



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 06:45 PM UTC

PDB ID : 6RXT / pdb_00006rxt
EMDB ID : EMD-10051
Title : Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from *Chaetomium thermophilum*, state A
Authors : Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on : 2019-06-10
Resolution : 7.00 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

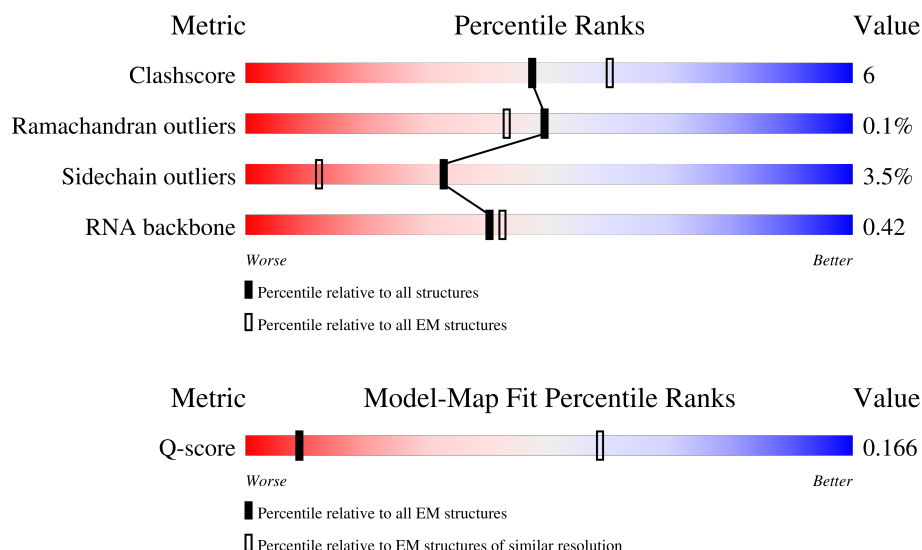
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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	483 (6.50 - 7.50)

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	UA	904	
2	UB	907	
3	UC	648	

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Mol	Chain	Length	Quality of chain
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	
9	UL	962	
10	UM	912	
11	UN	938	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	
26	CK	297	

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Mol	Chain	Length	Quality of chain
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Ca	255	
35	Cc	212	
36	Ce	203	
37	Cg	190	
38	Ch	151	
39	Ci	150	
40	Cj	143	
41	Cm	130	
42	Cn	145	
43	Cp	68	
44	CU	311	
45	C1	2352	
46	C2	230	
47	UH	930	
48	UE	410	
48	UI	410	

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Mol	Chain	Length	Quality of chain
49	US	549	
50	CI	156	
51	CX	480	
52	UP	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	GTP	CI	1201	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 169690 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	UA	839	Total	C	N	O	S	0	0
			6366	4101	1136	1105	24		

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	512	Total	C	N	O	S	0	0
			4079	2576	781	711	11		

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	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	UD	772	Total	C	N	O	S	0	0
			6071	3851	1093	1103	24		

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UF	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	UG	479	Total	C	N	O	S	0	0
			3717	2369	700	636	12		

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UJ	445	Total	C	N	O	S	0	0
			3377	2169	604	590	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UK	217	Total	C	N	O	S	0	0
			1687	1062	351	269	5		

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UL	785	Total	C	N	O	S	0	0
			6175	3940	1088	1130	17		

- Molecule 10 is a protein called Utp13".

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UM	729	Total	C	N	O	S	0	0
			5643	3590	995	1045	13		

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UN	154	Total	C	N	O	S	0	0
			1209	770	228	206	5		

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UO	504	Total	C	N	O	S	0	0
			3819	2422	699	684	14		

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UQ	789	Total	C	N	O	S	0	0
			6008	3831	1037	1119	21		

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UR	447	Total	C	N	O	S	0	0
			3491	2209	656	616	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UU	902	Total	C	N	O	S	0	0
			6734	4336	1236	1136	26		

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UX	190	Total	C	N	O	S	0	0
			1470	932	282	246	10		

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UZ	235	Total	C	N	O	S	0	0
			1815	1184	330	298	3		

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CA	242	Total	C	N	O	S	0	0
			1778	1149	327	293	9		
18	CB	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	CC	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	CD	420	Total	C	N	O	S	0	0
			3150	2023	560	557	10		

- Molecule 21 is a protein called snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	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	CG	378	Total	C	N	O	S	0	0
			2922	1865	527	517	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total	C	N	O	S	0	0
			6486	4169	1213	1077	27		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	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	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CM	445	Total	C	N	O	S	0	0
			3501	2195	672	619	15		

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CN	226	Total	C	N	O	S	0	0
			1762	1119	306	327	10		
29	CO	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	CP	201	Total	C	N	O	S	0	0
			1625	1047	286	283	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CQ	175	Total	C	N	O	S	0	0
			1361	862	250	242	7		

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CR	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		
32	CS	760	Total	C	N	O	S	0	0
			5989	3851	1024	1087	27		

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CT	131	Total	C	N	O	S	0	0
			1035	656	197	178	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ca	225	Total	C	N	O	S	0	0
			1821	1160	341	315	5		

- Molecule 35 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cc	192	Total	C	N	O	S	0	0
			1464	926	278	253	7		

- Molecule 36 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ce	159	Total	C	N	O		0	0
			1279	810	237	232			

- Molecule 37 is a protein called 40S ribosomal protein s9-like protein.

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

- Molecule 38 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ch	66	Total	C	N	O		0	0
			546	355	101	90			

- Molecule 39 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

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

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

- Molecule 41 is a protein called 40S ribosomal protein S22-like protein.

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

- Molecule 42 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

- Molecule 43 is a protein called 40S ribosomal protein S28-like protein.

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

- Molecule 44 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 45 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	C1	1152	Total	C	N	O	P	0	0
			24590	10964	4415	8059	1152		

- Molecule 46 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	C2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

- Molecule 47 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	UH	359	Total	C	N	O	S	0	0
			2809	1773	496	527	13		

- Molecule 48 is a protein called Utp5".

Mol	Chain	Residues	Atoms					AltConf	Trace
48	UE	125	Total	C	N	O	S	0	0
			972	608	183	175	6		
48	UI	125	Total	C	N	O	S	0	0
			972	608	183	175	6		

- Molecule 49 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 50 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 51 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	CX	267	Total	C	N	O	S	0	0
			2130	1384	374	362	10		

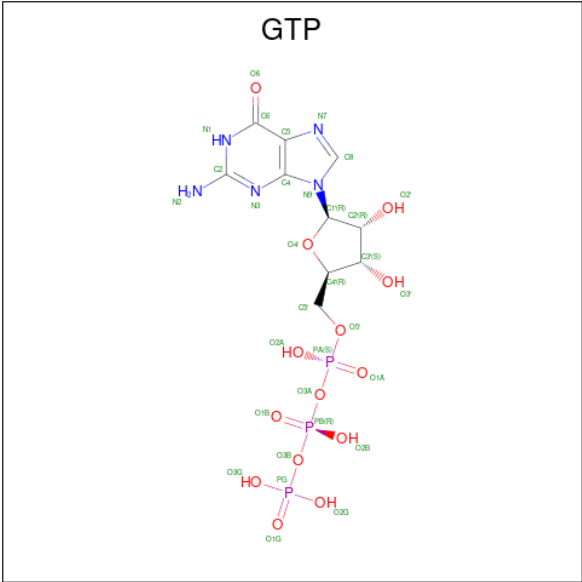
- Molecule 52 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	UP	54	Total	C	N	O	0	0
			422	264	88	70		

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	UX	1	Total	Zn	0
			1	1	

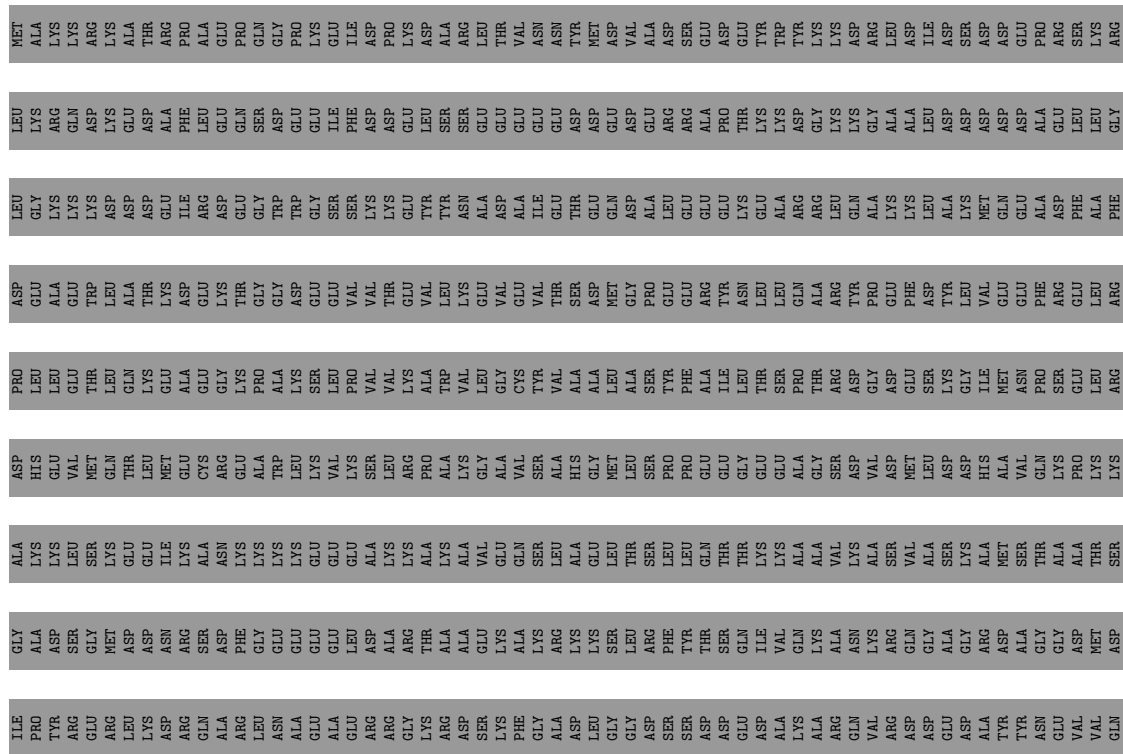
- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

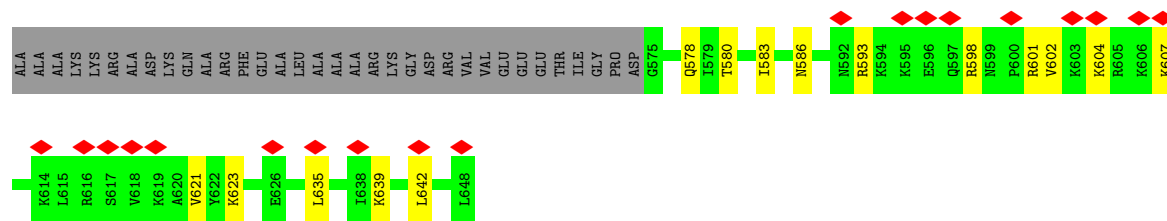


Mol	Chain	Residues	Atoms					AltConf
54	CI	1	Total	C	N	O	P	0
			32	10	5	14	3	

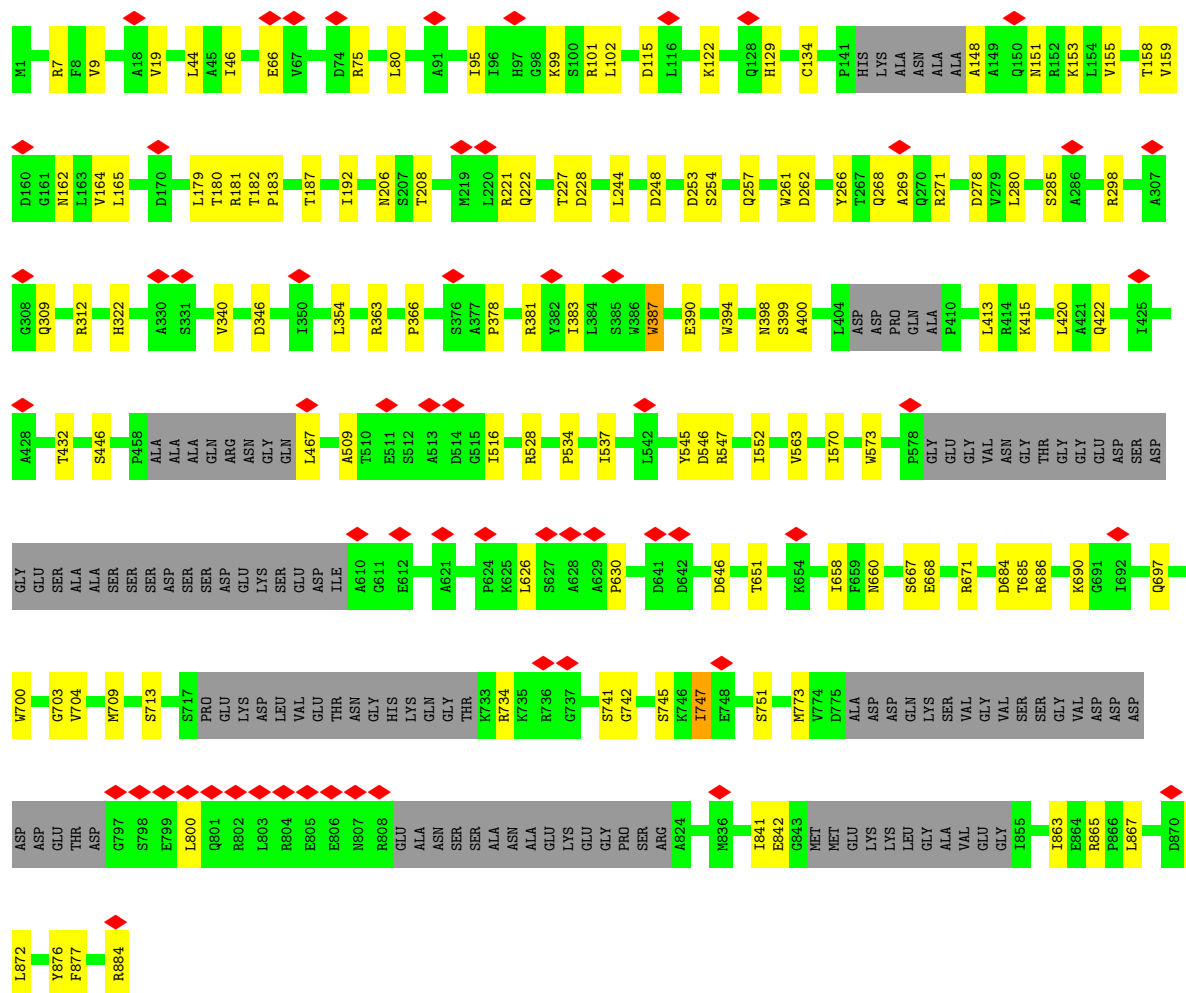
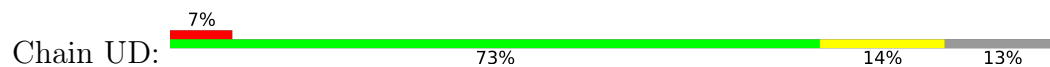
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	CI	1	Total	Mg	0
			1	1	

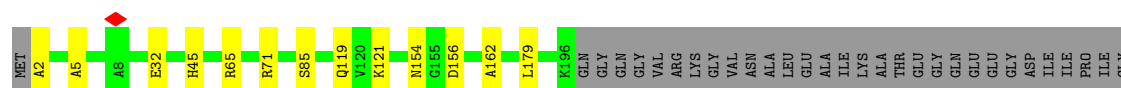
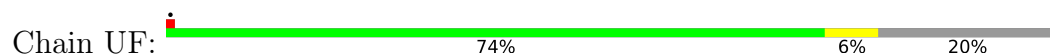


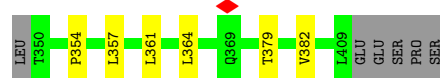
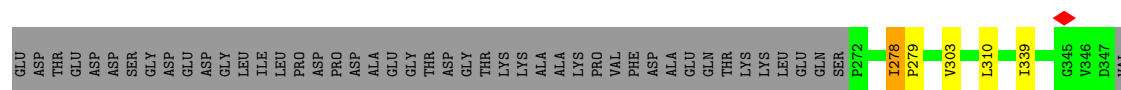


• Molecule 4: Utp4

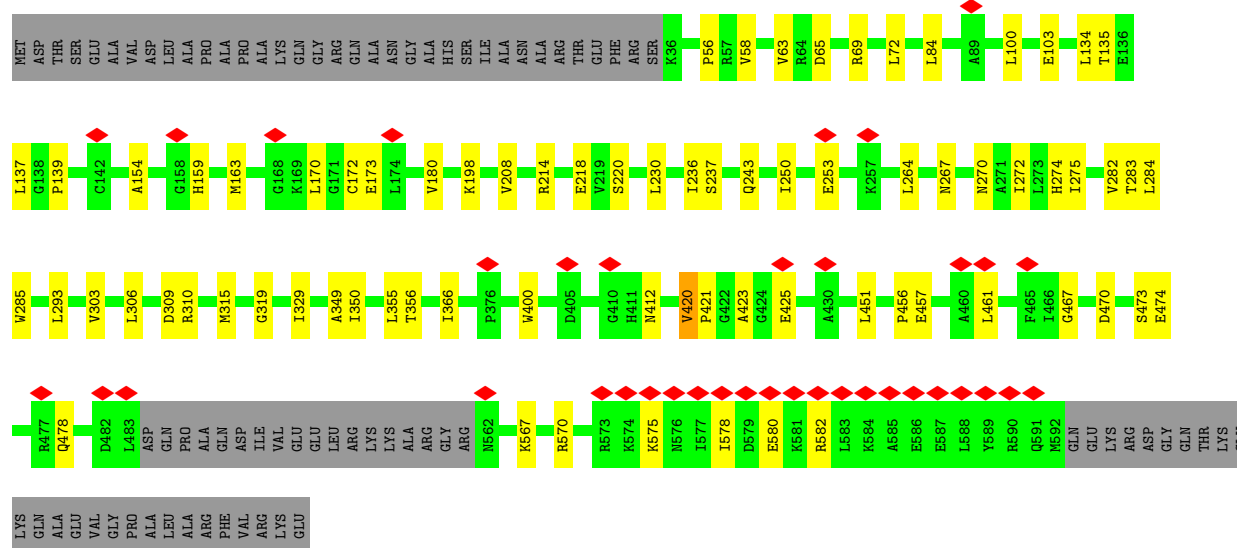
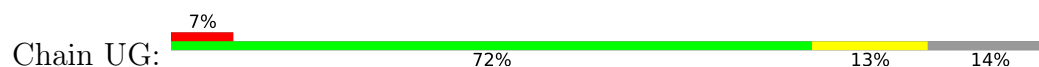


• Molecule 5: Utp6

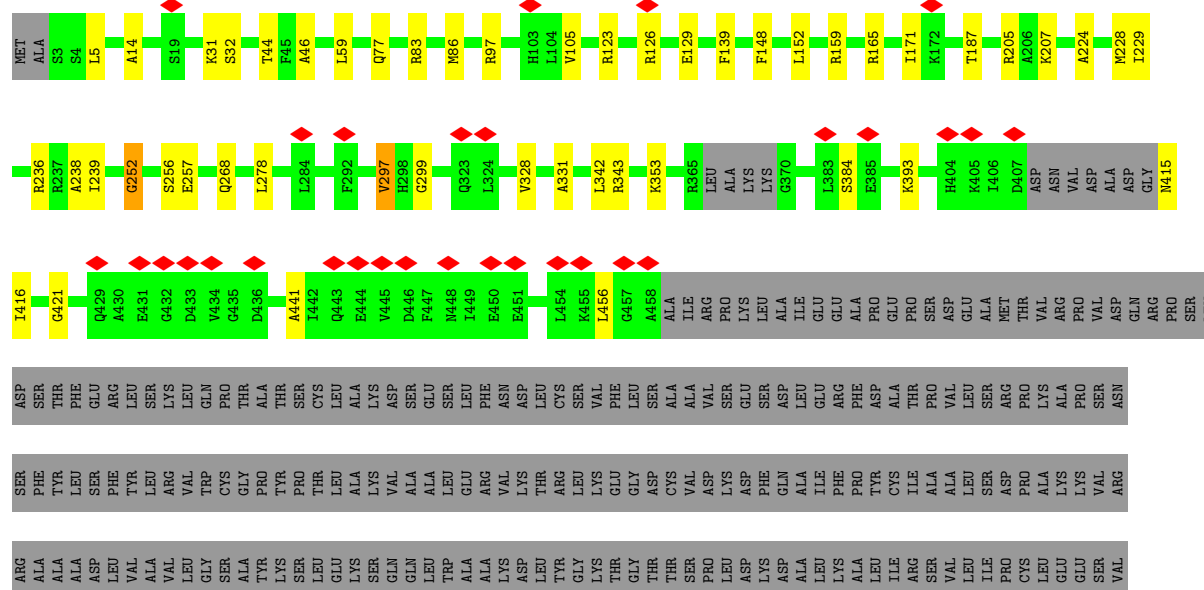




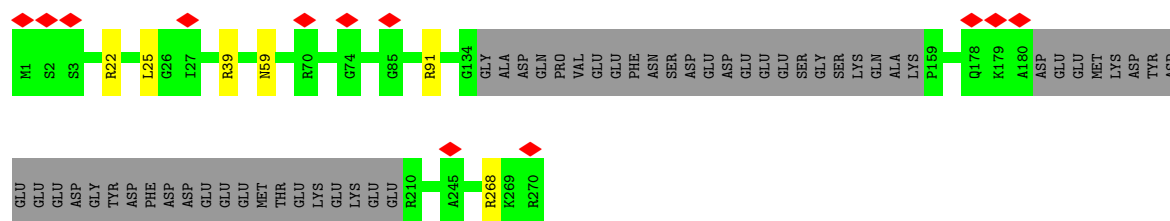
• Molecule 6: Utp7



• Molecule 7: UTP10

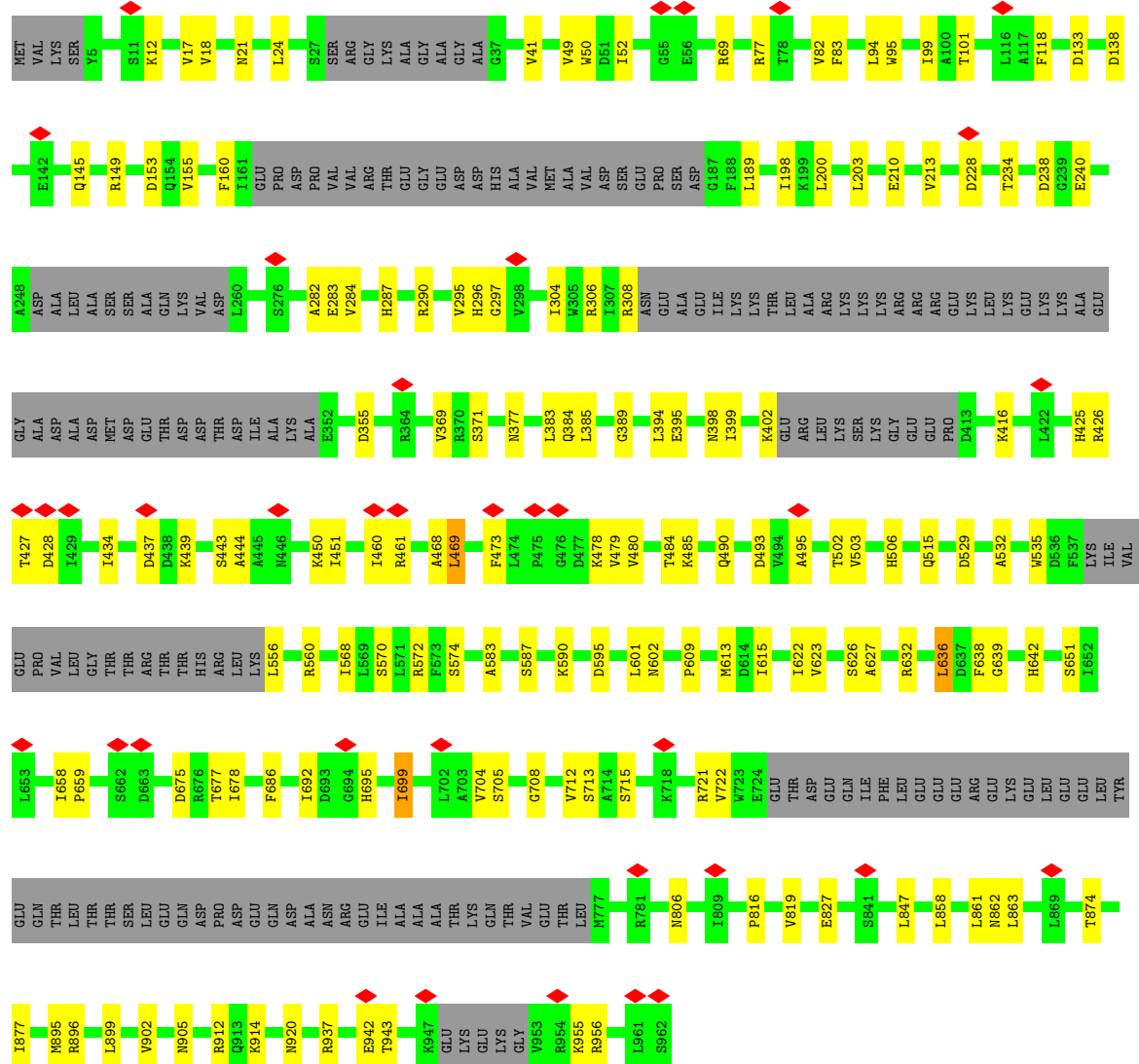






• Molecule 9: Utp12

Chain UL: 65% 16% 18%



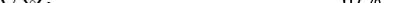
• Molecule 10: Utp13"

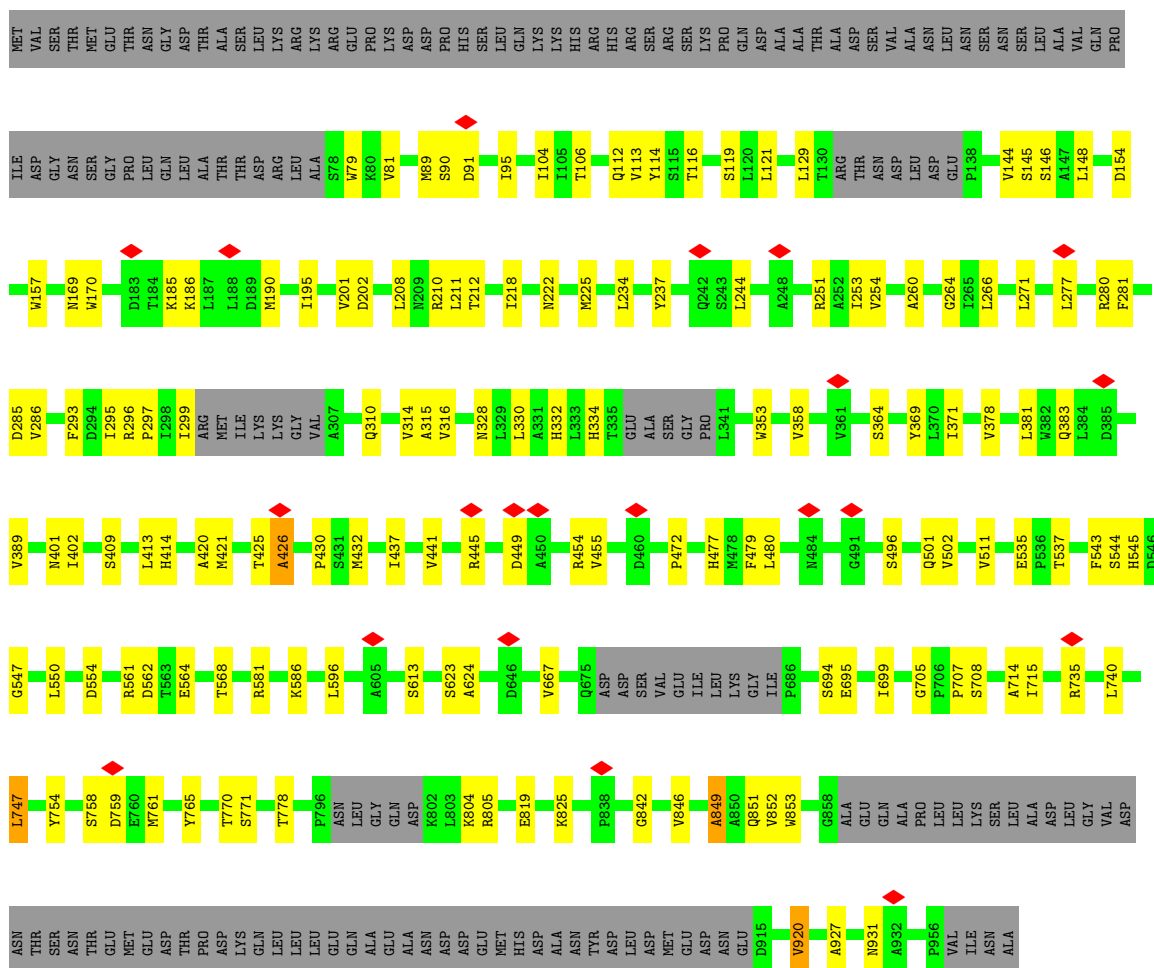
Chain UM: 18% 62% 17% 20%



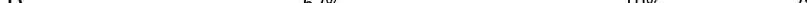


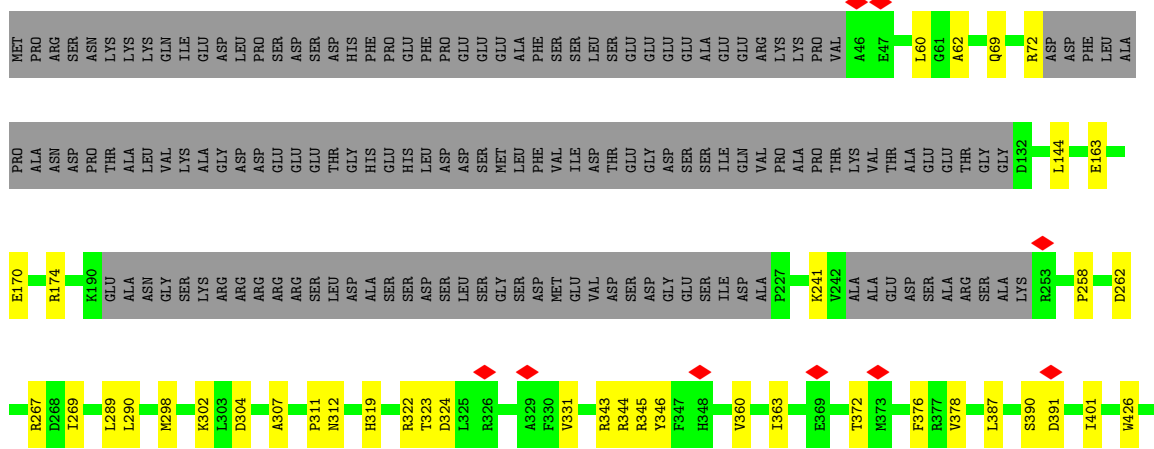
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ASP	ALA	ASP	PRO
ASP	ASP	LEU	LEU
ILE	GLY	ASP	ARG
LEU	ASP	HIS	ALA
LEU	ASP	PRO	HIS
ALA	SER	SER	GLY
THR	GLU	THR	ARG
ALA	GLU	SER	PRO
LEU	TRP	ALA	LEU
ASP	HIS	SER	LEU
GLN	VAL	ARG	PRO
TYR	GLY	ASN	SER
GLU	VAL	LYS	LEU
SER	THR	ARG	GLY
SER	GLY	GLN	SER
GLU	ALA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

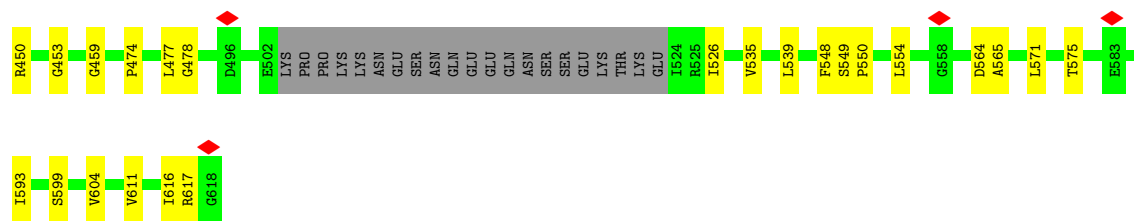
Chain UQ:  67% 15% 18%



- Molecule 14: Utp18

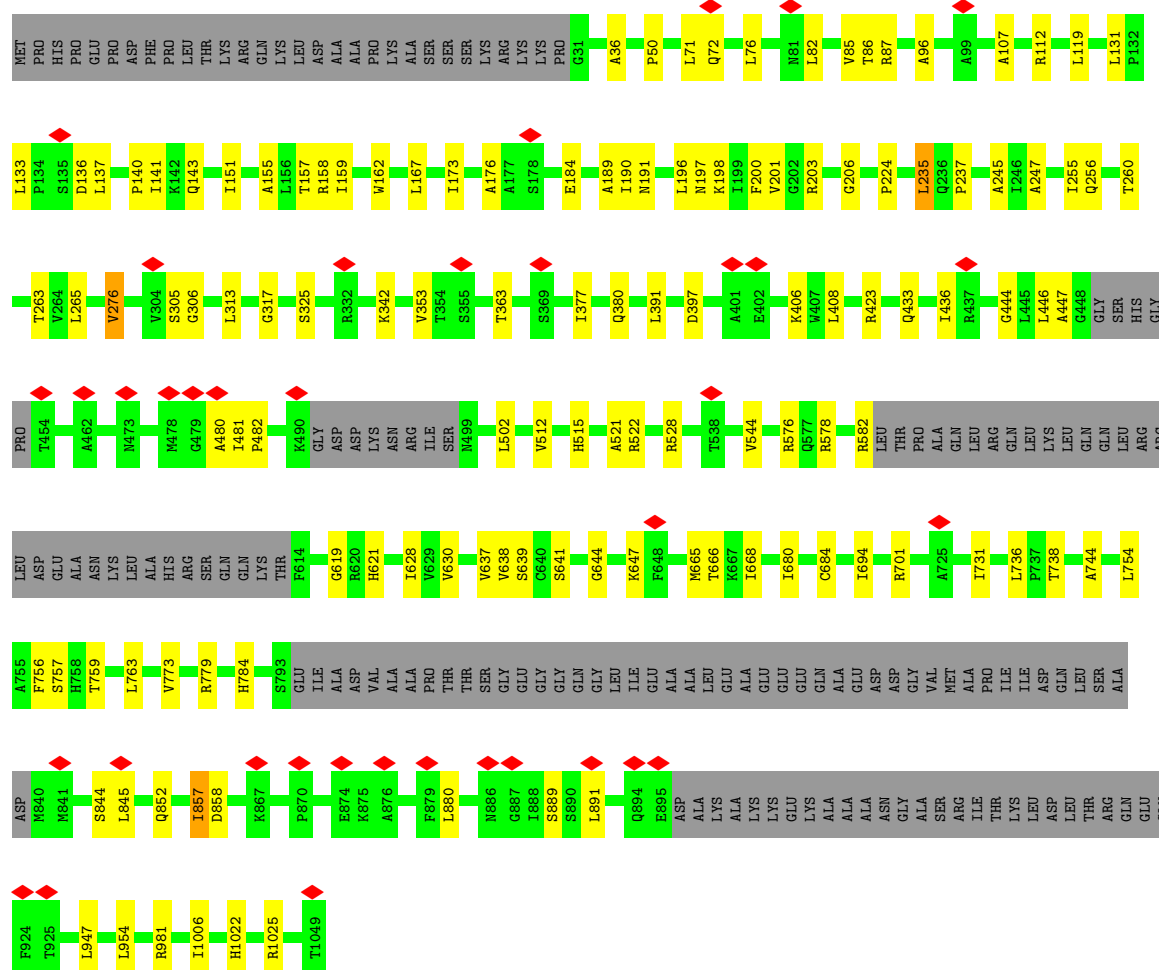
Chain UR: 





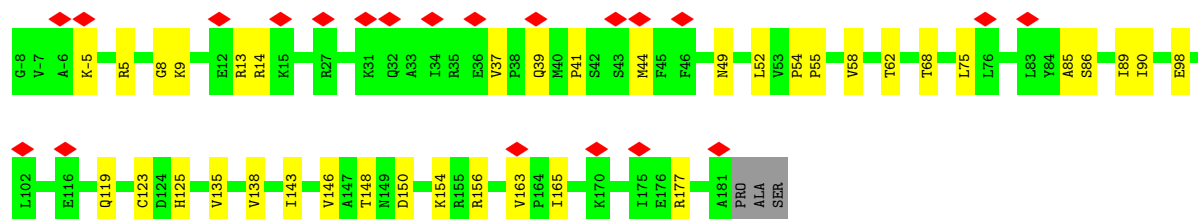
• Molecule 15: Putative U3 snoRNP protein

Chain UU: 74% 12% 14%



• Molecule 16: Utp24

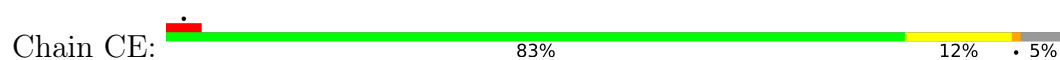
Chain UX: 11% 79% 19%

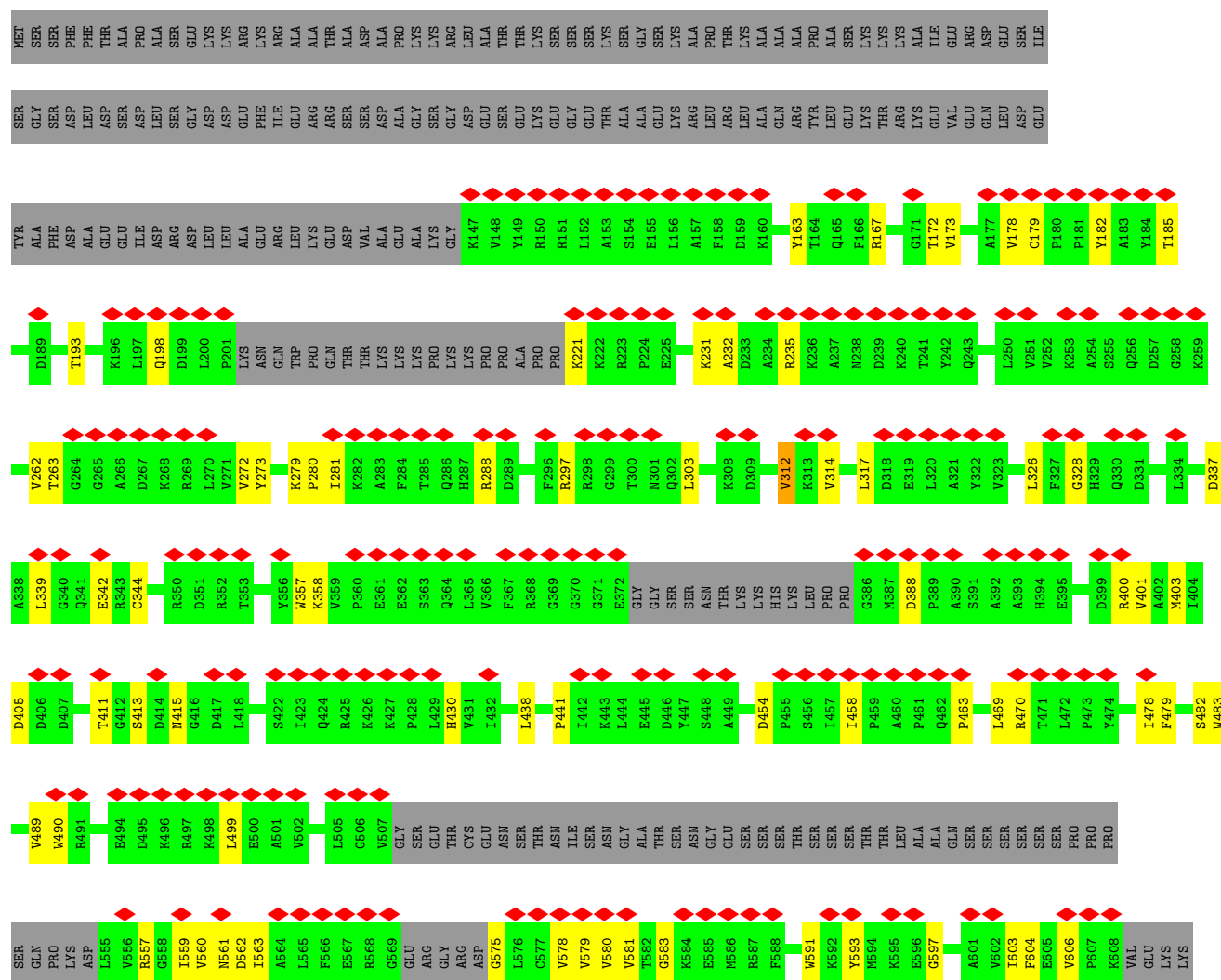


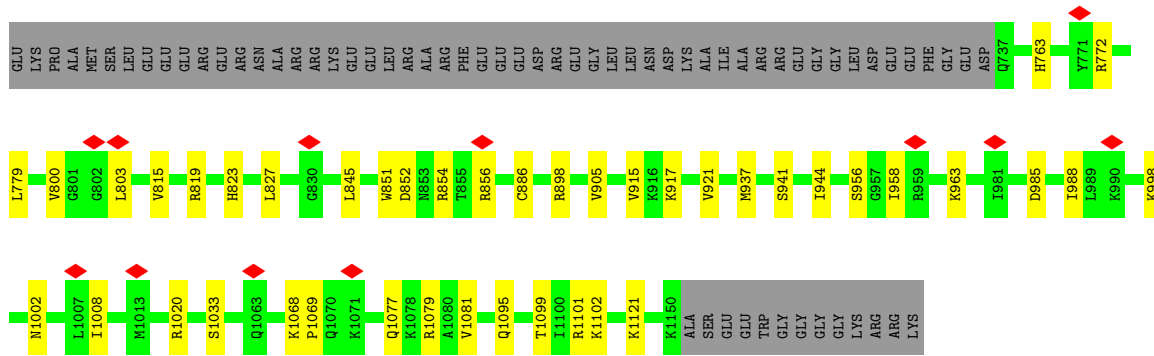
Chain UZ:



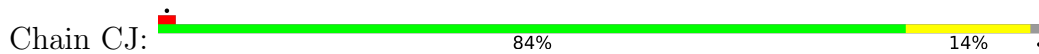
Chain CC:



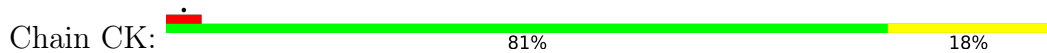




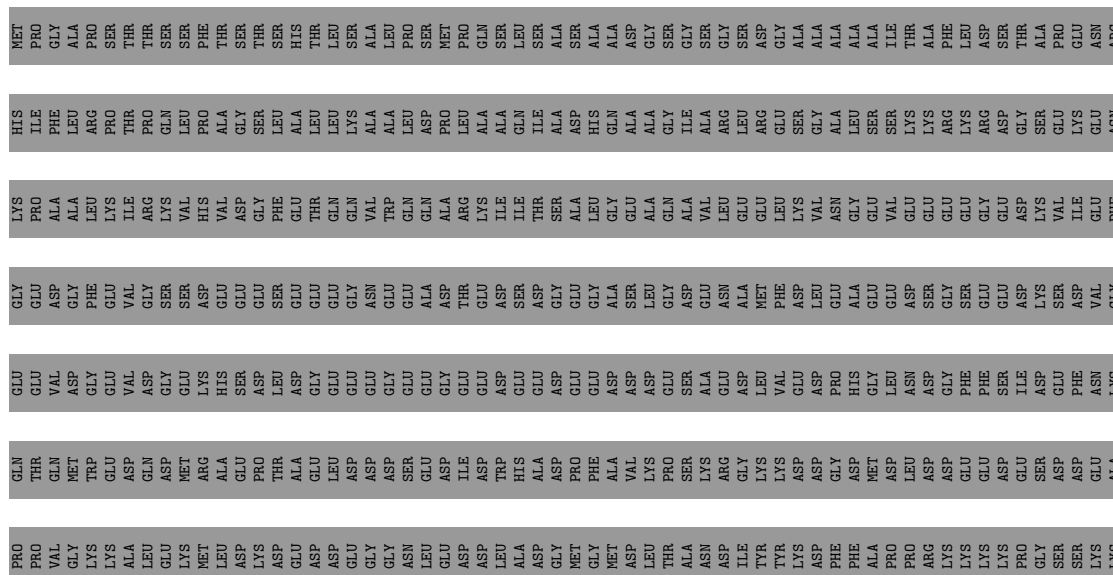
• Molecule 25: Imp3

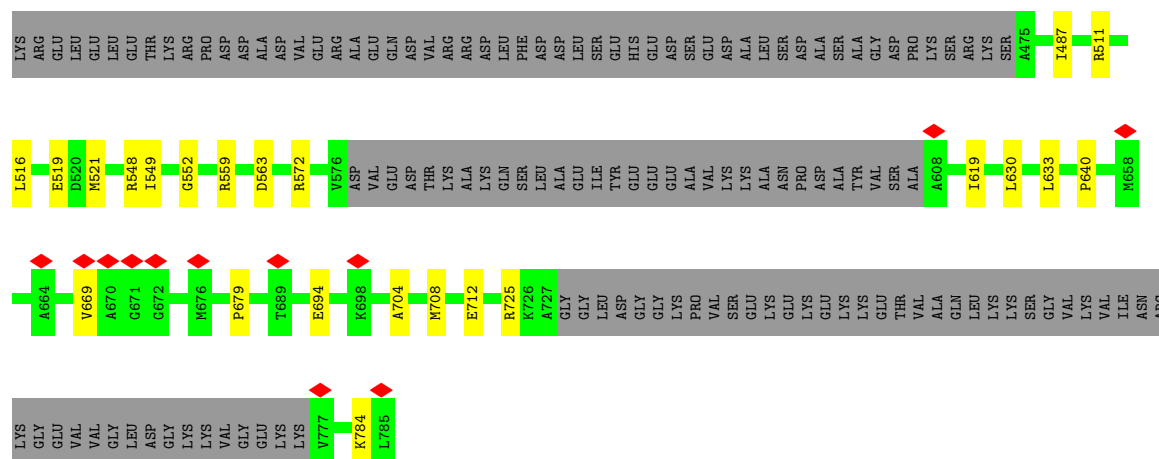


• Molecule 26: Putative U3 small nucleolar ribonucleoprotein

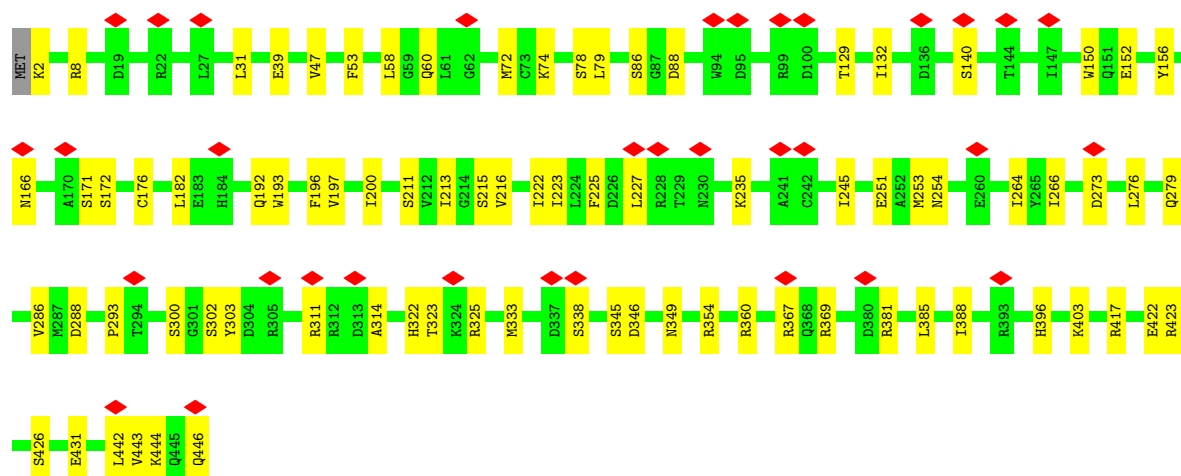
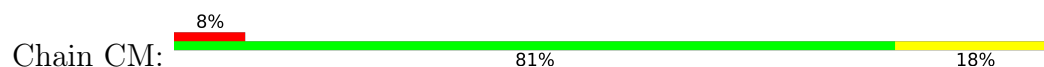


• Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein

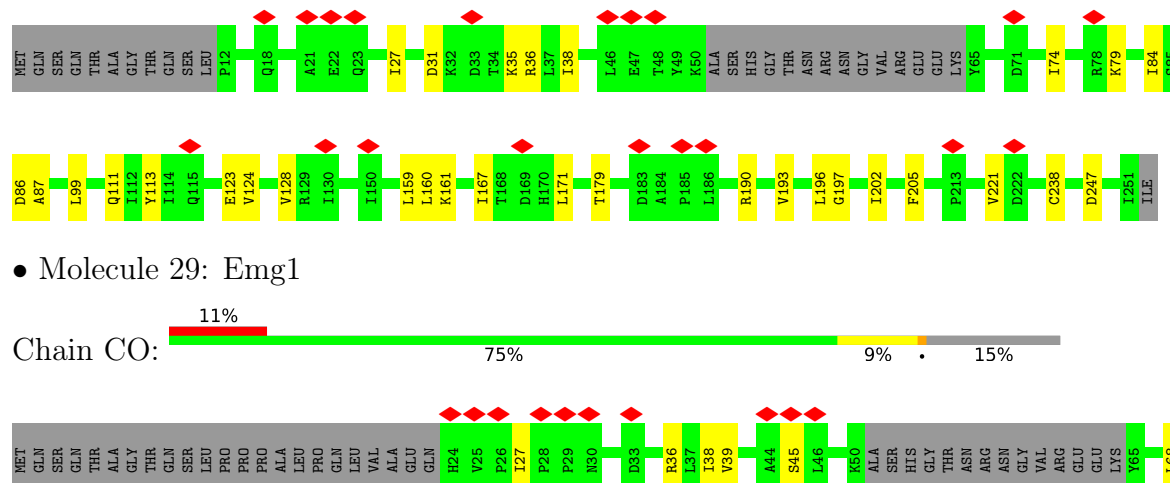
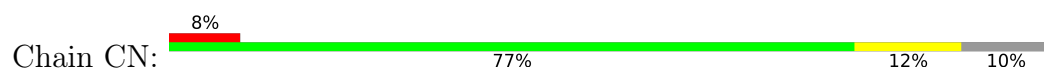




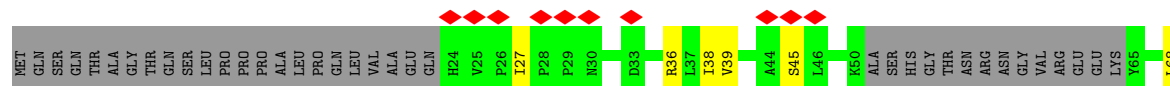
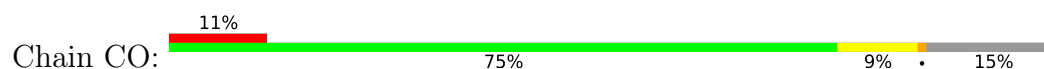
• Molecule 28: Sof1

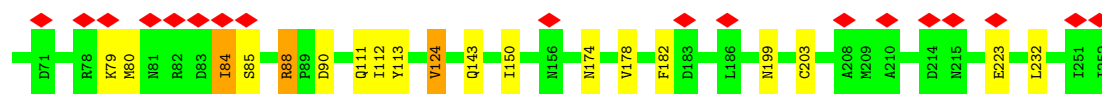


• Molecule 29: Emg1

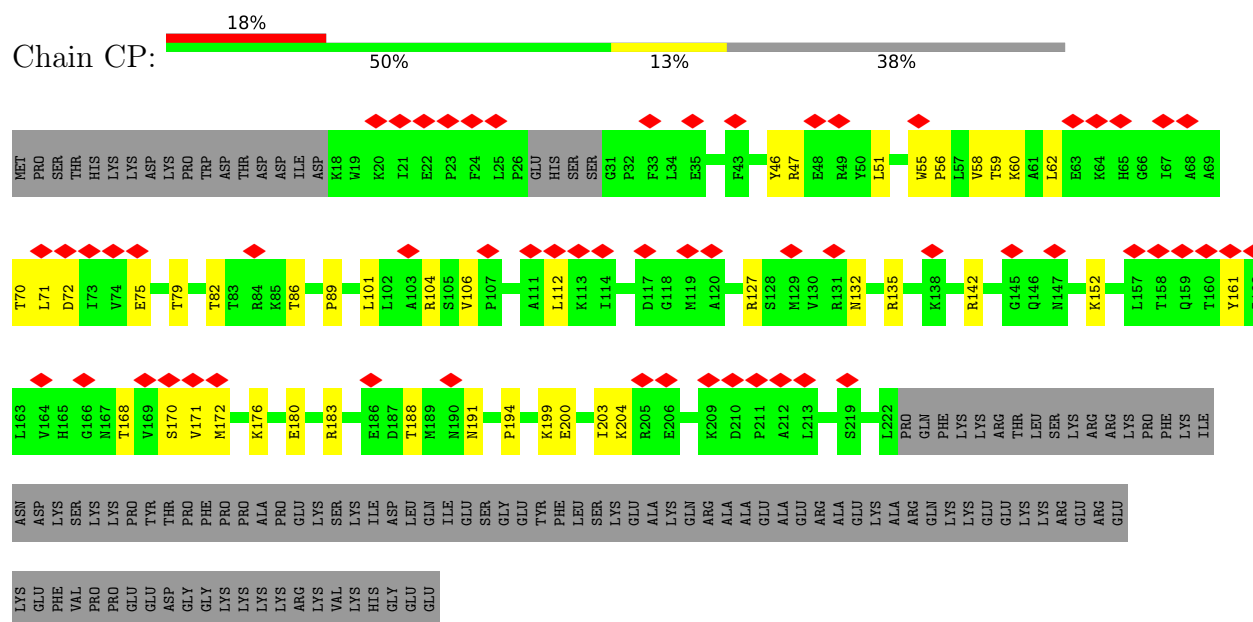


• Molecule 29: Emg1

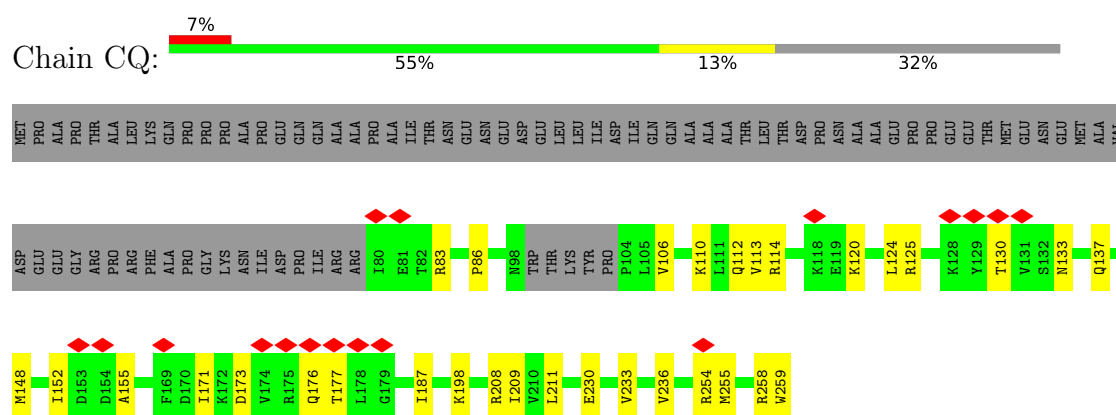




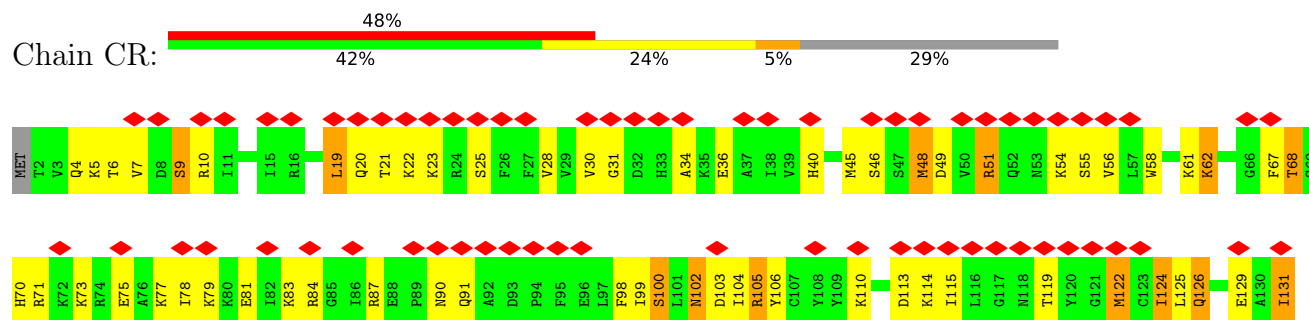
- Molecule 30: KRR1 small subunit processome component



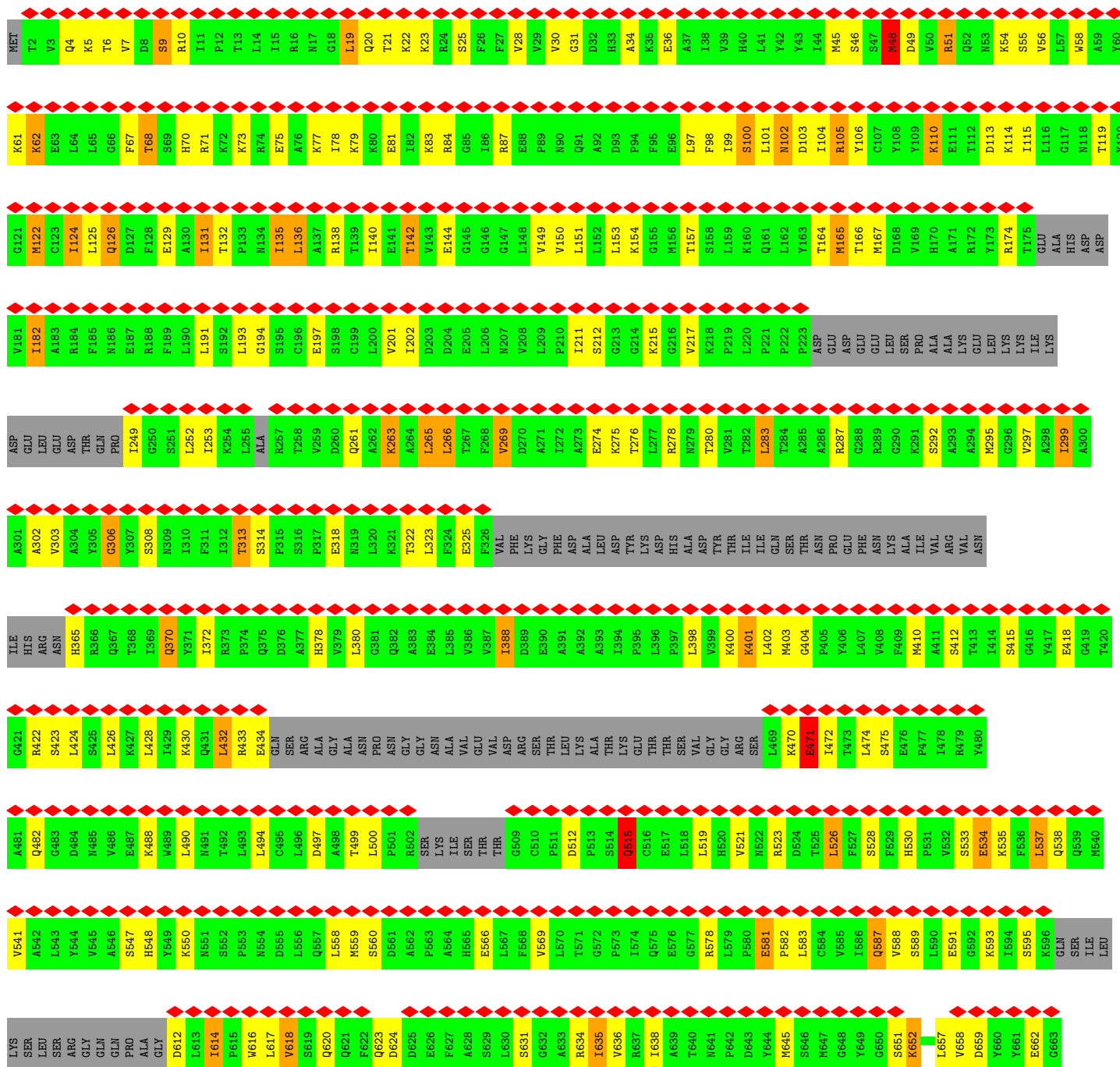
- Molecule 31: Pre-rRNA-processing protein PNO1

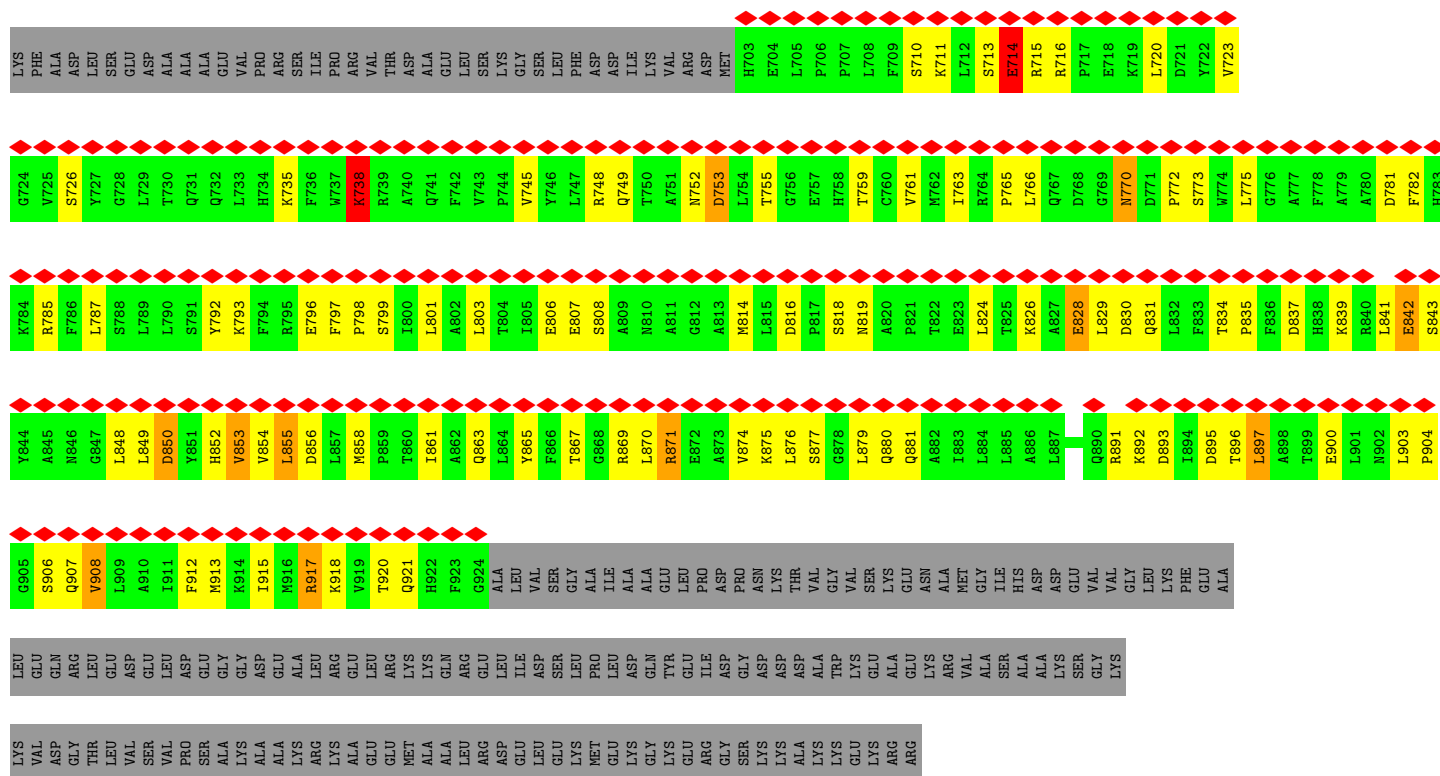


- Molecule 32: Kre33

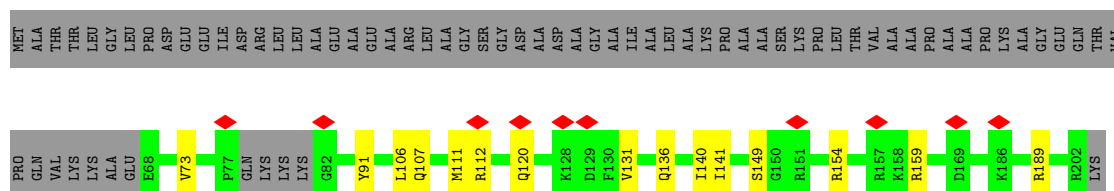




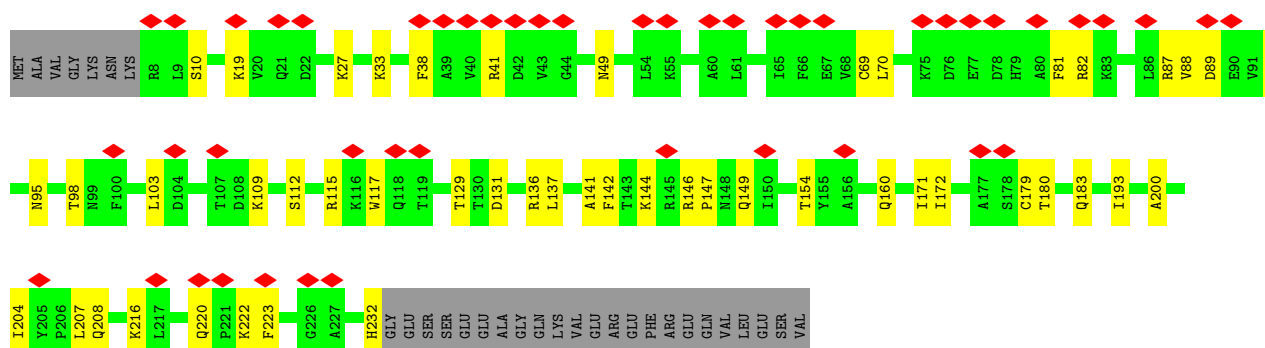
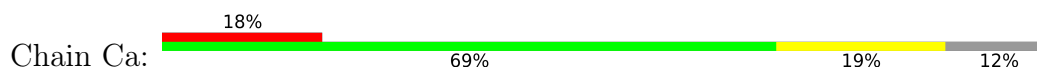




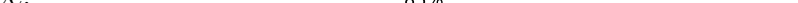
- Molecule 33: Fcf2

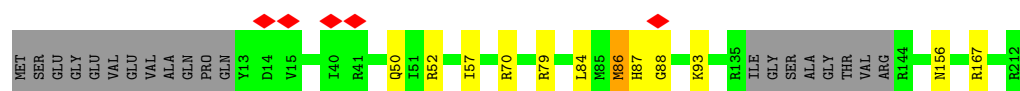


- Molecule 34: 40S ribosomal protein S1

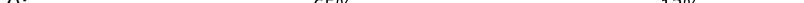


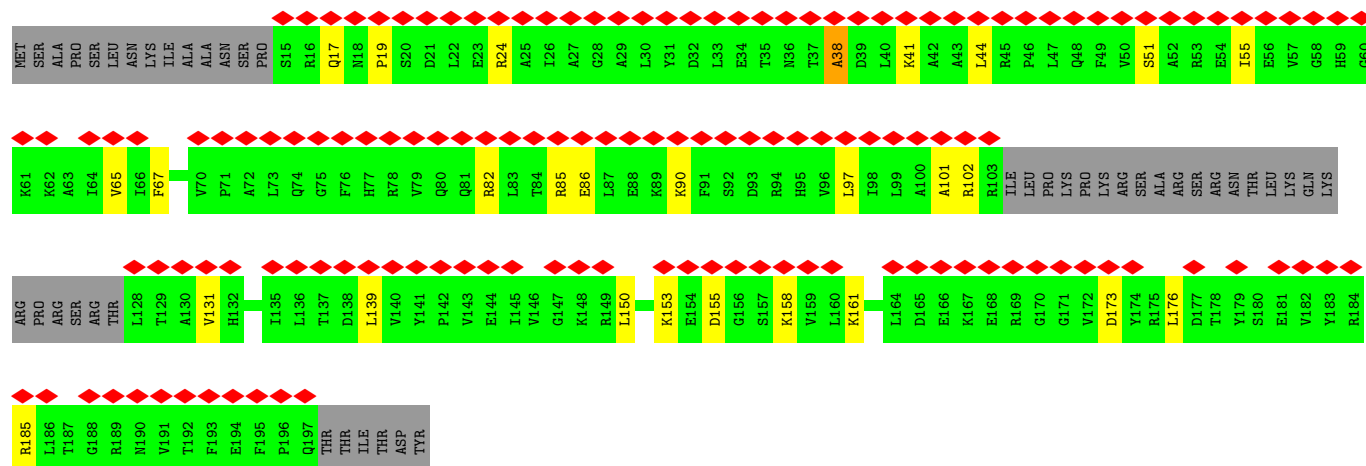
- Molecule 35: 40S ribosomal protein s5-like protein

Chain Cc:  85% 5% 9%

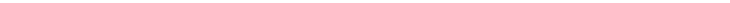


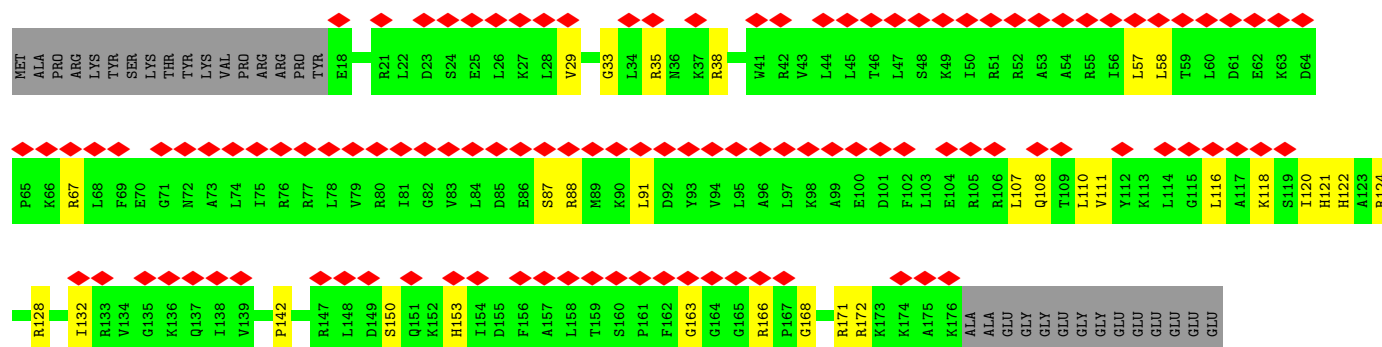
- Molecule 36: 40S ribosomal protein S7

Chain Ce: 



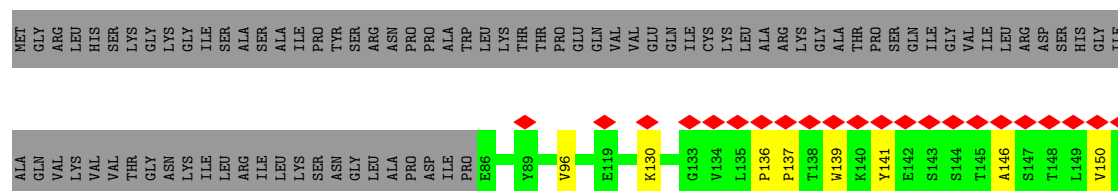
- Molecule 37: 40S ribosomal protein s9-like protein

Chain Cg: 

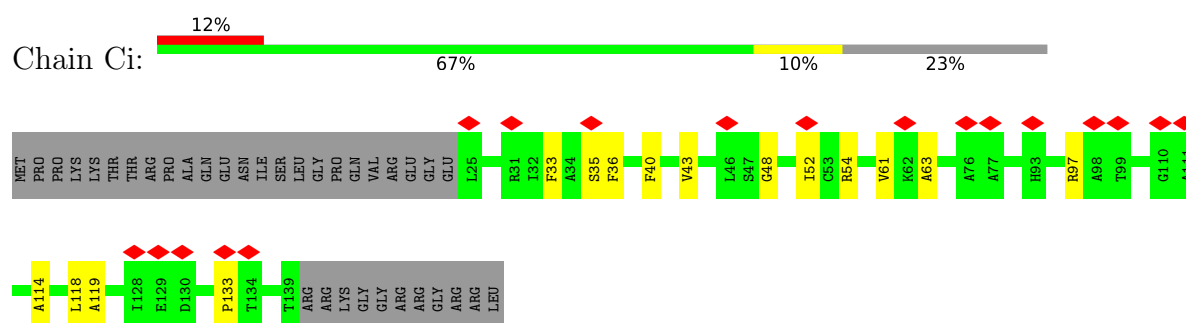


- Molecule 38: 40S ribosomal protein S13-like protein

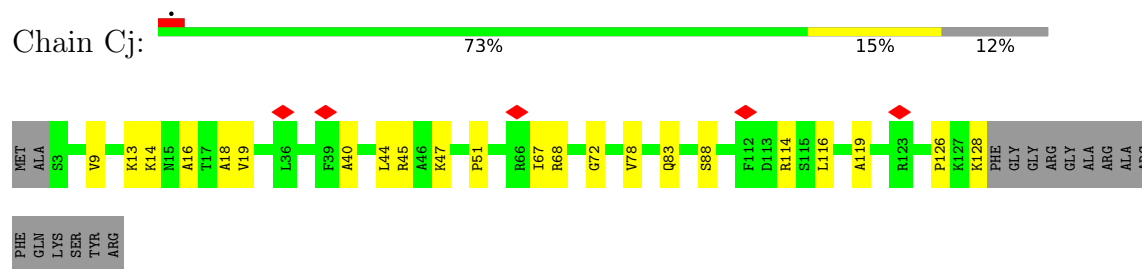
Chain Ch: 



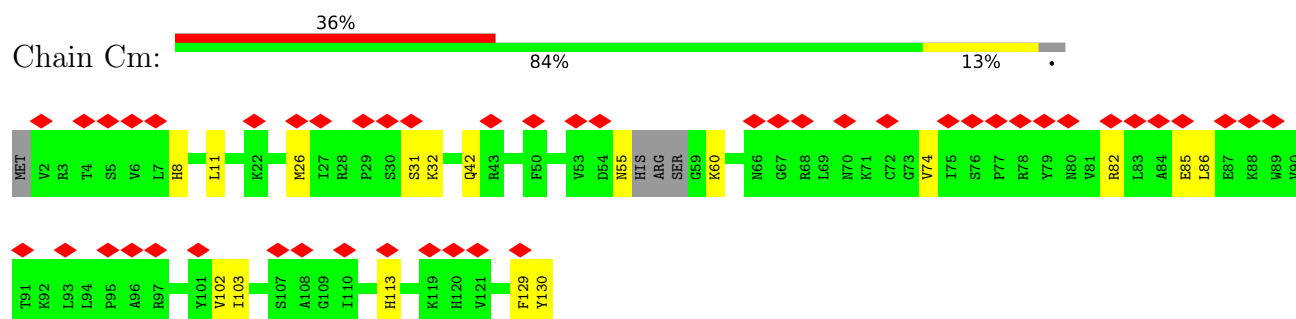
- Molecule 39: 40S ribosomal protein S14-like protein



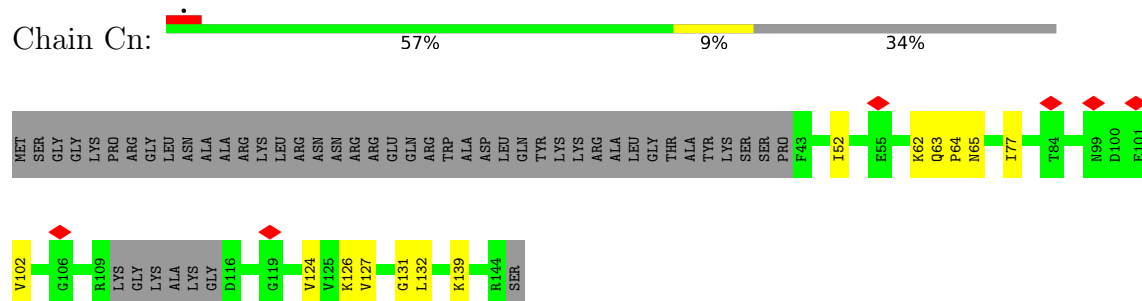
- Molecule 40: 40S ribosomal protein S16-like protein



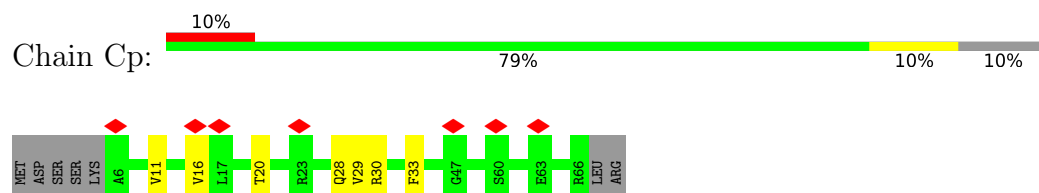
- Molecule 41: 40S ribosomal protein S22-like protein



- Molecule 42: 40S ribosomal protein s23-like protein

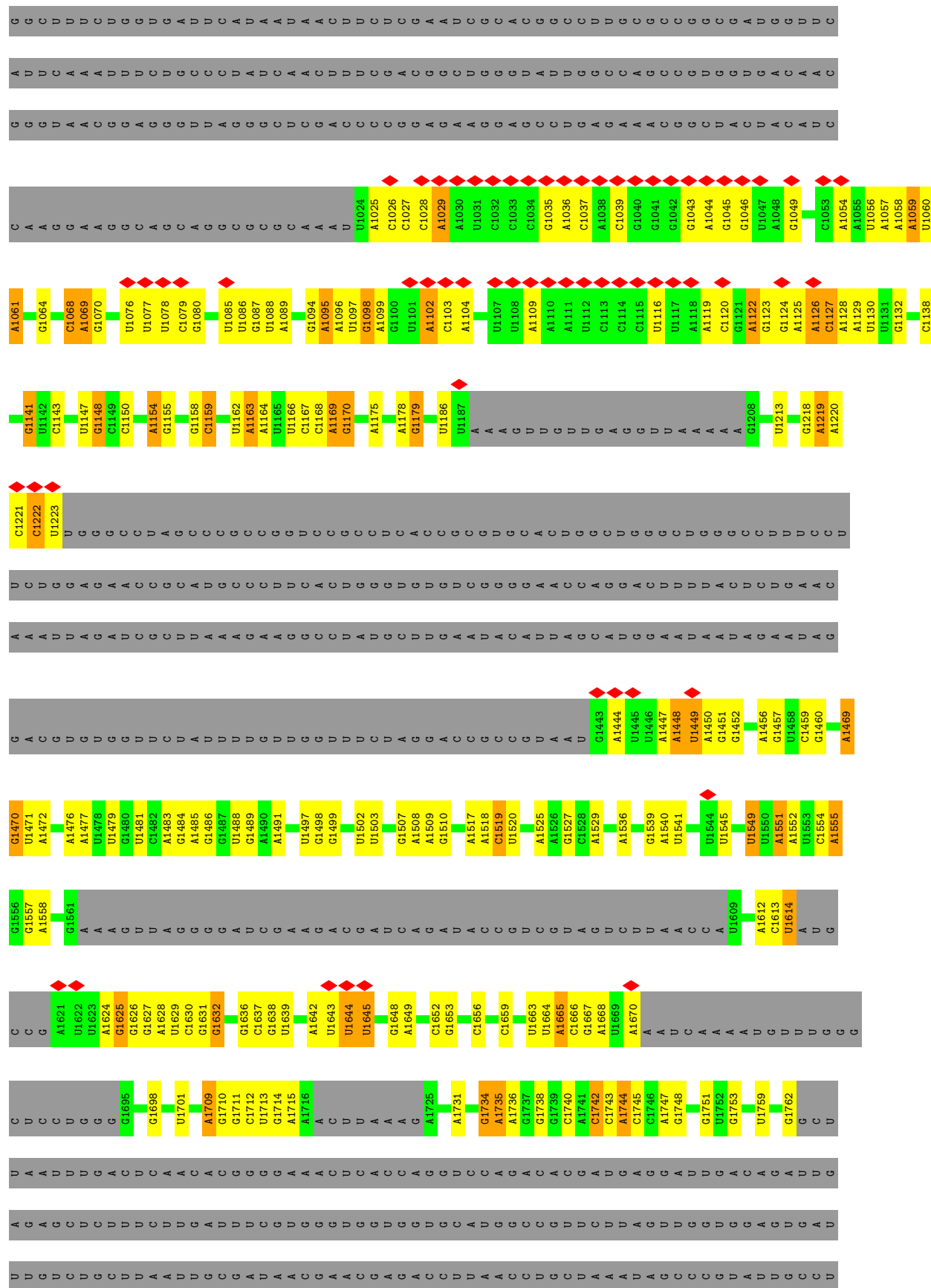


- Molecule 43: 40S ribosomal protein S28-like protein



Chain CU:









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8415	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	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	0.232	Depositor
Minimum map value	-0.184	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, GTP, MG

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	UA	0.42	0/6521	0.66	1/8867 (0.0%)
2	UB	0.28	0/4154	0.58	0/5583
3	UC	0.35	0/595	0.57	0/786
4	UD	0.32	0/6211	0.55	0/8408
5	UF	0.31	0/2657	0.58	0/3596
6	UG	0.42	0/3790	0.66	2/5120 (0.0%)
7	UJ	0.34	0/3435	0.59	1/4661 (0.0%)
8	UK	0.35	0/1701	0.51	0/2251
9	UL	0.33	0/6299	0.70	4/8531 (0.0%)
10	UM	0.29	0/5755	0.68	2/7827 (0.0%)
11	UN	0.37	0/1232	0.60	0/1662
12	UO	0.35	0/3903	0.63	0/5312
13	UQ	0.34	0/6136	0.64	5/8348 (0.1%)
14	UR	0.39	0/3564	0.60	0/4816
15	UU	0.40	0/6903	0.63	0/9392
16	UX	0.38	0/1493	0.63	1/2011 (0.0%)
17	UZ	0.29	0/1857	0.64	0/2526
18	CA	0.40	0/1814	0.60	2/2456 (0.1%)
18	CB	0.27	0/1853	0.54	0/2511
19	CC	0.33	0/2911	0.59	0/3937
20	CD	0.32	0/3205	0.66	3/4338 (0.1%)
21	CE	0.40	0/891	0.65	0/1214
21	CF	0.36	0/876	0.67	0/1195
22	CG	0.31	0/2983	0.62	2/4032 (0.0%)
23	CH	0.32	0/2939	0.59	0/3988
24	CI	0.37	0/6631	0.61	0/8943
25	CJ	0.43	0/1462	0.62	0/1967
26	CK	0.41	0/2376	0.64	1/3214 (0.0%)
27	CL	0.32	0/1812	0.54	0/2437
28	CM	0.42	0/3573	0.62	0/4829
29	CN	0.30	0/1797	0.59	0/2443
29	CO	0.25	0/1714	0.60	2/2325 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.32	0/1655	0.57	0/2229
31	CQ	0.26	0/1379	0.60	0/1850
32	CR	0.37	1/6108 (0.0%)	0.92	15/8266 (0.2%)
32	CS	0.37	1/6108 (0.0%)	0.92	15/8266 (0.2%)
33	CT	0.35	0/1053	0.64	0/1413
34	Ca	0.32	0/1850	0.64	0/2486
35	Cc	0.35	0/1485	0.56	0/2008
36	Ce	0.31	0/1298	0.76	2/1750 (0.1%)
37	Cg	0.36	0/1259	0.58	0/1687
38	Ch	0.25	0/557	0.54	0/749
39	Ci	0.31	0/819	0.58	0/1107
40	Cj	0.41	0/958	0.63	0/1293
41	Cm	0.33	0/1001	0.57	0/1345
42	Cn	0.37	0/712	0.55	0/954
43	Cp	0.35	0/458	0.57	0/617
44	CU	0.28	0/1350	0.60	0/1810
45	C1	0.32	0/27472	0.48	7/42792 (0.0%)
46	C2	0.32	0/5459	0.56	6/8498 (0.1%)
47	UH	0.27	0/2852	0.59	0/3846
48	UE	0.31	0/980	0.64	0/1316
48	UI	0.22	0/980	0.56	0/1316
49	US	0.28	0/3765	0.61	0/5100
50	Cl	0.24	0/638	0.70	0/857
51	CX	0.27	1/2180 (0.0%)	0.62	0/2956
52	UP	0.30	0/428	0.66	0/570
All	All	0.34	3/175847 (0.0%)	0.62	71/244607 (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	UA	0	1
4	UD	0	1
9	UL	0	2
10	UM	0	4
12	UO	0	1
13	UQ	0	4
14	UR	0	1
15	UU	0	3
17	UZ	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	CB	0	1
21	CF	0	1
22	CG	0	1
23	CH	0	1
24	CI	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cc	0	1
36	Ce	0	1
48	UE	0	1
49	US	0	1
50	Cl	0	1
All	All	0	42

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	CX	402	ALA	C-N	5.50	1.38	1.33
32	CR	714	GLU	CA-CB	5.26	1.59	1.52
32	CS	714	GLU	CA-CB	5.23	1.59	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	C2	2	G	OP1-P-OP2	-13.64	78.67	119.60
46	C2	2	G	O5'-P-OP1	-11.29	74.13	108.00
46	C2	1	A	OP2-P-O3'	-10.57	76.28	108.00
45	C1	55	G	OP1-P-O3'	-9.88	78.35	108.00
45	C1	45	U	OP1-P-O3'	-9.29	80.14	108.00
46	C2	1	A	OP1-P-O3'	9.19	135.56	108.00
20	CD	129	LEU	CA-C-N	8.67	125.70	120.24
20	CD	129	LEU	C-N-CA	8.67	125.70	120.24
46	C2	2	G	O5'-P-OP2	8.14	132.43	108.00
32	CR	714	GLU	CA-CB-CG	7.99	130.07	114.10
32	CR	471	GLU	CA-CB-CG	7.98	130.06	114.10
32	CS	471	GLU	CA-CB-CG	7.98	130.06	114.10
32	CS	714	GLU	CA-CB-CG	7.96	130.02	114.10
45	C1	45	U	OP2-P-O3'	-7.65	85.05	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	UQ	747	LEU	CA-C-N	7.47	135.81	121.54
13	UQ	747	LEU	C-N-CA	7.47	135.81	121.54
32	CS	515	GLN	CA-CB-CG	7.32	128.73	114.10
32	CR	515	GLN	CA-CB-CG	7.30	128.70	114.10
36	Ce	38	ALA	CA-C-N	7.26	134.77	121.70
36	Ce	38	ALA	C-N-CA	7.26	134.77	121.70
32	CS	370	GLN	CA-CB-CG	6.67	127.44	114.10
32	CR	370	GLN	CA-CB-CG	6.66	127.42	114.10
13	UQ	472	PRO	CA-C-N	6.64	134.23	121.54
13	UQ	472	PRO	C-N-CA	6.64	134.23	121.54
32	CR	797	PHE	N-CA-C	-6.58	102.30	108.22
32	CS	797	PHE	N-CA-C	-6.56	102.31	108.22
32	CS	738	LYS	CG-CD-CE	6.44	126.12	111.30
32	CR	738	LYS	CG-CD-CE	6.44	126.10	111.30
22	CG	358	LYS	CA-C-N	6.37	125.42	120.33
22	CG	358	LYS	C-N-CA	6.37	125.42	120.33
9	UL	437	ASP	CA-C-N	6.05	130.98	122.08
9	UL	437	ASP	C-N-CA	6.05	130.98	122.08
6	UG	575	LYS	CA-C-N	5.98	132.47	121.70
6	UG	575	LYS	C-N-CA	5.98	132.47	121.70
32	CR	51	ARG	N-CA-C	-5.94	106.58	113.88
32	CS	738	LYS	CD-CE-NZ	5.93	130.89	111.90
32	CR	738	LYS	CD-CE-NZ	5.93	130.89	111.90
32	CS	51	ARG	N-CA-C	-5.89	106.64	113.88
32	CS	714	GLU	CB-CG-CD	5.80	122.47	112.60
32	CR	714	GLU	CB-CG-CD	5.79	122.44	112.60
20	CD	189	TRP	CA-CB-CG	5.75	124.52	113.60
10	UM	672	ASP	CA-C-N	5.70	132.43	121.54
10	UM	672	ASP	C-N-CA	5.70	132.43	121.54
16	UX	143	ILE	N-CA-C	-5.68	107.74	113.20
29	CO	124	VAL	CA-C-N	5.68	130.12	121.03
29	CO	124	VAL	C-N-CA	5.68	130.12	121.03
32	CR	62	LYS	N-CA-C	-5.66	106.19	114.39
32	CS	62	LYS	N-CA-C	-5.63	106.23	114.39
9	UL	426	ARG	CA-C-N	-5.57	115.81	122.44
9	UL	426	ARG	C-N-CA	-5.57	115.81	122.44
32	CS	714	GLU	N-CA-CB	5.57	117.32	110.53
32	CR	714	GLU	N-CA-CB	5.55	117.30	110.53
18	CA	265	THR	CA-C-N	5.43	128.93	120.68
18	CA	265	THR	C-N-CA	5.43	128.93	120.68
32	CS	471	GLU	CB-CG-CD	5.40	121.78	112.60
32	CR	471	GLU	CB-CG-CD	5.38	121.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	C1	1163	A	P-O3'-C3'	5.35	128.22	120.20
45	C1	55	G	OP2-P-O3'	-5.28	92.15	108.00
46	C2	255	U	P-O3'-C3'	5.27	128.10	120.20
26	CK	89	LEU	CA-CB-CG	5.26	134.70	116.30
45	C1	209	A	P-O3'-C3'	5.25	128.07	120.20
32	CR	534	GLU	CB-CG-CD	5.21	121.46	112.60
1	UA	81	LEU	CA-CB-CG	5.20	134.50	116.30
32	CS	534	GLU	CB-CG-CD	5.20	121.44	112.60
32	CS	618	VAL	N-CA-CB	5.15	117.17	110.57
32	CR	618	VAL	N-CA-CB	5.15	117.16	110.57
32	CS	370	GLN	CB-CG-CD	5.14	121.33	112.60
32	CR	370	GLN	CB-CG-CD	5.13	121.33	112.60
7	UJ	252	GLY	N-CA-C	5.11	122.76	112.34
13	UQ	705	GLY	N-CA-C	5.08	122.71	112.34
45	C1	2219	C	C2'-C3'-O3'	5.07	121.31	113.70

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	293	GLU	Peptide
21	CF	60	GLN	Peptide
22	CG	178	VAL	Peptide
23	CH	143	HIS	Peptide
24	CI	851	TRP	Peptide
24	CI	852	ASP	Peptide
26	CK	261	PHE	Peptide
28	CM	140	SER	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
31	CQ	173	ASP	Peptide
32	CR	122	MET	Peptide
32	CR	306	GLY	Peptide
32	CR	432	LEU	Peptide
32	CS	122	MET	Peptide
32	CS	306	GLY	Peptide
32	CS	432	LEU	Peptide
35	Cc	86	MET	Peptide
36	Ce	38	ALA	Peptide
50	Cl	79	TYR	Peptide
1	UA	115	LEU	Peptide
4	UD	387	TRP	Peptide

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Mol	Chain	Res	Type	Group
48	UE	232	GLN	Peptide
9	UL	153	ASP	Peptide
9	UL	636	LEU	Peptide
10	UM	328	LEU	Peptide
10	UM	382	ILE	Peptide
10	UM	445	GLY	Peptide
10	UM	585	HIS	Peptide
12	UO	282	ALA	Peptide
13	UQ	237	TYR	Peptide
13	UQ	426	ALA	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
14	UR	616	ILE	Peptide
49	US	510	LYS	Peptide
15	UU	397	ASP	Peptide
15	UU	644	GLY	Peptide
15	UU	857	ILE	Peptide
17	UZ	103	ASP	Peptide
17	UZ	114	ASP	Peptide
17	UZ	273	GLN	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	UA	6366	0	6273	88	0
2	UB	4079	0	4201	45	0
3	UC	588	0	647	12	0
4	UD	6071	0	6080	86	0
5	UF	2591	0	2642	15	0
6	UG	3717	0	3756	48	0
7	UJ	3377	0	3472	31	0
8	UK	1687	0	1820	6	0
9	UL	6175	0	6188	94	0
10	UM	5643	0	5643	97	0
11	UN	1209	0	1234	10	0
12	UO	3819	0	3873	59	0
13	UQ	6008	0	6033	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	UR	3491	0	3507	44	0
15	UU	6734	0	6745	78	0
16	UX	1470	0	1533	20	0
17	UZ	1815	0	1896	30	0
18	CA	1778	0	1830	30	0
18	CB	1816	0	1847	28	0
19	CC	2866	0	2960	30	0
20	CD	3150	0	3262	46	0
21	CE	879	0	918	11	0
21	CF	864	0	900	4	0
22	CG	2922	0	2939	45	0
23	CH	2888	0	2979	56	0
24	CI	6486	0	6649	82	0
25	CJ	1434	0	1482	18	0
26	CK	2329	0	2373	34	0
27	CL	1786	0	1826	20	0
28	CM	3501	0	3498	54	0
29	CN	1762	0	1807	18	0
29	CO	1683	0	1726	14	0
30	CP	1625	0	1718	28	0
31	CQ	1361	0	1431	22	0
32	CR	5989	0	6130	110	0
32	CS	5989	0	6130	107	0
33	CT	1035	0	1063	15	0
34	Ca	1821	0	1936	38	0
35	Cc	1464	0	1504	10	0
36	Ce	1279	0	1322	17	0
37	Cg	1242	0	1354	23	0
38	Ch	546	0	580	6	0
39	Ci	808	0	831	10	0
40	Cj	943	0	1002	15	0
41	Cm	985	0	1021	12	0
42	Cn	702	0	750	12	0
43	Cp	455	0	482	5	0
44	CU	1337	0	1376	15	0
45	C1	24590	0	12457	216	0
46	C2	4891	0	2476	39	0
47	UH	2809	0	2843	55	0
48	UE	972	0	1032	12	0
48	UI	972	0	1032	13	0
49	US	3672	0	3679	64	0
50	Cl	633	0	676	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	CX	2130	0	2219	29	0
52	UP	422	0	457	10	0
53	UX	1	0	0	0	0
54	CI	32	0	12	11	0
55	CI	1	0	0	0	0
All	All	169690	0	158052	1941	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1941) 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)
47:UH:557:GLU:O	47:UH:565:GLY:HA2	1.36	1.25
47:UH:555:GLY:O	47:UH:567:LEU:HA	1.37	1.20
24:CI:80:GLY:HA2	54:CI:1201:GTP:O2A	1.01	1.15
24:CI:80:GLY:CA	54:CI:1201:GTP:O2A	1.95	1.14
17:UZ:280:ASN:ND2	17:UZ:282:TYR:HE2	1.47	1.11
45:C1:2085:G:N2	45:C1:2088:A:N7	2.10	0.99
45:C1:2237:G:H1	45:C1:2329:A:H61	1.07	0.99
46:C2:137:U:H3	46:C2:150:G:H1	1.02	0.98
17:UZ:280:ASN:HB2	17:UZ:282:TYR:CE2	2.00	0.97
47:UH:557:GLU:O	47:UH:565:GLY:CA	2.14	0.95
17:UZ:280:ASN:ND2	17:UZ:282:TYR:CE2	2.36	0.92
27:CL:548:ARG:O	27:CL:552:GLY:HA2	1.68	0.92
46:C2:200:U:H3	46:C2:246:G:H1	1.12	0.92
17:UZ:280:ASN:CG	17:UZ:282:TYR:HE2	1.83	0.85
45:C1:2238:A:H62	45:C1:2328:G:N2	1.76	0.84
45:C1:1448:A:N6	45:C1:1549:U:C4	2.46	0.84
45:C1:381:G:H21	45:C1:385:A:H62	1.28	0.81
17:UZ:280:ASN:CB	17:UZ:282:TYR:CE2	2.64	0.80
45:C1:2358:U:H3	45:C1:2369:G:H1	0.84	0.80
16:UX:49:ASN:HD22	16:UX:52:LEU:HD23	1.47	0.80
45:C1:2237:G:H1	45:C1:2329:A:N6	1.80	0.79
17:UZ:280:ASN:CG	17:UZ:282:TYR:CE2	2.60	0.79
13:UQ:330:LEU:O	13:UQ:334:HIS:HB2	1.85	0.77
5:UF:2:ALA:N	46:C2:39:U:HO2'	1.82	0.77
24:CI:81:LYS:NZ	54:CI:1201:GTP:O1B	2.18	0.77
24:CI:81:LYS:N	54:CI:1201:GTP:O2B	2.19	0.76
47:UH:555:GLY:O	47:UH:567:LEU:CA	2.28	0.75
12:UO:282:ALA:HB3	12:UO:287:ARG:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C1:381:G:N2	45:C1:385:A:H62	1.85	0.75
10:UM:452:SER:H	10:UM:482:VAL:HG23	1.51	0.74
45:C1:2238:A:N6	45:C1:2328:G:N2	2.37	0.71
24:CI:174:ASP:CG	54:CI:1201:GTP:HN21	1.99	0.71
18:CB:272:PHE:HB3	18:CB:289:GLN:HE22	1.55	0.70
12:UO:101:GLU:HB2	12:UO:119:ASP:HB2	1.75	0.69
20:CD:326:LYS:HB3	46:C2:91:G:H22	1.58	0.69
45:C1:1213:U:O2	45:C1:1555:A:N7	2.26	0.68
9:UL:895:MET:O	9:UL:899:LEU:HB2	1.94	0.68
10:UM:114:VAL:HA	10:UM:130:ALA:HA	1.75	0.68
30:CP:101:LEU:HD13	30:CP:172:MET:HE2	1.76	0.68
1:UA:559:ARG:HH22	1:UA:569:VAL:HG11	1.59	0.67
39:CI:33:PHE:HB3	39:CI:40:PHE:HB2	1.76	0.67
14:UR:322:ARG:HH21	45:C1:133:G:H22	1.42	0.67
15:UU:112:ARG:HE	15:UU:140:PRO:HD3	1.59	0.66
24:CI:80:GLY:HA2	54:CI:1201:GTP:PA	2.29	0.66
11:UN:916:GLN:HE22	45:C1:441:A:H62	1.43	0.66
5:UF:278:ILE:HG13	5:UF:279:PRO:HD3	1.78	0.66
13:UQ:496:SER:HB2	13:UQ:535:GLU:H	1.61	0.66
32:CS:903:LEU:HD21	32:CS:907:GLN:HB2	1.78	0.65
32:CR:903:LEU:HD21	32:CR:907:GLN:HB2	1.78	0.65
45:C1:1759:U:O4	45:C1:2047:G:O6	2.15	0.65
24:CI:123:LEU:HD22	24:CI:898:ARG:HD2	1.78	0.65
15:UU:189:ALA:HA	15:UU:200:PHE:O	1.97	0.65
45:C1:2238:A:N6	45:C1:2328:G:C2	2.63	0.65
18:CB:245:LEU:O	20:CD:123:ARG:NH2	2.30	0.65
32:CR:749:GLN:HE21	32:CS:852:HIS:HB3	1.61	0.65
1:UA:295:ILE:HB	1:UA:323:LEU:HD21	1.78	0.64
26:CK:123:ILE:HG23	26:CK:126:ASP:HB2	1.80	0.64
1:UA:544:GLN:OE1	40:Cj:114:ARG:NH2	2.30	0.64
28:CM:156:TYR:HA	28:CM:172:SER:HA	1.80	0.64
46:C2:127:A:N7	46:C2:187:U:O4	2.30	0.64
32:CS:614:ILE:HD11	32:CS:634:ARG:HB2	1.80	0.64
45:C1:1122:A:H5'	45:C1:1127:C:H41	1.63	0.64
24:CI:69:ARG:NH1	24:CI:230:LYS:O	2.30	0.64
17:UZ:243:ILE:HG21	17:UZ:266:LEU:HD11	1.80	0.64
32:CR:614:ILE:HD11	32:CR:634:ARG:HB2	1.80	0.64
12:UO:417:ARG:NH2	45:C1:129:G:O6	2.31	0.64
34:Ca:142:PHE:O	34:Ca:208:GLN:N	2.29	0.64
9:UL:515:GLN:HE21	9:UL:572:ARG:HG2	1.63	0.64
32:CR:912:PHE:HA	32:CR:915:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:131:LEU:HD21	15:UU:151:ILE:HD11	1.79	0.63
28:CM:58:LEU:HD21	28:CM:354:ARG:HH11	1.61	0.63
4:UD:244:LEU:HD12	4:UD:248:ASP:HB2	1.80	0.63
10:UM:283:LEU:HB2	10:UM:286:GLY:HA3	1.80	0.63
19:CC:222:VAL:O	19:CC:226:ILE:HB	1.98	0.63
12:UO:529:LYS:NZ	45:C1:112:C:O2'	2.30	0.63
15:UU:159:ILE:HB	15:UU:173:ILE:HB	1.81	0.63
17:UZ:115:GLU:HG2	17:UZ:221:VAL:HG21	1.79	0.63
32:CS:105:ARG:NH2	32:CS:106:TYR:O	2.32	0.63
45:C1:381:G:H21	45:C1:385:A:N6	1.97	0.63
9:UL:12:LYS:HB2	9:UL:722:VAL:HB	1.81	0.62
29:CO:27:ILE:HG21	29:CO:36:ARG:HE	1.64	0.62
45:C1:1665:A:N3	45:C1:1666:C:N4	2.47	0.62
10:UM:386:GLN:HE22	10:UM:703:SER:H	1.47	0.62
16:UX:39:GLN:HE22	18:CA:291:THR:H	1.46	0.62
19:CC:48:VAL:HG11	19:CC:134:ILE:HD11	1.80	0.62
30:CP:104:ARG:HH12	30:CP:170:SER:HB2	1.64	0.62
32:CR:623:GLN:H	32:CS:839:LYS:HZ3	1.47	0.62
8:UK:268:ARG:NH1	14:UR:539:LEU:O	2.32	0.62
32:CR:105:ARG:NH2	32:CR:106:TYR:O	2.32	0.62
10:UM:555:ASN:HD21	10:UM:557:LYS:HE3	1.64	0.62
15:UU:482:PRO:HD2	15:UU:502:LEU:HD21	1.81	0.62
32:CS:753:ASP:OD1	32:CS:753:ASP:N	2.30	0.62
10:UM:702:HIS:HD2	10:UM:705:THR:H	1.48	0.62
13:UQ:186:LYS:HB3	13:UQ:210:ARG:HD3	1.82	0.62
20:CD:81:LYS:HE3	20:CD:84:LYS:HD3	1.81	0.62
35:Cc:79:ARG:NH2	35:Cc:156:ASN:OD1	2.32	0.62
45:C1:69:U:H3	47:UH:884:SER:HG	1.45	0.62
1:UA:415:ARG:NH1	45:C1:2215:C:O2	2.33	0.62
28:CM:251:GLU:OE1	28:CM:254:ASN:ND2	2.32	0.62
32:CR:753:ASP:OD1	32:CR:753:ASP:N	2.30	0.62
2:UB:618:ILE:HG12	2:UB:639:LEU:HD22	1.82	0.62
32:CS:19:LEU:HD22	32:CS:49:ASP:HB3	1.82	0.62
32:CS:912:PHE:HA	32:CS:915:ILE:HD12	1.81	0.62
9:UL:601:LEU:HD11	9:UL:639:GLY:HA3	1.81	0.61
12:UO:129:GLY:H	12:UO:133:ARG:HB2	1.64	0.61
15:UU:889:SER:HB2	31:CQ:258:ARG:HG3	1.82	0.61
19:CC:227:GLY:HA2	19:CC:275:ARG:HH22	1.65	0.61
35:Cc:57:ILE:HD11	40:Cj:47:LYS:HG2	1.82	0.61
18:CA:111:VAL:HG21	33:CT:136:GLN:HG2	1.81	0.61
46:C2:160:U:H2'	46:C2:161:G:H8	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:208:THR:HG21	4:UD:222:GLN:HE21	1.63	0.61
1:UA:363:LYS:HG2	1:UA:379:THR:HG22	1.82	0.61
12:UO:458:THR:O	12:UO:462:HIS:ND1	2.33	0.61
32:CR:587:GLN:HG2	32:CR:636:VAL:HB	1.83	0.61
1:UA:418:ARG:NH2	1:UA:455:VAL:O	2.34	0.61
9:UL:699:ILE:HA	9:UL:715:SER:HA	1.83	0.61
20:CD:335:LYS:NZ	24:CI:1079:ARG:O	2.34	0.61
45:C1:66:G:OP2	47:UH:894:ARG:NH1	2.34	0.61
10:UM:459:LEU:HD13	10:UM:524:ILE:HD12	1.82	0.61
23:CH:152:THR:O	23:CH:156:ALA:HB3	2.01	0.61
24:CI:174:ASP:OD1	54:CI:1201:GTP:N2	2.27	0.61
36:Ce:51:SER:HB3	36:Ce:67:PHE:HB2	1.82	0.61
10:UM:666:PHE:N	10:UM:678:TRP:O	2.34	0.60
24:CI:56:VAL:HG12	42:Cn:52:ILE:HG12	1.83	0.60
45:C1:221:A:O2'	45:C1:224:C:N4	2.33	0.60
13:UQ:371:ILE:HG22	13:UQ:381:LEU:HG	1.83	0.60
32:CS:587:GLN:HG2	32:CS:636:VAL:HB	1.83	0.60
9:UL:238:ASP:HB3	9:UL:240:GLU:HG2	1.83	0.60
22:CG:557:ARG:HG3	22:CG:597:GLY:HA2	1.82	0.60
24:CI:81:LYS:NZ	54:CI:1201:GTP:O2G	2.21	0.60
45:C1:2085:G:N2	45:C1:2088:A:C5	2.70	0.60
49:US:194:ASP:OD2	49:US:197:ARG:NH2	2.35	0.60
12:UO:214:VAL:HG23	12:UO:235:ILE:HD13	1.83	0.60
32:CR:19:LEU:HD22	32:CR:49:ASP:HB3	1.82	0.60
1:UA:149:GLN:NE2	45:C1:267:U:OP2	2.33	0.60
10:UM:401:VAL:HA	10:UM:425:ASP:HA	1.83	0.60
6:UG:65:ASP:OD1	45:C1:582:G:N2	2.35	0.60
11:UN:312:ARG:NH1	28:CM:446:GLN:O	2.35	0.60
9:UL:816:PRO:HA	9:UL:819:VAL:HG22	1.84	0.59
13:UQ:413:LEU:O	13:UQ:420:ALA:HA	2.02	0.59
18:CB:250:GLY:HA2	18:CB:306:TYR:O	2.02	0.59
22:CG:388:ASP:OD1	22:CG:388:ASP:N	2.35	0.59
28:CM:369:ARG:HH11	45:C1:439:A:H5'	1.67	0.59
36:Ce:150:LEU:HD21	36:Ce:158:LYS:HD3	1.84	0.59
40:Cj:126:PRO:HB3	45:C1:2166:A:H5''	1.82	0.59
41:Cm:102:VAL:H	41:Cm:113:HIS:HD2	1.50	0.59
9:UL:434:ILE:HD11	9:UL:705:SER:HA	1.83	0.59
13:UQ:146:SER:HA	13:UQ:157:TRP:O	2.03	0.59
26:CK:269:THR:HG22	26:CK:280:VAL:HG12	1.85	0.59
4:UD:153:LYS:HD2	4:UD:165:LEU:HD21	1.83	0.59
4:UD:697:GLN:HE21	4:UD:713:SER:HB3	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:306:ARG:HH12	9:UL:402:LYS:HD3	1.65	0.59
22:CG:312:VAL:HG13	22:CG:326:LEU:HB2	1.83	0.59
29:CO:79:LYS:HD2	29:CO:80:MET:HG3	1.84	0.59
32:CS:765:PRO:HD2	32:CS:775:LEU:HD22	1.85	0.59
36:Ce:67:PHE:HB3	36:Ce:101:ALA:HB2	1.85	0.59
9:UL:658:ILE:HG22	9:UL:704:VAL:HG21	1.85	0.59
19:CC:391:ARG:HH21	21:CF:64:ILE:HG23	1.67	0.59
32:CR:313:THR:HB	32:CR:388:ILE:HG23	1.85	0.59
32:CS:658:VAL:O	32:CS:662:GLU:HB2	2.02	0.59
9:UL:369:VAL:HA	9:UL:389:GLY:HA2	1.85	0.59
20:CD:304:HIS:ND1	46:C2:93:G:O6	2.36	0.59
26:CK:238:GLU:OE2	26:CK:240:ARG:NH2	2.35	0.59
13:UQ:211:LEU:HD12	13:UQ:212:THR:HG23	1.85	0.59
20:CD:51:PHE:HB2	20:CD:72:LYS:HE2	1.84	0.59
33:CT:189:ARG:O	45:C1:2072:U:N3	2.34	0.59
15:UU:701:ARG:NH1	15:UU:736:LEU:O	2.36	0.59
22:CG:185:THR:HG1	22:CG:193:THR:HG1	1.49	0.59
32:CR:658:VAL:O	32:CR:662:GLU:HB2	2.02	0.59
32:CR:765:PRO:HD2	32:CR:775:LEU:HD22	1.85	0.59
37:Cg:118:LYS:H	37:Cg:122:HIS:HD2	1.50	0.59
32:CS:313:THR:HB	32:CS:388:ILE:HG23	1.85	0.58
1:UA:685:ASN:HA	1:UA:700:LEU:HD13	1.84	0.58
24:CI:1002:ASN:HD21	27:CL:487:ILE:HD11	1.67	0.58
36:Ce:102:ARG:HD2	36:Ce:131:VAL:HG13	1.85	0.58
13:UQ:454:ARG:HA	47:UH:887:GLU:HA	1.85	0.58
13:UQ:735:ARG:NH2	13:UQ:778:THR:OG1	2.36	0.58
24:CI:537:TRP:HB3	24:CI:561:ARG:HA	1.85	0.58
49:US:418:MET:HE3	49:US:478:ILE:HG23	1.85	0.58
2:UB:341:LYS:HG2	2:UB:344:ARG:HH21	1.67	0.58
10:UM:20:ILE:HG22	10:UM:371:GLY:HA2	1.84	0.58
15:UU:136:ASP:O	15:UU:158:ARG:NH1	2.33	0.58
18:CB:243:ALA:O	20:CD:120:ARG:NH2	2.36	0.58
37:Cg:124:ARG:NH1	45:C1:1059:A:OP2	2.37	0.58
1:UA:715:ILE:O	15:UU:701:ARG:NH2	2.37	0.58
2:UB:656:GLU:OE2	49:US:497:TYR:OH	2.21	0.58
10:UM:777:VAL:HG21	10:UM:794:VAL:HG21	1.86	0.58
4:UD:115:ASP:HB2	4:UD:122:LYS:HB2	1.84	0.58
4:UD:865:ARG:NH2	4:UD:871:ASP:OD2	2.37	0.58
29:CN:193:VAL:HA	29:CN:196:LEU:HG	1.85	0.58
15:UU:954:LEU:HD11	31:CQ:255:MET:HE2	1.85	0.58
24:CI:917:LYS:NZ	45:C1:1141:G:O3'	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CQ:112:GLN:HG3	31:CQ:125:ARG:HB3	1.85	0.58
31:CQ:176:GLN:HG2	31:CQ:177:THR:HG23	1.86	0.58
45:C1:9:G:N1	45:C1:27:A:N6	2.51	0.58
10:UM:821:ARG:NH2	45:C1:2221:G:OP2	2.36	0.58
15:UU:72:GLN:HG2	15:UU:85:VAL:HG23	1.86	0.58
23:CH:251:HIS:HB3	44:CU:111:MET:HG2	1.85	0.58
10:UM:126:LEU:HD23	10:UM:140:ILE:HG12	1.86	0.58
10:UM:695:ARG:HD2	34:Ca:10:SER:HB3	1.85	0.58
24:CI:179:PRO:O	24:CI:183:LYS:NZ	2.36	0.58
38:Ch:130:LYS:NZ	38:Ch:136:PRO:O	2.35	0.58
4:UD:684:ASP:HB2	4:UD:734:ARG:HD3	1.86	0.58
6:UG:270:ASN:ND2	6:UG:461:LEU:O	2.37	0.58
20:CD:125:HIS:HE1	20:CD:128:ASN:HD22	1.52	0.58
45:C1:1448:A:N6	45:C1:1549:U:N3	2.52	0.58
10:UM:624:ILE:HG23	10:UM:638:PHE:HB2	1.86	0.57
29:CN:31:ASP:O	29:CN:36:ARG:NH2	2.37	0.57
1:UA:472:SER:OG	1:UA:488:TRP:NE1	2.36	0.57
2:UB:618:ILE:HG23	2:UB:639:LEU:HB3	1.84	0.57
2:UB:730:THR:HG23	2:UB:780:LEU:HD22	1.84	0.57
12:UO:13:LEU:HD13	12:UO:493:ARG:HE	1.68	0.57
16:UX:68:THR:HG21	16:UX:75:LEU:HD13	1.86	0.57
32:CS:897:LEU:HD22	32:CS:908:VAL:HG11	1.86	0.57
2:UB:531:ILE:HA	2:UB:534:ILE:HD12	1.86	0.57
23:CH:36:ILE:HG22	23:CH:37:ARG:HG2	1.87	0.57
2:UB:685:PRO:HG2	2:UB:690:ARG:HH21	1.68	0.57
13:UQ:846:VAL:HG22	13:UQ:852:VAL:HG22	1.85	0.57
22:CG:167:ARG:NH2	46:C2:188:G:O6	2.38	0.57
1:UA:450:ILE:HG23	1:UA:464:LEU:HB2	1.86	0.57
26:CK:88:VAL:HA	26:CK:138:ASP:O	2.05	0.57
47:UH:550:ILE:HG21	47:UH:591:VAL:HG12	1.86	0.57
2:UB:88:PRO:HB3	45:C1:1762:G:H5"	1.85	0.57
10:UM:775:THR:HG22	10:UM:825:VAL:HG11	1.85	0.57
13:UQ:89:MET:HE1	13:UQ:420:ALA:HB2	1.85	0.57
18:CA:175:GLY:O	18:CA:202:ASN:ND2	2.38	0.57
47:UH:736:LEU:HD21	47:UH:792:TRP:HE1	1.69	0.57
6:UG:103:GLU:OE2	28:CM:2:LYS:N	2.37	0.57
15:UU:857:ILE:O	31:CQ:254:ARG:NH2	2.37	0.57
18:CA:247:LEU:O	19:CC:132:ARG:NH2	2.38	0.57
1:UA:264:HIS:HB2	1:UA:305:ILE:HD13	1.86	0.57
5:UF:65:ARG:NH1	5:UF:119:GLN:OE1	2.37	0.57
18:CA:110:SER:HB3	33:CT:141:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:849:LEU:HB2	32:CR:853:VAL:HG21	1.87	0.57
37:Cg:142:PRO:HD2	45:C1:1058:A:H5''	1.87	0.57
32:CS:714:GLU:OE1	32:CS:714:GLU:N	2.37	0.57
1:UA:467:HIS:O	26:CK:135:ARG:NH1	2.35	0.56
4:UD:187:THR:OG1	4:UD:206:ASN:ND2	2.38	0.56
9:UL:678:ILE:HB	9:UL:692:ILE:HB	1.87	0.56
20:CD:70:THR:HB	20:CD:73:LEU:HB2	1.87	0.56
29:CN:38:ILE:HA	29:CN:111:GLN:O	2.05	0.56
32:CR:530:HIS:HB3	32:CR:533:SER:HB3	1.86	0.56
32:CS:530:HIS:HB3	32:CS:533:SER:HB3	1.86	0.56
13:UQ:369:TYR:OH	13:UQ:383:GLN:NE2	2.38	0.56
13:UQ:543:PHE:HD1	13:UQ:550:LEU:HD13	1.69	0.56
19:CC:208:GLU:HA	19:CC:211:ARG:HE	1.70	0.56
24:CI:59:VAL:O	24:CI:239:ASN:ND2	2.39	0.56
29:CO:111:GLN:NE2	29:CO:113:TYR:OH	2.38	0.56
32:CR:499:THR:H	32:CR:538:GLN:HE22	1.53	0.56
32:CR:897:LEU:HD22	32:CR:908:VAL:HG11	1.86	0.56
32:CS:499:THR:H	32:CS:538:GLN:HE22	1.53	0.56
36:Ce:55:ILE:O	36:Ce:185:ARG:NH2	2.38	0.56
6:UG:425:GLU:O	28:CM:8:ARG:NH2	2.38	0.56
9:UL:133:ASP:OD1	9:UL:149:ARG:NH2	2.38	0.56
9:UL:282:ALA:H	9:UL:297:GLY:HA2	1.70	0.56
16:UX:8:GLY:O	16:UX:14:ARG:NH1	2.39	0.56
24:CI:90:ARG:O	32:CR:90:ASN:ND2	2.39	0.56
24:CI:291:VAL:HG13	24:CI:1008:ILE:HD11	1.88	0.56
3:UC:602:VAL:HG21	45:C1:1061:A:H5'	1.87	0.56
10:UM:759:VAL:HG22	10:UM:797:VAL:HG21	1.87	0.56
12:UO:147:VAL:HA	12:UO:164:SER:HA	1.87	0.56
29:CO:112:ILE:HB	29:CO:124:VAL:HB	1.88	0.56
32:CS:249:ILE:HA	32:CS:252:LEU:HD12	1.87	0.56
32:CS:302:ALA:O	32:CS:306:GLY:N	2.34	0.56
32:CS:591:GLU:OE1	32:CS:612:ASP:N	2.39	0.56
6:UG:267:ASN:ND2	6:UG:270:ASN:OD1	2.39	0.56
10:UM:46:THR:HG22	10:UM:53:ARG:HA	1.87	0.56
12:UO:164:SER:OG	12:UO:165:ASP:N	2.39	0.56
12:UO:203:ASN:HB2	12:UO:219:ALA:HB3	1.88	0.56
14:UR:302:LYS:NZ	14:UR:304:ASP:OD2	2.36	0.56
22:CG:172:THR:HG23	22:CG:583:GLY:HA3	1.87	0.56
32:CR:302:ALA:O	32:CR:306:GLY:N	2.34	0.56
32:CS:849:LEU:HB2	32:CS:853:VAL:HG21	1.87	0.56
51:CX:267:GLU:HA	51:CX:271:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:572:ARG:NH2	9:UL:613:MET:O	2.39	0.56
15:UU:665:MET:HG2	15:UU:666:THR:HG23	1.87	0.56
30:CP:70:THR:HG1	30:CP:79:THR:HG1	1.53	0.56
31:CQ:198:LYS:NZ	45:C1:2352:U:O2	2.38	0.56
23:CH:179:SER:HB2	23:CH:260:PRO:HG3	1.88	0.56
28:CM:322:HIS:NE2	28:CM:396:HIS:O	2.39	0.56
49:US:444:GLU:HB3	49:US:450:THR:HG22	1.87	0.56
1:UA:558:ARG:NH1	46:C2:62:A:OP2	2.37	0.56
4:UD:685:THR:O	45:C1:63:C:O2'	2.24	0.56
9:UL:18:VAL:HG21	9:UL:24:LEU:HD11	1.88	0.56
10:UM:145:VAL:O	45:C1:2359:A:O2'	2.24	0.56
23:CH:109:GLY:HA2	23:CH:138:ILE:HG23	1.87	0.56
30:CP:191:ASN:O	45:C1:1612:A:N6	2.39	0.56
38:Ch:96:VAL:HG11	38:Ch:150:VAL:HG11	1.88	0.56
1:UA:536:PHE:HB2	1:UA:546:SER:HB2	1.88	0.56
24:CI:921:VAL:HG22	24:CI:988:ILE:HG22	1.88	0.56
30:CP:104:ARG:NH2	30:CP:168:THR:OG1	2.39	0.56
32:CR:591:GLU:OE1	32:CR:612:ASP:N	2.39	0.56
47:UH:557:GLU:H	47:UH:566:ARG:H	1.53	0.56
4:UD:280:LEU:HD21	52:UP:347:LEU:HD21	1.86	0.55
4:UD:366:PRO:HB3	4:UD:704:VAL:HG11	1.89	0.55
9:UL:914:LYS:HZ1	10:UM:875:GLU:HG3	1.69	0.55
10:UM:477:GLY:O	10:UM:539:ARG:NH2	2.40	0.55
29:CO:178:VAL:HA	29:CO:223:GLU:O	2.06	0.55
42:Cn:102:VAL:HG22	42:Cn:127:VAL:HG22	1.88	0.55
13:UQ:699:ILE:HD11	13:UQ:714:ALA:HB1	1.89	0.55
25:CJ:85:MET:HE1	27:CL:630:LEU:HD22	1.88	0.55
4:UD:183:PRO:HB3	21:CE:17:LEU:HD22	1.88	0.55
4:UD:686:ARG:NH1	45:C1:63:C:O2	2.38	0.55
9:UL:384:GLN:NE2	9:UL:398:ASN:OD1	2.40	0.55
9:UL:473:PHE:HA	9:UL:480:VAL:HA	1.89	0.55
13:UQ:95:ILE:HG13	13:UQ:104:ILE:HB	1.88	0.55
28:CM:367:ARG:NH2	46:C2:38:G:OP1	2.38	0.55
24:CI:607:LYS:O	24:CI:611:SER:HB2	2.06	0.55
26:CK:94:ARG:NH2	45:C1:2189:C:OP2	2.39	0.55
29:CN:99:LEU:HD21	29:CN:238:CYS:HB3	1.89	0.55
32:CR:132:THR:H	32:CR:135:ILE:HD11	1.71	0.55
33:CT:107:GLN:NE2	45:C1:402:U:OP2	2.40	0.55
51:CX:419:GLN:O	51:CX:422:ARG:NH2	2.39	0.55
4:UD:75:ARG:HD3	52:UP:332:ALA:HB3	1.88	0.55
4:UD:399:SER:OG	4:UD:400:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CJ:115:MET:HB2	25:CJ:120:MET:HB2	1.88	0.55
28:CM:403:LYS:HD3	45:C1:1664:U:H4'	1.88	0.55
32:CR:249:ILE:HA	32:CR:252:LEU:HD12	1.87	0.55
14:UR:363:ILE:HG23	14:UR:401:ILE:HD11	1.87	0.55
15:UU:197:ASN:HD21	20:CD:446:GLY:HA2	1.72	0.55
24:CI:845:LEU:HD11	24:CI:998:LYS:HB2	1.87	0.55
25:CJ:54:LEU:HD21	25:CJ:82:LEU:HD21	1.89	0.55
26:CK:53:ARG:HD3	44:CU:210:ILE:HG21	1.87	0.55
32:CR:10:ARG:NH1	32:CR:215:LYS:O	2.40	0.55
1:UA:78:GLN:OE1	45:C1:257:G:N2	2.40	0.55
1:UA:444:SER:OG	1:UA:445:ILE:N	2.37	0.55
9:UL:377:ASN:ND2	9:UL:384:GLN:OE1	2.39	0.55
15:UU:668:ILE:HA	15:UU:684:CYS:HA	1.89	0.55
17:UZ:265:GLU:O	17:UZ:269:ARG:HB3	2.06	0.55
18:CB:222:MET:HE2	20:CD:124:GLN:HB2	1.89	0.55
32:CR:714:GLU:OE1	32:CR:714:GLU:N	2.37	0.55
12:UO:547:VAL:HG13	48:UE:239:LEU:HD22	1.89	0.55
13:UQ:581:ARG:NH2	13:UQ:613:SER:OG	2.38	0.55
34:Ca:87:ARG:HH22	34:Ca:220:GLN:HG3	1.72	0.55
41:Cm:55:ASN:ND2	45:C1:1449:U:O4	2.39	0.55
49:US:221:ASN:OD1	49:US:281:GLN:NE2	2.40	0.55
24:CI:344:MET:HB3	24:CI:353:ILE:HG22	1.89	0.55
32:CS:132:THR:H	32:CS:135:ILE:HD11	1.71	0.55
45:C1:1448:A:C6	45:C1:1549:U:O4	2.60	0.55
11:UN:903:LEU:O	28:CM:381:ARG:NH2	2.31	0.55
13:UQ:89:MET:HE2	13:UQ:414:HIS:HD2	1.72	0.55
20:CD:16:PHE:HA	20:CD:45:TYR:HA	1.88	0.55
26:CK:173:ARG:NH2	26:CK:182:GLY:O	2.40	0.55
29:CN:35:LYS:NZ	29:CN:197:GLY:O	2.40	0.54
45:C1:2358:U:O4	45:C1:2369:G:O6	2.25	0.54
47:UH:634:THR:O	47:UH:713:LYS:NZ	2.40	0.54
10:UM:155:LEU:HB3	10:UM:203:GLN:HB2	1.88	0.54
14:UR:550:PRO:HD2	14:UR:599:SER:HB2	1.89	0.54
16:UX:90:ILE:HG22	16:UX:119:GLN:HB2	1.89	0.54
18:CB:97:LEU:HD23	18:CB:200:ARG:HG2	1.87	0.54
23:CH:22:VAL:HG21	23:CH:116:PRO:HB3	1.88	0.54
32:CR:142:THR:O	32:CR:142:THR:OG1	2.24	0.54
32:CR:623:GLN:H	32:CS:839:LYS:NZ	2.04	0.54
35:Cc:50:GLN:HG2	35:Cc:52:ARG:HH11	1.73	0.54
49:US:205:LYS:HD2	49:US:267:GLU:HB3	1.88	0.54
1:UA:258:LEU:HA	1:UA:274:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:19:VAL:HG22	4:UD:46:ILE:HG12	1.88	0.54
10:UM:568:VAL:HG22	10:UM:589:VAL:HG11	1.89	0.54
23:CH:124:SER:OG	23:CH:199:GLN:NE2	2.40	0.54
28:CM:264:ILE:HB	28:CM:279:GLN:HB2	1.89	0.54
30:CP:183:ARG:NH2	45:C1:1488:U:OP1	2.39	0.54
32:CS:10:ARG:NH1	32:CS:215:LYS:O	2.40	0.54
34:Ca:172:ILE:HD13	34:Ca:193:ILE:HG21	1.88	0.54
1:UA:270:LEU:HD13	1:UA:284:MET:HE3	1.90	0.54
1:UA:509:LEU:HD11	1:UA:527:ILE:HD12	1.89	0.54
9:UL:21:ASN:OD1	9:UL:69:ARG:NH1	2.40	0.54
18:CB:218:MET:HE3	20:CD:10:SER:HA	1.89	0.54
34:Ca:69:CYS:SG	34:Ca:70:LEU:N	2.81	0.54
45:C1:1735:A:H2'	45:C1:1736:A:H8	1.72	0.54
1:UA:558:ARG:HB2	1:UA:566:ALA:HB2	1.90	0.54
2:UB:702:LEU:HD11	2:UB:728:THR:HG21	1.89	0.54
4:UD:162:ASN:HB3	4:UD:181:ARG:HB3	1.88	0.54
4:UD:646:ASP:HB3	4:UD:658:ILE:HD11	1.88	0.54
15:UU:391:LEU:HD22	15:UU:408:LEU:HD21	1.88	0.54
18:CB:204:ILE:HG22	20:CD:143:LEU:HG	1.88	0.54
23:CH:339:MET:HB3	23:CH:398:VAL:HG21	1.89	0.54
30:CP:152:LYS:HD2	44:CU:169:HIS:HD2	1.72	0.54
41:Cm:85:GLU:HA	44:CU:300:VAL:HG21	1.88	0.54
45:C1:22:U:H2'	45:C1:23:G:H8	1.73	0.54
49:US:357:ARG:NH1	49:US:395:SER:OG	2.40	0.54
4:UD:383:ILE:HD12	4:UD:863:ILE:HD11	1.89	0.54
7:UJ:252:GLY:O	7:UJ:256:SER:HB3	2.08	0.54
9:UL:284:VAL:HG22	9:UL:295:VAL:HG22	1.90	0.54
12:UO:162:SER:O	12:UO:169:VAL:HA	2.07	0.54
13:UQ:254:VAL:HG21	13:UQ:295:ILE:HG21	1.89	0.54
17:UZ:77:ARG:NH2	45:C1:373:C:O2'	2.41	0.54
18:CA:191:ARG:NH2	19:CC:171:HIS:O	2.41	0.54
20:CD:240:ALA:O	20:CD:244:SER:HB3	2.07	0.54
24:CI:173:LEU:HD23	24:CI:182:LEU:HD11	1.89	0.54
27:CL:712:GLU:OE1	45:C1:2222:C:N4	2.40	0.54
1:UA:170:SER:OG	1:UA:171:LYS:N	2.40	0.54
4:UD:546:ASP:OD1	4:UD:546:ASP:N	2.39	0.54
9:UL:460:ILE:HG13	9:UL:461:ARG:HG2	1.90	0.54
13:UQ:449:ASP:HB2	13:UQ:454:ARG:HE	1.72	0.54
22:CG:344:CYS:HB2	22:CG:357:TRP:HB2	1.90	0.54
43:Cp:20:THR:HG21	43:Cp:28:GLN:HB2	1.89	0.54
13:UQ:694:SER:OG	13:UQ:695:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:173:VAL:HG13	22:CG:581:VAL:HG13	1.89	0.54
24:CI:54:LEU:HB3	42:Cn:77:ILE:HG21	1.90	0.54
45:C1:495:G:N7	45:C1:504:C:N4	2.56	0.54
1:UA:170:SER:OG	1:UA:172:ASP:OD1	2.24	0.54
6:UG:264:LEU:HD13	6:UG:275:ILE:HG22	1.89	0.54
10:UM:459:LEU:HB2	10:UM:473:ALA:HB3	1.90	0.54
31:CQ:208:ARG:NH1	31:CQ:209:ILE:O	2.41	0.54
49:US:352:LEU:O	49:US:357:ARG:NH2	2.37	0.54
49:US:387:ARG:NH2	49:US:438:ASP:OD2	2.41	0.54
16:UX:13:ARG:HB3	25:CJ:19:ILE:HG13	1.89	0.54
17:UZ:64:LEU:HD12	17:UZ:281:PHE:HB3	1.89	0.54
28:CM:423:ARG:NH1	28:CM:431:GLU:O	2.41	0.54
7:UJ:126:ARG:NH2	7:UJ:129:GLU:OE1	2.40	0.53
9:UL:942:GLU:HG2	9:UL:943:THR:HG23	1.89	0.53
10:UM:375:GLU:HG3	10:UM:713:SER:HA	1.89	0.53
10:UM:592:VAL:HA	10:UM:616:LEU:O	2.08	0.53
9:UL:595:ASP:OD1	9:UL:595:ASP:N	2.41	0.53
9:UL:622:ILE:HD11	9:UL:636:LEU:HD13	1.90	0.53
13:UQ:208:LEU:HD12	13:UQ:244:LEU:HB2	1.90	0.53
17:UZ:217:ILE:HG13	17:UZ:218:PRO:HD3	1.90	0.53
45:C1:2177:G:O2'	45:C1:2183:A:N6	2.40	0.53
48:UI:156:VAL:O	48:UI:159:GLN:NE2	2.37	0.53
38:Ch:130:LYS:NZ	38:Ch:139:TRP:O	2.41	0.53
2:UB:339:ARG:HH21	2:UB:649:PHE:HZ	1.55	0.53
6:UG:137:LEU:HD13	6:UG:159:HIS:HB2	1.89	0.53
32:CR:620:GLN:O	32:CR:623:GLN:NE2	2.42	0.53
45:C1:1456:A:H2'	45:C1:1457:G:C8	2.43	0.53
12:UO:482:LEU:HD22	12:UO:505:LEU:HD13	1.90	0.53
13:UQ:251:ARG:HA	13:UQ:266:LEU:HD22	1.89	0.53
14:UR:474:PRO:HG2	14:UR:477:LEU:HB2	1.90	0.53
19:CC:212:ILE:HG23	19:CC:213:VAL:HG23	1.90	0.53
24:CI:1077:GLN:NE2	45:C1:366:G:OP1	2.41	0.53
30:CP:188:THR:HG23	30:CP:194:PRO:HD3	1.90	0.53
32:CS:166:THR:HG21	32:CS:211:ILE:HD12	1.91	0.53
15:UU:406:LYS:HB2	15:UU:423:ARG:HE	1.73	0.53
18:CB:239:VAL:HG21	18:CB:255:ILE:HD12	1.91	0.53
18:CB:265:THR:HG21	21:CE:124:ARG:HH11	1.72	0.53
23:CH:151:ASP:OD1	23:CH:154:ARG:NH2	2.42	0.53
1:UA:844:LEU:HD13	15:UU:1006:ILE:HD11	1.91	0.53
4:UD:278:ASP:N	4:UD:278:ASP:OD1	2.40	0.53
20:CD:217:ARG:NH2	20:CD:246:GLY:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:528:ARG:HH22	4:UD:547:ARG:HB3	1.73	0.53
6:UG:293:LEU:HD23	6:UG:461:LEU:HG	1.91	0.53
10:UM:697:TRP:HB2	10:UM:712:GLY:HA2	1.90	0.53
13:UQ:437:ILE:O	13:UQ:501:GLN:NE2	2.41	0.53
14:UR:267:ARG:O	14:UR:312:ASN:ND2	2.41	0.53
15:UU:82:LEU:O	45:C1:259:U:O2'	2.25	0.53
28:CM:171:SER:OG	28:CM:200:ILE:O	2.27	0.53
29:CN:190:ARG:NH1	29:CN:247:ASP:OD1	2.42	0.53
12:UO:126:PHE:HB3	12:UO:136:ILE:HA	1.91	0.53
15:UU:521:ALA:HB2	15:UU:544:VAL:HG11	1.91	0.53
16:UX:41:PRO:HG2	16:UX:44:MET:HG3	1.91	0.53
29:CO:143:GLN:HG3	29:CO:150:ILE:HD11	1.91	0.53
1:UA:319:LEU:HB3	1:UA:337:GLN:HE22	1.74	0.53
1:UA:548:VAL:HG23	1:UA:604:MET:HE3	1.91	0.53
14:UR:262:ASP:CB	14:UR:617:ARG:O	2.57	0.53
19:CC:195:ALA:HB1	19:CC:216:ASN:HB2	1.91	0.53
28:CM:417:ARG:NH1	45:C1:1627:G:OP1	2.41	0.53
35:Cc:87:HIS:HD2	35:Cc:167:ARG:HD2	1.74	0.53
47:UH:883:ARG:NH2	47:UH:887:GLU:OE2	2.42	0.53
4:UD:257:GLN:HE22	4:UD:271:ARG:HH21	1.57	0.52
17:UZ:282:TYR:CD1	17:UZ:292:PRO:HA	2.44	0.52
24:CI:63:PRO:HG2	24:CI:66:PRO:HA	1.91	0.52
19:CC:241:ALA:HA	19:CC:246:GLN:HB2	1.90	0.52
35:Cc:84:LEU:O	35:Cc:167:ARG:NH2	2.43	0.52
51:CX:371:LEU:HD21	51:CX:417:PHE:HB2	1.90	0.52
1:UA:635:PRO:HD2	1:UA:638:LEU:HD13	1.90	0.52
9:UL:587:SER:HA	9:UL:609:PRO:HA	1.91	0.52
10:UM:651:LEU:HG	10:UM:666:PHE:HA	1.91	0.52
18:CA:173:ILE:O	33:CT:91:TYR:OH	2.25	0.52
23:CH:296:GLU:OE1	23:CH:316:GLN:NE2	2.42	0.52
32:CR:876:LEU:HD12	32:CR:880:GLN:HE22	1.74	0.52
33:CT:189:ARG:NH2	45:C1:2072:U:O4	2.42	0.52
34:Ca:82:ARG:HB2	34:Ca:103:LEU:HD11	1.91	0.52
49:US:538:LEU:O	49:US:542:TRP:HB2	2.10	0.52
52:UP:337:LYS:O	52:UP:341:ASN:ND2	2.43	0.52
2:UB:618:ILE:O	2:UB:622:LEU:HB2	2.10	0.52
10:UM:711:ALA:HB2	10:UM:717:VAL:HG13	1.90	0.52
13:UQ:295:ILE:HG22	13:UQ:314:VAL:HG22	1.90	0.52
15:UU:71:LEU:H	15:UU:86:THR:HB	1.72	0.52
18:CB:250:GLY:CA	18:CB:306:TYR:O	2.58	0.52
32:CR:166:THR:HG21	32:CR:211:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:523:ARG:HA	32:CS:526:LEU:HB3	1.91	0.52
34:Ca:33:LYS:HA	34:Ca:41:ARG:O	2.09	0.52
1:UA:500:ARG:NH1	45:C1:1740:C:OP2	2.42	0.52
10:UM:628:ASN:HB3	10:UM:635:ILE:HD11	1.91	0.52
11:UN:905:VAL:N	28:CM:39:GLU:OE2	2.41	0.52
26:CK:237:ILE:HG23	26:CK:263:MET:HG3	1.91	0.52
28:CM:47:VAL:HG21	28:CM:388:ILE:HG23	1.92	0.52
45:C1:467:C:H4'	45:C1:468:C:H5'	1.91	0.52
45:C1:1457:G:N2	45:C1:1632:G:O2'	2.43	0.52
47:UH:554:PHE:HB3	47:UH:567:LEU:HD12	1.92	0.52
48:UI:185:ILE:O	48:UI:225:HIS:NE2	2.38	0.52
17:UZ:66:LEU:HD12	17:UZ:266:LEU:HD13	1.91	0.52
18:CA:222:MET:SD	19:CC:136:THR:OG1	2.64	0.52
19:CC:380:ARG:NH2	46:C2:111:G:O6	2.43	0.52
20:CD:6:LEU:HB3	20:CD:90:VAL:HG22	1.92	0.52
21:CE:53:VAL:O	21:CE:79:TYR:HA	2.10	0.52
32:CS:876:LEU:HD12	32:CS:880:GLN:HE22	1.74	0.52
49:US:139:LEU:HD23	49:US:184:HIS:HD2	1.75	0.52
1:UA:173:LEU:HA	1:UA:197:GLY:HA2	1.91	0.52
2:UB:652:ARG:O	2:UB:740:TRP:NE1	2.43	0.52
9:UL:41:VAL:HG11	9:UL:394:LEU:HD21	1.92	0.52
10:UM:563:SER:OG	10:UM:565:ASP:OD1	2.26	0.52
18:CA:286:PRO:HA	18:CA:304:CYS:HB3	1.92	0.52
28:CM:293:PRO:HG2	28:CM:338:SER:HB2	1.91	0.52
30:CP:132:ASN:HB3	30:CP:135:ARG:HB3	1.91	0.52
31:CQ:83:ARG:NH1	31:CQ:137:GLN:OE1	2.43	0.52
45:C1:1735:A:H2'	45:C1:1736:A:C8	2.45	0.52
2:UB:799:GLU:OE1	2:UB:802:HIS:NE2	2.43	0.52
13:UQ:91:ASP:O	13:UQ:401:ASN:ND2	2.43	0.52
20:CD:183:ALA:HB1	20:CD:204:ASN:HB2	1.91	0.52
32:CR:523:ARG:HA	32:CR:526:LEU:HB3	1.91	0.52
32:CR:749:GLN:HG2	32:CS:855:LEU:HD22	1.92	0.52
45:C1:1029:A:H61	45:C1:1046:G:H1'	1.73	0.52
1:UA:176:ARG:HG2	1:UA:190:VAL:HG23	1.91	0.52
15:UU:256:GLN:HG2	15:UU:263:THR:HA	1.91	0.52
18:CA:308:GLN:HE22	18:CA:313:GLY:HA2	1.74	0.52
36:Ce:17:GLN:HE21	36:Ce:51:SER:HA	1.75	0.52
37:Cg:108:GLN:HE21	37:Cg:120:ILE:HG22	1.75	0.52
47:UH:598:ASP:OD1	47:UH:598:ASP:N	2.34	0.52
2:UB:796:ARG:NH1	49:US:431:LEU:O	2.42	0.52
4:UD:363:ARG:NH2	4:UD:686:ARG:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:862:ASN:OD1	9:UL:905:ASN:ND2	2.43	0.52
20:CD:15:LEU:HD11	20:CD:76:LEU:HD21	1.91	0.52
24:CI:856:ARG:NH1	45:C1:1143:C:OP1	2.38	0.52
28:CM:72:MET:HE2	28:CM:333:MET:HE2	1.91	0.52
28:CM:216:VAL:HG12	28:CM:222:ILE:HG22	1.92	0.52
32:CS:30:VAL:HG22	32:CS:153:LEU:HD12	1.90	0.52
32:CS:194:GLY:HA2	32:CS:212:SER:HB3	1.92	0.52
34:Ca:204:ILE:O	45:C1:1648:G:O2'	2.28	0.52
45:C1:1613:C:H4'	45:C1:1614:U:H5'	1.92	0.52
2:UB:800:LEU:HD23	49:US:479:SER:HA	1.91	0.51
9:UL:427:THR:OG1	9:UL:428:ASP:N	2.43	0.51
9:UL:861:LEU:HD21	9:UL:877:ILE:HD11	1.92	0.51
12:UO:1:MET:HG3	13:UQ:430:PRO:HG3	1.92	0.51
26:CK:139:ILE:HG22	26:CK:155:SER:HB2	1.92	0.51
32:CR:824:LEU:HB3	32:CR:869:ARG:HB3	1.92	0.51
32:CR:826:LYS:HA	32:CR:829:LEU:HD12	1.93	0.51
51:CX:407:PRO:HB2	51:CX:409:ILE:HG22	1.92	0.51
1:UA:217:GLY:HA2	1:UA:258:LEU:HD23	1.91	0.51
10:UM:644:ASN:O	10:UM:671:ALA:N	2.42	0.51
14:UR:170:GLU:OE2	14:UR:174:ARG:NH2	2.43	0.51
24:CI:45:ARG:NH2	45:C1:615:A:OP1	2.43	0.51
32:CS:620:GLN:O	32:CS:623:GLN:NE2	2.42	0.51
40:Cj:83:GLN:HE22	40:Cj:119:ALA:HB2	1.75	0.51
45:C1:1138:C:N4	45:C1:1155:G:O6	2.43	0.51
4:UD:158:THR:OG1	4:UD:159:VAL:N	2.41	0.51
9:UL:626:SER:OG	9:UL:627:ALA:N	2.43	0.51
13:UQ:119:SER:HB3	13:UQ:432:MET:HG2	1.91	0.51
13:UQ:759:ASP:OD1	47:UH:543:ARG:NH1	2.43	0.51
47:UH:542:ASP:OD1	47:UH:542:ASP:N	2.43	0.51
3:UC:601:ARG:HH21	37:Cg:121:HIS:HD2	1.58	0.51
8:UK:91:ARG:NH1	24:CI:1068:LYS:O	2.41	0.51
22:CG:482:SER:OG	22:CG:483:TRP:N	2.42	0.51
47:UH:726:LEU:O	47:UH:730:PHE:HB2	2.11	0.51
3:UC:639:LYS:HD2	3:UC:642:LEU:HD22	1.92	0.51
10:UM:249:SER:O	10:UM:256:MET:HA	2.11	0.51
18:CB:180:VAL:O	18:CB:203:VAL:HA	2.11	0.51
28:CM:345:SER:OG	28:CM:346:ASP:N	2.42	0.51
32:CR:30:VAL:HG22	32:CR:153:LEU:HD12	1.91	0.51
32:CR:71:ARG:NH1	32:CR:100:SER:O	2.44	0.51
4:UD:509:ALA:HB1	4:UD:516:ILE:HD11	1.92	0.51
14:UR:258:PRO:O	14:UR:575:THR:OG1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CM:323:THR:HG22	28:CM:325:ARG:H	1.76	0.51
32:CS:824:LEU:HB3	32:CS:869:ARG:HB3	1.92	0.51
45:C1:2238:A:N6	45:C1:2328:G:H21	2.05	0.51
13:UQ:112:GLN:NE2	13:UQ:114:TYR:OH	2.44	0.51
15:UU:189:ALA:HB2	15:UU:201:VAL:HG12	1.93	0.51
15:UU:235:LEU:HA	15:UU:245:ALA:O	2.11	0.51
24:CI:937:MET:O	27:CL:511:ARG:NH2	2.35	0.51
46:C2:160:U:H2'	46:C2:161:G:C8	2.45	0.51
51:CX:342:ILE:HG12	51:CX:385:LEU:HD21	1.92	0.51
1:UA:531:ASP:O	1:UA:551:ARG:NH2	2.41	0.51
9:UL:444:ALA:HB1	9:UL:468:ALA:HB1	1.93	0.51
19:CC:20:VAL:HG11	19:CC:130:LEU:HD21	1.92	0.51
28:CM:78:SER:OG	28:CM:79:LEU:N	2.41	0.51
32:CR:194:GLY:HA2	32:CR:212:SER:HB3	1.92	0.51
45:C1:1626:G:H2'	45:C1:1627:G:C8	2.46	0.51
6:UG:100:LEU:HD23	6:UG:421:PRO:HG2	1.93	0.51
22:CG:297:ARG:NH1	22:CG:342:GLU:OE2	2.43	0.51
24:CI:963:LYS:NZ	45:C1:2181:U:OP2	2.44	0.51
28:CM:213:ILE:HD11	28:CM:227:LEU:HD12	1.93	0.51
34:Ca:216:LYS:NZ	45:C1:1470:G:OP1	2.39	0.51
45:C1:1625:G:N2	45:C1:1663:U:O2	2.44	0.51
2:UB:590:ASP:HA	2:UB:593:ILE:HG22	1.92	0.51
17:UZ:282:TYR:HE1	17:UZ:292:PRO:HB3	1.76	0.51
24:CI:252:ILE:O	24:CI:267:THR:OG1	2.27	0.51
36:Ce:41:LYS:HA	36:Ce:44:LEU:HD13	1.93	0.51
40:Cj:16:ALA:HB2	40:Cj:72:GLY:HA3	1.93	0.51
45:C1:493:G:H2'	45:C1:494:G:C8	2.45	0.51
45:C1:1747:A:N3	45:C1:2196:U:O2'	2.37	0.51
49:US:191:LYS:NZ	49:US:232:ASP:OD1	2.44	0.51
4:UD:876:TYR:HB3	52:UP:351:ARG:HD3	1.93	0.50
5:UF:32:GLU:HG2	14:UR:60:LEU:HD21	1.93	0.50
17:UZ:284:LYS:NZ	17:UZ:288:THR:O	2.45	0.50
42:Cn:65:ASN:HB2	45:C1:1154:A:H5'	1.93	0.50
44:CU:150:ASP:OD1	44:CU:150:ASP:N	2.40	0.50
44:CU:249:ARG:NH2	45:C1:1519:C:O2'	2.45	0.50
47:UH:754:ARG:O	48:UI:207:ARG:NH1	2.36	0.50
1:UA:466:GLY:O	1:UA:493:ARG:NH2	2.44	0.50
2:UB:726:LEU:HD22	2:UB:773:LEU:HD13	1.92	0.50
4:UD:19:VAL:HG13	4:UD:44:LEU:HD11	1.92	0.50
6:UG:58:VAL:HG11	6:UG:72:LEU:HD12	1.93	0.50
6:UG:139:PRO:HA	6:UG:412:ASN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CA:108:ARG:HG3	33:CT:141:ILE:HD12	1.93	0.50
23:CH:175:VAL:HG12	23:CH:192:VAL:HG12	1.92	0.50
29:CN:27:ILE:HD13	29:CN:36:ARG:HE	1.75	0.50
34:Ca:33:LYS:O	34:Ca:98:THR:OG1	2.28	0.50
34:Ca:131:ASP:OD2	34:Ca:180:THR:OG1	2.27	0.50
44:CU:191:THR:HA	44:CU:194:ARG:HE	1.76	0.50
44:CU:272:PRO:HB2	44:CU:275:LEU:HG	1.92	0.50
1:UA:568:ASN:ND2	46:C2:61:G:OP1	2.42	0.50
9:UL:451:ILE:HG12	9:UL:461:ARG:HB2	1.92	0.50
9:UL:574:SER:HA	9:UL:615:ILE:HD11	1.94	0.50
12:UO:404:ILE:HG23	14:UR:319:HIS:HD2	1.76	0.50
13:UQ:299:ILE:O	13:UQ:310:GLN:NE2	2.44	0.50
22:CG:337:ASP:HB3	22:CG:403:MET:HG3	1.93	0.50
22:CG:470:ARG:NH1	22:CG:563:ILE:O	2.44	0.50
32:CS:71:ARG:NH1	32:CS:100:SER:O	2.44	0.50
5:UF:154:ASN:ND2	5:UF:156:ASP:OD2	2.45	0.50
15:UU:157:THR:HG22	15:UU:184:GLU:HA	1.93	0.50
29:CN:124:VAL:HG22	29:CN:160:LEU:HD22	1.93	0.50
34:Ca:149:GLN:HE22	34:Ca:154:THR:HG22	1.75	0.50
45:C1:351:U:C4	45:C1:353:G:C6	3.00	0.50
45:C1:1744:A:H2'	45:C1:1745:C:H6	1.76	0.50
51:CX:234:ILE:HD12	51:CX:269:ILE:HD11	1.93	0.50
1:UA:112:VAL:HG13	1:UA:157:LEU:HD13	1.94	0.50
6:UG:63:VAL:O	6:UG:69:ARG:NH2	2.43	0.50
10:UM:619:SER:OG	10:UM:621:ASP:OD1	2.27	0.50
19:CC:240:LEU:HA	19:CC:243:VAL:HB	1.93	0.50
37:Cg:33:GLY:H	37:Cg:120:ILE:HG21	1.75	0.50
51:CX:313:SER:OG	51:CX:314:GLY:N	2.45	0.50
48:UI:214:LEU:HA	48:UI:217:TRP:HB2	1.94	0.50
4:UD:741:SER:OG	4:UD:742:GLY:N	2.42	0.50
7:UJ:236:ARG:HD2	7:UJ:239:ILE:HD12	1.93	0.50
10:UM:626:LEU:O	10:UM:635:ILE:N	2.44	0.50
24:CI:819:ARG:NH1	24:CI:823:HIS:O	2.44	0.50
25:CJ:61:LEU:HD23	27:CL:619:ILE:HD13	1.93	0.50
27:CL:572:ARG:NH1	45:C1:2213:U:OP1	2.45	0.50
32:CR:303:VAL:HB	32:CR:365:HIS:HE1	1.76	0.50
37:Cg:111:VAL:HG13	37:Cg:116:LEU:HD12	1.93	0.50
42:Cn:139:LYS:NZ	45:C1:618:C:O3'	2.45	0.50
49:US:461:VAL:HA	49:US:464:GLN:HG3	1.93	0.50
51:CX:414:LEU:HG	51:CX:449:ILE:HG21	1.91	0.50
1:UA:156:HIS:HB3	1:UA:169:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:668:GLU:HA	4:UD:671:ARG:HG2	1.93	0.50
6:UG:282:VAL:HG11	6:UG:306:LEU:HD21	1.93	0.50
15:UU:141:ILE:HA	15:UU:155:ALA:HA	1.92	0.50
15:UU:313:LEU:HA	15:UU:317:GLY:HA2	1.93	0.50
15:UU:433:GLN:HB2	15:UU:436:ILE:HD11	1.94	0.50
23:CH:228:ALA:HA	45:C1:1714:G:H22	1.77	0.50
31:CQ:171:ILE:HD11	31:CQ:236:VAL:HG11	1.94	0.50
32:CS:826:LYS:HA	32:CS:829:LEU:HD12	1.92	0.50
9:UL:861:LEU:HD22	9:UL:874:THR:HG23	1.94	0.50
10:UM:328:LEU:O	10:UM:330:GLU:N	2.45	0.50
10:UM:393:THR:OG1	10:UM:394:ASN:N	2.41	0.50
10:UM:702:HIS:CD2	10:UM:705:THR:H	2.28	0.50
12:UO:436:ALA:HB1	12:UO:456:LEU:HD11	1.93	0.50
13:UQ:195:ILE:O	13:UQ:201:VAL:HA	2.12	0.50
23:CH:168:PRO:HA	23:CH:171:ILE:HG12	1.92	0.50
35:Cc:93:LYS:NZ	45:C1:2110:C:OP1	2.43	0.50
45:C1:1759:U:O4	45:C1:2047:G:C6	2.65	0.50
4:UD:227:THR:OG1	14:UR:391:ASP:OD2	2.30	0.50
4:UD:378:PRO:HB3	4:UD:841:ILE:HA	1.92	0.50
12:UO:331:ASP:OD1	12:UO:331:ASP:N	2.38	0.50
20:CD:270:TYR:HD1	20:CD:273:GLN:HE21	1.58	0.50
29:CO:88:ARG:O	29:CO:90:ASP:N	2.44	0.50
32:CS:303:VAL:HB	32:CS:365:HIS:HE1	1.76	0.50
34:Ca:38:PHE:O	34:Ca:41:ARG:NH2	2.45	0.50
47:UH:575:SER:HA	47:UH:578:ILE:HG22	1.92	0.50
4:UD:269:ALA:O	4:UD:312:ARG:NH2	2.45	0.49
5:UF:361:LEU:HD23	5:UF:364:LEU:HD23	1.94	0.49
10:UM:398:ILE:HB	10:UM:429:LEU:HG	1.93	0.49
10:UM:559:PHE:O	10:UM:570:ILE:HA	2.11	0.49
17:UZ:105:GLN:NE2	17:UZ:127:VAL:O	2.45	0.49
32:CR:283:LEU:HD12	32:CR:472:ILE:HG12	1.93	0.49
1:UA:516:VAL:HG22	1:UA:527:ILE:HG22	1.93	0.49
8:UK:59:ASN:HD21	25:CJ:120:MET:HE2	1.77	0.49
9:UL:490:GLN:HG3	9:UL:502:THR:HG23	1.94	0.49
9:UL:615:ILE:HG22	9:UL:622:ILE:HG23	1.94	0.49
12:UO:339:GLN:NE2	50:Cl:5:SER:OG	2.46	0.49
13:UQ:144:VAL:O	13:UQ:445:ARG:NH2	2.45	0.49
17:UZ:282:TYR:OH	17:UZ:294:TYR:HE1	1.95	0.49
23:CH:261:LEU:HA	23:CH:271:LYS:O	2.12	0.49
46:C2:101:G:O6	46:C2:251:U:O4	2.29	0.49
9:UL:200:LEU:HB3	9:UL:210:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:896:ARG:HH22	10:UM:892:ASP:HB2	1.77	0.49
20:CD:363:ARG:NH1	46:C2:85:A:OP2	2.44	0.49
23:CH:235:MET:HE2	23:CH:279:LEU:HB2	1.94	0.49
51:CX:338:SER:HB3	51:CX:370:LEU:HD11	1.93	0.49
1:UA:278:ILE:HA	1:UA:294:SER:HA	1.94	0.49
6:UG:303:VAL:HA	6:UG:319:GLY:HA2	1.94	0.49
6:UG:567:LYS:HA	6:UG:570:ARG:HD2	1.94	0.49
9:UL:304:ILE:HD11	9:UL:385:LEU:HD22	1.95	0.49
10:UM:513:GLY:HA3	10:UM:547:ILE:HD11	1.95	0.49
22:CG:179:CYS:HB3	22:CG:182:TYR:HB2	1.94	0.49
39:CI:35:SER:OG	39:CI:36:PHE:N	2.45	0.49
2:UB:572:ARG:NH1	2:UB:609:GLN:OE1	2.45	0.49
4:UD:75:ARG:HG2	52:UP:334:LYS:HA	1.93	0.49
4:UD:387:TRP:NE1	4:UD:390:GLU:OE2	2.45	0.49
10:UM:755:ARG:HG3	10:UM:793:ALA:HB1	1.94	0.49
13:UQ:927:ALA:O	13:UQ:931:ASN:HB2	2.11	0.49
14:UR:343:ARG:HB2	14:UR:344:ARG:HH11	1.76	0.49
24:CI:1099:THR:HG22	45:C1:400:C:H5'	1.94	0.49
28:CM:132:ILE:HG12	28:CM:150:TRP:HB2	1.95	0.49
4:UD:7:ARG:HH21	47:UH:904:ARG:HB2	1.77	0.49
9:UL:138:ASP:HB2	9:UL:145:GLN:HE21	1.78	0.49
13:UQ:561:ARG:NH1	13:UQ:562:ASP:OD1	2.45	0.49
13:UQ:765:TYR:OH	13:UQ:819:GLU:O	2.31	0.49
22:CG:273:TYR:HA	22:CG:281:ILE:HG12	1.94	0.49
30:CP:82:THR:HB	30:CP:86:THR:HG21	1.95	0.49
32:CS:28:VAL:HG21	32:CS:193:LEU:HD11	1.95	0.49
32:CS:283:LEU:HD12	32:CS:472:ILE:HG12	1.93	0.49
48:UI:229:LEU:HG	48:UI:236:ILE:HG12	1.95	0.49
4:UD:383:ILE:HG12	4:UD:394:TRP:HB2	1.94	0.49
4:UD:390:GLU:OE1	4:UD:422:GLN:NE2	2.45	0.49
18:CA:102:SER:OG	18:CA:108:ARG:NH1	2.45	0.49
18:CB:106:GLU:OE2	18:CB:128:ARG:NH1	2.39	0.49
19:CC:199:ARG:HD2	19:CC:210:ILE:HD13	1.95	0.49
23:CH:117:LEU:HD21	23:CH:130:VAL:HG21	1.94	0.49
1:UA:216:ASP:OD1	1:UA:216:ASP:N	2.46	0.49
5:UF:354:PRO:HA	5:UF:357:LEU:HB2	1.95	0.49
10:UM:42:ASN:ND2	10:UM:58:GLN:OE1	2.46	0.49
15:UU:112:ARG:HH11	15:UU:140:PRO:HG3	1.77	0.49
17:UZ:282:TYR:HB3	17:UZ:290:ALA:HB1	1.95	0.49
17:UZ:282:TYR:CE1	17:UZ:292:PRO:HB3	2.47	0.49
18:CA:106:GLU:OE2	18:CA:128:ARG:NH1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CA:250:GLY:HA2	18:CA:306:TYR:O	2.13	0.49
24:CI:169:ILE:HG23	24:CI:206:LEU:HD13	1.93	0.49
29:CO:174:ASN:ND2	29:CO:199:ASN:O	2.46	0.49
40:Cj:40:ALA:HB3	40:Cj:45:ARG:HG3	1.94	0.49
46:C2:5:A:O2'	46:C2:6:C:O5'	2.26	0.49
4:UD:366:PRO:HG3	4:UD:704:VAL:HG21	1.94	0.49
10:UM:64:ILE:HA	10:UM:80:SER:HA	1.95	0.49
15:UU:621:HIS:CD2	15:UU:641:SER:HB2	2.48	0.49
21:CF:86:VAL:HG13	22:CG:591:TRP:HB3	1.95	0.49
28:CM:176:CYS:HB3	28:CM:192:GLN:HB3	1.95	0.49
32:CR:28:VAL:HG21	32:CR:193:LEU:HD11	1.95	0.49
32:CR:891:ARG:HB3	32:CS:792:TYR:HE1	1.76	0.49
45:C1:1221:C:N3	45:C1:1222:C:N4	2.61	0.49
49:US:196:ILE:O	49:US:200:THR:OG1	2.29	0.49
48:UI:210:ARG:HH22	48:UI:212:PHE:HB3	1.78	0.49
1:UA:220:PHE:HD2	1:UA:245:ILE:HD11	1.77	0.49
1:UA:242:GLN:OE1	1:UA:244:ARG:NH2	2.46	0.49
6:UG:134:LEU:HD21	7:UJ:5:LEU:HD13	1.95	0.49
13:UQ:544:SER:OG	13:UQ:545:HIS:N	2.45	0.49
17:UZ:272:PRO:HB2	45:C1:373:C:H5''	1.95	0.49
20:CD:86:VAL:HG23	20:CD:108:LYS:H	1.78	0.49
20:CD:345:TYR:HE1	20:CD:358:LYS:HD3	1.78	0.49
21:CE:55:LEU:HD23	21:CE:65:VAL:HB	1.94	0.49
22:CG:273:TYR:HB3	22:CG:280:PRO:HA	1.95	0.49
1:UA:8:SER:OG	1:UA:9:ASN:N	2.45	0.48
9:UL:847:LEU:O	43:Cp:30:ARG:NH2	2.44	0.48
12:UO:449:ASP:HB3	12:UO:452:ILE:HB	1.95	0.48
4:UD:877:PHE:HE2	52:UP:354:LYS:HD2	1.78	0.48
9:UL:283:GLU:HB2	9:UL:296:HIS:CE1	2.48	0.48
15:UU:757:SER:OG	15:UU:759:THR:O	2.27	0.48
18:CA:109:ILE:HG12	33:CT:140:ILE:HD13	1.95	0.48
29:CN:111:GLN:NE2	29:CN:113:TYR:OH	2.47	0.48
1:UA:204:SER:OG	1:UA:205:LYS:N	2.46	0.48
4:UD:285:SER:HB2	4:UD:354:LEU:HD21	1.95	0.48
7:UJ:32:SER:HB2	7:UJ:123:ARG:HH11	1.78	0.48
7:UJ:224:ALA:O	7:UJ:228:MET:HB2	2.12	0.48
15:UU:325:SER:HB3	15:UU:446:LEU:HG	1.94	0.48
21:CF:55:LEU:O	21:CF:81:TYR:HA	2.13	0.48
23:CH:323:GLN:HG3	23:CH:354:ARG:HB2	1.94	0.48
26:CK:108:ARG:HD3	26:CK:116:ARG:HB2	1.96	0.48
32:CR:313:THR:HG23	32:CR:372:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CR:850:ASP:N	32:CR:850:ASP:OD1	2.45	0.48
45:C1:2067:G:H1	45:C1:2174:C:H1'	1.78	0.48
4:UD:221:ARG:NH2	4:UD:266:TYR:O	2.47	0.48
13:UQ:455:VAL:HA	47:UH:888:ILE:HD11	1.96	0.48
15:UU:176:ALA:O	15:UU:203:ARG:NH1	2.39	0.48
15:UU:756:PHE:HD2	15:UU:763:LEU:HD12	1.78	0.48
22:CG:401:VAL:HG23	22:CG:411:THR:HG22	1.96	0.48
22:CG:478:ILE:HB	22:CG:490:TRP:HB2	1.96	0.48
26:CK:144:GLU:HA	26:CK:149:PRO:HA	1.93	0.48
32:CR:140:ILE:HG23	32:CR:149:VAL:HG21	1.96	0.48
34:Ca:89:ASP:HB3	34:Ca:223:PHE:HE1	1.78	0.48
45:C1:5:G:H1	45:C1:30:U:H3	1.61	0.48
12:UO:499:VAL:HG13	48:UE:259:LEU:HD13	1.96	0.48
15:UU:515:HIS:CD2	15:UU:522:ARG:HD3	2.49	0.48
25:CJ:87:ILE:HG21	25:CJ:101:VAL:HG23	1.96	0.48
32:CR:614:ILE:H	32:CR:614:ILE:HG12	1.45	0.48
34:Ca:136:ARG:NH2	45:C1:1469:A:OP1	2.46	0.48
44:CU:207:ASP:OD2	44:CU:218:SER:OG	2.32	0.48
46:C2:162:C:O2'	46:C2:164:U:OP2	2.27	0.48
1:UA:364:ILE:HD13	1:UA:399:THR:HG21	1.95	0.48
4:UD:552:ILE:HG12	4:UD:563:VAL:HG12	1.94	0.48
7:UJ:297:VAL:HG21	7:UJ:328:VAL:HA	1.95	0.48
8:UK:22:ARG:HE	8:UK:25:LEU:HD12	1.78	0.48
12:UO:171:LEU:O	12:UO:180:THR:N	2.47	0.48
32:CR:792:TYR:CE1	32:CS:891:ARG:HD2	2.49	0.48
35:Cc:86:MET:HE1	45:C1:2194:A:H8	1.79	0.48
49:US:499:SER:HA	49:US:502:GLU:HG2	1.95	0.48
1:UA:626:ASN:HB3	45:C1:256:U:H2'	1.94	0.48
1:UA:691:SER:OG	1:UA:692:THR:N	2.47	0.48
7:UJ:421:GLY:HA3	7:UJ:456:LEU:HG	1.94	0.48
15:UU:50:PRO:HB2	15:UU:342:LYS:HD2	1.95	0.48
16:UX:163:VAL:O	16:UX:177:ARG:NH1	2.47	0.48
24:CI:90:ARG:HH22	32:CR:91:GLN:HA	1.78	0.48
24:CI:1101:ARG:HD2	33:CT:111:MET:HG2	1.96	0.48
27:CL:519:GLU:HB2	27:CL:521:MET:HE2	1.96	0.48
33:CT:106:LEU:HD13	33:CT:131:VAL:HG22	1.95	0.48
39:Ci:48:GLY:O	45:C1:1503:U:O2'	2.31	0.48
45:C1:75:G:H5''	45:C1:76:U:H5''	1.96	0.48
47:UH:646:LYS:HB2	47:UH:730:PHE:HE1	1.78	0.48
4:UD:646:ASP:OD1	4:UD:660:ASN:ND2	2.47	0.48
12:UO:205:LEU:O	12:UO:216:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CA:123:THR:OG1	18:CA:124:LYS:N	2.44	0.48
20:CD:211:VAL:O	20:CD:254:TYR:OH	2.27	0.48
28:CM:360:ARG:NH1	46:C2:35:G:OP1	2.32	0.48
32:CR:70:HIS:HB3	32:CR:73:LYS:HG2	1.96	0.48
32:CS:140:ILE:HG23	32:CS:149:VAL:HG21	1.96	0.48
37:Cg:107:LEU:HD21	37:Cg:132:ILE:HD11	1.96	0.48
46:C2:153:G:C6	46:C2:176:U:O2	2.67	0.48
47:UH:700:ASP:OD1	47:UH:700:ASP:N	2.46	0.48
51:CX:278:ILE:HG12	51:CX:320:GLU:HG2	1.94	0.48
1:UA:582:MET:HG3	1:UA:682:PRO:HA	1.95	0.48
4:UD:570:ILE:HD11	4:UD:626:LEU:HD11	1.95	0.48
14:UR:322:ARG:O	14:UR:344:ARG:NH2	2.41	0.48
22:CG:163:TYR:HB3	22:CG:604:PHE:HB3	1.95	0.48
22:CG:413:SER:OG	22:CG:415:ASN:OD1	2.31	0.48
30:CP:46:TYR:HE2	34:Ca:117:TRP:HE1	1.60	0.48
31:CQ:152:ILE:HA	31:CQ:155:ALA:HB3	1.96	0.48
32:CS:850:ASP:OD1	32:CS:850:ASP:N	2.45	0.48
45:C1:1748:G:O2'	45:C1:2195:U:O2	2.31	0.48
46:C2:243:G:H2'	46:C2:244:G:C8	2.49	0.48
46:C2:259:A:H1'	46:C2:260:G:C2	2.47	0.48
1:UA:408:ALA:HB3	1:UA:418:ARG:HB2	1.94	0.48
6:UG:270:ASN:HB2	6:UG:272:ILE:HG12	1.96	0.48
9:UL:590:LYS:HD3	9:UL:602:ASN:HB3	1.96	0.48
12:UO:16:GLY:HA2	48:UE:244:ARG:HH12	1.79	0.48
14:UR:593:ILE:HG22	14:UR:604:VAL:HG22	1.95	0.48
18:CB:102:SER:OG	18:CB:108:ARG:NH1	2.44	0.48
28:CM:53:PHE:O	28:CM:360:ARG:NH2	2.46	0.48
30:CP:51:LEU:HB3	30:CP:71:LEU:HD11	1.95	0.48
32:CS:313:THR:HG23	32:CS:372:ILE:HG23	1.95	0.48
4:UD:253:ASP:OD1	4:UD:253:ASP:N	2.46	0.47
6:UG:578:ILE:HA	6:UG:582:ARG:HH21	1.79	0.47
10:UM:568:VAL:HB	10:UM:582:LEU:HB2	1.96	0.47
12:UO:333:HIS:HB3	12:UO:347:THR:HA	1.96	0.47
13:UQ:271:LEU:HD11	13:UQ:277:LEU:HD12	1.95	0.47
13:UQ:421:MET:HA	13:UQ:432:MET:O	2.13	0.47
15:UU:731:ILE:O	15:UU:744:ALA:HA	2.14	0.47
45:C1:1625:G:H2'	45:C1:1626:G:C8	2.49	0.47
46:C2:90:C:H1'	46:C2:91:G:H5'	1.95	0.47
1:UA:412:ILE:HG13	1:UA:413:ARG:HG2	1.95	0.47
3:UC:607:LYS:NZ	45:C1:1175:A:OP2	2.39	0.47
5:UF:5:ALA:HA	5:UF:45:HIS:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UR:69:GLN:OE1	14:UR:72:ARG:NH2	2.48	0.47
18:CB:247:LEU:O	20:CD:120:ARG:NH2	2.39	0.47
24:CI:84:LEU:HD21	24:CI:137:LEU:HD23	1.96	0.47
37:Cg:171:ARG:HD3	45:C1:1095:A:H5'	1.96	0.47
7:UJ:152:LEU:HG	7:UJ:171:ILE:HG12	1.96	0.47
13:UQ:426:ALA:HB1	14:UR:360:VAL:HG13	1.95	0.47
15:UU:353:VAL:HG13	15:UU:363:THR:HG22	1.96	0.47
18:CA:211:ARG:NH2	18:CA:232:GLN:OE1	2.45	0.47
45:C1:323:G:H2'	45:C1:324:G:H8	1.78	0.47
45:C1:597:G:H2'	45:C1:598:A:H8	1.80	0.47
45:C1:1056:U:H2'	45:C1:1057:A:H8	1.79	0.47
6:UG:309:ASP:HA	6:UG:350:ILE:HD11	1.96	0.47
10:UM:236:GLN:OE1	10:UM:252:ARG:NH1	2.47	0.47
18:CA:107:LYS:HB2	18:CA:129:ILE:HD12	1.97	0.47
20:CD:178:GLU:OE2	20:CD:267:ARG:NH1	2.46	0.47
22:CG:328:GLY:H	37:Cg:153:HIS:CE1	2.33	0.47
24:CI:386:LEU:HB2	32:CR:211:ILE:HG22	1.97	0.47
32:CR:378:HIS:ND1	32:CS:378:HIS:HB2	2.29	0.47
50:CI:46:VAL:HG12	50:CI:69:LEU:HD22	1.95	0.47
1:UA:505:GLU:OE2	35:Cc:70:ARG:NH2	2.46	0.47
3:UC:578:GLN:NE2	24:CI:144:TYR:OH	2.47	0.47
6:UG:467:GLY:HA2	28:CM:385:LEU:HD21	1.94	0.47
9:UL:77:ARG:NH2	9:UL:118:PHE:O	2.47	0.47
12:UO:48:SER:OG	12:UO:105:GLY:O	2.33	0.47
22:CG:454:ASP:OD1	22:CG:454:ASP:N	2.42	0.47
34:Ca:109:LYS:HA	34:Ca:112:SER:HB3	1.96	0.47
37:Cg:166:ARG:NH1	45:C1:1119:A:OP2	2.47	0.47
45:C1:1652:C:H2'	45:C1:1653:G:H8	1.79	0.47
9:UL:623:VAL:HA	9:UL:632:ARG:O	2.15	0.47
9:UL:638:PHE:HB3	23:CH:227:VAL:HG12	1.97	0.47
9:UL:827:GLU:HG2	9:UL:863:LEU:HD23	1.97	0.47
10:UM:105:ARG:HH22	45:C1:2369:G:H4'	1.78	0.47
10:UM:687:CYS:SG	10:UM:688:THR:N	2.87	0.47
15:UU:858:ASP:N	15:UU:858:ASP:OD1	2.44	0.47
22:CG:198:GLN:HE22	22:CG:221:LYS:HG2	1.80	0.47
24:CI:178:LYS:NZ	45:C1:1102:A:OP2	2.47	0.47
32:CR:792:TYR:HE1	32:CS:891:ARG:HD2	1.79	0.47
32:CS:400:LYS:HA	32:CS:403:MET:HB2	1.96	0.47
49:US:323:SER:HB2	49:US:363:LEU:HD11	1.97	0.47
1:UA:509:LEU:HD12	1:UA:513:VAL:HG22	1.97	0.47
6:UG:457:GLU:O	11:UN:879:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:UJ:393:LYS:HG2	7:UJ:441:ALA:HB2	1.95	0.47
9:UL:395:GLU:OE2	9:UL:416:LYS:NZ	2.48	0.47
12:UO:206:VAL:HG21	12:UO:247:LEU:HD11	1.97	0.47
13:UQ:104:ILE:HG12	13:UQ:113:VAL:HG12	1.97	0.47
13:UQ:328:ASN:O	13:UQ:332:HIS:ND1	2.42	0.47
15:UU:190:ILE:HG21	15:UU:237:PRO:HD3	1.96	0.47
15:UU:852:GLN:HG2	27:CL:669:VAL:HG13	1.97	0.47
18:CA:70:LYS:NZ	33:CT:159:ARG:O	2.39	0.47
28:CM:216:VAL:HG13	28:CM:245:ILE:HB	1.95	0.47
28:CM:354:ARG:HH22	28:CM:360:ARG:HA	1.78	0.47
32:CR:622:PHE:HA	32:CS:839:LYS:HZ3	1.79	0.47
32:CR:635:ILE:HD12	32:CR:635:ILE:HA	1.87	0.47
40:Cj:19:VAL:O	40:Cj:67:ILE:HA	2.15	0.47
41:Cm:31:SER:OG	41:Cm:32:LYS:N	2.47	0.47
43:Cp:11:VAL:HG23	43:Cp:33:PHE:HD1	1.79	0.47
45:C1:1509:A:H2'	45:C1:1510:G:C8	2.49	0.47
10:UM:47:GLU:H	10:UM:54:LEU:HD13	1.78	0.47
12:UO:190:VAL:HA	12:UO:209:SER:HA	1.97	0.47
13:UQ:253:ILE:HD11	13:UQ:281:PHE:HZ	1.80	0.47
24:CI:1020:ARG:NH1	45:C1:1162:U:OP1	2.40	0.47
37:Cg:168:GLY:O	37:Cg:172:ARG:HB2	2.14	0.47
44:CU:180:HIS:HD2	44:CU:182:GLN:H	1.63	0.47
45:C1:301:U:H2'	45:C1:302:A:H8	1.78	0.47
48:UI:194:GLY:HA3	48:UI:232:GLN:HE22	1.79	0.47
4:UD:298:ARG:NH2	4:UD:322:HIS:O	2.48	0.47
6:UG:310:ARG:HH12	28:CM:31:LEU:HG	1.80	0.47
7:UJ:97:ARG:HH22	14:UR:72:ARG:HB2	1.80	0.47
8:UK:22:ARG:NH2	24:CI:985:ASP:O	2.48	0.47
9:UL:99:ILE:HG12	9:UL:101:THR:HG23	1.97	0.47
15:UU:119:LEU:HD22	15:UU:131:LEU:HD22	1.97	0.47
17:UZ:104:PRO:HD2	17:UZ:212:ALA:HB2	1.96	0.47
23:CH:172:GLU:HB2	23:CH:195:ARG:HB2	1.96	0.47
24:CI:334:LEU:O	24:CI:341:ARG:NH2	2.42	0.47
24:CI:619:LEU:HA	24:CI:622:THR:HG22	1.96	0.47
29:CO:174:ASN:OD1	29:CO:174:ASN:N	2.48	0.47
32:CS:283:LEU:HD11	32:CS:474:LEU:HG	1.97	0.47
37:Cg:38:ARG:HH22	45:C1:1179:G:H5'	1.80	0.47
46:C2:135:U:H4'	46:C2:136:C:H4'	1.96	0.47
47:UH:587:SER:OG	47:UH:590:ASN:ND2	2.48	0.47
2:UB:587:THR:OG1	2:UB:588:VAL:N	2.45	0.47
7:UJ:205:ARG:NH2	7:UJ:257:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:UM:521:LYS:NZ	10:UM:573:VAL:O	2.38	0.47
12:UO:492:PRO:HB3	12:UO:495:ARG:HH21	1.80	0.47
16:UX:154:LYS:HG2	16:UX:165:ILE:HG21	1.97	0.47
23:CH:158:LEU:HA	23:CH:161:TYR:HD2	1.79	0.47
28:CM:60:GLN:NE2	28:CM:349:ASN:OD1	2.48	0.47
32:CS:738:LYS:HD3	32:CS:808:SER:HB3	1.97	0.47
47:UH:581:VAL:HG11	47:UH:626:LEU:HG	1.97	0.47
47:UH:836:ILE:HG22	48:UI:243:SER:HB3	1.96	0.47
1:UA:23:SER:HB2	1:UA:28:HIS:HB2	1.98	0.46
1:UA:54:HIS:NE2	1:UA:72:SER:OG	2.46	0.46
3:UC:604:LYS:HD3	37:Cg:29:VAL:HG11	1.96	0.46
6:UG:356:THR:O	6:UG:366:ILE:HA	2.15	0.46
10:UM:14:ALA:N	10:UM:719:PHE:O	2.47	0.46
10:UM:694:ASP:N	10:UM:694:ASP:OD1	2.48	0.46
25:CJ:37:MET:SD	45:C1:416:U:O2'	2.72	0.46
25:CJ:102:THR:HG22	25:CJ:104:SER:H	1.79	0.46
27:CL:725:ARG:NH2	45:C1:1731:A:OP2	2.47	0.46
28:CM:193:TRP:HB3	28:CM:196:PHE:HB2	1.97	0.46
32:CR:174:ARG:HB3	32:CR:182:ILE:HD11	1.96	0.46
1:UA:86:ARG:HH12	15:UU:784:HIS:HB3	1.81	0.46
1:UA:500:ARG:NH2	45:C1:2201:C:OP2	2.47	0.46
9:UL:695:HIS:NE2	9:UL:713:SER:OG	2.38	0.46
11:UN:901:LEU:HD12	11:UN:902:ARG:H	1.79	0.46
13:UQ:145:SER:HB2	13:UQ:190:MET:HG3	1.95	0.46
23:CH:167:PRO:HD2	23:CH:198:SER:HB2	1.98	0.46
29:CN:128:VAL:HG23	29:CN:159:LEU:HD13	1.98	0.46
30:CP:75:GLU:O	34:Ca:115:ARG:NH2	2.49	0.46
32:CS:70:HIS:HB3	32:CS:73:LYS:HG2	1.96	0.46
32:CS:749:GLN:HB3	32:CS:793:LYS:HD3	1.96	0.46
47:UH:906:ILE:O	47:UH:906:ILE:HG22	2.14	0.46
51:CX:225:PRO:HG2	51:CX:253:ILE:HG13	1.97	0.46
1:UA:562:ASP:OD1	25:CJ:144:ARG:NH2	2.48	0.46
4:UD:148:ALA:N	4:UD:151:ASN:O	2.47	0.46
10:UM:869:ARG:HH21	27:CL:679:PRO:HG2	1.80	0.46
12:UO:97:ARG:HE	12:UO:136:ILE:HD11	1.79	0.46
13:UQ:623:SER:OG	13:UQ:624:ALA:N	2.48	0.46
20:CD:189:TRP:HE1	20:CD:257:ILE:HA	1.80	0.46
21:CE:109:SER:HB2	21:CE:112:ASN:H	1.80	0.46
26:CK:131:ALA:HA	26:CK:136:LEU:HD12	1.98	0.46
26:CK:229:THR:O	26:CK:239:VAL:HA	2.15	0.46
32:CR:400:LYS:HA	32:CR:403:MET:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CS:174:ARG:HB3	32:CS:182:ILE:HD11	1.96	0.46
39:CI:61:VAL:HG12	39:CI:63:ALA:H	1.79	0.46
45:C1:1665:A:H1'	45:C1:1666:C:C4	2.51	0.46
49:US:313:SER:OG	49:US:314:GLY:N	2.48	0.46
4:UD:309:GLN:HG3	4:UD:312:ARG:HG3	1.95	0.46
10:UM:277:LEU:HD21	10:UM:291:SER:HB2	1.96	0.46
10:UM:336:CYS:HB3	10:UM:344:VAL:HB	1.96	0.46
10:UM:788:LEU:HD23	10:UM:832:ALA:HA	1.96	0.46
18:CB:180:VAL:HB	18:CB:203:VAL:HG12	1.97	0.46
20:CD:192:TRP:NE1	20:CD:247:THR:OG1	2.48	0.46
32:CR:283:LEU:HD11	32:CR:474:LEU:HG	1.96	0.46
34:Ca:144:LYS:HD3	34:Ca:208:GLN:HA	1.97	0.46
49:US:174:LEU:HD11	49:US:226:LEU:HD13	1.98	0.46
6:UG:163:MET:HA	6:UG:170:LEU:HA	1.98	0.46
9:UL:83:PHE:O	9:UL:94:LEU:HA	2.15	0.46
10:UM:374:ASP:HB2	34:Ca:19:LYS:HE2	1.96	0.46
12:UO:434:ALA:HA	12:UO:473:ARG:HH22	1.80	0.46
13:UQ:79:TRP:HZ3	13:UQ:842:GLY:HA2	1.80	0.46
18:CA:225:VAL:HA	18:CA:252:GLY:O	2.16	0.46
23:CH:227:VAL:O	45:C1:1714:G:N2	2.48	0.46
24:CI:278:ASN:HB3	24:CI:772:ARG:HA	1.98	0.46
24:CI:815:VAL:HG23	24:CI:905:VAL:HA	1.97	0.46
29:CN:205:PHE:HD2	29:CN:221:VAL:HG22	1.80	0.46
32:CS:98:PHE:O	32:CS:102:ASN:HB2	2.15	0.46
47:UH:641:LEU:HB2	47:UH:714:LEU:HD13	1.98	0.46
49:US:383:LYS:NZ	49:US:455:SER:OG	2.35	0.46
51:CX:246:ALA:O	51:CX:250:ALA:N	2.44	0.46
9:UL:160:PHE:HE1	9:UL:203:LEU:HD21	1.81	0.46
15:UU:76:LEU:HD21	15:UU:363:THR:HG21	1.98	0.46
16:UX:138:VAL:HG13	16:UX:163:VAL:HG11	1.97	0.46
32:CR:738:LYS:HD3	32:CR:808:SER:HB3	1.97	0.46
45:C1:1551:A:H2'	45:C1:1552:A:H8	1.81	0.46
4:UD:686:ARG:HH12	4:UD:745:SER:HB3	1.80	0.46
9:UL:583:ALA:HB2	9:UL:613:MET:HE3	1.98	0.46
12:UO:166:ASP:N	12:UO:166:ASP:OD1	2.40	0.46
13:UQ:185:LYS:NZ	13:UQ:211:LEU:O	2.40	0.46
17:UZ:60:THR:HB	17:UZ:286:PRO:HG3	1.98	0.46
18:CB:77:ARG:HH22	18:CB:146:GLU:HA	1.80	0.46
24:CI:854:ARG:NH1	42:Cn:62:LYS:O	2.49	0.46
32:CR:98:PHE:O	32:CR:102:ASN:HB2	2.15	0.46
32:CS:20:GLN:HG3	32:CS:21:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C1:468:C:O2'	45:C1:469:G:O4'	2.34	0.46
49:US:370:SER:OG	49:US:373:LEU:HD21	2.15	0.46
2:UB:729:ALA:HA	2:UB:732:ILE:HD12	1.96	0.46
9:UL:955:LYS:O	9:UL:956:ARG:NH1	2.49	0.46
13:UQ:409:SER:O	13:UQ:425:THR:OG1	2.23	0.46
14:UR:163:GLU:OE1	14:UR:174:ARG:NH1	2.49	0.46
14:UR:549:SER:HB2	14:UR:554:LEU:HB2	1.97	0.46
18:CA:250:GLY:N	18:CA:306:TYR:O	2.48	0.46
20:CD:13:TYR:HD2	20:CD:76:LEU:HD22	1.81	0.46
24:CI:280:ALA:H	24:CI:284:GLN:HE21	1.63	0.46
26:CK:244:TYR:HB3	26:CK:254:LEU:HD23	1.97	0.46
31:CQ:187:ILE:HB	31:CQ:211:LEU:HD21	1.98	0.46
32:CR:20:GLN:HG3	32:CR:21:THR:HG23	1.98	0.46
32:CR:749:GLN:HB3	32:CR:793:LYS:HD3	1.96	0.46
32:CS:798:PRO:HB2	32:CS:801:LEU:HB2	1.98	0.46
37:Cg:35:ARG:NH2	45:C1:1060:U:O4	2.44	0.46
45:C1:2085:G:N2	45:C1:2088:A:C8	2.81	0.46
2:UB:621:TYR:CZ	2:UB:625:LYS:HE2	2.51	0.46
2:UB:701:GLN:HB3	49:US:543:ASP:HB2	1.98	0.46
10:UM:588:GLY:O	10:UM:620:GLY:N	2.49	0.46
12:UO:467:ARG:HD2	12:UO:508:LEU:HD11	1.98	0.46
13:UQ:804:LYS:HE3	13:UQ:805:ARG:H	1.81	0.46
17:UZ:113:ALA:O	17:UZ:121:ARG:NH1	2.48	0.46
20:CD:224:ASP:OD1	20:CD:224:ASP:N	2.47	0.46
22:CG:272:VAL:HG21	22:CG:317:LEU:HD21	1.98	0.46
23:CH:336:LEU:HD12	23:CH:360:LEU:HD11	1.98	0.46
26:CK:89:LEU:HA	26:CK:115:ILE:O	2.16	0.46
30:CP:56:PRO:HA	30:CP:59:THR:HG22	1.98	0.46
32:CS:828:GLU:H	32:CS:828:GLU:HG2	1.62	0.46
39:CI:43:VAL:HG12	39:CI:52:ILE:HB	1.98	0.46
45:C1:2368:U:H2'	45:C1:2369:G:H8	1.81	0.46
47:UH:823:LEU:HD22	48:UI:260:LYS:HD2	1.98	0.46
4:UD:228:ASP:OD1	4:UD:228:ASP:N	2.37	0.46
4:UD:658:ILE:HG23	4:UD:667:SER:HB2	1.97	0.46
10:UM:560:ALA:HB2	10:UM:570:ILE:HG12	1.98	0.46
12:UO:215:ARG:HG2	12:UO:228:THR:HG23	1.97	0.46
18:CA:272:PHE:HB3	18:CA:289:GLN:HE22	1.80	0.46
18:CB:226:ILE:HG12	18:CB:247:LEU:HD13	1.98	0.46
32:CR:621:GLN:O	32:CS:839:LYS:NZ	2.48	0.46
36:Ce:97:LEU:HD21	36:Ce:139:LEU:HD23	1.98	0.46
47:UH:845:ARG:HB3	47:UH:873:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:UE:203:ARG:HB2	48:UE:214:LEU:HD21	1.98	0.46
4:UD:381:ARG:NH2	4:UD:398:ASN:O	2.49	0.45
9:UL:712:VAL:HA	9:UL:721:ARG:O	2.16	0.45
10:UM:254:LYS:HB3	10:UM:274:HIS:HB2	1.98	0.45
14:UR:289:LEU:HD21	14:UR:611:VAL:HG11	1.97	0.45
28:CM:223:ILE:HG22	28:CM:235:LYS:HB2	1.97	0.45
32:CS:142:THR:O	32:CS:142:THR:OG1	2.25	0.45
43:Cp:16:VAL:HA	43:Cp:29:VAL:HG23	1.97	0.45
49:US:368:LEU:HD23	49:US:373:LEU:HD13	1.98	0.45
49:US:522:HIS:HB3	49:US:525:THR:HB	1.97	0.45
1:UA:787:MET:HE2	1:UA:787:MET:HB3	1.89	0.45
6:UG:172:CYS:SG	6:UG:173:GLU:N	2.88	0.45
13:UQ:202:ASP:OD1	13:UQ:202:ASP:N	2.48	0.45
13:UQ:537:THR:O	13:UQ:554:ASP:HA	2.15	0.45
18:CA:156:VAL:HG22	18:CA:225:VAL:HB	1.97	0.45
18:CA:250:GLY:CA	18:CA:306:TYR:O	2.65	0.45
18:CB:191:ARG:HA	20:CD:154:LEU:HD21	1.98	0.45
20:CD:304:HIS:CD2	20:CD:322:LEU:HD22	2.52	0.45
22:CG:438:LEU:HA	22:CG:463:PRO:HA	1.97	0.45
24:CI:91:ARG:HB2	24:CI:219:ILE:HD12	1.99	0.45
35:Cc:86:MET:HE1	45:C1:2194:A:C8	2.51	0.45
45:C1:466:A:OP1	45:C1:467:C:N4	2.39	0.45
45:C1:1097:U:H2'	45:C1:1098:G:C8	2.50	0.45
45:C1:1459:C:H2'	45:C1:1460:G:C8	2.51	0.45
49:US:370:SER:OG	49:US:373:LEU:HG	2.16	0.45
1:UA:165:PHE:HE1	1:UA:183:GLU:HG3	1.81	0.45
5:UF:162:ALA:HB2	11:UN:359:PRO:HA	1.99	0.45
6:UG:214:ARG:NH2	45:C1:292:G:OP2	2.49	0.45
9:UL:198:ILE:HD11	9:UL:234:THR:HG21	1.98	0.45
10:UM:35:LEU:HD13	10:UM:48:LEU:HD21	1.97	0.45
10:UM:334:ILE:HG23	10:UM:346:TYR:HB2	1.98	0.45
13:UQ:477:HIS:HE1	13:UQ:511:VAL:HG21	1.81	0.45
15:UU:480:ALA:HB3	15:UU:528:ARG:HD2	1.98	0.45
19:CC:190:SER:HB2	19:CC:284:MET:HE1	1.98	0.45
22:CG:562:ASP:HB3	22:CG:581:VAL:HB	1.97	0.45
23:CH:98:ILE:HG23	23:CH:130:VAL:HA	1.97	0.45
32:CS:58:TRP:HE1	32:CS:126:GLN:HE21	1.64	0.45
45:C1:191:C:O2'	45:C1:192:A:N7	2.43	0.45
46:C2:101:G:H1	46:C2:251:U:H3	1.65	0.45
51:CX:329:ALA:O	51:CX:373:LYS:NZ	2.43	0.45
52:UP:350:ASP:OD1	52:UP:350:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:244:ARG:NH1	45:C1:282:C:OP2	2.49	0.45
6:UG:243:GLN:HB2	6:UG:250:ILE:HG22	1.99	0.45
14:UR:322:ARG:NH1	14:UR:346:TYR:OH	2.50	0.45
18:CB:163:SER:O	18:CB:163:SER:OG	2.30	0.45
24:CI:386:LEU:HD21	32:CR:190:LEU:HB3	1.97	0.45
31:CQ:86:PRO:HA	31:CQ:120:LYS:O	2.17	0.45
32:CR:789:LEU:HD12	32:CS:855:LEU:HD23	1.98	0.45
45:C1:1652:C:H2'	45:C1:1653:G:C8	2.52	0.45
47:UH:793:MET:HG3	48:UI:273:ARG:HD2	1.98	0.45
47:UH:826:VAL:HG12	48:UI:253:LEU:HD12	1.99	0.45
1:UA:540:SER:OG	1:UA:541:GLU:N	2.47	0.45
6:UG:243:GLN:HA	6:UG:250:ILE:HA	1.97	0.45
11:UN:364:THR:O	11:UN:364:THR:OG1	2.34	0.45
12:UO:30:PHE:HA	12:UO:348:ARG:HB2	1.99	0.45
12:UO:291:GLY:HA3	12:UO:317:ILE:HD11	1.97	0.45
13:UQ:480:LEU:HD11	13:UQ:501:GLN:HE21	1.82	0.45
15:UU:981:ARG:HD2	15:UU:981:ARG:HA	1.74	0.45
18:CB:93:CYS:HB3	18:CB:129:ILE:HD13	1.99	0.45
19:CC:244:LEU:HD23	19:CC:250:LYS:HG2	1.99	0.45
23:CH:375:TRP:CD1	23:CH:398:VAL:HG12	2.52	0.45
32:CR:58:TRP:HE1	32:CR:126:GLN:HE21	1.64	0.45
32:CR:828:GLU:H	32:CR:828:GLU:HG2	1.62	0.45
2:UB:828:ASN:OD1	2:UB:828:ASN:N	2.50	0.45
4:UD:690:LYS:HD2	4:UD:704:VAL:HG22	1.99	0.45
10:UM:813:LEU:O	10:UM:817:ASN:HB2	2.16	0.45
15:UU:377:ILE:HD11	15:UU:380:GLN:HB3	1.99	0.45
17:UZ:280:ASN:HB2	17:UZ:282:TYR:CZ	2.49	0.45
19:CC:280:ASN:HD21	20:CD:267:ARG:HD2	1.82	0.45
23:CH:121:ALA:O	23:CH:199:GLN:NE2	2.48	0.45
23:CH:132:PHE:HB2	23:CH:192:VAL:HG22	1.99	0.45
24:CI:941:SER:HA	24:CI:944:ILE:HD12	1.99	0.45
26:CK:117:LEU:HD11	40:Cj:126:PRO:HG2	1.97	0.45
32:CS:711:LYS:HA	32:CS:711:LYS:HD2	1.80	0.45
4:UD:528:ARG:NH1	4:UD:547:ARG:O	2.49	0.45
7:UJ:83:ARG:HA	7:UJ:86:MET:HE2	1.98	0.45
10:UM:393:THR:HG21	10:UM:399:ARG:HH22	1.82	0.45
13:UQ:95:ILE:HD12	13:UQ:148:LEU:HG	1.98	0.45
13:UQ:186:LYS:HD2	45:C1:46:C:H4'	1.99	0.45
13:UQ:222:ASN:HB2	13:UQ:225:MET:HB2	1.99	0.45
22:CG:575:GLY:N	22:CG:606:VAL:O	2.50	0.45
24:CI:84:LEU:HD22	24:CI:139:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CO:45:SER:HB2	29:CO:88:ARG:HB3	1.98	0.45
30:CP:60:LYS:HE2	30:CP:60:LYS:HB2	1.75	0.45
32:CS:398:LEU:HD12	32:CS:401:LYS:HE2	1.99	0.45
45:C1:495:G:N7	45:C1:503:G:N1	2.64	0.45
3:UC:593:ARG:NH1	45:C1:1130:U:OP2	2.49	0.45
9:UL:383:LEU:HB2	9:UL:399:ILE:HB	1.98	0.45
9:UL:675:ASP:OD2	9:UL:677:THR:OG1	2.32	0.45
12:UO:123:MET:HE2	12:UO:123:MET:HB3	1.80	0.45
15:UU:619:GLY:O	15:UU:647:LYS:NZ	2.40	0.45
21:CE:41:THR:HG23	21:CE:102:SER:HB2	1.98	0.45
23:CH:393:ASP:OD1	23:CH:393:ASP:N	2.50	0.45
24:CI:607:LYS:HB3	24:CI:607:LYS:HE2	1.83	0.45
24:CI:621:ARG:HD2	24:CI:621:ARG:HA	1.78	0.45
32:CS:110:LYS:HB3	32:CS:110:LYS:HE3	1.81	0.45
32:CS:839:LYS:HE3	32:CS:839:LYS:HB3	1.48	0.45
45:C1:1508:A:H2'	45:C1:1509:A:C8	2.52	0.45
48:UE:171:SER:O	49:US:299:LYS:NZ	2.37	0.45
49:US:430:LYS:O	49:US:430:LYS:NZ	2.49	0.45
51:CX:212:TYR:OH	51:CX:215:GLY:O	2.30	0.45
1:UA:312:LEU:O	1:UA:324:VAL:HA	2.16	0.45
2:UB:550:GLU:HG3	49:US:523:ILE:HB	1.99	0.45
3:UC:621:VAL:HG13	3:UC:623:LYS:HB2	1.99	0.45
4:UD:773:MET:HE2	4:UD:773:MET:HB3	1.74	0.45
6:UG:578:ILE:HD12	30:CP:72:ASP:HB2	1.99	0.45
7:UJ:415:ASN:HB3	7:UJ:416:ILE:H	1.61	0.45
19:CC:45:GLY:HA3	45:C1:435:A:N1	2.32	0.45
22:CG:235:ARG:HH22	46:C2:119:C:H2'	1.82	0.45
30:CP:199:LYS:HE3	30:CP:203:ILE:HD11	1.99	0.45
32:CS:165:MET:HE3	32:CS:165:MET:HB3	1.88	0.45
45:C1:96:C:O2'	45:C1:97:C:O5'	2.32	0.45
51:CX:259:PRO:HB3	51:CX:298:LYS:HG2	1.99	0.45
1:UA:223:LYS:HD3	1:UA:246:VAL:HG11	1.99	0.45
1:UA:291:HIS:HE1	1:UA:325:TRP:HE1	1.64	0.45
1:UA:630:MET:O	16:UX:-5:LYS:NZ	2.46	0.45
3:UC:635:LEU:O	33:CT:120:GLN:NE2	2.39	0.45
5:UF:179:LEU:HB3	5:UF:303:VAL:HG21	1.99	0.45
10:UM:578:VAL:HG12	10:UM:580:GLY:H	1.81	0.45
10:UM:589:VAL:HA	10:UM:619:SER:HA	1.98	0.45
12:UO:492:PRO:HA	12:UO:495:ARG:HB2	1.99	0.45
13:UQ:568:THR:HG22	48:UE:262:LYS:HE2	1.99	0.45
15:UU:680:ILE:HD11	15:UU:694:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:288:ARG:NH1	37:Cg:163:GLY:O	2.44	0.45
23:CH:48:PRO:HA	23:CH:51:ILE:HG22	1.98	0.45
23:CH:305:VAL:HG12	23:CH:307:GLU:H	1.80	0.45
38:Ch:141:TYR:HE1	38:Ch:146:ALA:HB2	1.82	0.45
40:Cj:51:PRO:HG3	40:Cj:116:LEU:HD22	1.98	0.45
43:Cp:11:VAL:HG23	43:Cp:33:PHE:HA	1.99	0.45
45:C1:301:U:C2	45:C1:341:G:N1	2.85	0.45
45:C1:1507:G:H2'	45:C1:1508:A:C8	2.52	0.45
47:UH:624:MET:HE3	47:UH:624:MET:HB3	1.79	0.45
1:UA:65:PRO:HG2	1:UA:106:PRO:HA	1.99	0.44
9:UL:287:HIS:CD2	9:UL:290:ARG:HB2	2.52	0.44
10:UM:150:SER:OG	10:UM:151:GLY:O	2.35	0.44
10:UM:205:GLY:HA3	10:UM:231:HIS:HB3	1.99	0.44
10:UM:635:ILE:HG22	10:UM:636:ARG:HG2	1.98	0.44
10:UM:840:ASN:O	10:UM:844:SER:OG	2.33	0.44
13:UQ:218:ILE:HG13	13:UQ:234:LEU:HB2	1.99	0.44
24:Cl:383:LYS:O	32:CR:215:LYS:NZ	2.46	0.44
26:CK:141:LEU:HB2	26:CK:153:THR:HB	1.97	0.44
32:CR:398:LEU:HD12	32:CR:401:LYS:HE2	1.99	0.44
34:Ca:129:THR:HG23	34:Ca:131:ASP:H	1.82	0.44
34:Ca:154:THR:O	34:Ca:154:THR:OG1	2.32	0.44
37:Cg:58:LEU:HD21	37:Cg:91:LEU:HB3	1.99	0.44
37:Cg:87:SER:OG	37:Cg:88:ARG:N	2.49	0.44
45:C1:9:G:H1	45:C1:27:A:N6	2.14	0.44
45:C1:2370:C:H2'	45:C1:2371:G:H8	1.82	0.44
49:US:266:GLN:HE22	49:US:299:LYS:HG3	1.82	0.44
4:UD:165:LEU:HD13	4:UD:179:LEU:HD21	2.00	0.44
4:UD:182:THR:HG21	4:UD:187:THR:HG21	1.99	0.44
10:UM:766:HIS:HA	10:UM:767:PRO:HD3	1.89	0.44
12:UO:293:LEU:HD11	50:Cl:4:VAL:HG22	1.98	0.44
15:UU:628:ILE:HG22	15:UU:639:SER:HB2	1.99	0.44
23:CH:168:PRO:HB3	44:CU:124:PRO:HG2	1.99	0.44
26:CK:196:PHE:HZ	26:CK:237:ILE:HD12	1.81	0.44
28:CM:288:ASP:O	28:CM:300:SER:HA	2.17	0.44
31:CQ:233:VAL:HA	31:CQ:236:VAL:HG22	1.99	0.44
32:CS:652:LYS:HD3	32:CS:652:LYS:HA	1.83	0.44
32:CS:917:ARG:HE	32:CS:917:ARG:HB2	1.36	0.44
45:C1:9:G:N1	45:C1:27:A:C6	2.85	0.44
45:C1:181:G:H3'	45:C1:182:C:H4'	1.99	0.44
45:C1:483:U:H4'	45:C1:484:G:H5''	2.00	0.44
48:UE:181:ILE:HD12	48:UE:216:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:US:208:LEU:HD21	49:US:223:VAL:HG11	1.99	0.44
49:US:302:MET:SD	49:US:302:MET:N	2.81	0.44
4:UD:747:ILE:HG21	4:UD:751:SER:HB2	2.00	0.44
9:UL:858:LEU:HD21	9:UL:899:LEU:HD13	1.99	0.44
10:UM:865:VAL:HG12	27:CL:679:PRO:HG3	1.98	0.44
12:UO:317:ILE:HG22	12:UO:338:MET:HG2	1.99	0.44
13:UQ:667:VAL:HG11	13:UQ:715:ILE:HD13	1.99	0.44
15:UU:36:ALA:HB2	15:UU:779:ARG:HH21	1.82	0.44
16:UX:135:VAL:HG11	16:UX:156:ARG:HE	1.81	0.44
22:CG:561:ASN:N	22:CG:581:VAL:O	2.49	0.44
30:CP:176:LYS:O	30:CP:180:GLU:HG2	2.17	0.44
32:CR:782:PHE:HA	32:CR:785:ARG:HB2	2.00	0.44
32:CS:635:ILE:HD12	32:CS:635:ILE:HA	1.87	0.44
37:Cg:57:LEU:HD22	37:Cg:67:ARG:HA	1.99	0.44
44:CU:115:GLU:HA	44:CU:118:VAL:HG12	1.99	0.44
45:C1:2370:C:H2'	45:C1:2371:G:C8	2.52	0.44
47:UH:638:SER:HB2	47:UH:721:GLU:HG2	2.00	0.44
1:UA:202:TYR:OH	1:UA:261:ALA:O	2.35	0.44
6:UG:253:GLU:OE2	45:C1:341:G:O2'	2.26	0.44
14:UR:241:LYS:HD3	14:UR:241:LYS:HA	1.81	0.44
15:UU:196:LEU:O	15:UU:198:LYS:NZ	2.44	0.44
16:UX:150:ASP:OD1	16:UX:150:ASP:N	2.41	0.44
20:CD:419:LEU:HD23	20:CD:423:GLY:HA2	1.98	0.44
22:CG:579:VAL:HG12	22:CG:603:ILE:HG23	1.99	0.44
24:CI:81:LYS:HZ3	54:CI:1201:GTP:PB	2.40	0.44
24:CI:269:GLU:HA	24:CI:779:LEU:O	2.18	0.44
24:CI:1121:LYS:HB2	24:CI:1121:LYS:HE2	1.81	0.44
32:CR:835:PRO:O	32:CR:839:LYS:HB2	2.18	0.44
32:CS:265:LEU:O	32:CS:269:VAL:HG23	2.17	0.44
39:CI:97:ARG:HH21	39:CI:133:PRO:HG3	1.82	0.44
47:UH:714:LEU:HD23	47:UH:779:LEU:HD11	1.98	0.44
51:CX:244:PRO:HB2	51:CX:287:HIS:HB2	1.99	0.44
51:CX:358:GLU:OE2	51:CX:391:ARG:NH1	2.48	0.44
9:UL:535:TRP:HB3	9:UL:556:LEU:HD13	1.99	0.44
9:UL:627:ALA:HA	9:UL:651:SER:HB2	2.00	0.44
19:CC:16:SER:HB3	19:CC:53:PHE:HD1	1.82	0.44
26:CK:238:GLU:HA	26:CK:262:THR:HA	1.98	0.44
28:CM:264:ILE:HD11	28:CM:286:VAL:HG11	1.99	0.44
29:CN:123:GLU:HG2	29:CN:161:LYS:HB3	1.98	0.44
32:CS:770:ASN:OD1	32:CS:770:ASN:N	2.50	0.44
32:CS:877:SER:O	32:CS:881:GLN:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C1:597:G:H2'	45:C1:598:A:C8	2.52	0.44
3:UC:586:ASN:ND2	42:Cn:139:LYS:O	2.37	0.44
6:UG:567:LYS:HA	6:UG:570:ARG:HB2	2.00	0.44
9:UL:899:LEU:HA	9:UL:902:VAL:HG12	2.00	0.44
12:UO:418:ARG:HH12	45:C1:75:G:H2'	1.82	0.44
26:CK:285:SER:O	26:CK:285:SER:OG	2.34	0.44
29:CN:86:ASP:OD1	29:CN:87:ALA:N	2.51	0.44
32:CR:819:ASN:HD22	32:CR:819:ASN:HA	1.61	0.44
32:CS:135:ILE:H	32:CS:135:ILE:HG13	1.47	0.44
47:UH:547:VAL:HG13	47:UH:594:ALA:HA	1.99	0.44
49:US:173:VAL:HG22	49:US:181:LEU:HD21	1.99	0.44
6:UG:349:ALA:O	6:UG:400:TRP:NE1	2.43	0.44
7:UJ:187:THR:HG22	7:UJ:224:ALA:HA	2.00	0.44
12:UO:454:LEU:HD22	12:UO:494:TYR:HD2	1.83	0.44
13:UQ:441:VAL:HG13	13:UQ:849:ALA:HA	2.00	0.44
14:UR:453:GLY:HA3	14:UR:526:ILE:HG13	1.99	0.44
15:UU:423:ARG:NH1	45:C1:258:C:N3	2.66	0.44
15:UU:891:LEU:HD13	31:CQ:259:TRP:HD1	1.82	0.44
23:CH:67:ASP:HB3	23:CH:76:THR:HG22	1.99	0.44
23:CH:68:VAL:HG13	23:CH:75:ILE:HG22	2.00	0.44
24:CI:286:VAL:HG13	24:CI:800:VAL:HG13	1.99	0.44
25:CJ:108:ARG:NH1	45:C1:350:U:OP1	2.36	0.44
32:CS:835:PRO:O	32:CS:839:LYS:HB2	2.18	0.44
49:US:370:SER:OG	49:US:373:LEU:CG	2.66	0.44
9:UL:189:LEU:HB2	9:UL:203:LEU:HD11	2.00	0.44
9:UL:503:VAL:HG11	9:UL:556:LEU:HD11	2.00	0.44
10:UM:335:LEU:HD11	10:UM:343:LEU:HD23	1.99	0.44
14:UR:324:ASP:OD1	14:UR:344:ARG:NH1	2.50	0.44
15:UU:391:LEU:HD21	15:UU:773:VAL:HG11	2.00	0.44
28:CM:311:ARG:HB2	28:CM:314:ALA:HB2	1.99	0.44
30:CP:161:TYR:O	30:CP:171:VAL:HA	2.17	0.44
32:CR:798:PRO:HB2	32:CR:801:LEU:HB2	1.98	0.44
45:C1:2:G:H2'	45:C1:3:G:C8	2.52	0.44
45:C1:616:U:H2'	45:C1:617:G:H8	1.83	0.44
45:C1:1219:A:N7	45:C1:1448:A:N6	2.66	0.44
2:UB:111:ASN:OD1	2:UB:111:ASN:N	2.47	0.44
4:UD:134:CYS:HB2	4:UD:192:ILE:HG22	2.00	0.44
6:UG:237:SER:HB3	45:C1:289:A:H2'	2.00	0.44
7:UJ:31:LYS:HD3	7:UJ:31:LYS:HA	1.86	0.44
7:UJ:165:ARG:HD2	7:UJ:165:ARG:HA	1.82	0.44
14:UR:345:ARG:HB2	45:C1:75:G:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UU:151:ILE:HG12	15:UU:162:TRP:HB2	2.00	0.44
15:UU:167:LEU:HD23	15:UU:167:LEU:HA	1.88	0.44
18:CB:157:LEU:HB3	18:CB:226:ILE:HD13	1.99	0.44
28:CM:253:MET:SD	28:CM:253:MET:N	2.90	0.44
32:CR:9:SER:O	32:CR:9:SER:OG	2.35	0.44
34:Ca:70:LEU:HD23	34:Ca:70:LEU:HA	1.88	0.44
34:Ca:137:LEU:HD13	34:Ca:172:ILE:HD11	2.00	0.44
34:Ca:160:GLN:NE2	34:Ca:204:ILE:O	2.45	0.44
37:Cg:171:ARG:HA	37:Cg:171:ARG:HD2	1.79	0.44
45:C1:1068:C:H2'	45:C1:1069:A:H8	1.82	0.44
45:C1:2057:G:H2'	45:C1:2058:A:C8	2.52	0.44
1:UA:11:LEU:O	1:UA:695:LEU:HB3	2.18	0.43
4:UD:9:VAL:HG21	4:UD:863:ILE:HD13	1.99	0.43
11:UN:366:GLY:N	11:UN:370:GLU:OE1	2.44	0.43
22:CG:430:HIS:CD2	22:CG:499:LEU:H	2.36	0.43
23:CH:219:ARG:HA	23:CH:251:HIS:O	2.18	0.43
24:CI:71:VAL:HG13	24:CI:135:ILE:HG13	2.00	0.43
26:CK:86:PRO:HD2	26:CK:213:PRO:HA	2.00	0.43
32:CR:303:VAL:HB	32:CR:365:HIS:CE1	2.53	0.43
36:Ce:153:LYS:O	41:Cm:42:GLN:NE2	2.51	0.43
46:C2:134:C:H4'	46:C2:181:A:H61	1.82	0.43
47:UH:495:GLU:OE2	47:UH:575:SER:OG	2.31	0.43
9:UL:484:THR:OG1	9:UL:485:LYS:N	2.51	0.43
10:UM:550:LEU:HD22	10:UM:559:PHE:HZ	1.82	0.43
10:UM:675:VAL:HG13	10:UM:689:LEU:HB2	2.00	0.43
10:UM:877:LEU:HD23	10:UM:877:LEU:HA	1.89	0.43
12:UO:470:LEU:HD13	12:UO:505:LEU:HG	2.00	0.43
13:UQ:114:TYR:HA	13:UQ:121:LEU:HA	2.00	0.43
16:UX:54:PRO:HB3	16:UX:85:ALA:HB1	2.00	0.43
18:CB:163:SER:N	18:CB:189:SER:OG	2.46	0.43
19:CC:307:GLN:HG3	19:CC:312:THR:HB	2.00	0.43
26:CK:252:VAL:HG21	27:CL:549:ILE:HG21	2.00	0.43
26:CK:272:THR:OG1	26:CK:273:LEU:N	2.51	0.43
32:CR:265:LEU:O	32:CR:269:VAL:HG23	2.17	0.43
32:CS:48:MET:HB3	32:CS:49:ASP:H	1.61	0.43
32:CS:616:TRP:O	32:CS:620:GLN:HB2	2.18	0.43
44:CU:235:LYS:HB2	44:CU:235:LYS:HE3	1.88	0.43
45:C1:61:G:H5''	47:UH:893:SER:HB2	1.99	0.43
45:C1:484:G:H2'	45:C1:485:G:C8	2.52	0.43
1:UA:3:THR:HG21	1:UA:607:LEU:HD13	1.99	0.43
3:UC:580:THR:HG22	3:UC:583:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:182:THR:O	21:CE:124:ARG:NH2	2.41	0.43
10:UM:135:ILE:HD11	10:UM:159:LEU:HD21	2.00	0.43
10:UM:289:MET:HB3	10:UM:301:TRP:HB2	1.99	0.43
12:UO:495:ARG:NH1	12:UO:533:GLU:OE1	2.47	0.43
13:UQ:543:PHE:HE2	13:UQ:547:GLY:HA2	1.83	0.43
27:CL:563:ASP:OD1	27:CL:563:ASP:N	2.44	0.43
32:CR:616:TRP:O	32:CR:620:GLN:HB2	2.18	0.43
32:CS:9:SER:O	32:CS:9:SER:OG	2.35	0.43
34:Ca:141:ALA:HB1	34:Ca:207:LEU:HD13	2.00	0.43
45:C1:61:G:O6	47:UH:904:ARG:NE	2.50	0.43
45:C1:301:U:O2	45:C1:341:G:C2	2.70	0.43
49:US:176:SER:O	49:US:182:ARG:NH2	2.44	0.43
49:US:299:LYS:HE3	49:US:299:LYS:HB2	1.77	0.43
51:CX:205:ILE:HD13	51:CX:208:ILE:HD12	1.99	0.43
2:UB:743:LEU:HD23	49:US:462:GLN:HE21	1.83	0.43
9:UL:532:ALA:HB2	9:UL:568:ILE:HD12	2.00	0.43
10:UM:20:ILE:HD12	10:UM:20:ILE:HA	1.90	0.43
14:UR:307:ALA:HB3	14:UR:311:PRO:HA	2.00	0.43
21:CE:115:ILE:HD13	21:CE:115:ILE:HA	1.84	0.43
23:CH:216:ARG:HB2	23:CH:286:SER:HB3	2.00	0.43
30:CP:47:ARG:HA	30:CP:47:ARG:HD2	1.75	0.43
30:CP:142:ARG:NH2	45:C1:1612:A:OP2	2.51	0.43
32:CR:79:LYS:HA	32:CR:79:LYS:HD3	1.85	0.43
32:CR:135:ILE:H	32:CR:135:ILE:HG13	1.47	0.43
32:CR:526:LEU:HG	32:CR:537:LEU:HD12	2.01	0.43
32:CS:68:THR:HG21	32:CS:73:LYS:HE2	2.00	0.43
47:UH:591:VAL:HG21	47:UH:609:ILE:HG21	1.99	0.43
49:US:299:LYS:HE2	49:US:302:MET:HE1	2.00	0.43
51:CX:368:LYS:O	51:CX:372:GLU:N	2.51	0.43
1:UA:353:GLN:HG2	1:UA:821:ARG:HH21	1.83	0.43
2:UB:672:ARG:HA	2:UB:672:ARG:HD3	1.84	0.43
7:UJ:139:PHE:HB3	7:UJ:148:PHE:HD1	1.82	0.43
24:CI:344:MET:HB2	24:CI:344:MET:HE3	1.72	0.43
24:CI:368:GLU:O	24:CI:369:ARG:NH1	2.46	0.43
30:CP:58:VAL:HG22	30:CP:112:LEU:HD21	1.99	0.43
32:CR:31:GLY:HA3	32:CR:34:ALA:HB2	2.01	0.43
32:CR:877:SER:O	32:CR:881:GLN:N	2.48	0.43
34:Ca:27:LYS:HD3	34:Ca:49:ASN:HA	2.01	0.43
45:C1:1630:C:H2'	45:C1:1631:G:H8	1.83	0.43
45:C1:2356:C:H2'	45:C1:2357:G:H8	1.84	0.43
47:UH:722:THR:O	47:UH:726:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:US:199:TYR:HA	49:US:202:GLU:HG2	2.01	0.43
49:US:430:LYS:HZ1	49:US:434:ASP:HB2	1.84	0.43
1:UA:73:ILE:HG21	1:UA:99:VAL:HB	2.01	0.43
1:UA:95:PHE:HB3	1:UA:115:LEU:HD21	1.99	0.43
2:UB:338:LYS:HA	2:UB:338:LYS:HD2	1.83	0.43
2:UB:591:LEU:HD21	2:UB:635:VAL:HG13	2.00	0.43
9:UL:479:VAL:HG12	9:UL:493:ASP:HB3	2.01	0.43
9:UL:920:ASN:ND2	10:UM:827:GLN:OE1	2.50	0.43
12:UO:273:GLN:HG2	48:UE:163:THR:HB	2.00	0.43
13:UQ:116:THR:HA	13:UQ:432:MET:HG3	2.01	0.43
13:UQ:554:ASP:OD2	13:UQ:586:LYS:NZ	2.52	0.43
16:UX:62:THR:HG21	16:UX:98:GLU:HB2	2.01	0.43
20:CD:153:LYS:HE3	20:CD:153:LYS:HB3	1.85	0.43
28:CM:215:SER:HB2	28:CM:223:ILE:HG13	2.01	0.43
32:CR:68:THR:HG21	32:CR:73:LYS:HE2	2.00	0.43
45:C1:2237:G:H2'	45:C1:2238:A:H8	1.83	0.43
1:UA:60:ARG:HD3	1:UA:60:ARG:HA	1.81	0.43
4:UD:346:ASP:OD1	4:UD:346:ASP:N	2.39	0.43
10:UM:813:LEU:HD23	10:UM:813:LEU:HA	1.82	0.43
15:UU:754:LEU:HD22	15:UU:763:LEU:HD21	2.00	0.43
16:UX:5:ARG:HA	16:UX:5:ARG:HD3	1.68	0.43
30:CP:200:GLU:HG2	30:CP:204:LYS:HE3	1.99	0.43
32:CS:738:LYS:NZ	32:CS:738:LYS:HB3	2.34	0.43
32:CS:893:ASP:O	32:CS:897:LEU:HB2	2.19	0.43
36:Ce:155:ASP:N	36:Ce:155:ASP:OD1	2.49	0.43
38:Ch:136:PRO:HA	38:Ch:137:PRO:HD3	1.88	0.43
41:Cm:11:LEU:HD22	41:Cm:74:VAL:HG13	2.01	0.43
41:Cm:26:MET:HG3	41:Cm:60:LYS:HD2	2.01	0.43
46:C2:153:G:O6	46:C2:176:U:O2	2.36	0.43
49:US:176:SER:HA	49:US:177:PRO:HD3	1.91	0.43
2:UB:557:HIS:HB2	2:UB:600:THR:HG22	2.00	0.43
4:UD:99:LYS:HE3	4:UD:101:ARG:HG2	2.01	0.43
6:UG:420:VAL:HA	6:UG:421:PRO:HD3	1.89	0.43
9:UL:469:LEU:HD13	9:UL:469:LEU:HA	1.80	0.43
14:UR:459:GLY:HA2	21:CE:87:ALA:HB2	2.01	0.43
15:UU:133:LEU:HD13	15:UU:137:LEU:HD23	2.00	0.43
22:CG:262:VAL:HG21	22:CG:303:LEU:HD21	2.01	0.43
22:CG:593:TYR:OH	46:C2:189:G:O2'	2.28	0.43
23:CH:151:ASP:OD2	23:CH:178:ARG:NH2	2.47	0.43
31:CQ:230:GLU:HA	31:CQ:233:VAL:HG22	2.00	0.43
32:CS:31:GLY:HA3	32:CS:34:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:C1:96:C:HO2'	45:C1:97:C:P	2.41	0.43
45:C1:331:C:N4	45:C1:332:U:O4	2.52	0.43
49:US:266:GLN:OE1	49:US:298:THR:OG1	2.29	0.43
1:UA:306:ASN:HB3	1:UA:309:GLY:H	1.84	0.43
1:UA:427:SER:O	1:UA:427:SER:OG	2.36	0.43
10:UM:560:ALA:HA	10:UM:569:LYS:O	2.19	0.43
13:UQ:81:VAL:HG21	13:UQ:825:LYS:HD2	2.00	0.43
20:CD:318:THR:OG1	46:C2:261:U:O2'	2.36	0.43
23:CH:270:LYS:O	45:C1:1715:A:N6	2.41	0.43
24:CI:80:GLY:CA	54:CI:1201:GTP:O2B	2.66	0.43
26:CK:153:THR:HG23	26:CK:164:MET:HG2	2.01	0.43
32:CR:738:LYS:NZ	32:CR:738:LYS:HB3	2.34	0.43
32:CR:855:LEU:HA	32:CR:858:MET:HG3	2.01	0.43
32:CR:893:ASP:O	32:CR:897:LEU:HB2	2.19	0.43
42:Cn:126:LYS:HG2	42:Cn:131:GLY:HA2	2.01	0.43
45:C1:2086:A:H5''	45:C1:2087:G:C8	2.54	0.43
45:C1:2351:G:H1'	45:C1:2352:U:H5	1.84	0.43
2:UB:550:GLU:OE2	49:US:523:ILE:N	2.52	0.43
6:UG:284:LEU:HA	6:UG:284:LEU:HD23	1.71	0.43
7:UJ:229:ILE:HD11	7:UJ:278:LEU:HD12	2.00	0.43
10:UM:21:TYR:HD1	10:UM:37:SER:HB3	1.84	0.43
12:UO:324:THR:HA	12:UO:331:ASP:HA	2.01	0.43
14:UR:426:TRP:HB3	14:UR:478:GLY:HA3	2.00	0.43
15:UU:578:ARG:HH21	15:UU:582:ARG:HG2	1.84	0.43
18:CB:156:VAL:HG22	18:CB:225:VAL:HB	1.99	0.43
26:CK:132:GLN:O	26:CK:135:ARG:NH2	2.52	0.43
32:CS:490:LEU:HA	32:CS:490:LEU:HD12	1.83	0.43
32:CS:526:LEU:HG	32:CS:537:LEU:HD12	2.01	0.43
41:Cm:103:ILE:HD11	41:Cm:129:PHE:HE2	1.84	0.43
45:C1:1742:C:N4	45:C1:2165:U:N3	2.67	0.43
45:C1:1753:G:N1	45:C1:2158:G:OP2	2.49	0.43
45:C1:2070:A:O2'	45:C1:2073:A:N1	2.52	0.43
46:C2:137:U:H2'	46:C2:138:A:C8	2.54	0.43
49:US:289:MET:HA	49:US:293:ILE:HB	2.00	0.43
2:UB:652:ARG:HD3	49:US:467:TYR:HA	2.01	0.42
4:UD:254:SER:OG	52:UP:349:ARG:NH2	2.52	0.42
10:UM:20:ILE:HD11	10:UM:46:THR:HG21	2.00	0.42
19:CC:310:LEU:HD23	19:CC:310:LEU:HA	1.92	0.42
22:CG:279:LYS:HB2	22:CG:279:LYS:HE2	1.87	0.42
25:CJ:96:ALA:O	25:CJ:100:ASN:HB3	2.19	0.42
32:CR:842:GLU:OE1	32:CR:920:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ca:92:GLN:HB2	34:Ca:95:ASN:HB3	2.00	0.42
41:Cm:82:ARG:O	41:Cm:86:LEU:N	2.52	0.42
45:C1:1169:A:O2'	45:C1:1170:G:N2	2.50	0.42
45:C1:2057:G:H2'	45:C1:2058:A:H8	1.83	0.42
51:CX:379:TRP:HA	51:CX:382:ILE:HD12	2.00	0.42
1:UA:149:GLN:HE21	45:C1:266:C:H3'	1.84	0.42
2:UB:616:LEU:HD21	49:US:500:LEU:HB3	2.01	0.42
2:UB:655:PRO:HD2	49:US:467:TYR:HE2	1.85	0.42
4:UD:432:THR:N	4:UD:446:SER:O	2.53	0.42
7:UJ:77:GLN:NE2	14:UR:62:ALA:H	2.18	0.42
9:UL:658:ILE:HA	9:UL:659:PRO:HD3	1.87	0.42
9:UL:912:ARG:HE	10:UM:828:ARG:HH12	1.67	0.42
10:UM:340:ASP:O	34:Ca:19:LYS:NZ	2.52	0.42
14:UR:564:ASP:OD2	45:C1:241:G:N2	2.44	0.42
23:CH:361:LEU:HD13	24:CI:546:MET:HG2	2.01	0.42
28:CM:211:SER:HB2	28:CM:227:LEU:HB3	2.01	0.42
29:CO:38:ILE:O	29:CO:203:CYS:HA	2.19	0.42
32:CR:295:MET:O	32:CR:299:ILE:HG23	2.19	0.42
32:CS:782:PHE:HA	32:CS:785:ARG:HB2	1.99	0.42
32:CS:855:LEU:HA	32:CS:858:MET:HG3	2.01	0.42
34:Ca:179:CYS:HB2	34:Ca:183:GLN:HB2	2.01	0.42
45:C1:62:U:C2	47:UH:894:ARG:HG3	2.54	0.42
45:C1:1457:G:N2	45:C1:1541:U:O2	2.52	0.42
49:US:488:ASN:OD1	49:US:488:ASN:N	2.51	0.42
51:CX:193:GLU:HB3	51:CX:194:ILE:H	1.66	0.42
4:UD:534:PRO:HD2	4:UD:537:ILE:HD12	2.00	0.42
4:UD:884:ARG:HD3	4:UD:884:ARG:HA	1.86	0.42
6:UG:474:GLU:OE1	6:UG:478:GLN:NE2	2.52	0.42
13:UQ:90:SER:OG	13:UQ:106:THR:O	2.37	0.42
13:UQ:154:ASP:HA	13:UQ:170:TRP:NE1	2.33	0.42
15:UU:247:ALA:HB1	15:UU:276:VAL:HG13	2.02	0.42
18:CA:249:GLN:HG2	19:CC:39:LYS:HD2	2.01	0.42
23:CH:152:THR:O	23:CH:156:ALA:CB	2.67	0.42
24:CI:369:ARG:HD3	24:CI:369:ARG:HA	1.78	0.42
32:CS:113:ASP:OD1	32:CS:113:ASP:N	2.51	0.42
32:CS:295:MET:O	32:CS:299:ILE:HG23	2.19	0.42
45:C1:1557:G:H2'	45:C1:1558:A:H8	1.83	0.42
49:US:92:LEU:HD23	49:US:92:LEU:HA	1.89	0.42
1:UA:16:CYS:SG	1:UA:17:ARG:N	2.92	0.42
2:UB:645:GLN:NE2	49:US:536:SER:OG	2.45	0.42
4:UD:690:LYS:H	4:UD:703:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:UG:274:HIS:CE1	6:UG:284:LEU:HD21	2.55	0.42
11:UN:304:LYS:HA	11:UN:304:LYS:HD2	1.79	0.42
12:UO:145:GLN:HE22	49:US:413:LEU:HG	1.84	0.42
15:UU:87:ARG:HA	15:UU:87:ARG:HD3	1.81	0.42
16:UX:55:PRO:HA	16:UX:86:SER:O	2.18	0.42
21:CE:21:LEU:HD23	21:CE:118:LEU:HD21	2.01	0.42
22:CG:483:TRP:HB3	22:CG:559:ILE:HG12	2.01	0.42
31:CQ:106:VAL:HG12	31:CQ:112:GLN:HA	2.02	0.42
31:CQ:110:LYS:O	31:CQ:130:THR:OG1	2.36	0.42
32:CR:138:ARG:O	32:CR:142:THR:HG22	2.19	0.42
39:CI:54:ARG:NH1	45:C1:1502:U:O2	2.53	0.42
45:C1:320:A:H1'	45:C1:321:G:C2	2.54	0.42
1:UA:21:LEU:HD23	1:UA:21:LEU:HA	1.92	0.42
1:UA:818:VAL:HA	1:UA:821:ARG:HG2	2.00	0.42
2:UB:700:ARG:HG3	2:UB:724:ALA:HB2	2.00	0.42
7:UJ:297:VAL:HG13	7:UJ:331:ALA:HB3	2.02	0.42
7:UJ:342:LEU:HD23	7:UJ:342:LEU:HA	1.91	0.42
9:UL:24:LEU:HD13	9:UL:371:SER:HB3	2.02	0.42
9:UL:570:SER:O	9:UL:583:ALA:HB3	2.20	0.42
9:UL:806:ASN:OD1	9:UL:806:ASN:N	2.51	0.42
13:UQ:364:SER:O	13:UQ:364:SER:OG	2.32	0.42
21:CE:110:ASP:OD1	21:CE:114:LYS:NZ	2.52	0.42
24:CI:171:THR:OG1	24:CI:172:HIS:N	2.51	0.42
24:CI:1033:SER:OG	45:C1:1159:C:O2	2.35	0.42
32:CR:113:ASP:OD1	32:CR:113:ASP:N	2.51	0.42
32:CR:471:GLU:OE1	32:CR:472:ILE:N	2.52	0.42
39:CI:114:ALA:O	39:CI:118:LEU:HB2	2.19	0.42
47:UH:621:ASP:OD1	47:UH:623:THR:OG1	2.33	0.42
9:UL:24:LEU:HG	9:UL:41:VAL:HG12	2.01	0.42
13:UQ:293:PHE:HA	13:UQ:315:ALA:O	2.20	0.42
15:UU:96:ALA:HB3	15:UU:107:ALA:HB3	2.02	0.42
15:UU:305:SER:OG	15:UU:306:GLY:N	2.53	0.42
17:UZ:97:VAL:HA	17:UZ:152:VAL:O	2.20	0.42
17:UZ:169:LYS:HG2	17:UZ:173:LYS:HB3	2.02	0.42
18:CB:164:GLY:HA2	18:CB:167:VAL:HG12	2.01	0.42
24:CI:559:ARG:HE	24:CI:559:ARG:HB2	1.57	0.42
32:CR:515:GLN:N	32:CR:515:GLN:OE1	2.53	0.42
32:CR:623:GLN:N	32:CS:839:LYS:HZ3	2.17	0.42
32:CS:865:TYR:CE1	32:CS:871:ARG:HB2	2.55	0.42
42:Cn:63:GLN:HA	42:Cn:64:PRO:HD3	1.90	0.42
48:UI:154:GLY:HA2	48:UI:184:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:534:LEU:HD21	1:UA:578:ILE:HG21	2.02	0.42
2:UB:784:LEU:HD23	2:UB:784:LEU:HA	1.92	0.42
4:UD:381:ARG:NH1	4:UD:842:GLU:O	2.52	0.42
4:UD:420:LEU:HD21	4:UD:467:LEU:HD21	2.00	0.42
5:UF:85:SER:O	5:UF:85:SER:OG	2.36	0.42
5:UF:339:ILE:HG12	5:UF:364:LEU:HA	2.01	0.42
6:UG:84:LEU:HD12	6:UG:84:LEU:HA	1.90	0.42
6:UG:198:LYS:O	6:UG:218:GLU:N	2.48	0.42
9:UL:425:HIS:NE2	9:UL:450:LYS:HB2	2.35	0.42
19:CC:87:PRO:HG2	19:CC:96:VAL:HG21	2.02	0.42
23:CH:122:PRO:HB3	23:CH:166:ILE:HG12	2.00	0.42
23:CH:131:ARG:NH1	23:CH:193:GLU:OE1	2.53	0.42
28:CM:197:VAL:HG21	36:Ce:161:LYS:HD3	2.02	0.42
40:Cj:9:VAL:HG21	40:Cj:88:SER:HA	2.00	0.42
45:C1:1026:C:O2'	45:C1:1109:A:N1	2.52	0.42
45:C1:1629:U:H2'	45:C1:1630:C:C6	2.54	0.42
49:US:342:LYS:HD2	49:US:342:LYS:HA	1.81	0.42
51:CX:234:ILE:O	51:CX:237:THR:OG1	2.36	0.42
51:CX:323:ILE:HD12	51:CX:323:ILE:HA	1.89	0.42
4:UD:80:LEU:HD22	4:UD:102:LEU:HD11	2.02	0.42
7:UJ:14:ALA:O	7:UJ:159:ARG:NH2	2.53	0.42
9:UL:228:ASP:OD1	9:UL:228:ASP:N	2.47	0.42
9:UL:705:SER:HB2	9:UL:708:GLY:H	1.84	0.42
14:UR:548:PHE:HE1	14:UR:571:LEU:HD11	1.85	0.42
18:CA:106:GLU:H	18:CA:106:GLU:HG2	1.65	0.42
23:CH:128:LEU:O	23:CH:195:ARG:HA	2.19	0.42
24:CI:287:HIS:HB2	24:CI:803:LEU:HD21	2.00	0.42
31:CQ:113:VAL:O	31:CQ:114:ARG:NH1	2.47	0.42
32:CS:138:ARG:O	32:CS:142:THR:HG22	2.19	0.42
32:CS:515:GLN:OE1	32:CS:515:GLN:N	2.53	0.42
32:CS:614:ILE:H	32:CS:614:ILE:HG12	1.45	0.42
34:Ca:81:PHE:CG	34:Ca:109:LYS:HD2	2.54	0.42
36:Ce:90:LYS:HE3	36:Ce:90:LYS:HB3	1.88	0.42
40:Cj:44:LEU:HB3	40:Cj:78:VAL:HG11	2.02	0.42
45:C1:2359:A:H2'	45:C1:2360:G:C8	2.55	0.42
47:UH:731:LYS:HB2	47:UH:734:GLU:HG3	2.01	0.42
47:UH:780:MET:HE1	47:UH:819:ILE:HD11	2.02	0.42
3:UC:598:ARG:HH12	45:C1:1126:A:H62	1.68	0.42
5:UF:310:LEU:HD23	5:UF:310:LEU:HA	1.91	0.42
6:UG:470:ASP:HB3	6:UG:473:SER:HB3	2.02	0.42
9:UL:402:LYS:HB3	9:UL:402:LYS:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:UL:861:LEU:HD23	9:UL:861:LEU:HA	1.86	0.42
10:UM:83:LEU:HD12	10:UM:108:LYS:HD3	2.02	0.42
12:UO:210:TYR:HB3	49:US:374:PRO:HB3	2.02	0.42
14:UR:345:ARG:NH1	45:C1:75:G:OP1	2.43	0.42
28:CM:302:SER:OG	28:CM:303:TYR:N	2.53	0.42
29:CN:179:THR:HG22	29:CN:221:VAL:HG11	2.02	0.42
31:CQ:145:ALA:HA	31:CQ:148:MET:HG2	2.02	0.42
32:CR:662:GLU:OE1	32:CR:767:GLN:NE2	2.45	0.42
36:Ce:173:ASP:HA	36:Ce:176:LEU:HG	2.01	0.42
45:C1:1148:G:O4'	45:C1:2179:C:N4	2.53	0.42
47:UH:811:PHE:O	47:UH:815:PHE:HB2	2.20	0.42
48:UE:232:GLN:O	48:UE:234:ASP:N	2.52	0.42
49:US:458:TRP:HA	49:US:461:VAL:HG12	2.02	0.42
2:UB:747:ILE:HG23	2:UB:788:LEU:HD22	2.02	0.42
7:UJ:238:ALA:HB3	15:UU:444:GLY:HA3	2.01	0.42
13:UQ:502:VAL:HG23	13:UQ:511:VAL:HB	2.02	0.42
15:UU:576:ARG:HA	15:UU:576:ARG:HD3	1.74	0.42
18:CA:66:LYS:NZ	33:CT:149:SER:O	2.44	0.42
18:CB:188:ARG:HA	18:CB:191:ARG:HD2	2.02	0.42
24:CI:308:THR:O	24:CI:310:ALA:N	2.53	0.42
28:CM:166:ASN:HB3	28:CM:182:LEU:HB2	2.01	0.42
28:CM:338:SER:O	28:CM:338:SER:OG	2.29	0.42
31:CQ:133:ASN:OD1	31:CQ:133:ASN:N	2.53	0.42
32:CR:839:LYS:HE3	32:CR:839:LYS:HB3	1.48	0.42
34:Ca:171:ILE:HD11	34:Ca:200:ALA:HB3	2.02	0.42
36:Ce:82:ARG:HA	36:Ce:85:ARG:HB2	2.02	0.42
7:UJ:59:LEU:HD21	7:UJ:105:VAL:HG23	2.02	0.41
10:UM:794:VAL:HA	10:UM:797:VAL:HG12	2.02	0.41
13:UQ:296:ARG:HA	13:UQ:297:PRO:HD3	1.91	0.41
13:UQ:754:TYR:HA	13:UQ:761:MET:HA	2.02	0.41
14:UR:376:PHE:HB3	14:UR:387:LEU:HD23	2.01	0.41
15:UU:143:GLN:NE2	15:UU:189:ALA:O	2.53	0.41
19:CC:23:GLN:H	19:CC:23:GLN:HG3	1.72	0.41
19:CC:205:HIS:CE1	19:CC:229:LYS:HE3	2.54	0.41
22:CG:339:LEU:HD23	22:CG:339:LEU:HA	1.86	0.41
22:CG:560:VAL:HG13	22:CG:580:VAL:HG13	2.01	0.41
27:CL:708:MET:HE2	27:CL:708:MET:HB3	1.83	0.41
32:CR:874:VAL:HG13	32:CR:876:LEU:HD22	2.02	0.41
45:C1:1507:G:H2'	45:C1:1508:A:H8	1.83	0.41
45:C1:2356:C:H2'	45:C1:2357:G:C8	2.55	0.41
46:C2:200:U:O4	46:C2:246:G:O6	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:UH:498:MET:HE1	47:UH:549:ALA:HB2	2.01	0.41
48:UE:182:GLN:HE22	48:UE:216:ARG:HH12	1.67	0.41
4:UD:262:ASP:OD1	14:UR:450:ARG:NH1	2.52	0.41
4:UD:563:VAL:HG22	4:UD:573:TRP:HZ3	1.85	0.41
5:UF:71:ARG:HH22	5:UF:85:SER:HB2	1.85	0.41
6:UG:283:THR:OG1	6:UG:285:TRP:NE1	2.53	0.41
6:UG:315:MET:HB2	6:UG:329:ILE:HD11	2.02	0.41
7:UJ:207:LYS:HE2	7:UJ:207:LYS:HB2	1.92	0.41
7:UJ:268:GLN:NE2	7:UJ:299:GLY:O	2.50	0.41
7:UJ:353:LYS:HB3	7:UJ:353:LYS:HE3	1.87	0.41
9:UL:425:HIS:NE2	9:UL:443:SER:HB2	2.36	0.41
13:UQ:260:ALA:HA	13:UQ:285:ASP:HA	2.01	0.41
13:UQ:735:ARG:HB2	13:UQ:747:LEU:HG	2.02	0.41
14:UR:290:LEU:HD11	14:UR:298:MET:HE2	2.02	0.41
17:UZ:279:ARG:HG3	17:UZ:280:ASN:H	1.85	0.41
19:CC:165:LYS:HE2	19:CC:165:LYS:HB2	1.84	0.41
19:CC:197:ARG:NH2	20:CD:174:GLU:OE2	2.53	0.41
23:CH:150:ILE:HD13	23:CH:150:ILE:HA	1.89	0.41
23:CH:375:TRP:O	24:CI:763:HIS:NE2	2.53	0.41
28:CM:266:ILE:O	28:CM:276:LEU:N	2.53	0.41
32:CR:865:TYR:CE1	32:CR:871:ARG:HB2	2.55	0.41
32:CS:303:VAL:HB	32:CS:365:HIS:CE1	2.53	0.41
41:Cm:103:ILE:HD11	41:Cm:129:PHE:CE2	2.56	0.41
45:C1:172:C:H2'	45:C1:173:G:C8	2.55	0.41
45:C1:2328:G:H2'	45:C1:2329:A:C8	2.55	0.41
45:C1:2363:G:N7	45:C1:2365:A:N6	2.68	0.41
1:UA:115:LEU:O	1:UA:118:LYS:N	2.53	0.41
2:UB:605:ASP:OD1	2:UB:605:ASP:N	2.51	0.41
10:UM:806:ILE:HD11	10:UM:837:HIS:CE1	2.55	0.41
12:UO:430:GLN:OE1	12:UO:432:ARG:NH2	2.54	0.41
13:UQ:330:LEU:O	13:UQ:334:HIS:CB	2.64	0.41
13:UQ:770:THR:OG1	13:UQ:771:SER:N	2.53	0.41
13:UQ:920:VAL:HG11	14:UR:575:THR:HG21	2.01	0.41
15:UU:255:ILE:HG12	15:UU:265:LEU:HB2	2.02	0.41
18:CB:83:VAL:HG12	18:CB:92:LEU:HD12	2.02	0.41
20:CD:258:LYS:HE3	20:CD:258:LYS:HB3	1.83	0.41
22:CG:469:LEU:HA	22:CG:479:PHE:O	2.21	0.41
23:CH:110:ILE:HD12	23:CH:110:ILE:HA	1.93	0.41
24:CI:1102:LYS:HB3	24:CI:1102:LYS:HE2	1.87	0.41
26:CK:76:GLU:OE2	26:CK:203:ARG:NH2	2.53	0.41
26:CK:140:ILE:HG22	26:CK:154:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CL:516:LEU:HD12	27:CL:521:MET:HE1	2.02	0.41
27:CL:694:GLU:HA	27:CL:704:ALA:HA	2.02	0.41
27:CL:784:LYS:HE3	27:CL:784:LYS:HB3	1.87	0.41
32:CS:283:LEU:HA	32:CS:472:ILE:O	2.20	0.41
32:CS:581:GLU:HA	32:CS:582:PRO:HD3	1.97	0.41
34:Ca:146:ARG:HD3	34:Ca:147:PRO:HD2	2.03	0.41
34:Ca:222:LYS:HD3	34:Ca:223:PHE:H	1.85	0.41
40:Cj:126:PRO:HD2	40:Cj:128:LYS:HE3	2.01	0.41
47:UH:615:ILE:HD13	47:UH:647:LEU:HD11	2.02	0.41
47:UH:900:ILE:HD13	47:UH:900:ILE:HA	1.88	0.41
49:US:89:VAL:HG12	49:US:148:ALA:HB2	2.01	0.41
49:US:146:LEU:HD23	49:US:146:LEU:HA	1.93	0.41
48:UI:180:ILE:O	48:UI:184:THR:OG1	2.34	0.41
1:UA:327:TRP:HZ3	15:UU:880:LEU:HD13	1.85	0.41
2:UB:13:LEU:HD22	2:UB:18:LEU:HD12	2.02	0.41
4:UD:261:TRP:HA	4:UD:268:GLN:HA	2.03	0.41
7:UJ:44:THR:HG23	7:UJ:46:ALA:H	1.85	0.41
9:UL:478:LYS:HE3	9:UL:495:ALA:HB3	2.01	0.41
10:UM:774:PHE:HA	10:UM:777:VAL:HG12	2.01	0.41
12:UO:169:VAL:HG22	12:UO:183:PHE:HB2	2.03	0.41
13:UQ:851:GLN:HG3	13:UQ:853:TRP:HZ3	1.85	0.41
20:CD:108:LYS:HA	20:CD:108:LYS:HD3	1.90	0.41
20:CD:186:VAL:HA	20:CD:189:TRP:HB3	2.03	0.41
23:CH:219:ARG:HD2	44:CU:111:MET:HE3	2.02	0.41
23:CH:339:MET:HE1	23:CH:349:LEU:HB2	2.02	0.41
24:CI:380:GLN:HE21	32:CR:207:ASN:ND2	2.19	0.41
28:CM:354:ARG:HH22	28:CM:360:ARG:HD3	1.86	0.41
32:CR:874:VAL:HG22	32:CR:876:LEU:HB3	2.03	0.41
32:CS:422:ARG:HH21	32:CS:422:ARG:HD3	1.75	0.41
32:CS:471:GLU:OE1	32:CS:472:ILE:N	2.52	0.41
32:CS:917:ARG:HA	32:CS:920:THR:HG22	2.02	0.41
40:Cj:18:ALA:HA	40:Cj:68:ARG:O	2.21	0.41
46:C2:49:U:H2'	46:C2:50:G:H8	1.86	0.41
46:C2:158:C:H2'	46:C2:159:G:C8	2.55	0.41
47:UH:639:SER:OG	47:UH:640:GLU:OE1	2.35	0.41
4:UD:867:LEU:HD23	4:UD:867:LEU:HA	1.83	0.41
9:UL:642:HIS:HB3	9:UL:686:PHE:CE2	2.56	0.41
10:UM:382:ILE:HD12	10:UM:462:VAL:HG11	2.01	0.41
13:UQ:286:VAL:HG11	13:UQ:316:VAL:HG11	2.03	0.41
13:UQ:758:SER:O	47:UH:596:LYS:NZ	2.40	0.41
19:CC:185:ASP:OD1	19:CC:317:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CH:245:GLN:HB2	23:CH:246:LEU:HD12	2.03	0.41
25:CJ:38:ILE:HG22	25:CJ:40:LYS:H	1.85	0.41
25:CJ:108:ARG:HA	25:CJ:113:VAL:HG21	2.02	0.41
33:CT:154:ARG:N	46:C2:249:U:OP1	2.54	0.41
40:Cj:47:LYS:HA	40:Cj:47:LYS:HD2	1.68	0.41
45:C1:346:C:O2'	45:C1:347:C:O5'	2.34	0.41
45:C1:1476:A:H2'	45:C1:1477:A:H8	1.85	0.41
45:C1:1734:G:H2'	45:C1:1735:A:H8	1.85	0.41
45:C1:2175:A:H2'	45:C1:2176:A:C8	2.55	0.41
49:US:484:LYS:HA	49:US:484:LYS:HD2	1.85	0.41
51:CX:310:LEU:HD12	51:CX:315:THR:HB	2.02	0.41
1:UA:454:SER:HB3	1:UA:457:THR:HB	2.02	0.41
4:UD:66:GLU:OE1	4:UD:545:TYR:OH	2.27	0.41
4:UD:413:LEU:HD23	4:UD:413:LEU:HA	1.93	0.41
4:UD:700:TRP:CD2	4:UD:709:MET:HB3	2.56	0.41
4:UD:800:LEU:HD23	4:UD:800:LEU:HA	1.94	0.41
8:UK:39:ARG:HA	8:UK:39:ARG:HD3	1.88	0.41
13:UQ:129:LEU:HD12	13:UQ:129:LEU:HA	1.92	0.41
15:UU:844:SER:OG	15:UU:845:LEU:N	2.54	0.41
21:CF:114:LYS:O	21:CF:118:LEU:HB2	2.20	0.41
23:CH:236:ILE:HG12	23:CH:252:ILE:HB	2.03	0.41
25:CJ:68:ASN:HB3	25:CJ:71:ARG:HB3	2.03	0.41
26:CK:94:ARG:HA	26:CK:94:ARG:HD3	1.90	0.41
26:CK:100:LEU:HD22	26:CK:144:GLU:HG2	2.02	0.41
28:CM:273:ASP:OD1	28:CM:444:LYS:NZ	2.42	0.41
29:CN:74:ILE:HA	29:CN:84:ILE:HD11	2.03	0.41
45:C1:1644:U:O2'	45:C1:1645:U:O2	2.29	0.41
49:US:153:LEU:HD23	49:US:153:LEU:HA	1.92	0.41
49:US:250:LYS:HB2	49:US:253:HIS:HB2	2.03	0.41
51:CX:386:VAL:HG13	51:CX:433:LEU:HD21	2.03	0.41
2:UB:23:LYS:HB3	2:UB:27:GLN:HB2	2.01	0.41
2:UB:734:LYS:HD2	2:UB:734:LYS:HA	1.93	0.41
6:UG:220:SER:HB3	6:UG:236:ILE:HG12	2.02	0.41
9:UL:82:VAL:HA	9:UL:95:TRP:O	2.21	0.41
9:UL:642:HIS:HB3	9:UL:686:PHE:HE2	1.84	0.41
10:UM:150:SER:OG	10:UM:151:GLY:N	2.54	0.41
12:UO:317:ILE:HA	12:UO:338:MET:HA	2.01	0.41
13:UQ:264:GLY:HA2	13:UQ:280:ARG:O	2.20	0.41
16:UX:9:LYS:HE2	16:UX:9:LYS:HB3	1.75	0.41
20:CD:6:LEU:HB2	20:CD:88:LEU:HD11	2.02	0.41
23:CH:377:ILE:HG23	23:CH:394:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CI:80:GLY:C	54:CI:1201:GTP:O2B	2.62	0.41
26:CK:230:PHE:HB3	26:CK:237:ILE:HD11	2.03	0.41
30:CP:51:LEU:O	30:CP:55:TRP:HB2	2.20	0.41
30:CP:127:ARG:HD2	30:CP:127:ARG:HA	1.78	0.41
31:CQ:113:VAL:HG23	31:CQ:124:LEU:HD23	2.02	0.41
32:CR:917:ARG:HE	32:CR:917:ARG:HB2	1.36	0.41
32:CS:842:GLU:OE1	32:CS:920:THR:OG1	2.36	0.41
34:Ca:89:ASP:HB3	34:Ca:223:PHE:CE1	2.56	0.41
40:Cj:13:LYS:HG3	40:Cj:14:LYS:H	1.86	0.41
45:C1:1045:G:H2'	45:C1:1046:G:C8	2.56	0.41
51:CX:415:LEU:HD13	51:CX:449:ILE:HG12	2.03	0.41
52:UP:328:ASP:OD1	52:UP:328:ASP:N	2.43	0.41
1:UA:398:PHE:CE2	1:UA:433:VAL:HG21	2.55	0.41
4:UD:155:VAL:HG22	4:UD:165:LEU:HD12	2.02	0.41
6:UG:567:LYS:HE3	6:UG:567:LYS:HB2	1.92	0.41
9:UL:17:VAL:HG23	9:UL:50:TRP:CE2	2.55	0.41
10:UM:645:VAL:HA	10:UM:670:GLY:HA2	2.02	0.41
14:UR:331:VAL:HG22	14:UR:378:VAL:HG11	2.02	0.41
15:UU:191:ASN:OD1	15:UU:191:ASN:N	2.40	0.41
26:CK:85:ASP:OD1	27:CL:559:ARG:NH2	2.53	0.41
26:CK:90:VAL:HA	26:CK:140:ILE:HG13	2.02	0.41
28:CM:74:LYS:H	28:CM:74:LYS:HG2	1.69	0.41
28:CM:422:GLU:O	28:CM:426:SER:CB	2.68	0.41
32:CR:283:LEU:HA	32:CR:472:ILE:O	2.20	0.41
32:CR:559:MET:HG2	32:CR:587:GLN:HE22	1.86	0.41
34:Ca:144:LYS:HA	34:Ca:208:GLN:HB2	2.02	0.41
36:Ce:65:VAL:HA	36:Ce:97:LEU:O	2.20	0.41
38:Ch:96:VAL:HG22	38:Ch:146:ALA:HB1	2.02	0.41
45:C1:1539:G:H2'	45:C1:1540:A:C8	2.56	0.41
45:C1:2085:G:C2	45:C1:2088:A:N7	2.86	0.41
47:UH:721:GLU:HA	47:UH:724:LYS:HG2	2.03	0.41
1:UA:180:LEU:HA	1:UA:180:LEU:HD23	1.84	0.41
1:UA:773:LEU:HG	1:UA:797:LEU:HD11	2.03	0.41
2:UB:584:LEU:HD11	2:UB:625:LYS:HB2	2.03	0.41
7:UJ:238:ALA:HB1	15:UU:447:ALA:HB3	2.02	0.41
9:UL:439:LYS:HE3	9:UL:439:LYS:HB2	1.84	0.41
9:UL:937:ARG:HA	9:UL:937:ARG:HD3	1.78	0.41
10:UM:155:LEU:O	10:UM:203:GLN:N	2.54	0.41
10:UM:710:SER:OG	10:UM:718:THR:OG1	2.38	0.41
12:UO:146:PRO:O	12:UO:165:ASP:N	2.46	0.41
13:UQ:479:PHE:HE2	13:UQ:596:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UR:144:LEU:HD23	14:UR:144:LEU:HA	1.93	0.41
14:UR:372:THR:HG22	14:UR:390:SER:HB3	2.03	0.41
14:UR:539:LEU:HD22	14:UR:565:ALA:HB1	2.03	0.41
15:UU:481:ILE:O	15:UU:528:ARG:NH2	2.54	0.41
18:CB:185:PHE:HB2	18:CB:209:ASP:HA	2.02	0.41
22:CG:400:ARG:HE	22:CG:400:ARG:HB3	1.73	0.41
22:CG:403:MET:HE2	22:CG:403:MET:HB3	1.95	0.41
22:CG:405:ASP:OD1	22:CG:405:ASP:N	2.53	0.41
24:CI:854:ARG:HH12	42:Cn:64:PRO:HA	1.86	0.41
25:CJ:54:LEU:HD23	25:CJ:101:VAL:HG21	2.03	0.41
25:CJ:131:ILE:HG22	25:CJ:136:VAL:HB	2.02	0.41
28:CM:213:ILE:HB	28:CM:225:PHE:HB2	2.02	0.41
28:CM:442:LEU:HD23	28:CM:443:VAL:HG13	2.03	0.41
30:CP:62:LEU:HD23	30:CP:62:LEU:HA	1.85	0.41
30:CP:106:VAL:HG11	30:CP:172:MET:HE3	2.03	0.41
32:CR:490:LEU:HA	32:CR:490:LEU:HD12	1.83	0.41
32:CR:523:ARG:NH1	32:CR:559:MET:O	2.54	0.41
32:CR:581:GLU:HA	32:CR:582:PRO:HD3	1.97	0.41
32:CR:855:LEU:HA	32:CR:858:MET:HE2	2.03	0.41
32:CS:523:ARG:NH1	32:CS:559:MET:O	2.54	0.41
32:CS:874:VAL:HG22	32:CS:876:LEU:HB3	2.03	0.41
34:Ca:160:GLN:HE22	45:C1:1649:A:H5'	1.85	0.41
37:Cg:128:ARG:HA	37:Cg:128:ARG:HD2	1.90	0.41
45:C1:68:U:O4	47:UH:883:ARG:NE	2.40	0.41
45:C1:1096:A:H2'	45:C1:1097:U:O4'	2.21	0.41
45:C1:1709:A:H4'	45:C1:1710:G:H5'	2.03	0.41
46:C2:145:A:H2'	46:C2:146:A:H8	1.86	0.41
47:UH:867:LEU:HD23	47:UH:867:LEU:HA	1.90	0.41
48:UE:159:GLN:O	48:UE:163:THR:HG22	2.21	0.41
49:US:301:GLU:OE2	49:US:332:ARG:NE	2.43	0.41
49:US:362:ARG:NH2	49:US:494:ASP:OD2	2.53	0.41
51:CX:194:ILE:HD13	51:CX:194:ILE:HA	1.97	0.41
2:UB:804:ARG:NH1	29:CO:182:PHE:O	2.43	0.41
5:UF:379:THR:HA	5:UF:382:VAL:HG12	2.03	0.41
6:UG:230:LEU:HD21	6:UG:456:PRO:HB3	2.02	0.41
6:UG:355:LEU:HD12	6:UG:423:ALA:HB2	2.03	0.41
12:UO:44:ILE:HG12	12:UO:77:ALA:HB2	2.02	0.41
12:UO:50:PRO:HG2	12:UO:70:ASN:HD21	1.85	0.41
13:UQ:543:PHE:CE2	13:UQ:547:GLY:HA2	2.55	0.41
16:UX:123:CYS:HB2	16:UX:125:HIS:HD2	1.86	0.41
17:UZ:235:LEU:HD23	17:UZ:235:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CA:85:ARG:HH11	33:CT:112:ARG:HH22	1.69	0.41
18:CA:230:VAL:HG23	18:CA:235:GLN:HG3	2.02	0.41
20:CD:122:ILE:O	20:CD:126:LEU:HB2	2.21	0.41
20:CD:292:LEU:HD23	20:CD:292:LEU:HA	1.95	0.41
24:CI:183:LYS:HE2	45:C1:1049:G:H5''	2.03	0.41
26:CK:294:LYS:HB3	26:CK:294:LYS:HE3	1.88	0.41
29:CN:167:ILE:HG13	29:CN:171:LEU:HG	2.03	0.41
31:CQ:255:MET:HE3	31:CQ:255:MET:HB2	1.90	0.41
32:CR:263:LYS:HA	32:CR:266:LEU:HD12	2.02	0.41
32:CS:559:MET:HG2	32:CS:587:GLN:HE22	1.86	0.41
32:CS:855:LEU:HA	32:CS:858:MET:HE2	2.03	0.41
35:Cc:87:HIS:HB3	35:Cc:88:GLY:H	1.75	0.41
45:C1:314:A:H2'	45:C1:315:G:H8	1.86	0.41
46:C2:201:A:H2'	46:C2:202:C:C6	2.57	0.41
6:UG:451:LEU:HD23	6:UG:451:LEU:HA	1.93	0.40
7:UJ:343:ARG:NH2	7:UJ:384:SER:O	2.50	0.40
9:UL:560:ARG:NH1	9:UL:595:ASP:O	2.43	0.40
12:UO:332:ARG:HA	12:UO:332:ARG:HD3	1.92	0.40
13:UQ:402:ILE:HG22	13:UQ:413:LEU:HD22	2.02	0.40
15:UU:151:ILE:HD13	15:UU:151:ILE:HG21	1.85	0.40
15:UU:630:VAL:HG13	15:UU:637:VAL:HG12	2.03	0.40
23:CH:218:ILE:O	23:CH:250:VAL:HA	2.21	0.40
23:CH:281:LEU:HB3	23:CH:317:LEU:HD22	2.03	0.40
24:CI:1095:GLN:O	24:CI:1099:THR:HG23	2.22	0.40
30:CP:89:PRO:HG2	39:CI:119:ALA:HB3	2.02	0.40
32:CR:743:VAL:HG21	32:CR:775:LEU:HD21	2.03	0.40
32:CR:917:ARG:HA	32:CR:920:THR:HG22	2.03	0.40
32:CS:782:PHE:HA	32:CS:785:ARG:HD2	2.03	0.40
45:C1:399:G:H2'	45:C1:400:C:C6	2.56	0.40
49:US:460:ILE:HG21	49:US:478:ILE:HD12	2.03	0.40
1:UA:16:CYS:HB3	1:UA:34:GLY:H	1.86	0.40
4:UD:129:HIS:CD2	4:UD:164:VAL:HG11	2.56	0.40
4:UD:346:ASP:HA	4:UD:872:LEU:HD22	2.03	0.40
6:UG:154:ALA:HB1	6:UG:180:VAL:HG11	2.02	0.40
9:UL:308:ARG:NH1	9:UL:355:ASP:OD1	2.55	0.40
10:UM:781:ARG:HE	10:UM:781:ARG:HB2	1.73	0.40
15:UU:206:GLY:HA3	15:UU:224:PRO:HG3	2.03	0.40
15:UU:1022:HIS:HD2	15:UU:1025:ARG:HH21	1.69	0.40
19:CC:206:PHE:HE2	19:CC:209:LEU:HD13	1.87	0.40
20:CD:339:PRO:HA	46:C2:89:A:H3'	2.03	0.40
22:CG:231:LYS:NZ	22:CG:232:ALA:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CG:479:PHE:HB3	22:CG:563:ILE:HD13	2.03	0.40
25:CJ:149:LEU:HD13	27:CL:633:LEU:HD21	2.03	0.40
28:CM:86:SER:OG	28:CM:88:ASP:OD1	2.28	0.40
29:CN:196:LEU:HD21	29:CN:202:ILE:HD12	2.03	0.40
29:CO:68:LEU:HD12	29:CO:68:LEU:HA	1.89	0.40
32:CR:40:HIS:HB3	32:CR:206:LEU:HD11	2.03	0.40
32:CS:716:ARG:HA	32:CS:716:ARG:HD2	1.94	0.40
37:Cg:110:LEU:HD23	37:Cg:110:LEU:HA	1.85	0.40
45:C1:114:U:O2'	48:UE:210:ARG:NH1	2.54	0.40
51:CX:325:SER:HB2	51:CX:369:VAL:HG11	2.02	0.40
4:UD:876:TYR:CZ	52:UP:348:ARG:HD3	2.56	0.40
9:UL:506:HIS:ND1	9:UL:529:ASP:OD1	2.55	0.40
12:UO:95:ILE:HD13	12:UO:126:PHE:HE1	1.86	0.40
13:UQ:169:ASN:N	13:UQ:169:ASN:OD1	2.53	0.40
14:UR:269:ILE:HD13	14:UR:269:ILE:HA	1.93	0.40
20:CD:182:MET:HE1	20:CD:267:ARG:HG3	2.03	0.40
23:CH:52:SER:HB3	23:CH:102:ILE:HG22	2.03	0.40
23:CH:225:THR:HG22	23:CH:257:ASP:HB2	2.02	0.40
32:CR:131:ILE:HD12	32:CR:136:LEU:HD12	2.02	0.40
32:CR:782:PHE:HA	32:CR:785:ARG:HD2	2.03	0.40
32:CS:79:LYS:HA	32:CS:79:LYS:HD3	1.85	0.40
32:CS:97:LEU:O	32:CS:101:LEU:HB2	2.21	0.40
32:CS:124:ILE:HG12	32:CS:150:VAL:HB	2.03	0.40
32:CS:131:ILE:HD12	32:CS:136:LEU:HD12	2.03	0.40
36:Ce:19:PRO:HG2	36:Ce:24:ARG:HH21	1.86	0.40
36:Ce:86:GLU:O	36:Ce:90:LYS:HB2	2.21	0.40
37:Cg:150:SER:O	37:Cg:150:SER:OG	2.36	0.40
41:Cm:8:HIS:HB2	41:Cm:74:VAL:HG21	2.03	0.40
46:C2:128:C:H2'	46:C2:129:U:C6	2.56	0.40
1:UA:6:LYS:HA	1:UA:6:LYS:HD3	1.87	0.40
1:UA:312:LEU:HD12	1:UA:325:TRP:HD1	1.86	0.40
13:UQ:353:TRP:NE1	45:C1:72:U:OP1	2.51	0.40
14:UR:322:ARG:NH2	45:C1:76:U:OP2	2.54	0.40
16:UX:146:VAL:HG12	16:UX:148:THR:HG23	2.03	0.40
20:CD:220:ALA:O	20:CD:238:LYS:NZ	2.52	0.40
24:CI:104:ILE:O	24:CI:115:THR:HA	2.22	0.40
24:CI:956:SER:HB2	24:CI:958:ILE:HD12	2.03	0.40
28:CM:152:GLU:O	28:CM:156:TYR:OH	2.37	0.40
29:CO:232:LEU:HD12	29:CO:232:LEU:HA	1.90	0.40
39:CI:133:PRO:HB2	45:C1:1472:A:H5''	2.03	0.40
41:Cm:130:TYR:HE2	44:CU:274:ASP:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Cn:132:LEU:HD12	42:Cn:132:LEU:HA	1.93	0.40
45:C1:495:G:C8	45:C1:503:G:N2	2.83	0.40
45:C1:1744:A:H2'	45:C1:1745:C:C6	2.56	0.40
47:UH:909:ILE:HB	47:UH:926:VAL:HG13	2.03	0.40
2:UB:113:VAL:HG23	23:CH:63:GLY:HA2	2.04	0.40
4:UD:415:LYS:HA	4:UD:415:LYS:HD3	1.94	0.40
4:UD:630:PRO:HA	4:UD:651:THR:HA	2.03	0.40
12:UO:144:LYS:HE3	12:UO:144:LYS:HB3	1.88	0.40
12:UO:457:LEU:HD23	12:UO:457:LEU:HA	1.94	0.40
13:UQ:740:LEU:HA	13:UQ:740:LEU:HD12	1.86	0.40
15:UU:947:LEU:HD23	15:UU:947:LEU:HA	1.95	0.40
17:UZ:147:PHE:HB2	17:UZ:171:PHE:HD1	1.86	0.40
18:CA:283:LYS:HD3	18:CA:307:LEU:HD11	2.04	0.40
22:CG:441:PRO:HB2	22:CG:458:ILE:HD11	2.03	0.40
23:CH:336:LEU:HD23	23:CH:336:LEU:HA	1.84	0.40
24:CI:1069:PRO:HB3	45:C1:364:C:H5''	2.04	0.40
29:CN:79:LYS:HE3	29:CN:79:LYS:HB3	1.90	0.40
32:CR:58:TRP:HA	32:CR:124:ILE:HG22	2.04	0.40
32:CR:293:ALA:O	32:CR:297:VAL:HG12	2.22	0.40
32:CS:263:LYS:HA	32:CS:266:LEU:HD12	2.02	0.40
34:Ca:98:THR:H	34:Ca:232:HIS:CE1	2.40	0.40
42:Cn:102:VAL:HG13	42:Cn:124:VAL:HG13	2.02	0.40
45:C1:345:U:N3	45:C1:346:C:N4	2.70	0.40
46:C2:3:C:H2'	46:C2:4:G:H8	1.86	0.40
49:US:163:ARG:H	49:US:163:ARG:HG3	1.74	0.40
49:US:196:ILE:O	49:US:200:THR:CB	2.69	0.40
51:CX:290:ASN:HA	51:CX:293:LYS:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	835/904 (92%)	768 (92%)	67 (8%)	0	100	100
2	UB	502/907 (55%)	470 (94%)	32 (6%)	0	100	100
3	UC	72/648 (11%)	64 (89%)	8 (11%)	0	100	100
4	UD	754/884 (85%)	722 (96%)	32 (4%)	0	100	100
5	UF	325/414 (78%)	310 (95%)	14 (4%)	1 (0%)	36	72
6	UG	475/558 (85%)	441 (93%)	32 (7%)	2 (0%)	30	67
7	UJ	439/1802 (24%)	422 (96%)	17 (4%)	0	100	100
8	UK	211/270 (78%)	210 (100%)	1 (0%)	0	100	100
9	UL	767/962 (80%)	711 (93%)	56 (7%)	0	100	100
10	UM	705/912 (77%)	656 (93%)	48 (7%)	1 (0%)	48	83
11	UN	150/938 (16%)	146 (97%)	3 (2%)	1 (1%)	18	56
12	UO	498/557 (89%)	474 (95%)	24 (5%)	0	100	100
13	UQ	775/960 (81%)	712 (92%)	61 (8%)	2 (0%)	36	72
14	UR	437/618 (71%)	416 (95%)	21 (5%)	0	100	100
15	UU	890/1049 (85%)	832 (94%)	58 (6%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	215 (94%)	14 (6%)	0	100	100
18	CA	238/313 (76%)	225 (94%)	13 (6%)	0	100	100
18	CB	235/313 (75%)	220 (94%)	15 (6%)	0	100	100
19	CC	383/523 (73%)	367 (96%)	16 (4%)	0	100	100
20	CD	416/582 (72%)	393 (94%)	23 (6%)	0	100	100
21	CE	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	16	54
22	CG	368/630 (58%)	343 (93%)	25 (7%)	0	100	100
23	CH	383/411 (93%)	346 (90%)	36 (9%)	1 (0%)	36	72
24	CI	812/1163 (70%)	760 (94%)	50 (6%)	2 (0%)	43	78
25	CJ	177/183 (97%)	166 (94%)	11 (6%)	0	100	100
26	CK	295/297 (99%)	284 (96%)	11 (4%)	0	100	100
27	CL	225/785 (29%)	212 (94%)	12 (5%)	1 (0%)	30	67
28	CM	443/446 (99%)	417 (94%)	26 (6%)	0	100	100
29	CN	222/252 (88%)	210 (95%)	12 (5%)	0	100	100
29	CO	211/252 (84%)	197 (93%)	12 (6%)	2 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	CP	197/322 (61%)	191 (97%)	6 (3%)	0	100	100
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	24	63
32	CS	746/1073 (70%)	682 (91%)	60 (8%)	4 (0%)	24	63
33	CT	127/203 (63%)	119 (94%)	8 (6%)	0	100	100
34	Ca	223/255 (88%)	212 (95%)	11 (5%)	0	100	100
35	Cc	188/212 (89%)	179 (95%)	9 (5%)	0	100	100
36	Ce	155/203 (76%)	139 (90%)	16 (10%)	0	100	100
37	Cg	157/190 (83%)	152 (97%)	5 (3%)	0	100	100
38	Ch	64/151 (42%)	61 (95%)	3 (5%)	0	100	100
39	Ci	113/150 (75%)	106 (94%)	7 (6%)	0	100	100
40	Cj	124/143 (87%)	116 (94%)	8 (6%)	0	100	100
41	Cm	122/130 (94%)	117 (96%)	5 (4%)	0	100	100
42	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
43	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
44	CU	168/311 (54%)	156 (93%)	12 (7%)	0	100	100
47	UH	349/930 (38%)	340 (97%)	9 (3%)	0	100	100
48	UE	121/410 (30%)	117 (97%)	4 (3%)	0	100	100
48	UI	121/410 (30%)	121 (100%)	0	0	100	100
49	US	443/549 (81%)	415 (94%)	28 (6%)	0	100	100
50	Cl	78/156 (50%)	73 (94%)	5 (6%)	0	100	100
51	CX	265/480 (55%)	255 (96%)	10 (4%)	0	100	100
52	UP	52/364 (14%)	46 (88%)	5 (10%)	1 (2%)	6	32
All	All	17778/27558 (64%)	16693 (94%)	1062 (6%)	23 (0%)	49	83

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
6	UG	580	GLU
13	UQ	708	SER
6	UG	56	PRO
32	CR	48	MET
32	CS	48	MET

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Mol	Chain	Res	Type
11	UN	902	ARG
27	CL	640	PRO
5	UF	121	LYS
10	UM	329	PRO
13	UQ	564	GLU
24	CI	309	PRO
52	UP	329	PRO
32	CR	772	PRO
32	CS	772	PRO
23	CH	258	PRO
32	CR	904	PRO
32	CS	904	PRO
21	CF	61	PRO
32	CR	404	GLY
32	CS	404	GLY
29	CO	84	ILE
24	CI	308	THR

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	UA	651/775 (84%)	649 (100%)	2 (0%)	86	86
2	UB	425/788 (54%)	425 (100%)	0	100	100
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	649 (99%)	4 (1%)	78	83
5	UF	248/341 (73%)	247 (100%)	1 (0%)	84	84
6	UG	373/474 (79%)	370 (99%)	3 (1%)	73	80
7	UJ	351/1526 (23%)	350 (100%)	1 (0%)	86	86
8	UK	159/227 (70%)	159 (100%)	0	100	100
9	UL	667/821 (81%)	661 (99%)	6 (1%)	70	79
10	UM	606/770 (79%)	599 (99%)	7 (1%)	63	75
11	UN	123/765 (16%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	UO	404/456 (89%)	395 (98%)	9 (2%)	45	64
13	UQ	650/817 (80%)	646 (99%)	4 (1%)	78	83
14	UR	360/524 (69%)	358 (99%)	2 (1%)	78	83
15	UU	672/863 (78%)	666 (99%)	6 (1%)	70	79
16	UX	150/167 (90%)	147 (98%)	3 (2%)	48	66
17	UZ	186/329 (56%)	184 (99%)	2 (1%)	65	76
18	CA	175/228 (77%)	172 (98%)	3 (2%)	53	69
18	CB	195/228 (86%)	193 (99%)	2 (1%)	68	78
19	CC	287/435 (66%)	287 (100%)	0	100	100
20	CD	319/489 (65%)	318 (100%)	1 (0%)	86	86
21	CE	91/108 (84%)	90 (99%)	1 (1%)	65	76
21	CF	88/108 (82%)	87 (99%)	1 (1%)	65	76
22	CG	299/525 (57%)	294 (98%)	5 (2%)	53	69
23	CH	303/320 (95%)	299 (99%)	4 (1%)	61	74
24	CI	661/1009 (66%)	653 (99%)	8 (1%)	63	75
25	CJ	147/169 (87%)	146 (99%)	1 (1%)	76	81
26	CK	245/266 (92%)	238 (97%)	7 (3%)	37	58
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	363 (100%)	1 (0%)	86	86
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	192 (100%)	1 (0%)	81	83
30	CP	177/287 (62%)	177 (100%)	0	100	100
31	CQ	145/215 (67%)	145 (100%)	0	100	100
32	CR	654/916 (71%)	446 (68%)	208 (32%)	0	2
32	CS	654/916 (71%)	446 (68%)	208 (32%)	0	2
33	CT	108/167 (65%)	107 (99%)	1 (1%)	70	79
34	Ca	198/223 (89%)	197 (100%)	1 (0%)	81	83
35	Cc	149/178 (84%)	149 (100%)	0	100	100
36	Ce	137/177 (77%)	137 (100%)	0	100	100
37	Cg	122/162 (75%)	122 (100%)	0	100	100
38	Ch	58/130 (45%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Ci	78/117 (67%)	78 (100%)	0	100	100
40	Cj	92/115 (80%)	92 (100%)	0	100	100
41	Cm	103/113 (91%)	103 (100%)	0	100	100
42	Cn	70/116 (60%)	70 (100%)	0	100	100
43	Cp	46/61 (75%)	46 (100%)	0	100	100
44	CU	137/260 (53%)	137 (100%)	0	100	100
47	UH	301/788 (38%)	298 (99%)	3 (1%)	68	78
48	UE	105/346 (30%)	105 (100%)	0	100	100
48	UI	105/346 (30%)	105 (100%)	0	100	100
49	US	404/493 (82%)	403 (100%)	1 (0%)	87	87
50	Cl	71/135 (53%)	71 (100%)	0	100	100
51	CX	227/411 (55%)	227 (100%)	0	100	100
52	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	14674/23259 (63%)	14167 (96%)	507 (4%)	32	53

All (507) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	346	LEU
1	UA	450	ILE
4	UD	95	ILE
4	UD	180	THR
4	UD	340	VAL
4	UD	747	ILE
5	UF	278	ILE
6	UG	135	THR
6	UG	208	VAL
6	UG	420	VAL
7	UJ	297	VAL
9	UL	49	VAL
9	UL	52	ILE
9	UL	155	VAL
9	UL	213	VAL
9	UL	469	LEU
9	UL	699	ILE
10	UM	35	LEU
10	UM	400	ILE

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Mol	Chain	Res	Type
10	UM	403	VAL
10	UM	450	SER
10	UM	546	ASP
10	UM	675	VAL
10	UM	780	THR
12	UO	5	VAL
12	UO	75	VAL
12	UO	147	VAL
12	UO	150	THR
12	UO	257	VAL
12	UO	299	VAL
12	UO	320	LEU
12	UO	489	VAL
12	UO	534	VAL
13	UQ	358	VAL
13	UQ	378	VAL
13	UQ	389	VAL
13	UQ	920	VAL
14	UR	323	THR
14	UR	535	VAL
15	UU	235	LEU
15	UU	260	THR
15	UU	276	VAL
15	UU	512	VAL
15	UU	638	VAL
15	UU	738	THR
16	UX	37	VAL
16	UX	58	VAL
16	UX	89	ILE
17	UZ	175	THR
17	UZ	280	ASN
18	CA	91	LEU
18	CA	292	LEU
18	CA	304	CYS
18	CB	125	THR
18	CB	293	GLU
20	CD	86	VAL
21	CE	53	VAL
21	CF	67	HIS
22	CG	263	THR
22	CG	312	VAL
22	CG	314	VAL

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Mol	Chain	Res	Type
22	CG	489	VAL
22	CG	578	VAL
23	CH	85	THR
23	CH	98	ILE
23	CH	157	VAL
23	CH	250	VAL
24	CI	197	LEU
24	CI	252	ILE
24	CI	354	THR
24	CI	380	GLN
24	CI	827	LEU
24	CI	886	CYS
24	CI	915	VAL
24	CI	1081	VAL
25	CJ	158	VAL
26	CK	88	VAL
26	CK	91	THR
26	CK	148	THR
26	CK	218	THR
26	CK	231	VAL
26	CK	237	ILE
26	CK	262	THR
28	CM	129	THR
29	CO	39	VAL
32	CR	4	GLN
32	CR	5	LYS
32	CR	6	THR
32	CR	7	VAL
32	CR	9	SER
32	CR	19	LEU
32	CR	22	LYS
32	CR	23	LYS
32	CR	25	SER
32	CR	36	GLU
32	CR	45	MET
32	CR	46	SER
32	CR	48	MET
32	CR	51	ARG
32	CR	54	LYS
32	CR	55	SER
32	CR	56	VAL
32	CR	61	LYS

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Mol	Chain	Res	Type
32	CR	62	LYS
32	CR	67	PHE
32	CR	68	THR
32	CR	75	GLU
32	CR	77	LYS
32	CR	78	ILE
32	CR	81	GLU
32	CR	83	LYS
32	CR	84	ARG
32	CR	87	ARG
32	CR	99	ILE
32	CR	100	SER
32	CR	102	ASN
32	CR	103	ASP
32	CR	104	ILE
32	CR	105	ARG
32	CR	110	LYS
32	CR	114	LYS
32	CR	115	ILE
32	CR	119	THR
32	CR	122	MET
32	CR	124	ILE
32	CR	125	LEU
32	CR	126	GLN
32	CR	129	GLU
32	CR	131	ILE
32	CR	135	ILE
32	CR	136	LEU
32	CR	142	THR
32	CR	144	GLU
32	CR	151	LEU
32	CR	154	LYS
32	CR	157	THR
32	CR	164	THR
32	CR	165	MET
32	CR	167	MET
32	CR	182	ILE
32	CR	191	LEU
32	CR	197	GLU
32	CR	201	VAL
32	CR	202	ILE
32	CR	217	VAL

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Mol	Chain	Res	Type
32	CR	253	ILE
32	CR	261	GLN
32	CR	263	LYS
32	CR	265	LEU
32	CR	266	LEU
32	CR	269	VAL
32	CR	274	GLU
32	CR	275	LYS
32	CR	276	THR
32	CR	278	ARG
32	CR	280	THR
32	CR	283	LEU
32	CR	287	ARG
32	CR	292	SER
32	CR	297	VAL
32	CR	299	ILE
32	CR	308	SER
32	CR	313	THR
32	CR	314	SER
32	CR	318	GLU
32	CR	322	THR
32	CR	323	LEU
32	CR	325	GLU
32	CR	370	GLN
32	CR	380	LEU
32	CR	388	ILE
32	CR	401	LYS
32	CR	402	LEU
32	CR	410	MET
32	CR	412	SER
32	CR	415	SER
32	CR	418	GLU
32	CR	423	SER
32	CR	424	LEU
32	CR	426	LEU
32	CR	428	LEU
32	CR	430	LYS
32	CR	432	LEU
32	CR	433	ARG
32	CR	434	GLU
32	CR	470	LYS
32	CR	471	GLU

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Mol	Chain	Res	Type
32	CR	475	SER
32	CR	482	GLN
32	CR	488	LYS
32	CR	494	LEU
32	CR	497	ASP
32	CR	500	LEU
32	CR	512	ASP
32	CR	515	GLN
32	CR	519	LEU
32	CR	521	VAL
32	CR	526	LEU
32	CR	528	SER
32	CR	534	GLU
32	CR	535	LYS
32	CR	537	LEU
32	CR	541	VAL
32	CR	547	SER
32	CR	548	HIS
32	CR	550	LYS
32	CR	558	LEU
32	CR	560	SER
32	CR	566	GLU
32	CR	569	VAL
32	CR	578	ARG
32	CR	581	GLU
32	CR	583	LEU
32	CR	587	GLN
32	CR	588	VAL
32	CR	589	SER
32	CR	593	LYS
32	CR	595	SER
32	CR	614	ILE
32	CR	617	LEU
32	CR	618	VAL
32	CR	624	ASP
32	CR	631	SER
32	CR	635	ILE
32	CR	638	ILE
32	CR	645	MET
32	CR	651	SER
32	CR	652	LYS
32	CR	657	LEU

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Mol	Chain	Res	Type
32	CR	659	ASP
32	CR	710	SER
32	CR	713	SER
32	CR	714	GLU
32	CR	715	ARG
32	CR	720	LEU
32	CR	723	VAL
32	CR	726	SER
32	CR	735	LYS
32	CR	738	LYS
32	CR	745	VAL
32	CR	748	ARG
32	CR	752	ASN
32	CR	753	ASP
32	CR	755	THR
32	CR	759	THR
32	CR	761	VAL
32	CR	763	ILE
32	CR	766	LEU
32	CR	770	ASN
32	CR	773	SER
32	CR	781	ASP
32	CR	787	LEU
32	CR	796	GLU
32	CR	799	SER
32	CR	803	LEU
32	CR	806	GLU
32	CR	807	GLU
32	CR	814	MET
32	CR	816	ASP
32	CR	818	SER
32	CR	819	ASN
32	CR	828	GLU
32	CR	830	ASP
32	CR	831	GLN
32	CR	834	THR
32	CR	837	ASP
32	CR	841	LEU
32	CR	842	GLU
32	CR	843	SER
32	CR	848	LEU
32	CR	850	ASP

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Mol	Chain	Res	Type
32	CR	853	VAL
32	CR	854	VAL
32	CR	855	LEU
32	CR	856	ASP
32	CR	861	ILE
32	CR	863	GLN
32	CR	867	THR
32	CR	870	LEU
32	CR	871	ARG
32	CR	875	LYS
32	CR	879	LEU
32	CR	892	LYS
32	CR	895	ASP
32	CR	896	THR
32	CR	897	LEU
32	CR	900	GLU
32	CR	906	SER
32	CR	908	VAL
32	CR	913	MET
32	CR	917	ARG
32	CR	918	LYS
32	CR	921	GLN
32	CS	4	GLN
32	CS	5	LYS
32	CS	6	THR
32	CS	7	VAL
32	CS	9	SER
32	CS	19	LEU
32	CS	22	LYS
32	CS	23	LYS
32	CS	25	SER
32	CS	36	GLU
32	CS	45	MET
32	CS	46	SER
32	CS	48	MET
32	CS	51	ARG
32	CS	54	LYS
32	CS	55	SER
32	CS	56	VAL
32	CS	61	LYS
32	CS	62	LYS
32	CS	67	PHE

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Mol	Chain	Res	Type
32	CS	68	THR
32	CS	75	GLU
32	CS	77	LYS
32	CS	78	ILE
32	CS	81	GLU
32	CS	83	LYS
32	CS	84	ARG
32	CS	87	ARG
32	CS	99	ILE
32	CS	100	SER
32	CS	102	ASN
32	CS	103	ASP
32	CS	104	ILE
32	CS	105	ARG
32	CS	110	LYS
32	CS	114	LYS
32	CS	115	ILE
32	CS	119	THR
32	CS	122	MET
32	CS	124	ILE
32	CS	125	LEU
32	CS	126	GLN
32	CS	129	GLU
32	CS	131	ILE
32	CS	135	ILE
32	CS	136	LEU
32	CS	142	THR
32	CS	144	GLU
32	CS	151	LEU
32	CS	154	LYS
32	CS	157	THR
32	CS	164	THR
32	CS	165	MET
32	CS	167	MET
32	CS	182	ILE
32	CS	191	LEU
32	CS	197	GLU
32	CS	201	VAL
32	CS	202	ILE
32	CS	217	VAL
32	CS	253	ILE
32	CS	261	GLN

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Mol	Chain	Res	Type
32	CS	263	LYS
32	CS	265	LEU
32	CS	266	LEU
32	CS	269	VAL
32	CS	274	GLU
32	CS	275	LYS
32	CS	276	THR
32	CS	278	ARG
32	CS	280	THR
32	CS	283	LEU
32	CS	287	ARG
32	CS	292	SER
32	CS	297	VAL
32	CS	299	ILE
32	CS	308	SER
32	CS	313	THR
32	CS	314	SER
32	CS	318	GLU
32	CS	322	THR
32	CS	323	LEU
32	CS	325	GLU
32	CS	370	GLN
32	CS	380	LEU
32	CS	388	ILE
32	CS	401	LYS
32	CS	402	LEU
32	CS	410	MET
32	CS	412	SER
32	CS	415	SER
32	CS	418	GLU
32	CS	423	SER
32	CS	424	LEU
32	CS	426	LEU
32	CS	428	LEU
32	CS	430	LYS
32	CS	432	LEU
32	CS	433	ARG
32	CS	434	GLU
32	CS	470	LYS
32	CS	471	GLU
32	CS	475	SER
32	CS	482	GLN

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Mol	Chain	Res	Type
32	CS	488	LYS
32	CS	494	LEU
32	CS	497	ASP
32	CS	500	LEU
32	CS	512	ASP
32	CS	515	GLN
32	CS	519	LEU
32	CS	521	VAL
32	CS	526	LEU
32	CS	528	SER
32	CS	534	GLU
32	CS	535	LYS
32	CS	537	LEU
32	CS	541	VAL
32	CS	547	SER
32	CS	548	HIS
32	CS	550	LYS
32	CS	558	LEU
32	CS	560	SER
32	CS	566	GLU
32	CS	569	VAL
32	CS	578	ARG
32	CS	581	GLU
32	CS	583	LEU
32	CS	587	GLN
32	CS	588	VAL
32	CS	589	SER
32	CS	593	LYS
32	CS	595	SER
32	CS	614	ILE
32	CS	617	LEU
32	CS	618	VAL
32	CS	624	ASP
32	CS	631	SER
32	CS	635	ILE
32	CS	638	ILE
32	CS	645	MET
32	CS	651	SER
32	CS	652	LYS
32	CS	657	LEU
32	CS	659	ASP
32	CS	710	SER

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Mol	Chain	Res	Type
32	CS	713	SER
32	CS	714	GLU
32	CS	715	ARG
32	CS	720	LEU
32	CS	723	VAL
32	CS	726	SER
32	CS	735	LYS
32	CS	738	LYS
32	CS	745	VAL
32	CS	748	ARG
32	CS	752	ASN
32	CS	753	ASP
32	CS	755	THR
32	CS	759	THR
32	CS	761	VAL
32	CS	763	ILE
32	CS	766	LEU
32	CS	770	ASN
32	CS	773	SER
32	CS	781	ASP
32	CS	787	LEU
32	CS	796	GLU
32	CS	799	SER
32	CS	803	LEU
32	CS	806	GLU
32	CS	807	GLU
32	CS	814	MET
32	CS	816	ASP
32	CS	818	SER
32	CS	819	ASN
32	CS	828	GLU
32	CS	830	ASP
32	CS	831	GLN
32	CS	834	THR
32	CS	837	ASP
32	CS	841	LEU
32	CS	842	GLU
32	CS	843	SER
32	CS	848	LEU
32	CS	850	ASP
32	CS	853	VAL
32	CS	854	VAL

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Mol	Chain	Res	Type
32	CS	855	LEU
32	CS	856	ASP
32	CS	861	ILE
32	CS	863	GLN
32	CS	867	THR
32	CS	870	LEU
32	CS	871	ARG
32	CS	875	LYS
32	CS	879	LEU
32	CS	892	LYS
32	CS	895	ASP
32	CS	896	THR
32	CS	897	LEU
32	CS	900	GLU
32	CS	906	SER
32	CS	908	VAL
32	CS	913	MET
32	CS	917	ARG
32	CS	918	LYS
32	CS	921	GLN
33	CT	73	VAL
34	Ca	88	VAL
47	UH	599	VAL
47	UH	726	LEU
47	UH	926	VAL
49	US	174	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	110	HIS
1	UA	249	HIS
1	UA	291	HIS
1	UA	336	GLN
1	UA	381	HIS
1	UA	615	ASN
1	UA	685	ASN
2	UB	33	ASN
2	UB	525	ASN
2	UB	645	GLN
2	UB	759	HIS
3	UC	578	GLN

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Mol	Chain	Res	Type
4	UD	23	HIS
4	UD	124	HIS
4	UD	206	ASN
4	UD	222	GLN
4	UD	324	HIS
4	UD	548	ASN
4	UD	688	GLN
4	UD	697	GLN
4	UD	714	GLN
4	UD	807	ASN
5	UF	62	ASN
5	UF	319	HIS
6	UG	49	GLN
6	UG	159	HIS
6	UG	175	GLN
6	UG	190	GLN
6	UG	206	ASN
6	UG	221	HIS
6	UG	267	ASN
6	UG	270	ASN
6	UG	378	GLN
6	UG	391	GLN
6	UG	455	GLN
6	UG	478	GLN
7	UJ	15	ASN
7	UJ	77	GLN
7	UJ	131	ASN
7	UJ	184	GLN
7	UJ	245	HIS
8	UK	9	GLN
8	UK	13	HIS
9	UL	107	ASN
9	UL	377	ASN
9	UL	384	GLN
9	UL	453	ASN
9	UL	515	GLN
9	UL	517	HIS
9	UL	642	HIS
9	UL	661	ASN
9	UL	823	ASN
9	UL	832	ASN
9	UL	905	ASN

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Mol	Chain	Res	Type
10	UM	30	ASN
10	UM	386	GLN
10	UM	394	ASN
10	UM	455	ASN
10	UM	466	ASN
10	UM	548	ASN
10	UM	641	HIS
10	UM	772	ASN
10	UM	808	GLN
11	UN	358	GLN
11	UN	879	ASN
11	UN	916	GLN
12	UO	46	HIS
12	UO	253	ASN
12	UO	284	GLN
12	UO	329	HIS
12	UO	333	HIS
12	UO	339	GLN
12	UO	393	ASN
12	UO	524	GLN
13	UQ	112	GLN
13	UQ	262	HIS
13	UQ	310	GLN
13	UQ	328	ASN
13	UQ	383	GLN
13	UQ	414	HIS
13	UQ	474	ASN
13	UQ	477	HIS
13	UQ	501	GLN
13	UQ	509	GLN
13	UQ	520	ASN
13	UQ	557	GLN
13	UQ	606	HIS
13	UQ	675	GLN
13	UQ	783	ASN
14	UR	238	ASN
14	UR	364	GLN
14	UR	399	ASN
14	UR	411	GLN
14	UR	498	ASN
14	UR	560	GLN
15	UU	117	GLN

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Mol	Chain	Res	Type
15	UU	197	ASN
15	UU	236	GLN
15	UU	328	ASN
15	UU	621	HIS
15	UU	1002	HIS
15	UU	1022	HIS
16	UX	39	GLN
16	UX	49	ASN
16	UX	119	GLN
17	UZ	76	HIS
17	UZ	90	ASN
17	UZ	105	GLN
17	UZ	234	HIS
18	CA	289	GLN
18	CB	289	GLN
19	CC	22	HIS
19	CC	67	ASN
19	CC	171	HIS
19	CC	173	ASN
19	CC	321	HIS
19	CC	410	GLN
19	CC	413	GLN
20	CD	128	ASN
20	CD	137	ASN
20	CD	142	ASN
20	CD	256	ASN
20	CD	263	GLN
20	CD	273	GLN
20	CD	422	ASN
21	CE	27	GLN
21	CF	60	GLN
22	CG	169	ASN
22	CG	245	HIS
22	CG	364	GLN
22	CG	424	GLN
22	CG	430	HIS
22	CG	561	ASN
23	CH	43	ASN
23	CH	129	ASN
23	CH	199	GLN
23	CH	207	HIS
23	CH	233	ASN

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Mol	Chain	Res	Type
24	CI	121	ASN
24	CI	165	ASN
24	CI	284	GLN
24	CI	747	GLN
24	CI	767	GLN
24	CI	791	ASN
24	CI	853	ASN
24	CI	930	ASN
24	CI	1002	ASN
24	CI	1029	GLN
24	CI	1030	ASN
24	CI	1077	GLN
25	CJ	99	HIS
25	CJ	135	HIS
26	CK	48	ASN
26	CK	121	ASN
26	CK	159	HIS
26	CK	225	ASN
26	CK	295	ASN
27	CL	480	GLN
28	CM	14	GLN
28	CM	77	ASN
28	CM	120	ASN
28	CM	184	HIS
28	CM	230	ASN
28	CM	243	ASN
29	CN	111	GLN
29	CN	164	GLN
29	CO	111	GLN
29	CO	146	HIS
29	CO	243	HIS
31	CQ	247	ASN
32	CR	40	HIS
32	CR	207	ASN
32	CR	261	GLN
32	CR	309	ASN
32	CR	485	ASN
32	CR	565	HIS
32	CR	587	GLN
32	CR	655	GLN
32	CR	749	GLN
32	CR	758	HIS

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Mol	Chain	Res	Type
32	CR	819	ASN
32	CR	863	GLN
32	CR	880	GLN
32	CR	881	GLN
32	CS	309	ASN
32	CS	482	GLN
32	CS	485	ASN
32	CS	565	HIS
32	CS	587	GLN
32	CS	655	GLN
32	CS	703	HIS
32	CS	749	GLN
32	CS	758	HIS
32	CS	819	ASN
32	CS	863	GLN
32	CS	880	GLN
32	CS	881	GLN
34	Ca	149	GLN
34	Ca	182	HIS
34	Ca	183	GLN
35	Cc	87	HIS
35	Cc	103	HIS
35	Cc	126	ASN
36	Ce	17	GLN
36	Ce	36	ASN
36	Ce	95	HIS
36	Ce	197	GLN
37	Cg	121	HIS
40	Cj	83	GLN
40	Cj	107	GLN
41	Cm	16	ASN
41	Cm	66	ASN
41	Cm	113	HIS
42	Cn	63	GLN
42	Cn	94	ASN
44	CU	169	HIS
47	UH	563	ASN
47	UH	590	ASN
47	UH	702	HIS
47	UH	898	HIS
48	UE	269	GLN
49	US	151	GLN

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Mol	Chain	Res	Type
49	US	184	HIS
49	US	225	ASN
49	US	253	HIS
49	US	274	HIS
49	US	419	HIS
50	Cl	19	ASN
50	Cl	21	ASN
51	CX	263	GLN
51	CX	322	GLN
51	CX	352	GLN
51	CX	364	ASN
48	UI	174	GLN
48	UI	232	GLN
48	UI	237	ASN
52	UP	341	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	C1	1134/2352 (48%)	347 (30%)	26 (2%)
46	C2	226/230 (98%)	68 (30%)	4 (1%)
All	All	1360/2582 (52%)	415 (30%)	30 (2%)

All (415) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	C1	4	G
45	C1	5	G
45	C1	7	A
45	C1	13	G
45	C1	14	G
45	C1	15	G
45	C1	16	U
45	C1	17	C
45	C1	18	G
45	C1	19	C
45	C1	20	C
45	C1	26	C
45	C1	38	G
45	C1	40	A
45	C1	41	G

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Mol	Chain	Res	Type
45	C1	47	G
45	C1	49	G
45	C1	56	C
45	C1	60	A
45	C1	61	G
45	C1	63	C
45	C1	66	G
45	C1	68	U
45	C1	71	A
45	C1	72	U
45	C1	73	A
45	C1	74	C
45	C1	75	G
45	C1	77	C
45	C1	89	G
45	C1	90	A
45	C1	93	G
45	C1	97	C
45	C1	104	U
45	C1	105	A
45	C1	121	G
45	C1	126	C
45	C1	127	C
45	C1	128	G
45	C1	134	C
45	C1	136	C
45	C1	143	A
45	C1	150	C
45	C1	152	G
45	C1	154	C
45	C1	155	G
45	C1	158	C
45	C1	159	C
45	C1	160	C
45	C1	161	A
45	C1	162	G
45	C1	166	A
45	C1	169	G
45	C1	170	C
45	C1	182	C
45	C1	183	C
45	C1	193	U

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Mol	Chain	Res	Type
45	C1	201	G
45	C1	202	A
45	C1	203	C
45	C1	205	C
45	C1	206	C
45	C1	207	U
45	C1	208	A
45	C1	209	A
45	C1	210	G
45	C1	216	A
45	C1	220	A
45	C1	221	A
45	C1	225	C
45	C1	234	G
45	C1	242	U
45	C1	243	U
45	C1	244	G
45	C1	257	G
45	C1	265	G
45	C1	266	C
45	C1	267	U
45	C1	268	G
45	C1	269	G
45	C1	273	G
45	C1	276	C
45	C1	277	U
45	C1	278	A
45	C1	281	U
45	C1	282	C
45	C1	283	A
45	C1	285	A
45	C1	290	C
45	C1	291	C
45	C1	292	G
45	C1	308	U
45	C1	310	G
45	C1	311	G
45	C1	312	G
45	C1	319	U
45	C1	320	A
45	C1	322	C
45	C1	323	G

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Mol	Chain	Res	Type
45	C1	325	C
45	C1	333	C
45	C1	334	U
45	C1	339	C
45	C1	340	G
45	C1	346	C
45	C1	347	C
45	C1	349	C
45	C1	351	U
45	C1	362	G
45	C1	372	U
45	C1	382	U
45	C1	383	G
45	C1	384	C
45	C1	386	G
45	C1	398	C
45	C1	402	U
45	C1	403	G
45	C1	404	C
45	C1	416	U
45	C1	425	C
45	C1	427	G
45	C1	435	A
45	C1	436	A
45	C1	440	G
45	C1	441	A
45	C1	442	U
45	C1	443	G
45	C1	454	C
45	C1	458	A
45	C1	459	C
45	C1	468	C
45	C1	469	G
45	C1	474	A
45	C1	475	C
45	C1	484	G
45	C1	491	G
45	C1	492	C
45	C1	497	A
45	C1	499	G
45	C1	500	C
45	C1	501	U

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Mol	Chain	Res	Type
45	C1	502	A
45	C1	504	C
45	C1	581	C
45	C1	582	G
45	C1	583	A
45	C1	584	U
45	C1	585	A
45	C1	586	G
45	C1	587	U
45	C1	594	G
45	C1	595	U
45	C1	609	A
45	C1	610	G
45	C1	613	A
45	C1	614	U
45	C1	621	G
45	C1	624	U
45	C1	628	A
45	C1	1025	A
45	C1	1027	C
45	C1	1028	C
45	C1	1029	A
45	C1	1035	G
45	C1	1036	A
45	C1	1037	C
45	C1	1039	C
45	C1	1043	G
45	C1	1044	A
45	C1	1054	A
45	C1	1059	A
45	C1	1061	A
45	C1	1064	G
45	C1	1069	A
45	C1	1070	G
45	C1	1076	U
45	C1	1077	U
45	C1	1078	U
45	C1	1079	C
45	C1	1080	G
45	C1	1085	U
45	C1	1086	U
45	C1	1088	U

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Mol	Chain	Res	Type
45	C1	1089	A
45	C1	1094	G
45	C1	1095	A
45	C1	1098	G
45	C1	1099	A
45	C1	1102	A
45	C1	1103	C
45	C1	1104	A
45	C1	1116	U
45	C1	1120	C
45	C1	1122	A
45	C1	1123	G
45	C1	1124	G
45	C1	1125	A
45	C1	1126	A
45	C1	1127	C
45	C1	1128	A
45	C1	1129	A
45	C1	1132	G
45	C1	1141	G
45	C1	1147	U
45	C1	1148	G
45	C1	1150	C
45	C1	1154	A
45	C1	1158	G
45	C1	1159	C
45	C1	1163	A
45	C1	1164	A
45	C1	1166	U
45	C1	1167	C
45	C1	1168	C
45	C1	1169	A
45	C1	1170	G
45	C1	1178	A
45	C1	1179	G
45	C1	1186	U
45	C1	1218	G
45	C1	1219	A
45	C1	1220	A
45	C1	1222	C
45	C1	1223	U
45	C1	1444	A

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Mol	Chain	Res	Type
45	C1	1447	A
45	C1	1448	A
45	C1	1449	U
45	C1	1450	A
45	C1	1451	G
45	C1	1452	G
45	C1	1469	A
45	C1	1470	G
45	C1	1471	U
45	C1	1479	U
45	C1	1481	U
45	C1	1483	A
45	C1	1484	G
45	C1	1486	G
45	C1	1489	G
45	C1	1491	A
45	C1	1497	U
45	C1	1498	G
45	C1	1499	G
45	C1	1517	A
45	C1	1518	A
45	C1	1519	C
45	C1	1520	U
45	C1	1525	A
45	C1	1527	G
45	C1	1529	A
45	C1	1536	A
45	C1	1545	U
45	C1	1549	U
45	C1	1551	A
45	C1	1554	C
45	C1	1555	A
45	C1	1614	U
45	C1	1624	A
45	C1	1625	G
45	C1	1628	A
45	C1	1632	G
45	C1	1636	G
45	C1	1637	C
45	C1	1639	U
45	C1	1642	A
45	C1	1643	U

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Mol	Chain	Res	Type
45	C1	1644	U
45	C1	1645	U
45	C1	1656	C
45	C1	1659	C
45	C1	1665	A
45	C1	1667	G
45	C1	1668	A
45	C1	1670	A
45	C1	1698	G
45	C1	1701	U
45	C1	1709	A
45	C1	1711	G
45	C1	1712	C
45	C1	1713	U
45	C1	1735	A
45	C1	1738	G
45	C1	1742	C
45	C1	1743	C
45	C1	1744	A
45	C1	1751	G
45	C1	2047	G
45	C1	2054	A
45	C1	2055	C
45	C1	2056	U
45	C1	2057	G
45	C1	2061	G
45	C1	2070	A
45	C1	2072	U
45	C1	2073	A
45	C1	2074	C
45	C1	2075	U
45	C1	2077	C
45	C1	2078	C
45	C1	2085	G
45	C1	2086	A
45	C1	2087	G
45	C1	2088	A
45	C1	2107	A
45	C1	2109	A
45	C1	2115	U
45	C1	2118	U
45	C1	2120	C

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Mol	Chain	Res	Type
45	C1	2121	U
45	C1	2156	A
45	C1	2157	G
45	C1	2166	A
45	C1	2167	G
45	C1	2173	G
45	C1	2177	G
45	C1	2178	U
45	C1	2183	A
45	C1	2184	G
45	C1	2185	C
45	C1	2190	G
45	C1	2197	A
45	C1	2201	C
45	C1	2202	C
45	C1	2210	U
45	C1	2211	U
45	C1	2212	G
45	C1	2213	U
45	C1	2214	A
45	C1	2215	C
45	C1	2216	A
45	C1	2220	C
45	C1	2222	C
45	C1	2223	C
45	C1	2227	C
45	C1	2238	A
45	C1	2328	G
45	C1	2329	A
45	C1	2330	G
45	C1	2351	G
45	C1	2362	U
45	C1	2363	G
45	C1	2364	A
45	C1	2365	A
45	C1	2366	C
45	C1	2373	A
45	C1	2374	G
46	C2	5	A
46	C2	8	A
46	C2	15	A
46	C2	23	A

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Mol	Chain	Res	Type
46	C2	24	U
46	C2	28	U
46	C2	29	A
46	C2	33	U
46	C2	36	U
46	C2	37	U
46	C2	39	U
46	C2	48	G
46	C2	57	A
46	C2	58	A
46	C2	62	A
46	C2	63	G
46	C2	81	G
46	C2	90	C
46	C2	91	G
46	C2	92	A
46	C2	95	U
46	C2	100	G
46	C2	104	C
46	C2	111	G
46	C2	118	C
46	C2	124	U
46	C2	125	U
46	C2	126	U
46	C2	127	A
46	C2	128	C
46	C2	135	U
46	C2	136	C
46	C2	140	C
46	C2	142	G
46	C2	145	A
46	C2	147	G
46	C2	148	G
46	C2	153	G
46	C2	160	U
46	C2	162	C
46	C2	163	C
46	C2	164	U
46	C2	165	C
46	C2	166	G
46	C2	167	U
46	C2	168	C

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Mol	Chain	Res	Type
46	C2	170	C
46	C2	178	U
46	C2	179	A
46	C2	181	A
46	C2	182	G
46	C2	187	U
46	C2	188	G
46	C2	189	G
46	C2	190	C
46	C2	198	U
46	C2	199	G
46	C2	200	U
46	C2	201	A
46	C2	205	C
46	C2	244	G
46	C2	247	G
46	C2	255	U
46	C2	256	G
46	C2	259	A
46	C2	260	G
46	C2	261	U
46	C2	262	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	C1	88	C
45	C1	89	G
45	C1	96	C
45	C1	135	A
45	C1	150	C
45	C1	205	C
45	C1	209	A
45	C1	277	U
45	C1	281	U
45	C1	424	U
45	C1	582	G
45	C1	593	G
45	C1	1068	C
45	C1	1077	U
45	C1	1085	U
45	C1	1087	G

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Mol	Chain	Res	Type
45	C1	1163	A
45	C1	1485	A
45	C1	1638	G
45	C1	1712	C
45	C1	1734	G
45	C1	2054	A
45	C1	2077	C
45	C1	2156	A
45	C1	2177	G
45	C1	2219	C
46	C2	23	A
46	C2	35	G
46	C2	91	G
46	C2	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	GTP	CI	1201	-	33,34,34	1.09	3 (9%)	50,54,54	1.80	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	GTP	CI	1201	-	-	2/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CI	1201	GTP	C6-N1	-2.77	1.33	1.38
54	CI	1201	GTP	C5-C4	2.74	1.46	1.38
54	CI	1201	GTP	C5-N7	-2.27	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CI	1201	GTP	C5-C4-N3	-6.31	118.34	128.39
54	CI	1201	GTP	C2-N3-C4	5.13	121.14	112.30
54	CI	1201	GTP	N9-C4-N3	4.67	135.29	125.95
54	CI	1201	GTP	C6-C5-N7	3.33	136.34	130.29
54	CI	1201	GTP	C4-C5-N7	-2.60	106.56	110.67
54	CI	1201	GTP	O6-C6-C5	-2.24	120.62	126.53
54	CI	1201	GTP	C5-C6-N1	2.18	118.81	113.25
54	CI	1201	GTP	C3'-C2'-C1'	2.02	105.29	101.46
54	CI	1201	GTP	C2-N1-C6	-2.02	121.45	125.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	CI	1201	GTP	O4'-C4'-C5'-O5'
54	CI	1201	GTP	C3'-C4'-C5'-O5'

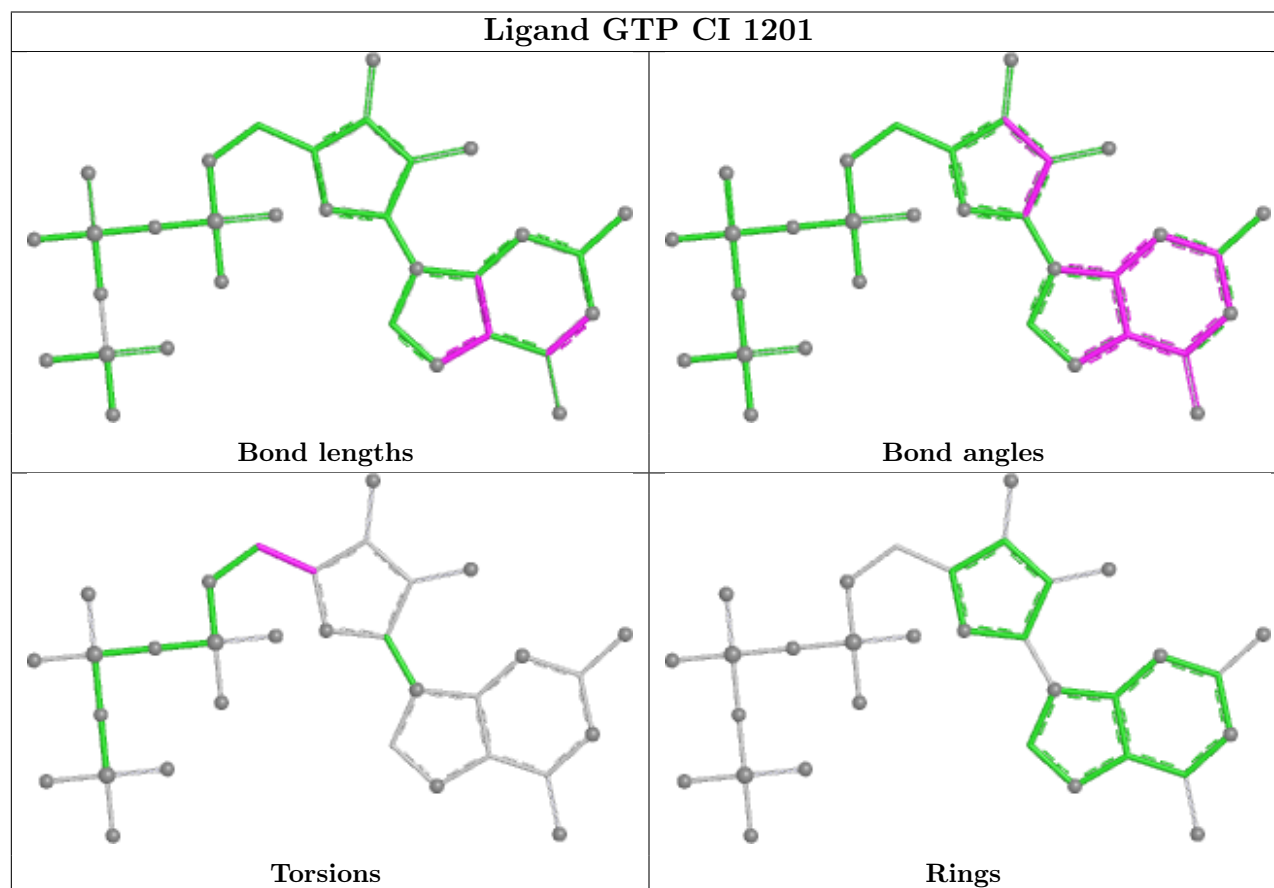
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CI	1201	GTP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.77
1	C2	105:C	O3'	110:A	P	16.05
1	C2	119:C	O3'	123:A	P	11.95

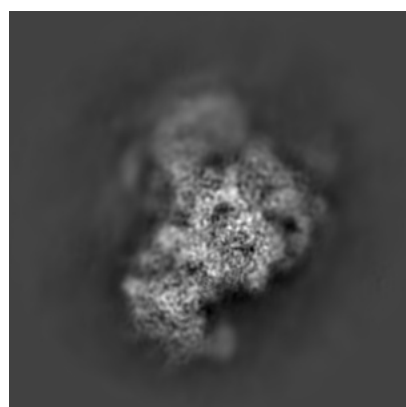
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10051. These allow visual inspection of the internal detail of the map and identification of artifacts.

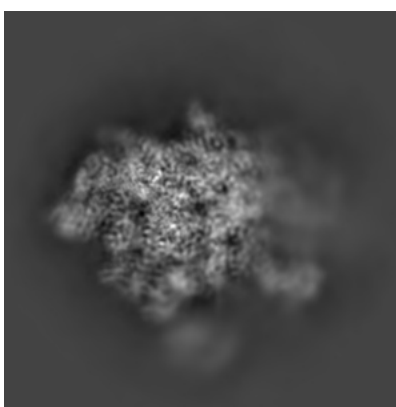
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

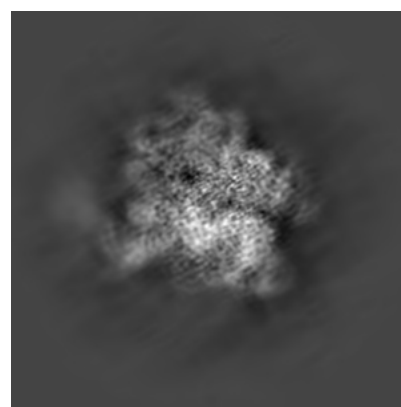
6.1.1 Primary map



X



Y

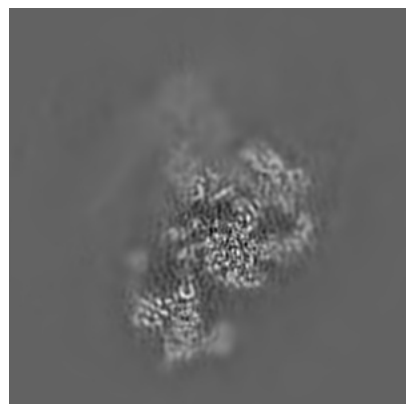


Z

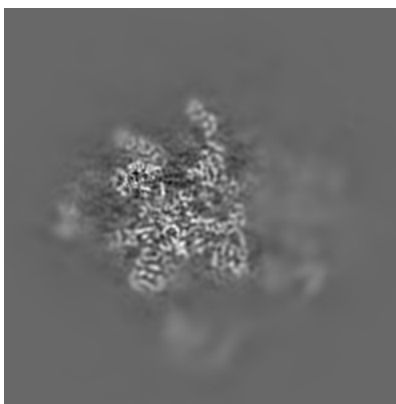
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

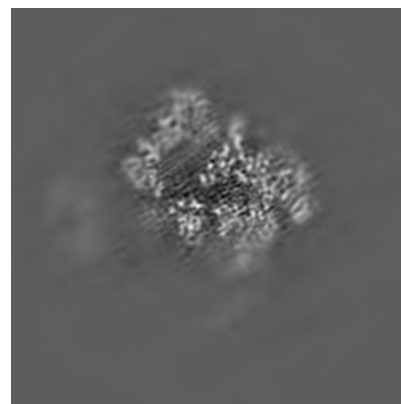
6.2.1 Primary map



X Index: 240



Y Index: 240

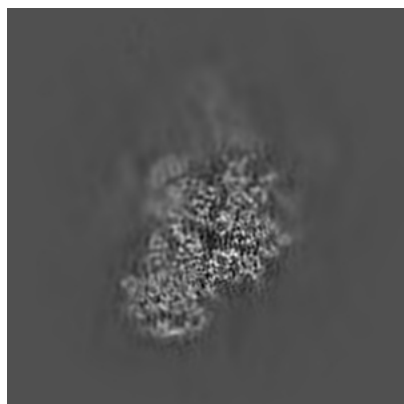


Z Index: 240

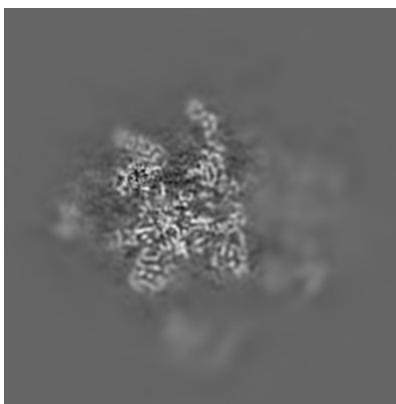
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

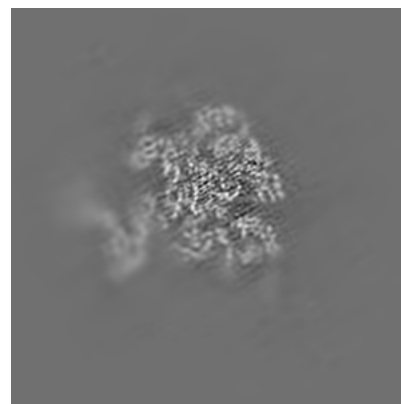
6.3.1 Primary map



X Index: 280



Y Index: 241

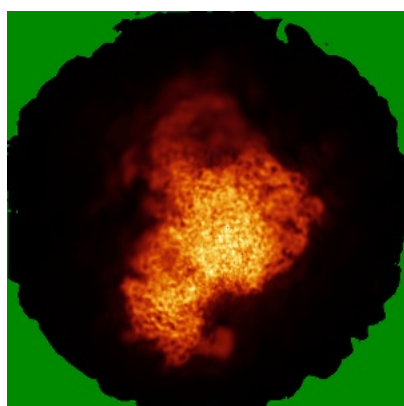


Z Index: 204

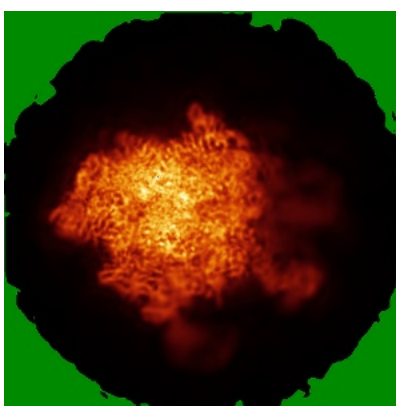
The images above show the largest variance slices of the map in three orthogonal directions.

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

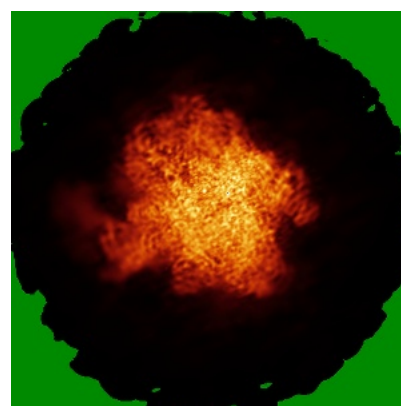
6.4.1 Primary map



X



Y



Z

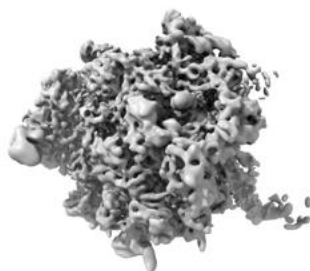
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

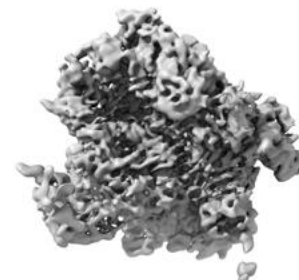
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

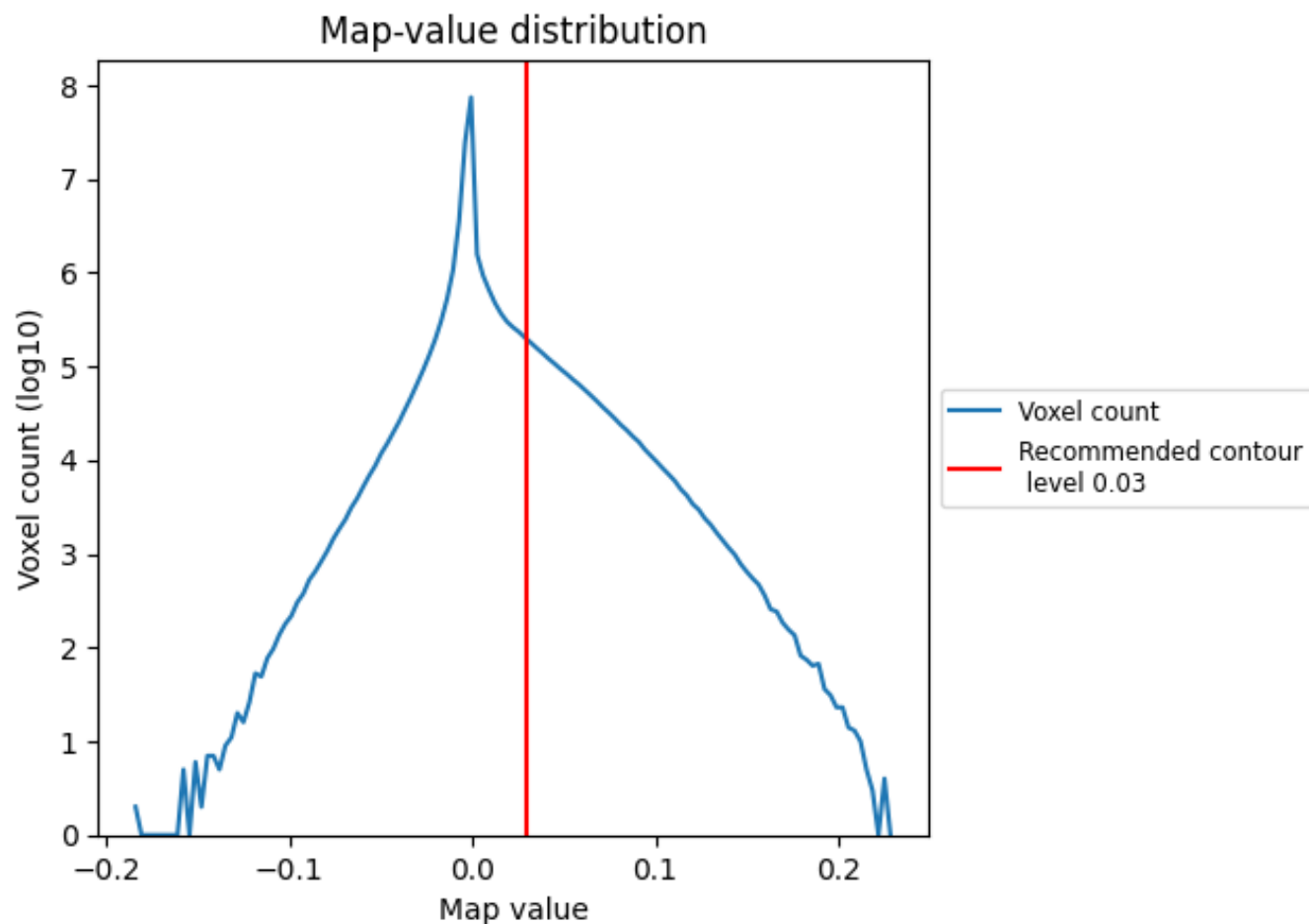
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

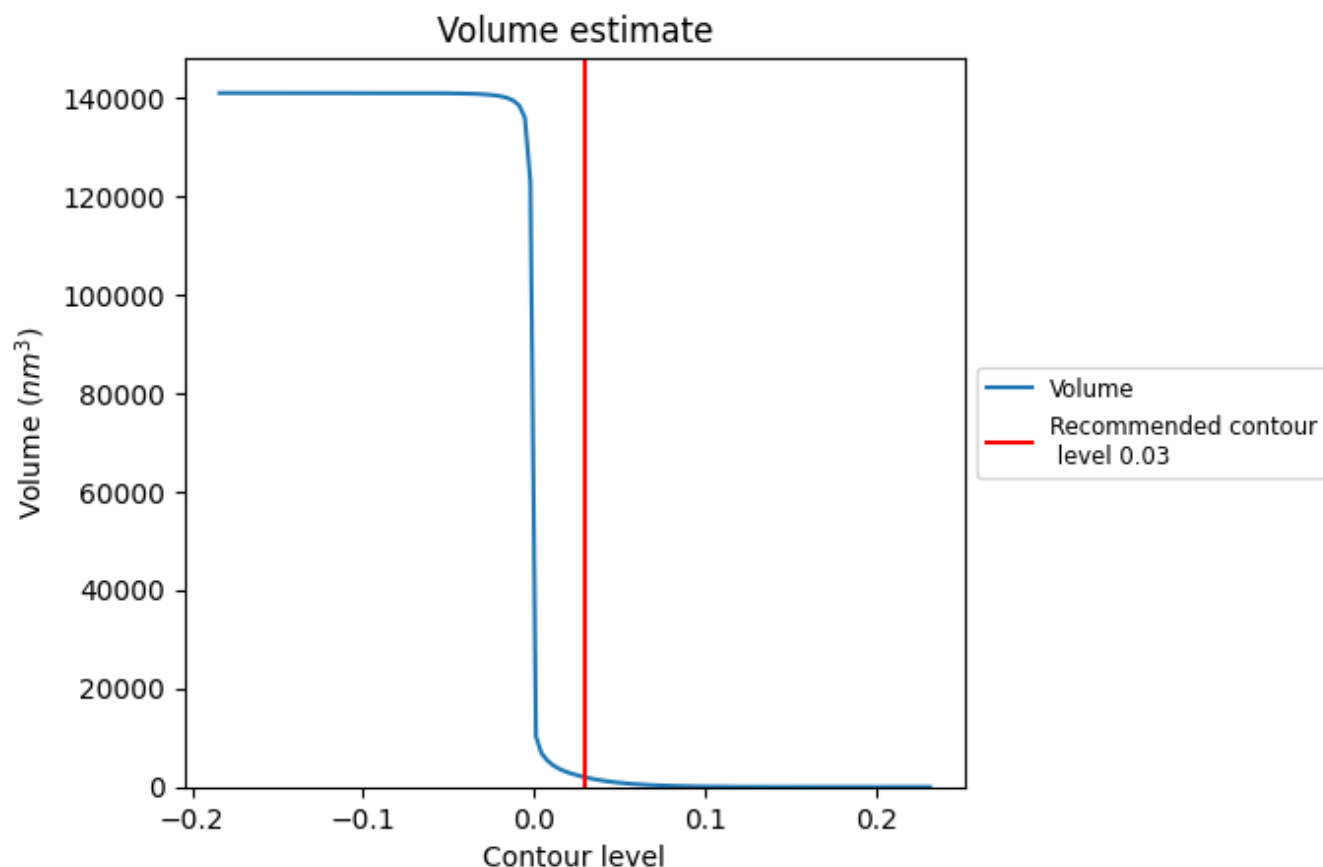
This section contains the results of statistical analysis of the map.

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.

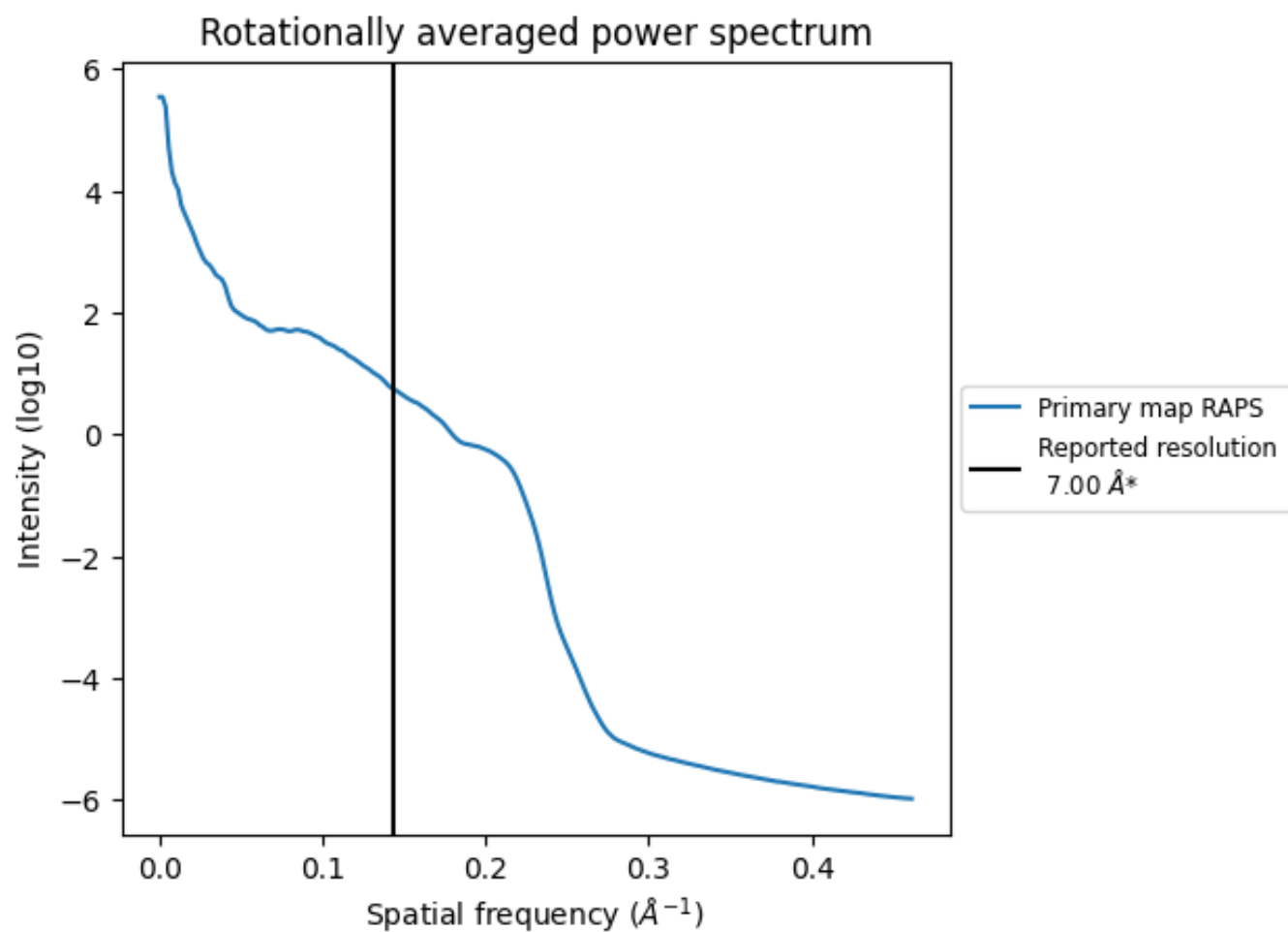
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1958 nm^3 ; this corresponds to an approximate mass of 1768 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 ⓘ

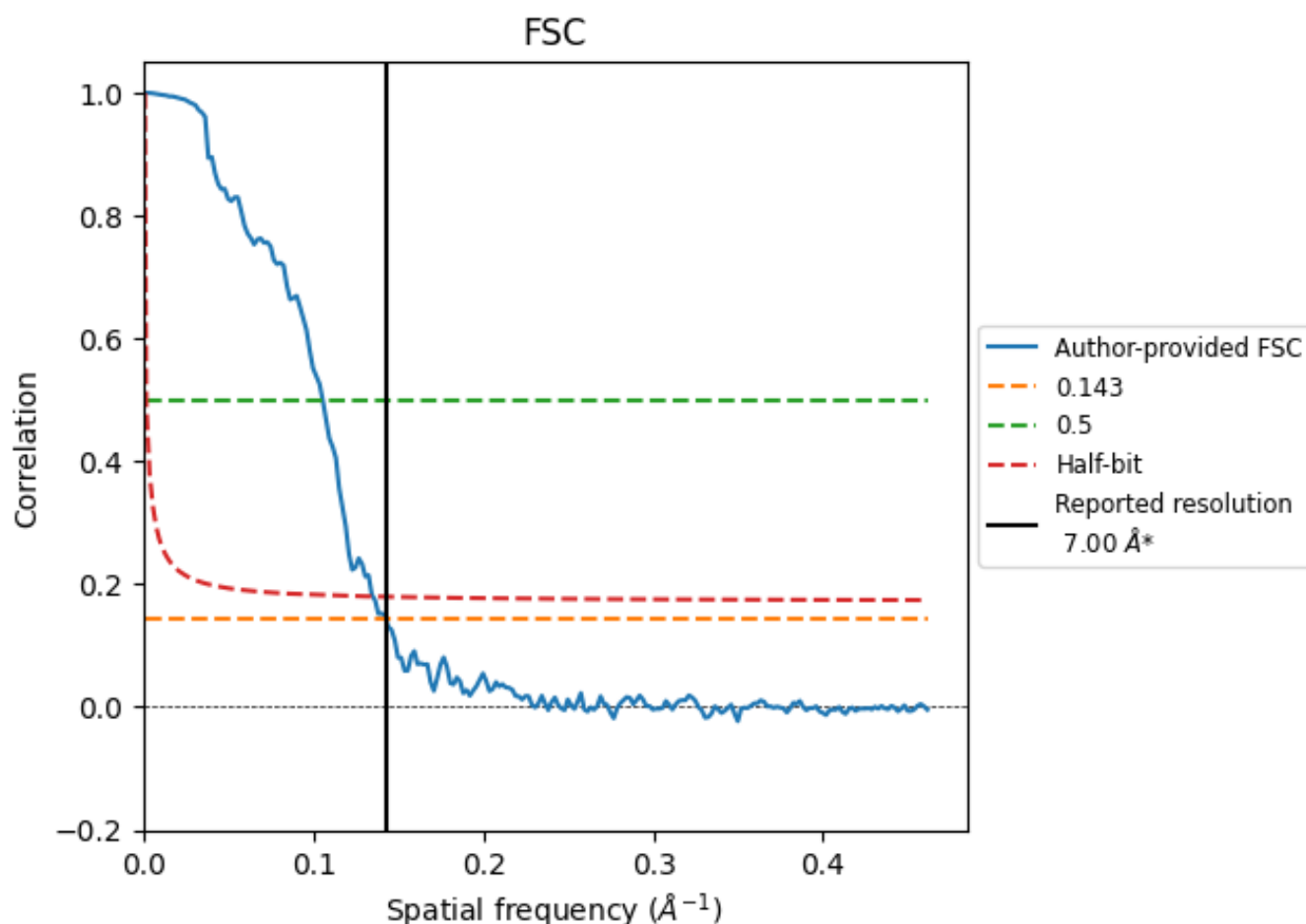


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 Å⁻¹

8.2 Resolution estimates [i](#)

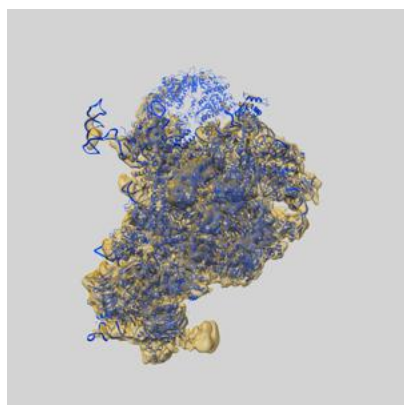
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	7.00	9.47	7.40
Unmasked-calculated*	-	-	-

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

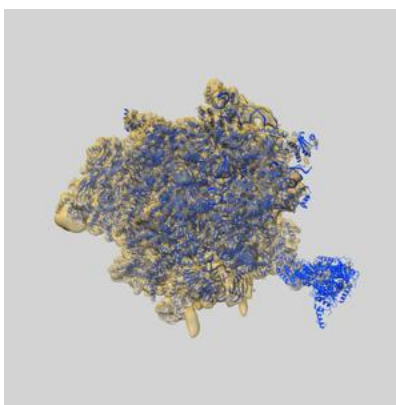
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10051 and PDB model 6RXT. Per-residue inclusion information can be found in section [3](#) on page [15](#).

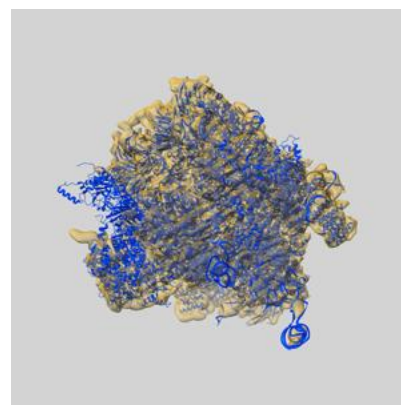
9.1 Map-model overlay [i](#)



X



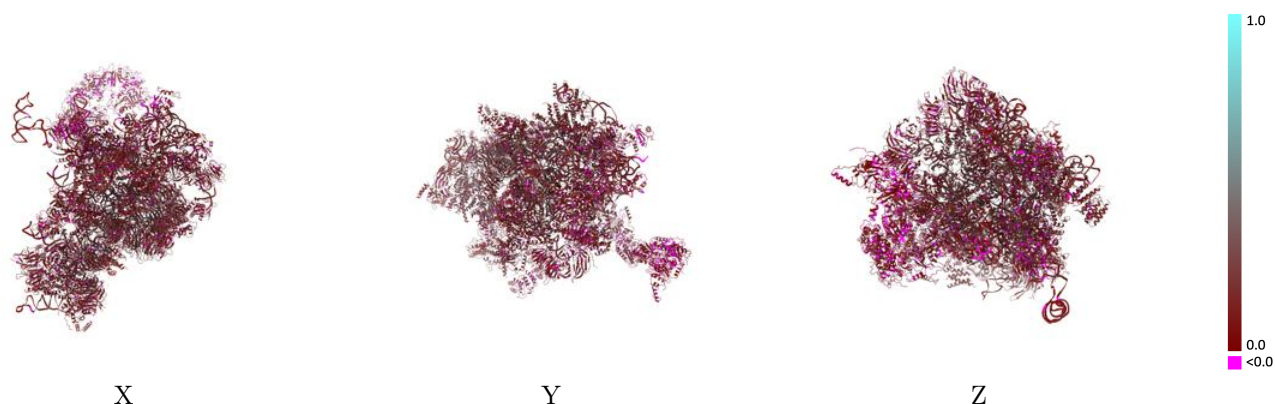
Y



Z

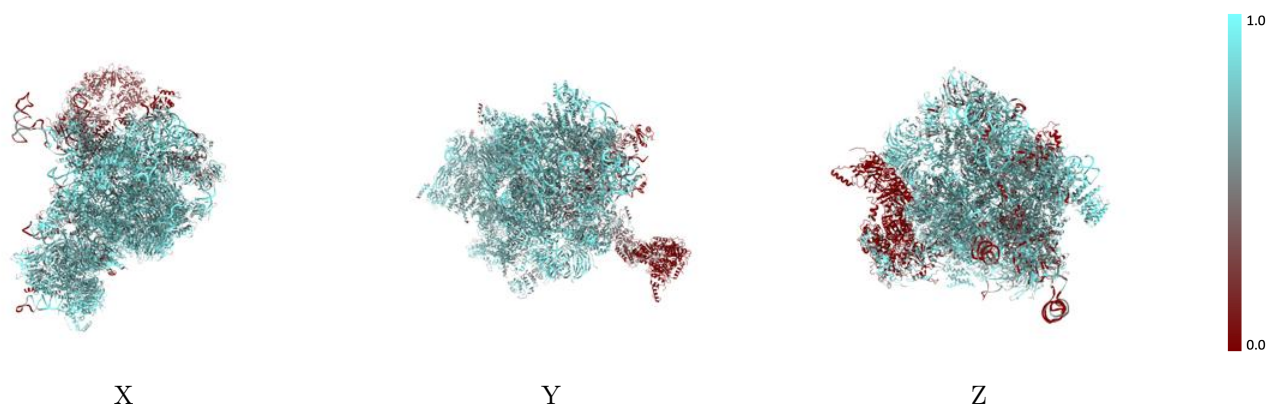
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



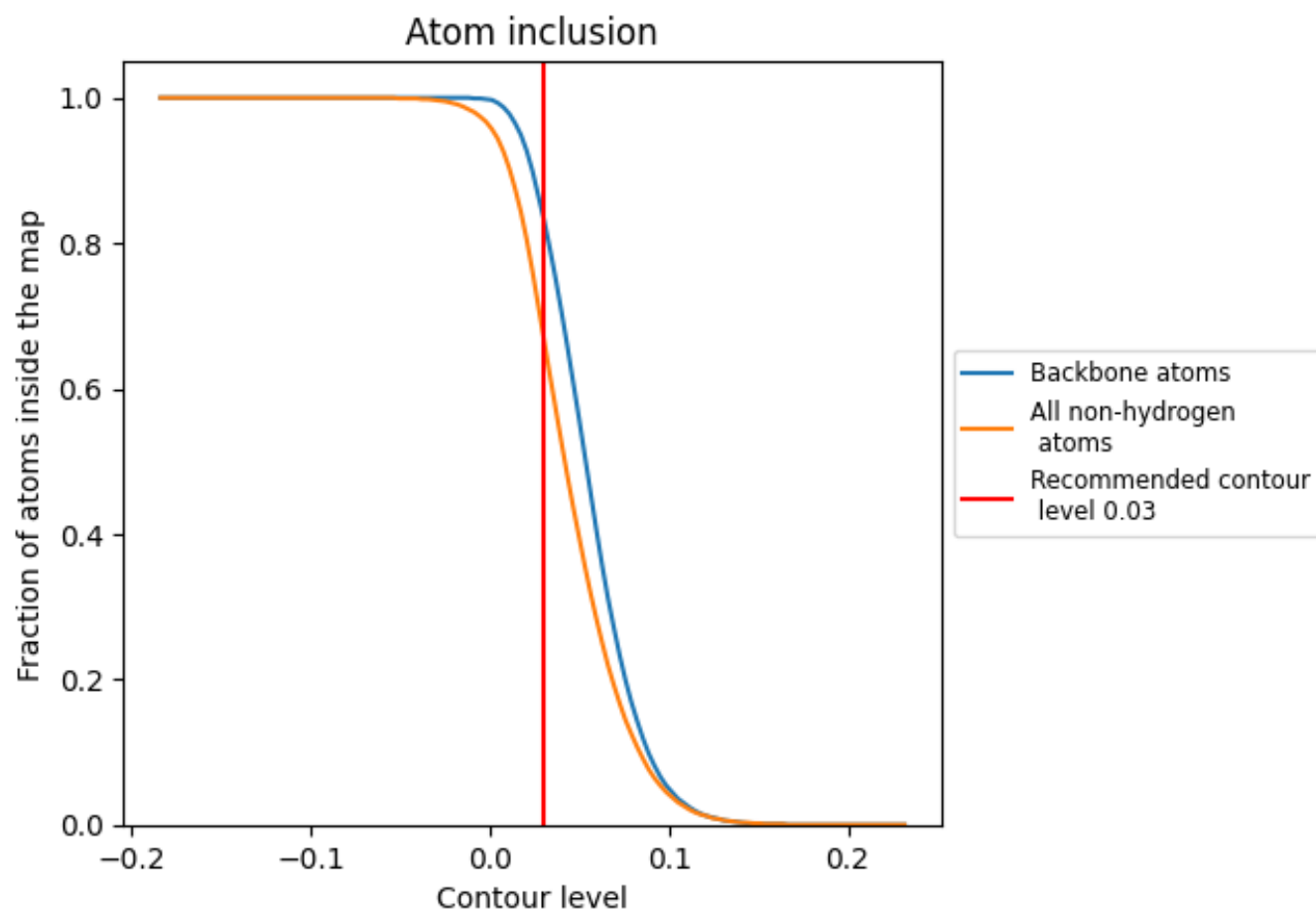
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 67% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.1660
C1	 0.8420	 0.2100
C2	 0.7280	 0.1970
CA	 0.7010	 0.1750
CB	 0.6540	 0.1480
CC	 0.6640	 0.1560
CD	 0.7060	 0.1610
CE	 0.7090	 0.1920
CF	 0.5920	 0.1310
CG	 0.4090	 0.0860
CH	 0.6830	 0.1430
CI	 0.6700	 0.1600
CJ	 0.7190	 0.2240
CK	 0.6880	 0.2120
CL	 0.7070	 0.1960
CM	 0.7080	 0.1460
CN	 0.6700	 0.1560
CO	 0.6970	 0.1380
CP	 0.5310	 0.1470
CQ	 0.7070	 0.1590
CR	 0.2890	 0.0920
CS	 0.0150	 0.0450
CT	 0.6710	 0.1670
CU	 0.5220	 0.1560
CX	 0.6420	 0.0950
Ca	 0.6210	 0.1280
Cc	 0.6990	 0.1800
Ce	 0.1150	 0.0970
Cg	 0.2770	 0.1210
Ch	 0.4740	 0.1070
Ci	 0.6500	 0.1360
Cj	 0.7220	 0.2320
Cl	 0.3870	 0.1290
Cm	 0.4820	 0.1310
Cn	 0.6610	 0.1730



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Chain	Atom inclusion	Q-score
Cp	 0.7150	 0.1790
UA	 0.7410	 0.2100
UB	 0.7300	 0.1640
UC	 0.5660	 0.1530
UD	 0.7270	 0.1680
UE	 0.6910	 0.1540
UF	 0.7680	 0.1560
UG	 0.7000	 0.1990
UH	 0.7500	 0.1490
UI	 0.7160	 0.1460
UJ	 0.7050	 0.1730
UK	 0.7070	 0.1910
UL	 0.7640	 0.1500
UM	 0.6370	 0.1240
UN	 0.7150	 0.1700
UO	 0.7170	 0.1750
UP	 0.7050	 0.1730
UQ	 0.7570	 0.1870
UR	 0.7620	 0.2290
US	 0.7280	 0.1490
UU	 0.7640	 0.2090
UX	 0.6630	 0.1610
UZ	 0.6900	 0.1550