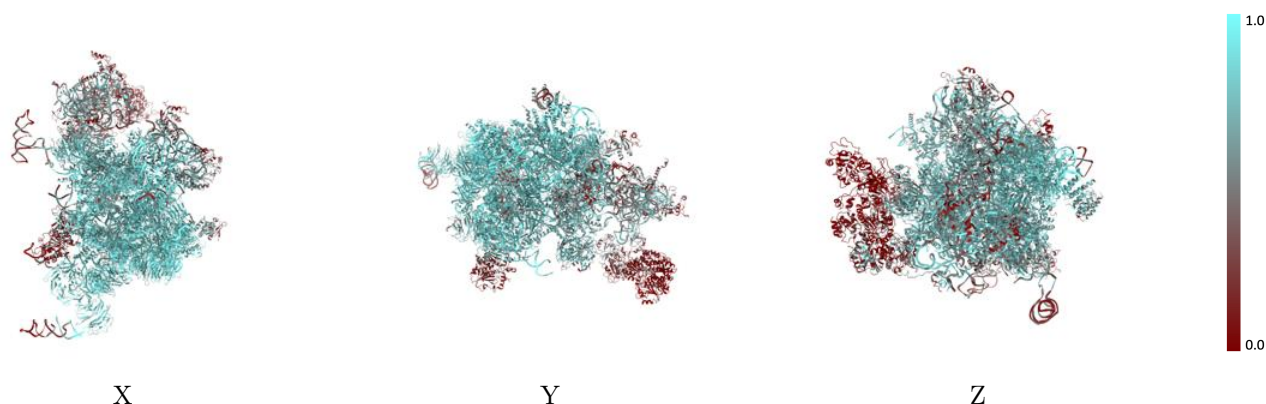
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



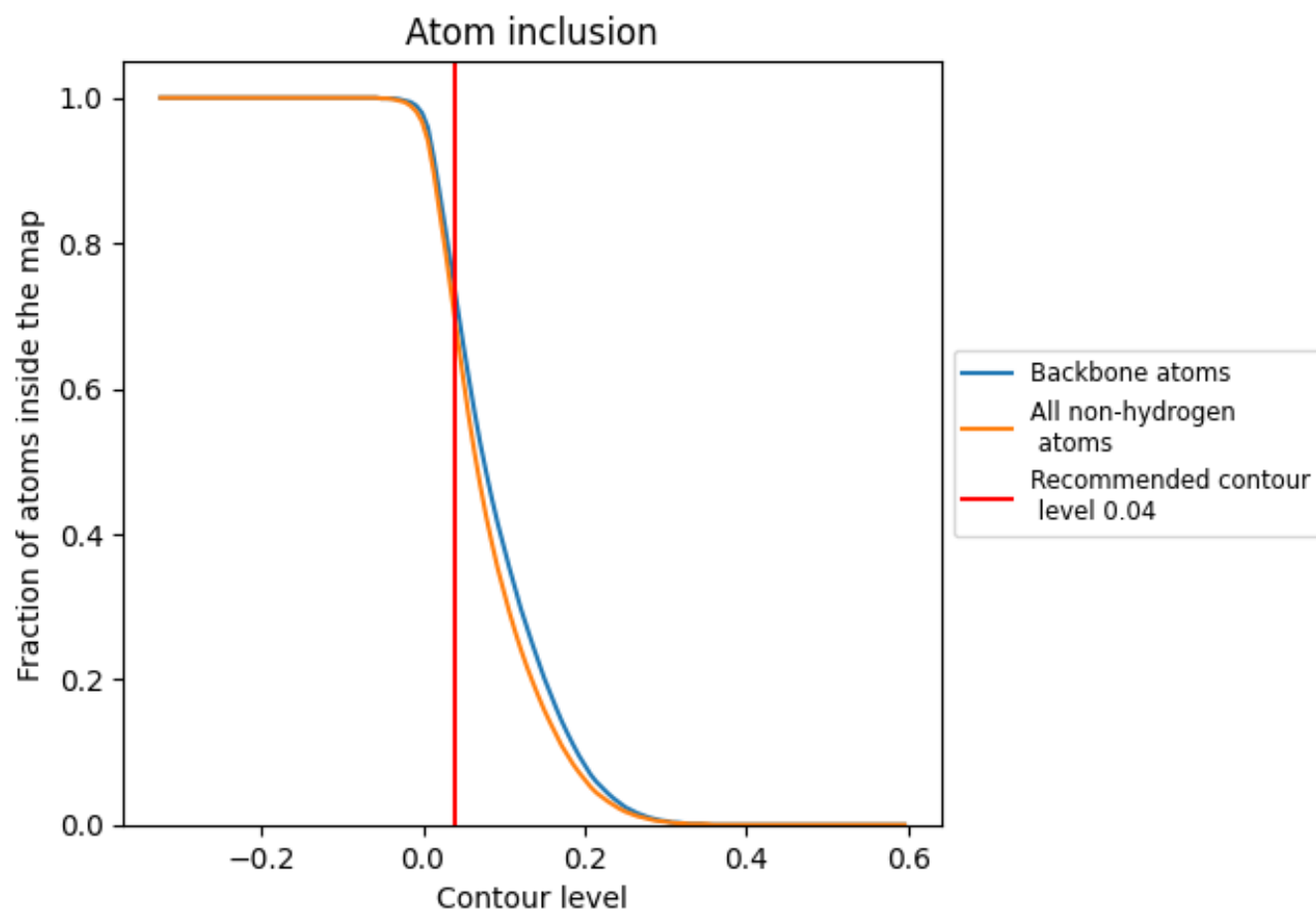
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.3820
0	 0.7120	 0.4640
1	 0.7330	 0.3550
2	 0.7240	 0.3600
A	 0.8650	 0.4950
B	 0.7520	 0.4400
C	 0.8250	 0.4940
D	 0.8140	 0.4580
E	 0.7670	 0.3920
F	 0.8920	 0.5210
G	 0.8690	 0.4970
H	 0.8380	 0.4990
I	 0.6940	 0.3900
J	 0.7810	 0.4010
K	 0.8400	 0.4800
L	 0.6570	 0.3730
M	 0.8070	 0.4230
N	 0.8740	 0.5100
O	 0.8820	 0.5000
P	 0.8120	 0.4790
Q	 0.6090	 0.3400
R	 0.8710	 0.5060
S	 0.2730	 0.2150
T	 0.7630	 0.4080
U	 0.5740	 0.3530
V	 0.8010	 0.4560
W	 0.6850	 0.3740
X	 0.6950	 0.3800
Y	 0.6760	 0.3870
Z	 0.8120	 0.4610
a	 0.8960	 0.5260
b	 0.8090	 0.4820
c	 0.7780	 0.4460
d	 0.8740	 0.5080
e	 0.3280	 0.2480



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Chain	Atom inclusion	Q-score
f	 0.0890	 0.0800
g	 0.5350	 0.3700
h	 0.4820	 0.2610
i	 0.2140	 0.1550
j	 0.0390	 0.0820
k	 0.8280	 0.4800
l	 0.4560	 0.2900
m	 0.4330	 0.2260
n	 0.8200	 0.4630
o	 0.4030	 0.1770
p	 0.4310	 0.2430
q	 0.3830	 0.1720
r	 0.8210	 0.4630
s	 0.4440	 0.2070
t	 0.5710	 0.3280
u	 0.8700	 0.5000
v	 0.3860	 0.1660
w	 0.7540	 0.4290
x	 0.8430	 0.4850
y	 0.4620	 0.2300
z	 0.7820	 0.4430