Full wwPDB EM Validation Report ⓘ

Jan 7, 2025 – 07:35 pm GMT

PDB ID	:	9FNY
EMDB ID	:	EMD-50611
Title	:	PF30S-PF30S dimer mediated by aRDF from P. furiosus (Structure I)
Authors	:	Hassan, A.H.; Demo, G.
Deposited on	:	2024-06-11
Resolution	:	3.20 Å(reported)
Based on initial models	:	4V6U, ., 7ZHG

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:

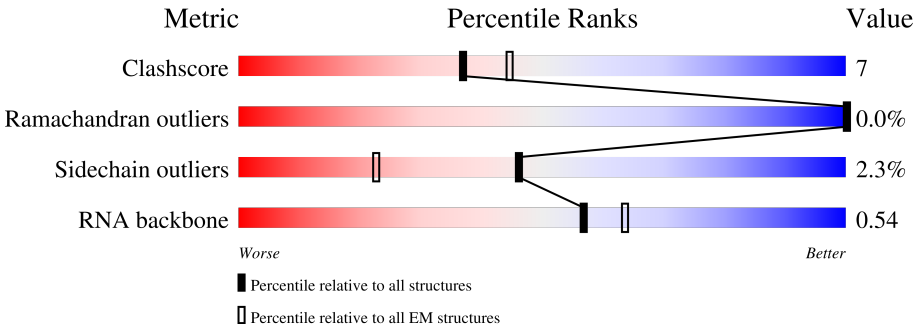
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A1	60	5% 75% 25%
1	B1	60	12% 90% 10%
2	A2	37	62% 32% 5%
2	B2	37	84% 11% 5%
3	A3	306	75% 22%
3	A4	306	76% 19% 5%
3	B3	306	77% 19%

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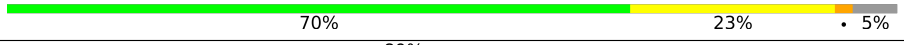
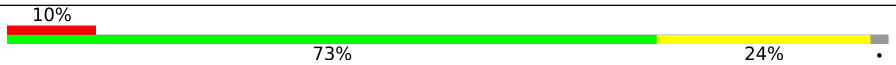
Mol	Chain	Length	Quality of chain
3	B4	306	
4	A5	123	
4	B5	123	
5	AA	1495	
5	BA	1495	
6	AB	202	
6	BB	202	
7	AC	210	
7	BC	210	
8	AD	198	
8	BD	198	
9	AE	180	
9	BE	180	
10	AF	243	
10	BF	243	
11	AG	236	
11	BG	236	
12	AH	125	
12	BH	125	
13	AI	215	
13	BI	215	
14	AJ	130	
14	BJ	130	
15	AK	127	
15	BK	127	

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Mol	Chain	Length	Quality of chain
16	AL	135	76% 19% 5%
16	BL	135	14% 73% 21% 5%
17	AM	102	23% 71% 28%
17	BM	102	24% 76% 24%
18	AN	137	75% 18% 7%
18	BN	137	71% 21% 7%
19	AO	147	72% 25%
19	BO	147	71% 25%
20	AP	148	8% 64% 24% 11%
20	BP	148	59% 65% 23% 11%
21	AQ	56	64% 21% 11%
21	BQ	56	7% 61% 25% 11%
22	AR	158	80% 18%
22	BR	158	80% 18%
23	AS	113	69% 27%
23	BS	113	82% 14%
24	AT	67	81% 13% 6%
24	BT	67	13% 79% 15% 6%
25	AU	132	20% 66% 21% 13%
25	BU	132	63% 72% 15% 13%
26	AV	150	81% 17%
26	BV	150	19% 80% 19%
27	AW	99	69% 23% 6%
27	BW	99	78% 15% 6%
28	AX	50	42% 68% 22% 10%

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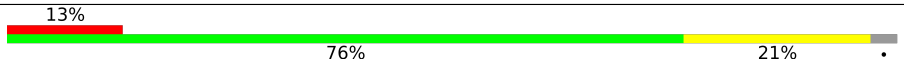
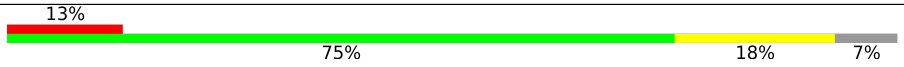
Mol	Chain	Length	Quality of chain
28	BX	50	
29	AY	63	
29	BY	63	
30	AZ	71	
30	BZ	71	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 130968 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 RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		
1	B1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		

- Molecule 2 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		
2	B2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		

- Molecule 3 is a protein called Archaeal Ribosome Dimerizing Factor (aRDF).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	298	Total	C	N	O	S	0	0
			2372	1535	395	438	4		
3	A4	292	Total	C	N	O	S	0	0
			2329	1509	388	428	4		
3	B3	295	Total	C	N	O	S	0	0
			2353	1524	391	434	4		
3	B4	290	Total	C	N	O	S	0	0
			2312	1497	385	426	4		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	301	HIS	-	expression tag	UNP Q8U3B0
A3	302	HIS	-	expression tag	UNP Q8U3B0
A3	303	HIS	-	expression tag	UNP Q8U3B0
A3	304	HIS	-	expression tag	UNP Q8U3B0
A3	305	HIS	-	expression tag	UNP Q8U3B0

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Chain	Residue	Modelled	Actual	Comment	Reference
A3	306	HIS	-	expression tag	UNP Q8U3B0
A4	301	HIS	-	expression tag	UNP Q8U3B0
A4	302	HIS	-	expression tag	UNP Q8U3B0
A4	303	HIS	-	expression tag	UNP Q8U3B0
A4	304	HIS	-	expression tag	UNP Q8U3B0
A4	305	HIS	-	expression tag	UNP Q8U3B0
A4	306	HIS	-	expression tag	UNP Q8U3B0
B3	301	HIS	-	expression tag	UNP Q8U3B0
B3	302	HIS	-	expression tag	UNP Q8U3B0
B3	303	HIS	-	expression tag	UNP Q8U3B0
B3	304	HIS	-	expression tag	UNP Q8U3B0
B3	305	HIS	-	expression tag	UNP Q8U3B0
B3	306	HIS	-	expression tag	UNP Q8U3B0
B4	301	HIS	-	expression tag	UNP Q8U3B0
B4	302	HIS	-	expression tag	UNP Q8U3B0
B4	303	HIS	-	expression tag	UNP Q8U3B0
B4	304	HIS	-	expression tag	UNP Q8U3B0
B4	305	HIS	-	expression tag	UNP Q8U3B0
B4	306	HIS	-	expression tag	UNP Q8U3B0

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		
4	B5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		
5	BA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	197	Total	C	N	O	S	0	0
			1579	1022	271	282	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	197	Total 1579	C 1022	N 271	O 282	S 4	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	195	Total 1532	C 980	N 283	O 266	S 3	0	0
7	BC	195	Total 1532	C 980	N 283	O 266	S 3	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	184	Total 1511	C 978	N 263	O 265	S 5	0	0
8	BD	184	Total 1511	C 978	N 263	O 265	S 5	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	173	Total 1455	C 915	N 282	O 254	S 4	0	0
9	BE	173	Total 1455	C 915	N 282	O 254	S 4	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	242	Total 1981	C 1280	N 356	O 340	S 5	0	0
10	BF	242	Total 1981	C 1280	N 356	O 340	S 5	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	227	Total 1794	C 1134	N 335	O 318	S 7	0	0
11	BG	227	Total 1794	C 1134	N 335	O 318	S 7	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		
12	BH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		
13	BI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		
14	BJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 15 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AK	124	Total	C	N	O	0	0
			977	607	204	166		
15	BK	124	Total	C	N	O	0	0
			977	607	204	166		

- Molecule 16 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		
16	BL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		
17	BM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		
18	BN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		
19	BO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		
20	BP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		

- Molecule 21 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		
21	BQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		

- Molecule 22 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		
23	BS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		

- Molecule 24 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		
24	BT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		
25	BU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		

- Molecule 26 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	AV	148	Total	C	N	O	0	0
			1209	781	218	210		
26	BV	148	Total	C	N	O	0	0
			1209	781	218	210		

- Molecule 27 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		
27	BW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		
28	BX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		
29	BY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

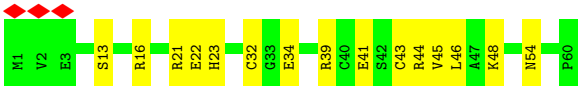
Mol	Chain	Residues	Atoms				AltConf	Trace
30	AZ	66	Total	C	N	O	0	0
			523	320	104	99		
30	BZ	66	Total	C	N	O	0	0
			523	320	104	99		

3 Residue-property plots (i)

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

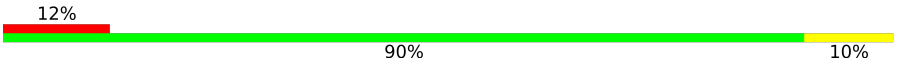
• Molecule 1: RNA-binding protein

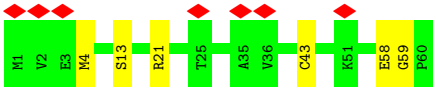
Chain A1:



• Molecule 1: RNA-binding protein

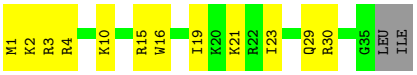
Chain B1:





• Molecule 2: Small ribosomal subunit protein eS32

Chain A2:

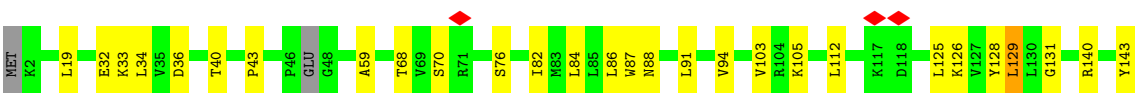


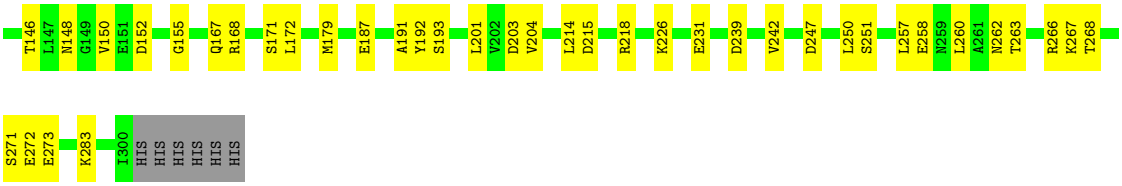
• Molecule 2: Small ribosomal subunit protein eS32

Chain B2:

• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

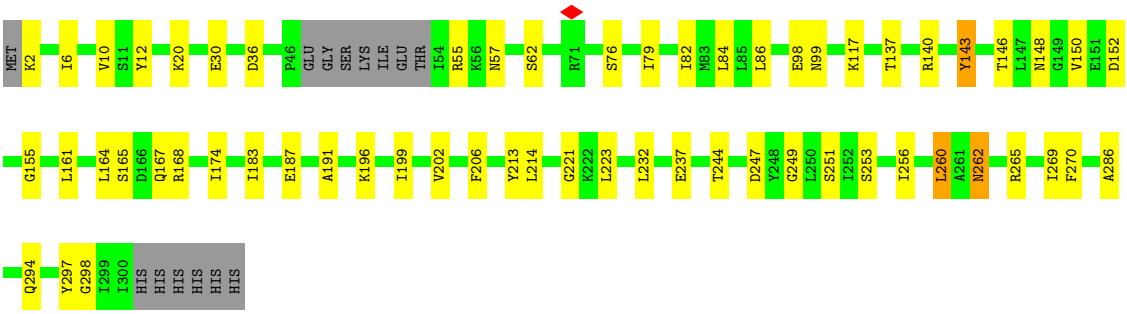
Chain A3:





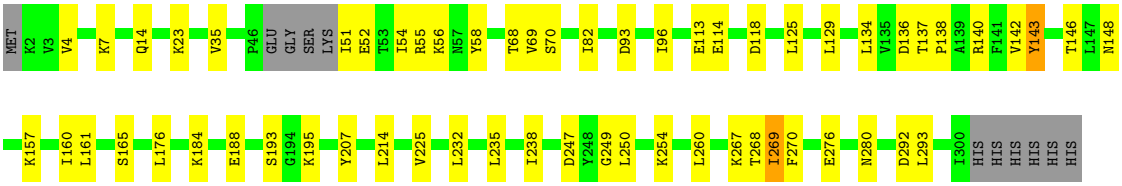
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain A4:



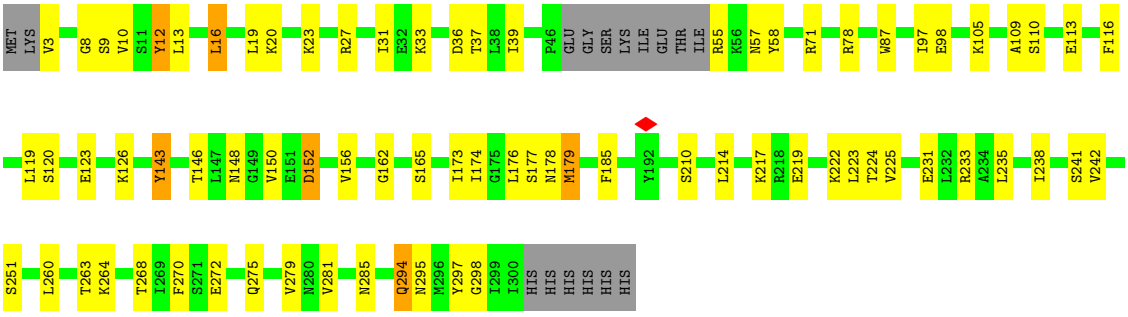
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B3:



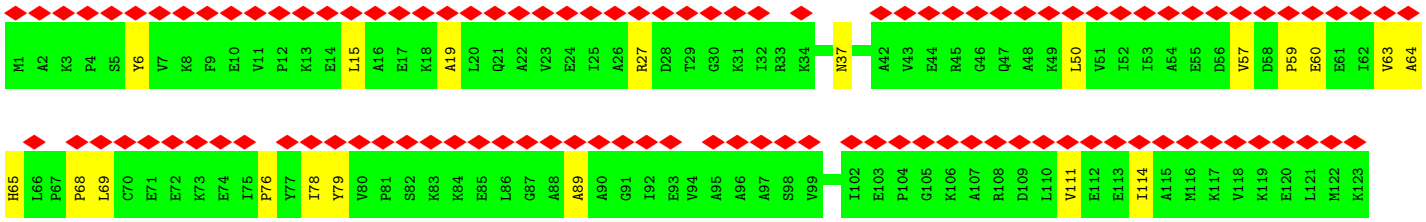
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B4:



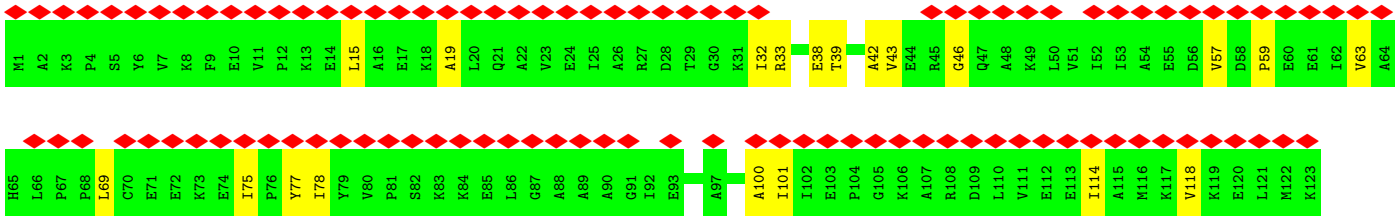
• Molecule 4: Large ribosomal subunit protein eL8

Chain A5:



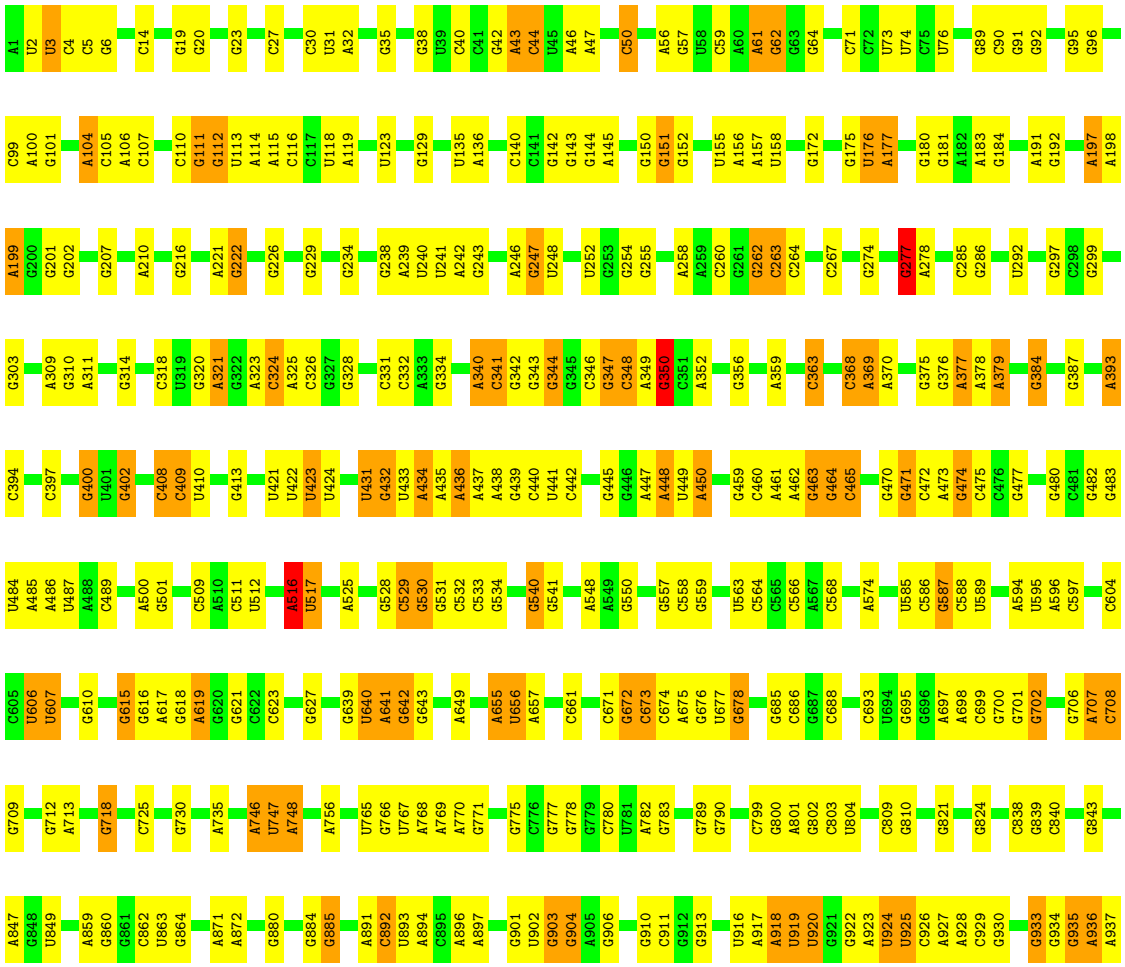
• Molecule 4: Large ribosomal subunit protein eL8

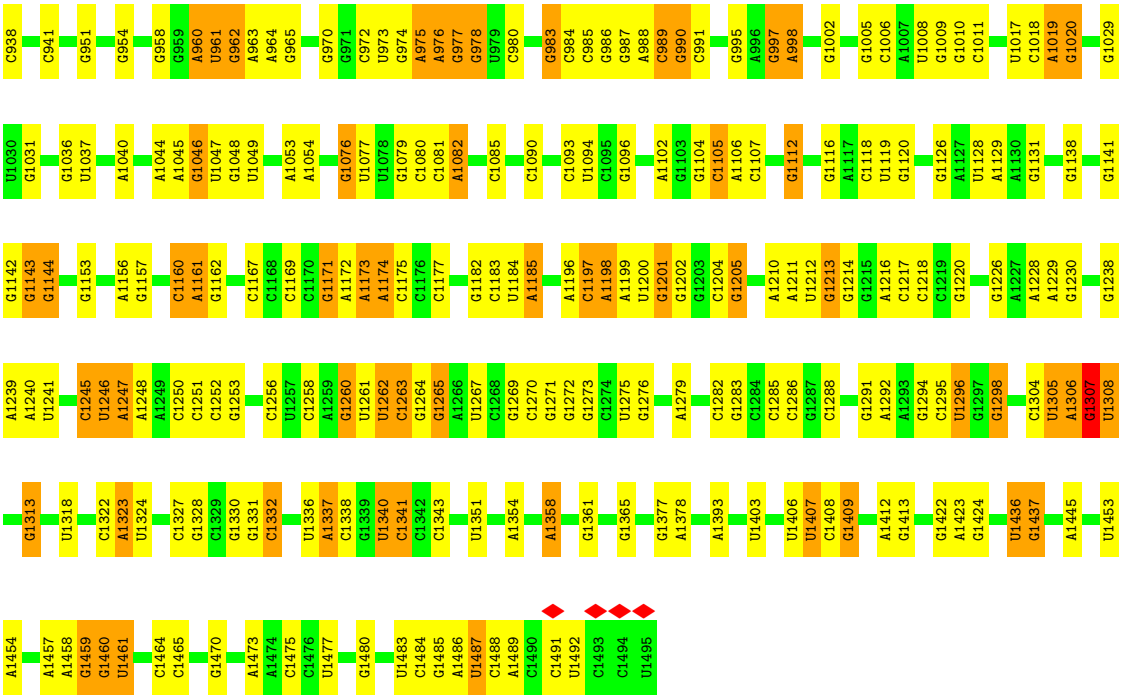
Chain B5:



• Molecule 5: 16S rRNA

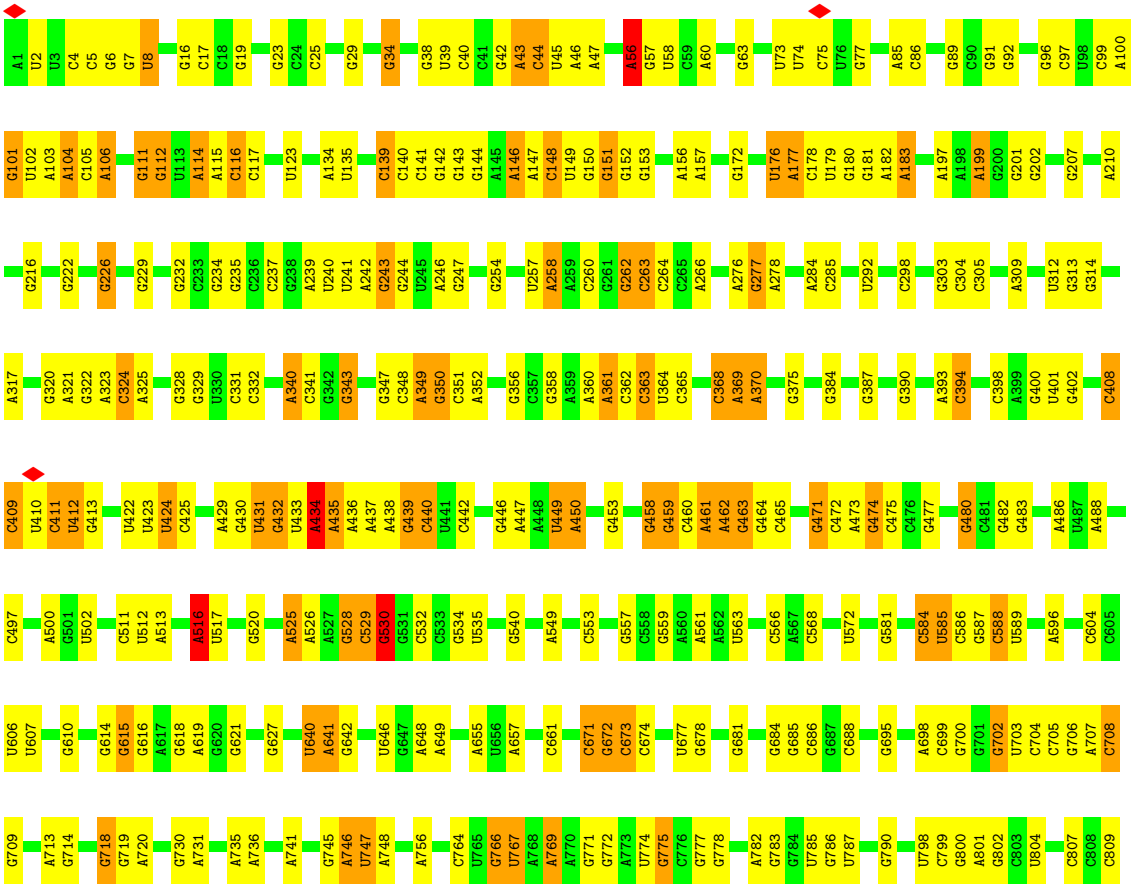
Chain AA:

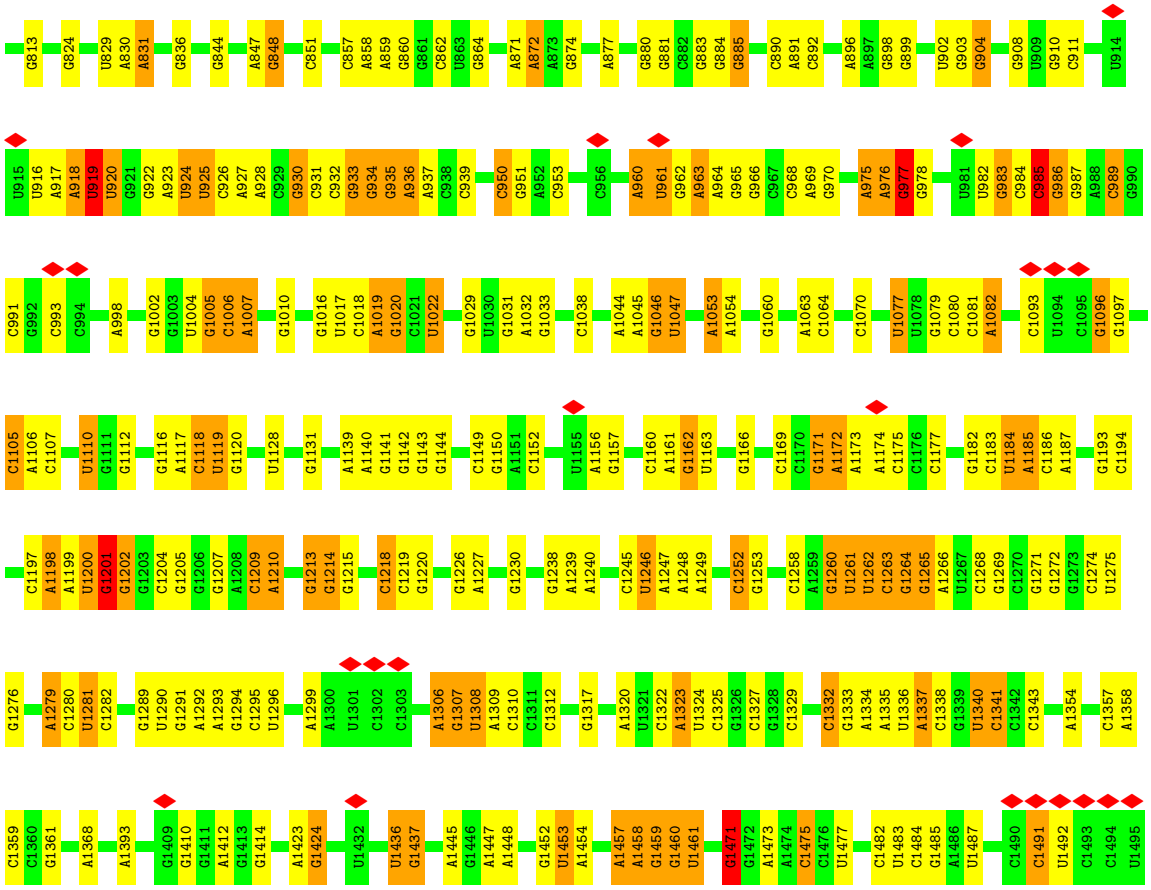




• Molecule 5: 16S rRNA

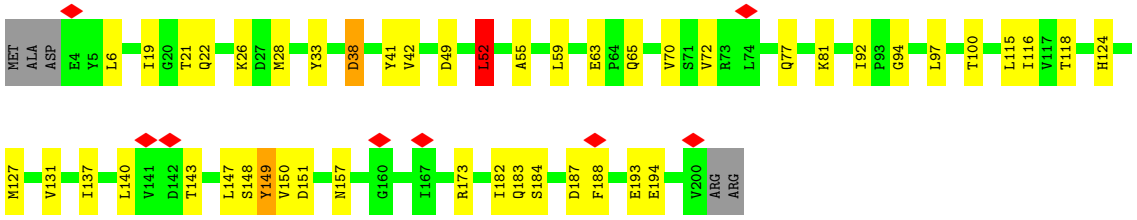
Chain BA:





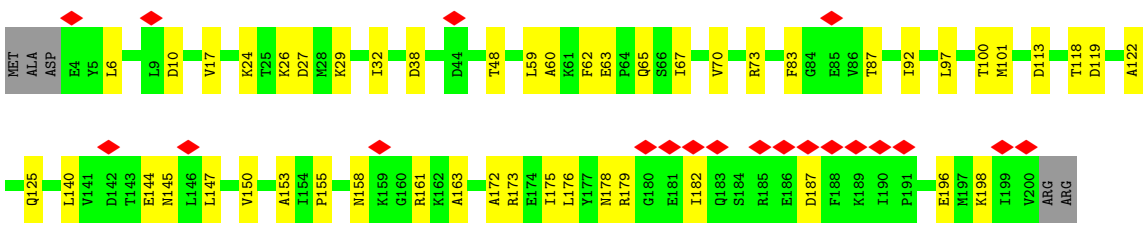
• Molecule 6: Small ribosomal subunit protein uS2

Chain AB:



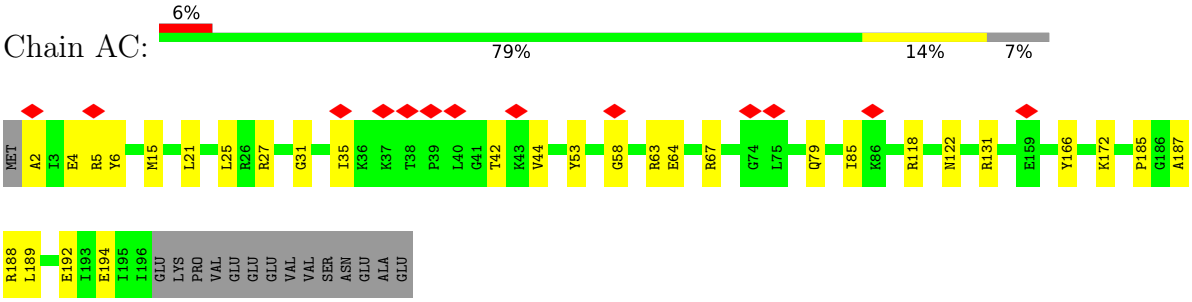
• Molecule 6: Small ribosomal subunit protein uS2

Chain BB:



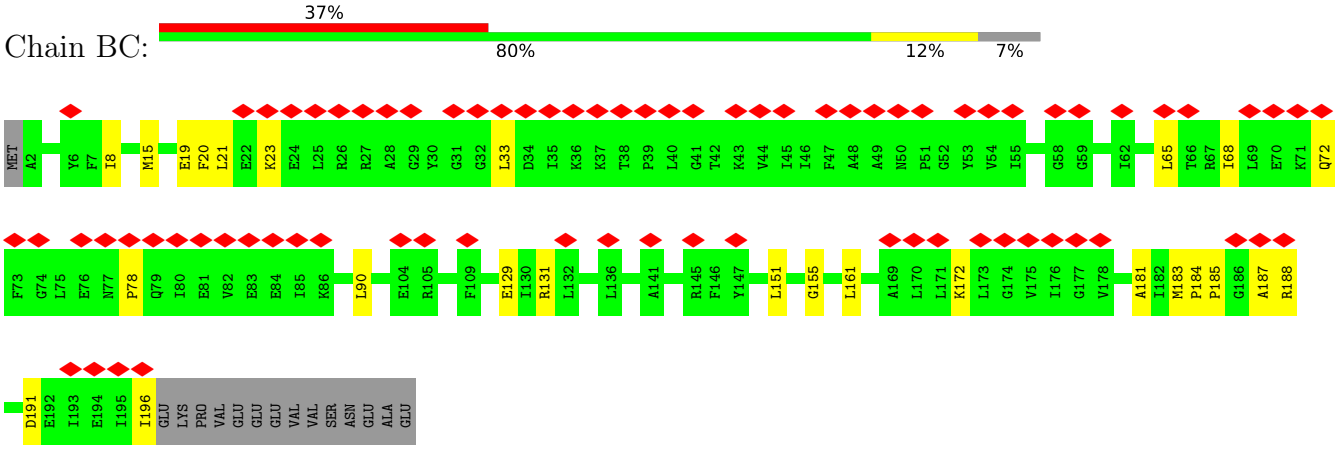
• Molecule 7: Small ribosomal subunit protein uS3

Chain AC:



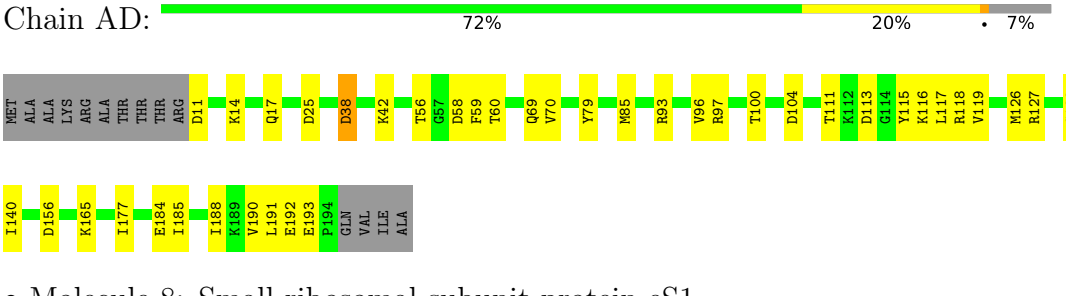
• Molecule 7: Small ribosomal subunit protein uS3

Chain BC:



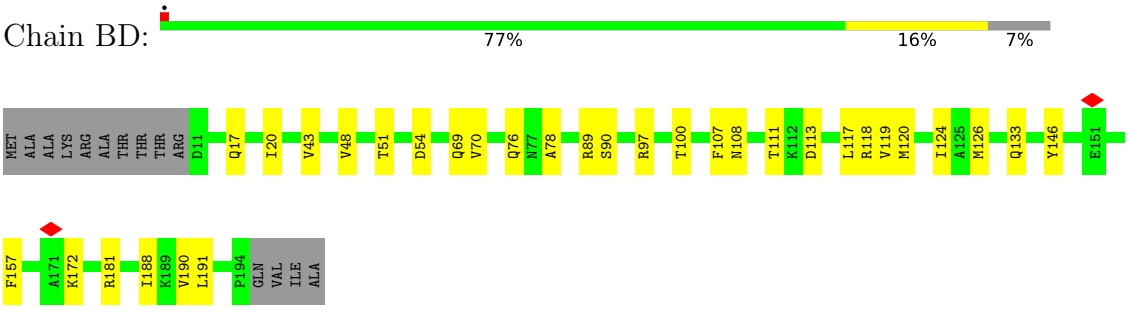
• Molecule 8: Small ribosomal subunit protein eS1

Chain AD:



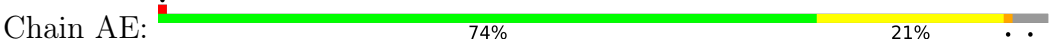
• Molecule 8: Small ribosomal subunit protein eS1

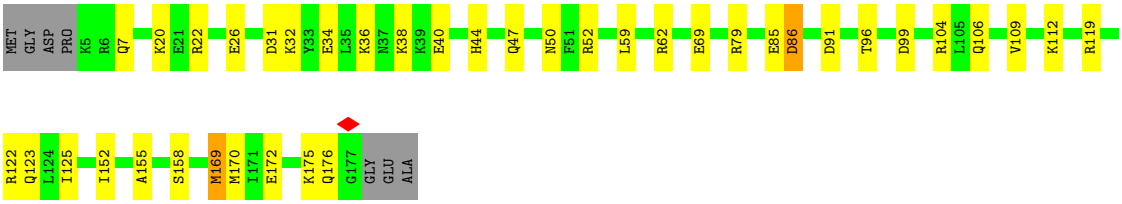
Chain BD:



• Molecule 9: Small ribosomal subunit protein uS4

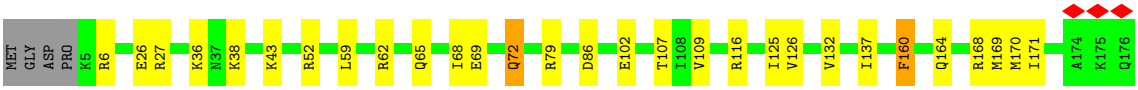
Chain AE:





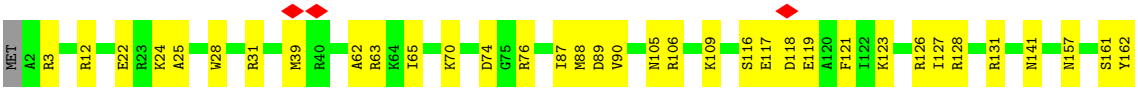
• Molecule 9: Small ribosomal subunit protein uS4

Chain BE:



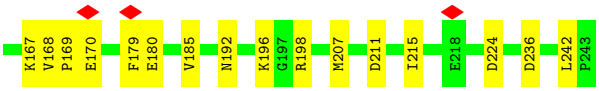
• Molecule 10: Small ribosomal subunit protein eS4

Chain AF:



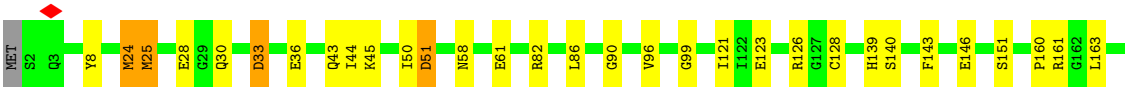
• Molecule 10: Small ribosomal subunit protein eS4

Chain BF:



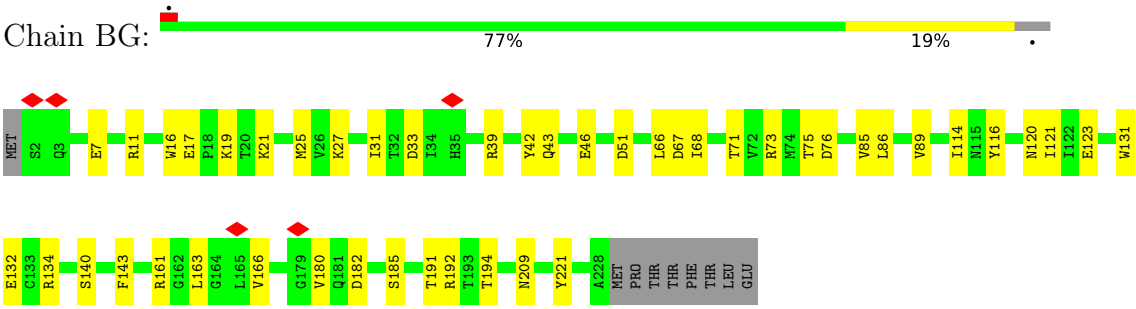
• Molecule 11: Small ribosomal subunit protein uS5

Chain AG:



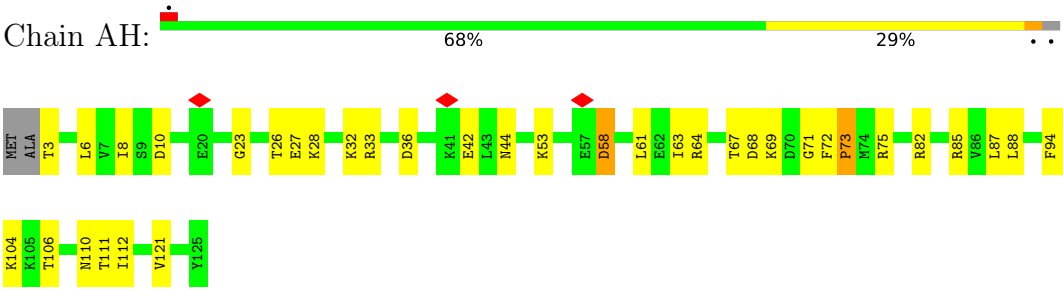
• Molecule 11: Small ribosomal subunit protein uS5

Chain BG:



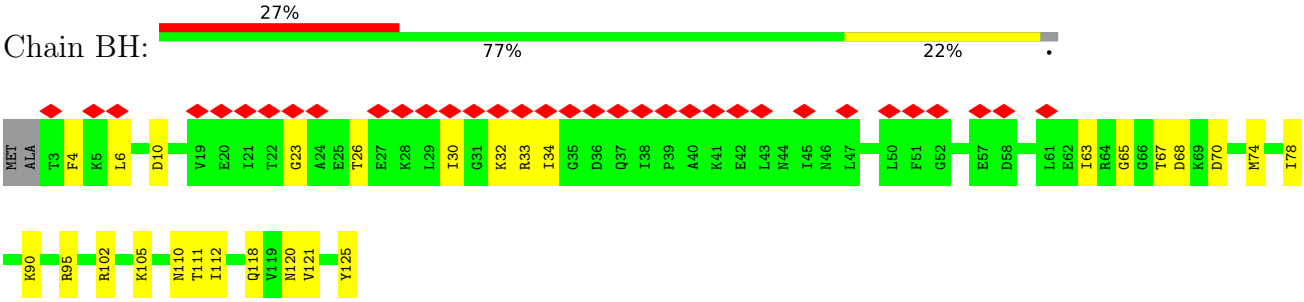
• Molecule 12: Small ribosomal subunit protein eS6

Chain AH:



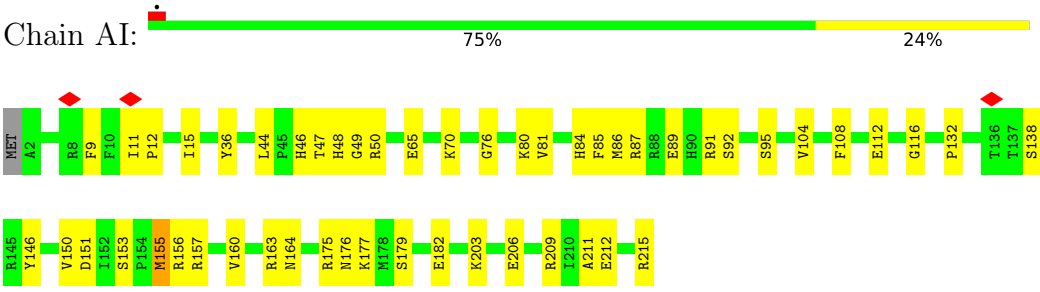
• Molecule 12: Small ribosomal subunit protein eS6

Chain BH:



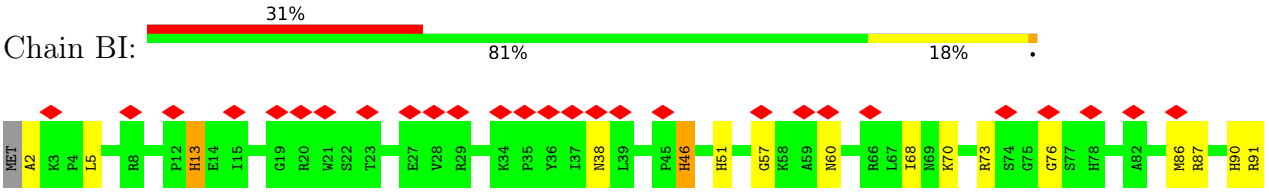
• Molecule 13: Small ribosomal subunit protein uS7

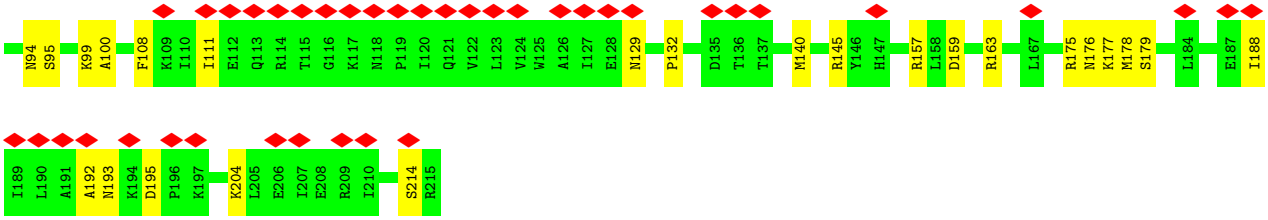
Chain AI:



• Molecule 13: Small ribosomal subunit protein uS7

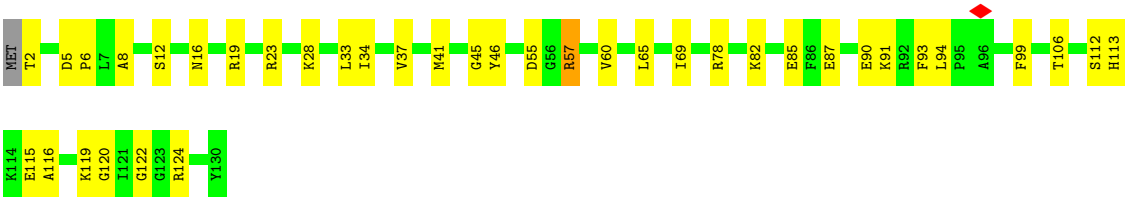
Chain BI:





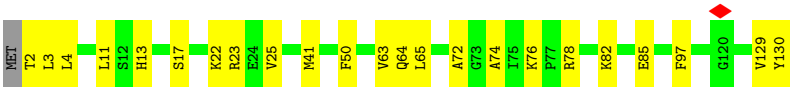
• Molecule 14: Small ribosomal subunit protein uS8

Chain AJ:



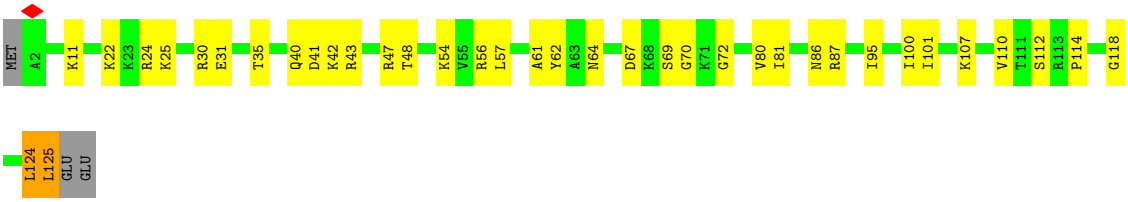
• Molecule 14: Small ribosomal subunit protein uS8

Chain BJ:



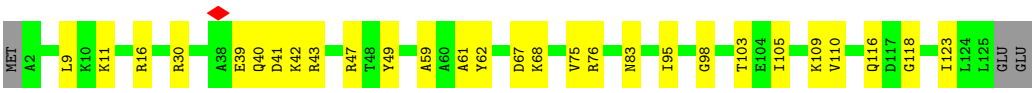
• Molecule 15: Small ribosomal subunit protein eS8

Chain AK:



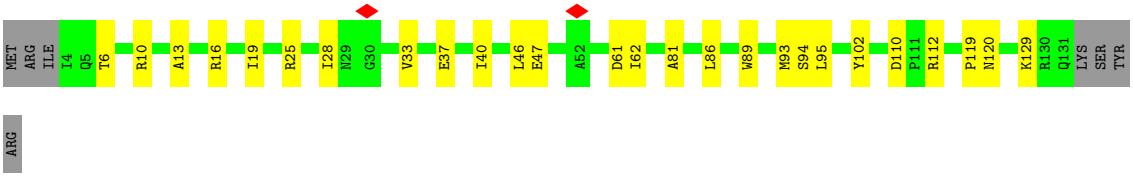
• Molecule 15: Small ribosomal subunit protein eS8

Chain BK:

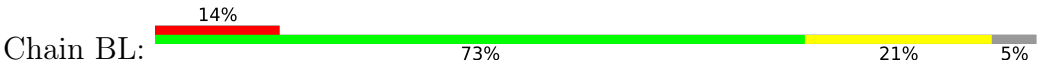


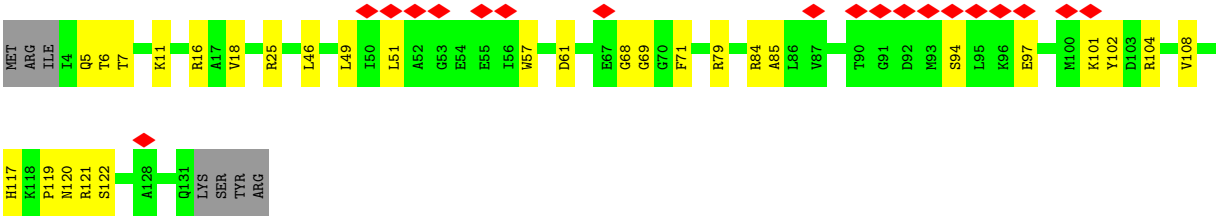
• Molecule 16: Small ribosomal subunit protein uS9

Chain AL:

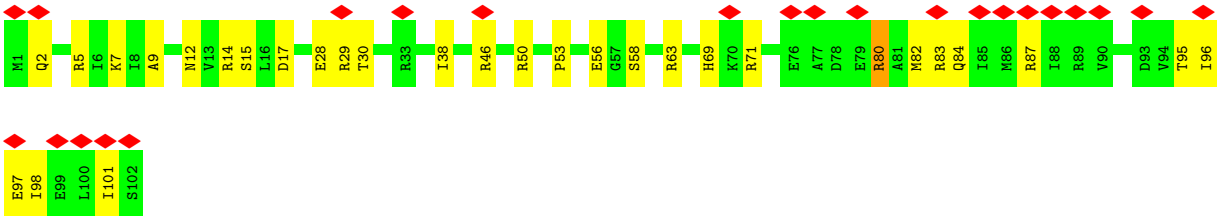


• Molecule 16: Small ribosomal subunit protein uS9

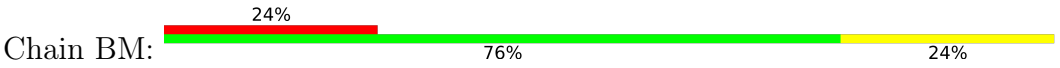


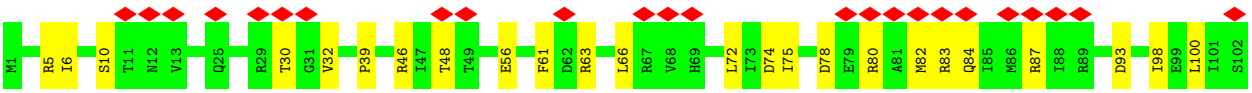


• Molecule 17: Small ribosomal subunit protein uS10

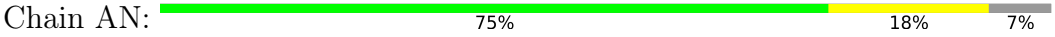


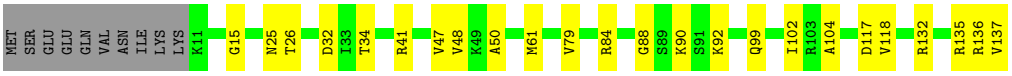
• Molecule 17: Small ribosomal subunit protein uS10





• Molecule 18: Small ribosomal subunit protein uS11

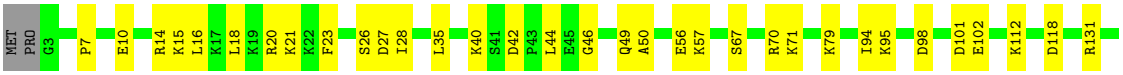


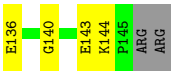


• Molecule 18: Small ribosomal subunit protein uS11

• Molecule 19: Small ribosomal subunit protein uS12

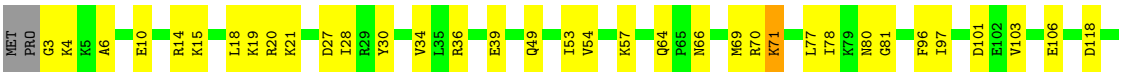
Chain AO:

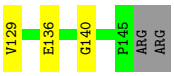




• Molecule 19: Small ribosomal subunit protein uS12

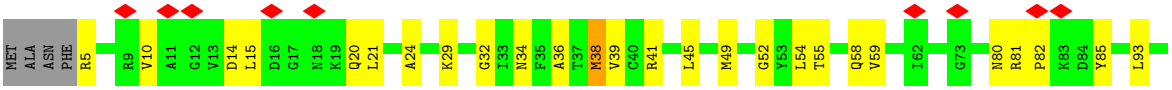
Chain BO:

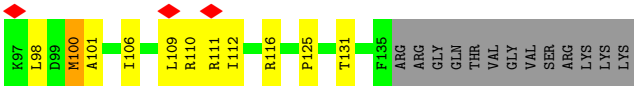




• Molecule 20: Small ribosomal subunit protein uS13

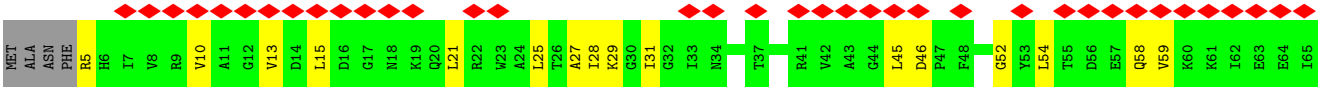
Chain AP:

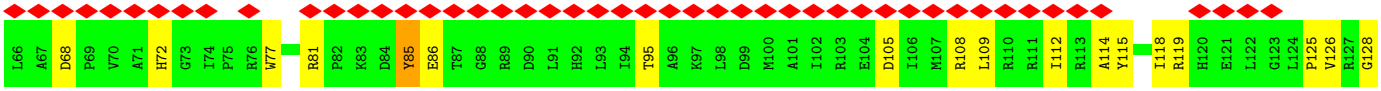


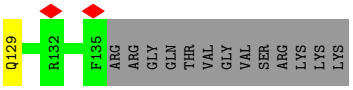


• Molecule 20: Small ribosomal subunit protein uS13

Chain BP:

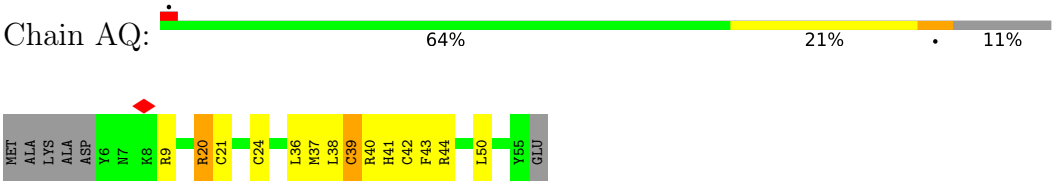






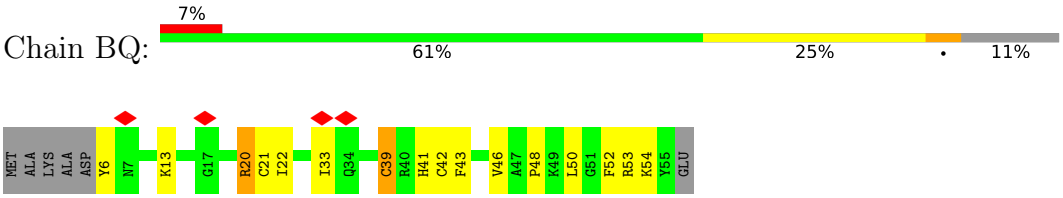
• Molecule 21: Small ribosomal subunit protein uS14

Chain AQ:



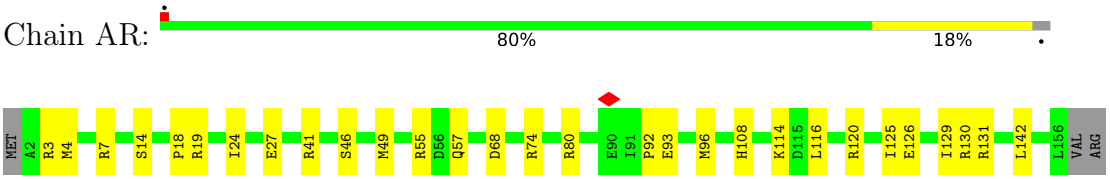
• Molecule 21: Small ribosomal subunit protein uS14

Chain BQ:



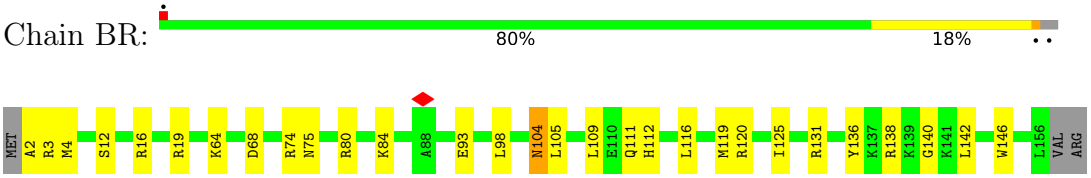
• Molecule 22: Small ribosomal subunit protein uS15

Chain AR:



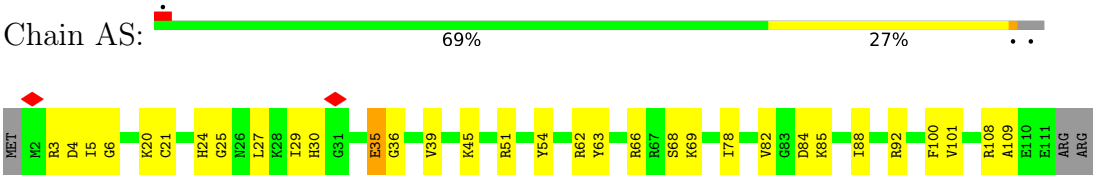
• Molecule 22: Small ribosomal subunit protein uS15

Chain BR:



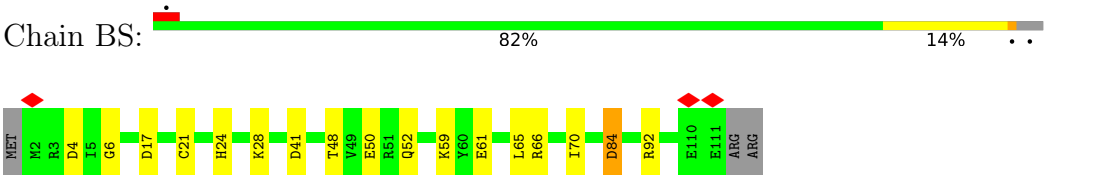
• Molecule 23: Small ribosomal subunit protein uS17

Chain AS:



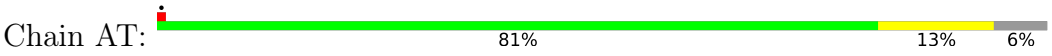
• Molecule 23: Small ribosomal subunit protein uS17

Chain BS:



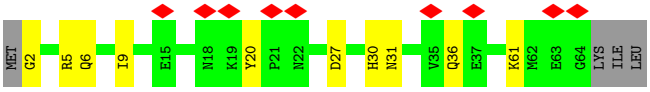
• Molecule 24: Small ribosomal subunit protein eS17

Chain AT:



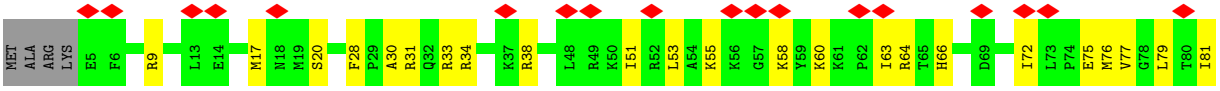
• Molecule 24: Small ribosomal subunit protein eS17

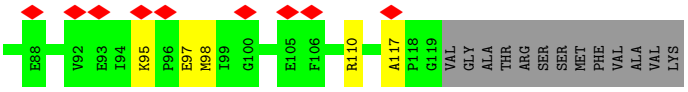
Chain BT:



• Molecule 25: Small ribosomal subunit protein uS19

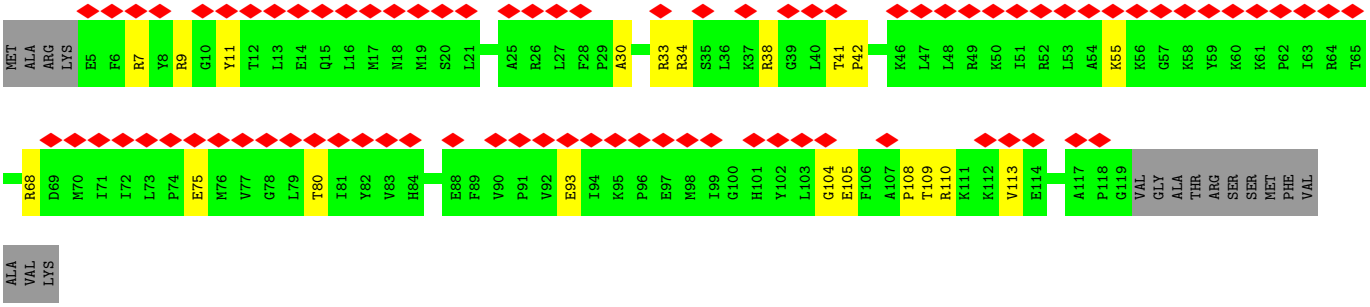
Chain AU:





• Molecule 25: Small ribosomal subunit protein uS19

Chain BU:

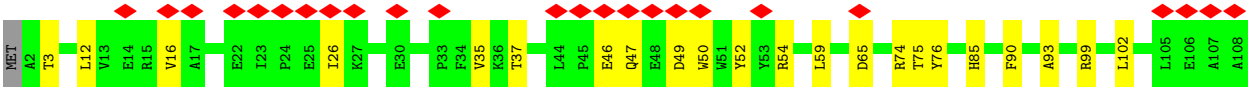


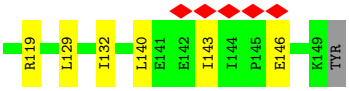
• Molecule 26: Small ribosomal subunit protein eS19

Chain AV:

• Molecule 26: Small ribosomal subunit protein eS19

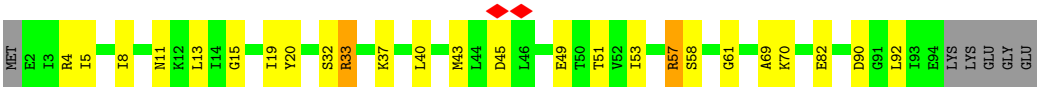
Chain BV:





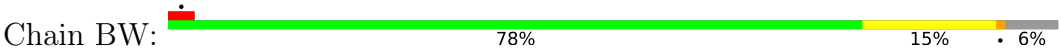
• Molecule 27: Small ribosomal subunit protein eS24

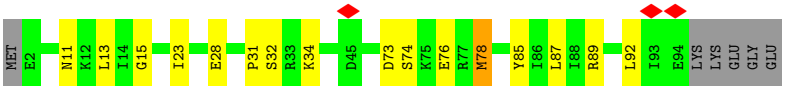
Chain AW:



• Molecule 27: Small ribosomal subunit protein eS24

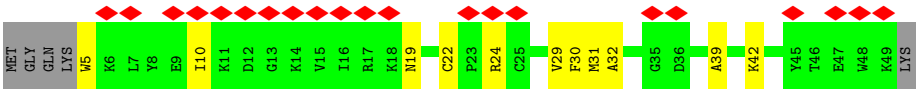
Chain BW:





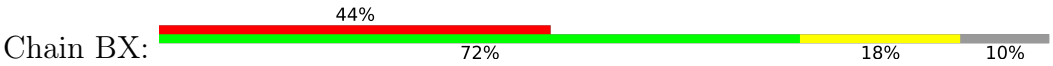
• Molecule 28: Small ribosomal subunit protein eS31

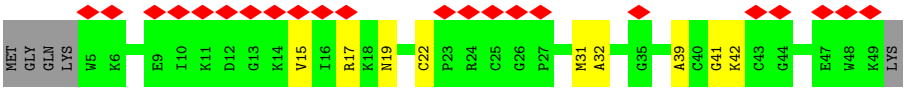
Chain AX:



• Molecule 28: Small ribosomal subunit protein eS31

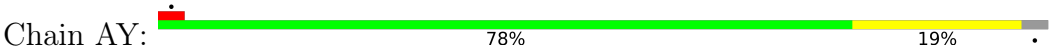
Chain BX:

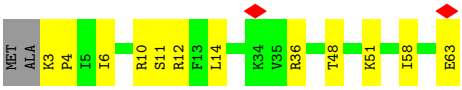




• Molecule 29: Small ribosomal subunit protein eS27

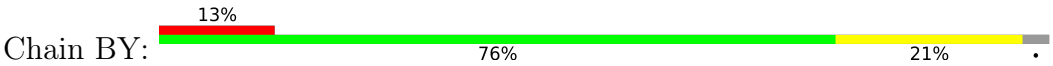
Chain AY:

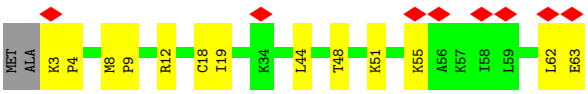




• Molecule 29: Small ribosomal subunit protein eS27

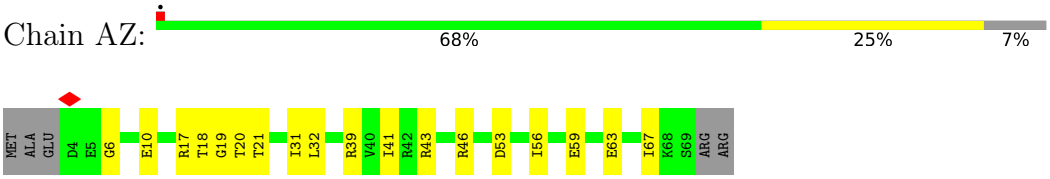
Chain BY:





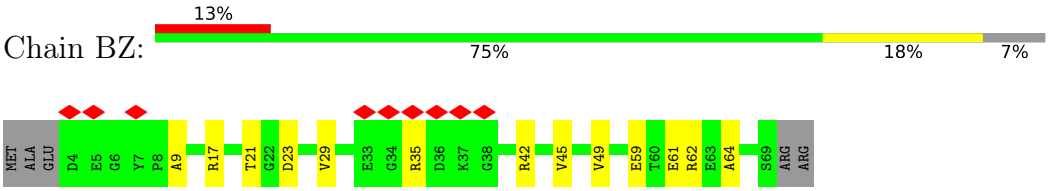
• Molecule 30: Small ribosomal subunit protein eS28

Chain AZ:



• Molecule 30: Small ribosomal subunit protein eS28

Chain BZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.071	Depositor
Minimum map value	-6.271	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.802	Depositor
Recommended contour level	3	Depositor
Map size (Å)	480.384, 480.384, 480.384	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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	A1	0.34	0/485	0.60	0/656
1	B1	0.31	0/485	0.58	0/656
2	A2	0.47	0/341	0.83	0/440
2	B2	0.39	0/341	0.86	0/440
3	A3	0.36	0/2404	0.60	1/3229 (0.0%)
3	A4	0.35	0/2361	0.59	1/3172 (0.0%)
3	B3	0.32	0/2385	0.57	0/3205
3	B4	0.33	0/2344	0.59	0/3150
4	A5	0.28	0/951	0.53	0/1281
4	B5	0.28	0/951	0.50	0/1281
5	AA	0.64	0/35966	0.91	18/56138 (0.0%)
5	BA	0.55	0/35966	0.91	37/56138 (0.1%)
6	AB	0.31	0/1610	0.59	1/2177 (0.0%)
6	BB	0.31	0/1610	0.61	0/2177
7	AC	0.29	0/1554	0.61	0/2087
7	BC	0.30	0/1554	0.64	0/2087
8	AD	0.32	0/1537	0.61	0/2060
8	BD	0.32	0/1537	0.60	0/2060
9	AE	0.33	0/1478	0.64	0/1980
9	BE	0.29	0/1478	0.63	0/1980
10	AF	0.32	0/2030	0.61	0/2739
10	BF	0.30	0/2030	0.60	0/2739
11	AG	0.34	0/1824	0.62	0/2457
11	BG	0.30	0/1824	0.63	0/2457
12	AH	0.31	0/986	0.65	1/1320 (0.1%)
12	BH	0.32	0/986	0.63	0/1320
13	AI	0.30	0/1765	0.62	0/2371
13	BI	0.29	0/1765	0.60	0/2371
14	AJ	0.36	0/1049	0.63	0/1408
14	BJ	0.34	0/1049	0.63	0/1408
15	AK	0.29	0/986	0.65	0/1315
15	BK	0.29	0/986	0.67	0/1315
16	AL	0.27	0/1021	0.67	0/1369
16	BL	0.31	0/1021	0.68	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AM	0.29	0/830	0.73	0/1113
17	BM	0.27	0/830	0.68	0/1113
18	AN	0.33	0/972	0.68	0/1309
18	BN	0.33	0/972	0.68	1/1309 (0.1%)
19	AO	0.36	0/1134	0.66	0/1508
19	BO	0.33	0/1134	0.63	0/1508
20	AP	0.28	0/1070	0.69	1/1440 (0.1%)
20	BP	0.30	0/1070	0.67	0/1440
21	AQ	0.31	0/426	0.73	0/562
21	BQ	0.32	0/426	0.75	0/562
22	AR	0.32	0/1311	0.66	0/1763
22	BR	0.32	0/1311	0.63	0/1763
23	AS	0.36	0/925	0.63	0/1249
23	BS	0.35	0/925	0.61	0/1249
24	AT	0.29	0/528	0.60	0/701
24	BT	0.28	0/528	0.61	0/701
25	AU	0.28	0/968	0.65	0/1293
25	BU	0.31	0/968	0.65	2/1293 (0.2%)
26	AV	0.27	0/1238	0.55	0/1668
26	BV	0.27	0/1238	0.57	0/1668
27	AW	0.32	0/790	0.58	0/1061
27	BW	0.32	0/790	0.65	0/1061
28	AX	0.29	0/381	0.62	0/509
28	BX	0.27	0/381	0.58	0/509
29	AY	0.31	0/472	0.63	0/634
29	BY	0.31	0/472	0.62	0/634
30	AZ	0.29	0/525	0.70	0/703
30	BZ	0.27	0/525	0.69	0/703
All	All	0.48	0/139800	0.79	63/203378 (0.0%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AA	71	C	N3-C2-O2	-9.71	115.10	121.90
5	BA	140	C	N3-C2-O2	-9.11	115.53	121.90
5	BA	449	U	C2-N1-C1'	8.81	128.27	117.70
5	BA	985	C	N3-C2-O2	-8.45	115.99	121.90
5	BA	1118	C	C2-N1-C1'	8.34	127.98	118.80
5	AA	718	G	N3-C4-C5	7.10	132.15	128.60
5	AA	303	G	C4-N9-C1'	7.06	135.68	126.50
5	BA	449	U	N3-C2-O2	-6.80	117.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BA	985	C	N1-C2-O2	6.79	122.98	118.90
5	BA	8	U	C5-C4-O4	-6.73	121.86	125.90
5	AA	718	G	N3-C4-N9	-6.59	122.04	126.00
5	BA	303	G	C4-N9-C1'	6.41	134.84	126.50
5	AA	277	G	C8-N9-C4	-6.32	103.87	106.40
25	BU	108	PRO	N-CD-CG	-6.27	93.79	103.20
25	BU	108	PRO	CA-N-CD	-6.25	102.74	111.50
5	BA	1201	G	C4-N9-C1'	6.21	134.58	126.50
5	BA	1118	C	C6-N1-C1'	-6.17	113.39	120.80
5	BA	7	G	N1-C6-O6	-6.15	116.21	119.90
5	BA	1471	G	N3-C4-N9	-6.15	122.31	126.00
5	BA	139	C	N1-C2-O2	6.13	122.58	118.90
5	AA	71	C	C6-N1-C2	-6.04	117.88	120.30
5	BA	516	A	C4-N9-C1'	6.03	137.15	126.30
5	BA	140	C	C2-N3-C4	-6.00	116.90	119.90
5	BA	530	G	N3-C4-C5	6.00	131.60	128.60
5	BA	140	C	N1-C2-N3	5.96	123.37	119.20
20	AP	125	PRO	CA-N-CD	-5.93	103.19	111.50
12	AH	73	PRO	CA-N-CD	-5.87	103.29	111.50
5	BA	449	U	N1-C2-O2	5.85	126.90	122.80
5	BA	140	C	C6-N1-C2	-5.82	117.97	120.30
5	AA	718	G	C2-N3-C4	-5.78	109.01	111.90
5	AA	303	G	C8-N9-C4	-5.78	104.09	106.40
5	BA	1201	G	C8-N9-C1'	-5.76	119.51	127.00
5	BA	434	A	C8-N9-C4	-5.73	103.51	105.80
5	BA	516	A	C8-N9-C1'	-5.68	117.47	127.70
5	BA	530	G	N3-C4-N9	-5.67	122.60	126.00
5	BA	718	G	N3-C4-C5	5.60	131.40	128.60
3	A3	129	LEU	CA-CB-CG	5.53	128.03	115.30
5	AA	303	G	N7-C8-N9	5.53	115.86	113.10
5	AA	718	G	N3-C2-N2	-5.52	116.03	119.90
5	BA	151	G	C6-N1-C2	-5.48	121.81	125.10
5	BA	919	U	P-O3'-C3'	5.47	126.27	119.70
5	BA	449	U	C6-N1-C1'	-5.47	113.54	121.20
5	BA	7	G	C5-C6-O6	5.46	131.88	128.60
5	BA	708	C	C2-N1-C1'	5.40	124.74	118.80
5	BA	614	G	C4-N9-C1'	5.39	133.50	126.50
5	BA	303	G	N3-C4-C5	-5.38	125.91	128.60
5	BA	1475	C	N3-C2-O2	-5.34	118.16	121.90
5	BA	718	G	N3-C4-N9	-5.33	122.80	126.00
5	BA	303	G	C8-N9-C1'	-5.32	120.08	127.00
5	AA	1201	G	C4-N9-C1'	5.31	133.41	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A4	260	LEU	CB-CG-CD2	-5.30	101.99	111.00
5	AA	363	C	C6-N1-C2	-5.25	118.20	120.30
5	AA	303	G	C8-N9-C1'	-5.21	120.23	127.00
5	AA	708	C	C2-N1-C1'	5.21	124.53	118.80
5	AA	1307	G	P-O3'-C3'	5.18	125.91	119.70
5	AA	350	G	C4-N9-C1'	5.16	133.21	126.50
6	AB	52	LEU	CA-CB-CG	5.09	127.02	115.30
5	BA	56	A	P-O3'-C3'	5.09	125.81	119.70
5	BA	977	G	P-O3'-C3'	5.09	125.81	119.70
5	AA	303	G	N3-C4-C5	-5.08	126.06	128.60
5	BA	141	C	C2-N3-C4	-5.06	117.37	119.90
18	BN	61	MET	CA-CB-CG	5.03	121.85	113.30
5	AA	516	A	C4-N9-C1'	5.01	135.31	126.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	471	0	457	8	0
1	B1	471	0	457	3	0
2	A2	335	0	396	11	0
2	B2	335	0	396	4	0
3	A3	2372	0	2526	42	0
3	A4	2329	0	2481	38	0
3	B3	2353	0	2505	35	0
3	B4	2312	0	2457	48	0
4	A5	939	0	994	15	0
4	B5	939	0	994	13	0
5	AA	32135	0	16231	381	0
5	BA	32135	0	16231	384	0
6	AB	1579	0	1638	28	0
6	BB	1579	0	1638	29	0
7	AC	1532	0	1622	21	0
7	BC	1532	0	1622	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AD	1511	0	1595	29	0
8	BD	1511	0	1595	20	0
9	AE	1455	0	1531	28	0
9	BE	1455	0	1531	21	0
10	AF	1981	0	2051	35	0
10	BF	1981	0	2051	30	0
11	AG	1794	0	1850	29	0
11	BG	1794	0	1850	29	0
12	AH	971	0	1027	27	0
12	BH	971	0	1027	20	0
13	AI	1728	0	1775	32	0
13	BI	1728	0	1775	33	0
14	AJ	1028	0	1065	29	0
14	BJ	1028	0	1065	18	0
15	AK	977	0	1064	27	0
15	BK	977	0	1064	17	0
16	AL	1006	0	1052	17	0
16	BL	1006	0	1052	21	0
17	AM	822	0	870	19	0
17	BM	822	0	870	14	0
18	AN	954	0	981	16	0
18	BN	954	0	981	22	0
19	AO	1118	0	1214	25	0
19	BO	1118	0	1214	27	0
20	AP	1052	0	1094	25	0
20	BP	1052	0	1094	22	0
21	AQ	417	0	445	11	0
21	BQ	417	0	445	11	0
22	AR	1283	0	1358	23	0
22	BR	1283	0	1358	23	0
23	AS	903	0	922	28	0
23	BS	903	0	922	15	0
24	AT	522	0	557	6	0
24	BT	522	0	557	7	0
25	AU	948	0	1007	25	0
25	BU	948	0	1007	18	0
26	AV	1209	0	1254	22	0
26	BV	1209	0	1254	19	0
27	AW	774	0	794	17	0
27	BW	774	0	794	11	0
28	AX	369	0	361	9	0
28	BX	369	0	361	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	AY	465	0	507	10	0
29	BY	465	0	507	7	0
30	AZ	523	0	551	13	0
30	BZ	523	0	551	10	0
All	All	130968	0	102495	1633	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 7.

All (1633) 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)
5:BA:777:G:HO2'	14:BJ:2:THR:N	1.53	1.04
5:AA:777:G:HO2'	14:AJ:2:THR:N	1.65	0.94
5:BA:1264:G:H21	5:BA:1293:A:N6	1.65	0.93
5:BA:1264:G:H21	5:BA:1293:A:H62	1.10	0.91
5:AA:516:A:OP2	19:AO:20:ARG:NH1	2.07	0.88
5:BA:1248:A:HO2'	5:BA:1312:C:HO2'	0.99	0.87
5:BA:1044:A:O2'	5:BA:1045:A:O4'	1.92	0.86
5:BA:106:A:H62	5:BA:235:G:N2	1.72	0.86
5:BA:1477:U:OP1	18:BN:136:ARG:NH1	2.08	0.86
5:BA:262:G:O2'	5:BA:264:C:OP2	1.93	0.85
5:BA:516:A:OP2	19:BO:20:ARG:NH1	2.09	0.85
5:AA:262:G:O2'	5:AA:264:C:OP2	1.93	0.85
5:BA:559:G:N2	5:BA:587:G:OP2	2.10	0.85
5:BA:1162:G:O2'	5:BA:1163:U:O4'	1.96	0.84
3:A4:232:LEU:HD23	3:A4:260:LEU:HD21	1.61	0.83
5:BA:1260:G:O2'	5:BA:1263:C:N4	2.12	0.83
5:AA:1460:G:O2'	5:AA:1461:U:OP2	1.97	0.82
5:AA:619:A:N7	5:AA:678:G:O6	2.11	0.82
5:BA:1264:G:N2	5:BA:1293:A:H62	1.77	0.82
5:AA:1305:U:O2'	5:AA:1337:A:N1	2.10	0.82
5:BA:1177:C:O2'	21:BQ:6:TYR:O	1.97	0.82
5:BA:46:A:O2'	5:BA:356:G:N2	2.12	0.82
5:AA:671:C:O2'	5:AA:688:C:O4'	1.98	0.81
5:AA:1365:G:O2'	5:AA:1473:A:O2'	1.97	0.81
5:BA:1215:G:O2'	5:BA:1218:C:O2	1.98	0.81
5:BA:1332:C:O2'	13:BI:95:SER:O	1.99	0.81
5:AA:674:C:O2'	8:AD:100:THR:O	1.98	0.80
2:A2:1:MET:N	5:AA:862:C:OP2	2.14	0.80
5:AA:400:G:N2	5:AA:450:A:N7	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:106:A:N6	5:BA:235:G:H21	1.78	0.80
5:AA:615:G:O6	5:AA:698:A:N1	2.16	0.80
5:BA:260:C:O2'	23:BS:92:ARG:NH1	2.15	0.79
5:BA:226:G:OP1	10:BF:31:ARG:NH2	2.15	0.79
2:B2:34:ARG:NH2	5:BA:851:C:OP1	2.15	0.79
1:B1:13:SER:OG	1:B1:43:CYS:SG	2.40	0.79
5:BA:1274:C:OP2	25:BU:34:ARG:NE	2.16	0.79
5:AA:433:U:O2	5:AA:434:A:O2'	2.01	0.79
5:BA:352:A:N3	5:BA:364:U:O2'	2.14	0.79
19:BO:70:ARG:NH2	19:BO:118:ASP:OD2	2.16	0.79
5:BA:1063:A:O2'	7:BC:191:ASP:OD1	2.01	0.78
5:AA:559:G:N2	5:AA:587:G:OP2	2.16	0.78
5:BA:1193:G:OP1	16:BL:121:ARG:NH2	2.17	0.78
5:BA:150:G:OP2	12:BH:95:ARG:NH2	2.15	0.78
21:BQ:48:PRO:O	21:BQ:53:ARG:NH2	2.17	0.78
5:AA:197:A:O2'	5:AA:198:A:O4'	2.00	0.78
5:AA:1458:A:OP1	5:AA:1486:A:O2'	2.02	0.78
3:B4:219:GLU:OE2	3:B4:224:THR:OG1	2.00	0.78
5:BA:199:A:N1	5:BA:216:G:O2'	2.16	0.78
5:BA:1200:U:OP2	13:BI:179:SER:OG	2.01	0.78
5:AA:920:U:OP1	5:AA:1183:C:O2'	1.99	0.78
5:AA:983:G:O2'	5:AA:984:C:O4'	2.01	0.78
5:BA:1120:G:OP1	24:BT:5:ARG:NH2	2.17	0.78
19:AO:23:PHE:O	19:AO:26:SER:OG	2.01	0.78
5:BA:180:G:N2	5:BA:183:A:OP2	2.18	0.77
18:BN:88:GLY:O	18:BN:92:LYS:NZ	2.16	0.77
3:B4:238:ILE:O	3:B4:241:SER:OG	2.01	0.77
5:AA:918:A:O2'	5:AA:920:U:OP2	2.01	0.77
5:AA:528:G:N3	5:AA:529:C:N4	2.31	0.77
12:AH:10:ASP:OD2	12:AH:53:LYS:NZ	2.17	0.77
5:BA:112:G:N2	5:BA:229:G:O6	2.17	0.77
5:AA:1269:G:N2	20:AP:80:ASN:O	2.18	0.77
5:BA:1029:G:N2	5:BA:1032:A:OP2	2.18	0.77
5:BA:1306:A:OP2	5:BA:1337:A:N6	2.18	0.77
5:AA:746:A:O2'	5:AA:748:A:N7	2.17	0.76
5:AA:902:U:O4	5:AA:903:G:O6	2.04	0.76
5:BA:898:G:O2'	13:BI:73:ARG:NH2	2.18	0.76
5:AA:897:A:N3	5:AA:1336:U:O2'	2.17	0.76
10:BF:116:SER:OG	10:BF:118:ASP:OD1	2.03	0.76
5:AA:566:C:O2'	9:AE:69:GLU:OE2	2.04	0.76
5:BA:1004:U:O2	5:BA:1166:G:O6	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1458:A:N6	5:AA:1487:U:O2	2.19	0.76
5:BA:606:U:O4	5:BA:706:G:O2'	2.03	0.76
25:BU:80:THR:OG1	25:BU:93:GLU:OE1	2.03	0.76
5:AA:181:G:O2'	23:AS:4:ASP:OD2	2.04	0.76
2:A2:4:ARG:NH2	5:AA:847:A:O2'	2.19	0.76
5:BA:969:A:N6	5:BA:977:G:O6	2.19	0.76
5:BA:1335:A:O2'	13:BI:73:ARG:NH2	2.19	0.76
5:BA:144:G:N2	5:BA:147:A:OP2	2.19	0.76
15:AK:67:ASP:OD2	15:AK:69:SER:OG	2.03	0.75
5:BA:561:A:O2'	10:BF:13:LEU:O	2.04	0.75
5:AA:1307:G:N2	5:AA:1308:U:O4	2.18	0.75
5:BA:351:C:O2'	5:BA:384:G:N3	2.19	0.75
5:AA:110:C:OP1	5:AA:558:C:O2'	2.04	0.75
3:A4:62:SER:OG	5:AA:725:C:OP1	2.03	0.75
5:AA:1160:C:OP1	5:AA:1161:A:O2'	2.04	0.75
5:AA:258:A:OP2	15:AK:54:LYS:NZ	2.18	0.75
5:AA:473:A:H62	5:AA:482:G:N2	1.84	0.75
5:BA:1461:U:O2	18:BN:136:ARG:NH1	2.20	0.75
29:BY:9:PRO:O	29:BY:12:ARG:NH2	2.20	0.75
5:AA:1488:C:O2'	5:AA:1489:A:O4'	2.02	0.74
2:B2:6:ARG:NH2	5:BA:844:G:O3'	2.20	0.74
3:B4:233:ARG:NH1	3:B4:263:THR:O	2.20	0.74
1:A1:13:SER:OG	1:A1:43:CYS:SG	2.44	0.74
5:AA:894:A:O2'	5:AA:1343:C:N3	2.19	0.74
5:BA:1276:G:O6	25:BU:38:ARG:NH1	2.20	0.74
5:AA:1487:U:O2'	5:AA:1488:C:O4'	2.03	0.74
5:BA:1207:G:OP2	26:BV:76:TYR:OH	2.05	0.74
11:BG:7:GLU:OE2	11:BG:11:ARG:NH2	2.21	0.74
5:AA:1351:U:O2'	5:AA:1487:U:OP1	2.04	0.74
5:AA:1279:A:OP2	25:AU:31:ARG:NH2	2.20	0.74
5:BA:881:G:O2'	5:BA:1359:C:OP2	2.05	0.74
5:AA:780:C:O2	14:AJ:16:ASN:ND2	2.21	0.74
8:AD:97:ARG:O	8:AD:100:THR:OG1	2.05	0.74
5:BA:25:C:OP1	9:BE:6:ARG:NH1	2.21	0.74
5:AA:892:C:O2'	5:AA:1304:C:OP2	2.05	0.73
17:AM:30:THR:O	17:AM:80:ARG:NH2	2.21	0.73
5:BA:902:U:OP2	13:BI:87:ARG:NH1	2.21	0.73
8:BD:51:THR:OG1	8:BD:54:ASP:OD2	2.05	0.73
5:AA:615:G:N2	5:AA:790:G:O3'	2.20	0.73
5:BA:671:C:O2'	5:BA:688:C:O4'	2.04	0.73
18:BN:107:ARG:O	30:BZ:35:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AC:187:ALA:O	7:AC:188:ARG:NH1	2.20	0.73
19:BO:6:ALA:O	19:BO:19:LYS:NZ	2.21	0.73
5:AA:1332:C:O2	13:AI:95:SER:OG	2.07	0.73
20:AP:5:ARG:N	20:AP:52:GLY:O	2.21	0.73
5:AA:180:G:N2	5:AA:183:A:OP2	2.21	0.73
13:AI:36:TYR:OH	30:AZ:53:ASP:OD1	2.06	0.73
5:AA:156:A:O2'	5:AA:157:A:O4'	2.04	0.73
5:BA:730:G:N2	5:BA:756:A:OP2	2.20	0.73
15:BK:76:ARG:O	15:BK:103:THR:OG1	2.06	0.73
5:AA:123:U:OP1	10:AF:76:ARG:NH1	2.22	0.72
5:AA:913:G:O2'	25:AU:117:ALA:O	2.07	0.72
17:BM:83:ARG:O	17:BM:87:ARG:NH1	2.23	0.72
5:AA:1327:C:OP1	16:AL:120:ASN:N	2.23	0.72
20:BP:86:GLU:OE1	25:BU:7:ARG:NH2	2.22	0.72
14:AJ:85:GLU:OE1	14:AJ:85:GLU:N	2.22	0.72
15:AK:42:LYS:NZ	15:AK:43:ARG:O	2.22	0.72
10:BF:151:SER:OG	10:BF:154:GLU:OE1	2.07	0.72
1:A1:23:HIS:O	1:A1:44:ARG:NH1	2.22	0.72
3:A4:98:GLU:OE2	3:A4:99:ASN:ND2	2.22	0.72
18:BN:42:TRP:NE1	18:BN:70:GLU:OE1	2.22	0.72
5:AA:433:U:O2'	5:AA:436:A:N7	2.23	0.72
9:AE:169:MET:N	9:AE:169:MET:SD	2.63	0.72
14:AJ:82:LYS:N	14:AJ:85:GLU:OE2	2.23	0.72
21:AQ:39:CYS:SG	21:AQ:42:CYS:N	2.62	0.72
5:BA:785:U:O2	5:BA:813:G:O6	2.08	0.72
21:BQ:39:CYS:SG	21:BQ:42:CYS:N	2.62	0.72
5:AA:176:U:O2'	5:AA:177:A:OP1	2.06	0.72
5:BA:899:G:OP1	13:BI:163:ARG:NE	2.21	0.72
3:B4:270:PHE:O	3:B4:275:GLN:NE2	2.23	0.72
5:BA:1333:G:OP1	13:BI:46:HIS:NE2	2.23	0.72
13:BI:76:GLY:N	13:BI:86:MET:O	2.22	0.72
19:AO:15:LYS:NZ	19:AO:15:LYS:O	2.23	0.71
5:BA:1307:G:N2	5:BA:1334:A:OP2	2.23	0.71
24:BT:27:ASP:O	24:BT:31:ASN:ND2	2.23	0.71
5:AA:746:A:O2'	5:AA:747:U:OP2	2.08	0.71
5:AA:935:G:OP2	5:AA:1318:U:O2'	2.07	0.71
5:AA:1288:C:OP1	20:AP:34:ASN:ND2	2.23	0.71
11:AG:28:GLU:OE1	11:AG:30:GLN:NE2	2.23	0.71
3:B3:125:LEU:O	3:B3:129:LEU:HD12	1.90	0.71
25:BU:55:LYS:NZ	25:BU:75:GLU:O	2.21	0.71
5:AA:1197:C:O2'	5:AA:1260:G:N2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1275:U:C2	5:AA:1279:A:N6	2.58	0.71
10:BF:12:ARG:NH1	10:BF:28:TRP:O	2.22	0.71
15:BK:9:LEU:O	15:BK:16:ARG:NH1	2.24	0.71
5:BA:176:U:O2'	5:BA:177:A:OP1	2.05	0.71
5:AA:1213:G:OP1	17:AM:46:ARG:NH2	2.24	0.71
5:BA:566:C:O2'	9:BE:69:GLU:OE1	2.07	0.71
5:BA:1197:C:O2'	5:BA:1260:G:N2	2.23	0.71
5:AA:5:C:OP2	11:AG:191:THR:OG1	2.08	0.71
5:AA:311:A:OP2	15:AK:22:LYS:NZ	2.24	0.71
8:AD:38:ASP:OD2	8:AD:42:LYS:NZ	2.24	0.71
5:BA:616:G:O2'	5:BA:790:G:OP1	2.08	0.71
5:BA:1275:U:C2	5:BA:1279:A:N6	2.59	0.71
5:AA:463:G:OP1	9:AE:20:LYS:NZ	2.24	0.71
12:AH:26:THR:OG1	12:AH:27:GLU:OE1	2.09	0.71
9:BE:160:PHE:O	9:BE:168:ARG:NH1	2.23	0.71
5:AA:234:G:OP1	23:AS:66:ARG:NH1	2.24	0.71
5:AA:1201:G:OP1	13:AI:91:ARG:NH1	2.23	0.71
3:B3:214:LEU:HD21	3:B3:225:VAL:HG13	1.72	0.71
12:BH:10:ASP:OD1	12:BH:125:TYR:OH	2.08	0.71
10:AF:195:ARG:NH2	10:AF:221:GLU:OE1	2.24	0.70
5:AA:1262:U:O2'	5:AA:1263:C:OP1	2.09	0.70
13:AI:81:VAL:O	13:AI:84:HIS:ND1	2.24	0.70
2:A2:2:LYS:NZ	5:AA:863:U:OP2	2.21	0.70
5:AA:1183:C:OP2	25:AU:110:ARG:NH2	2.24	0.70
22:AR:126:GLU:OE1	22:AR:130:ARG:NH1	2.25	0.70
5:AA:369:A:N6	5:AA:387:G:N3	2.39	0.70
5:AA:471:G:N3	19:AO:67:SER:OG	2.24	0.70
9:AE:104:ARG:NH2	9:AE:106:GLN:OE1	2.24	0.70
23:AS:88:ILE:HD11	23:AS:100:PHE:HB3	1.73	0.70
5:BA:234:G:OP1	23:BS:66:ARG:NH1	2.23	0.70
3:A4:12:TYR:OH	3:A4:30:GLU:OE1	2.07	0.70
5:AA:1327:C:O2'	17:AM:63:ARG:NH2	2.24	0.70
5:BA:896:A:O2'	30:BZ:21:THR:OG1	2.06	0.70
3:A3:266:ARG:NH1	3:A3:267:LYS:O	2.25	0.70
5:BA:134:A:N6	5:BA:157:A:OP2	2.24	0.70
5:BA:904:G:N2	5:BA:1294:G:O2'	2.24	0.70
24:AT:27:ASP:O	24:AT:31:ASN:ND2	2.24	0.70
16:BL:79:ARG:NH2	16:BL:102:TYR:OH	2.25	0.70
3:B4:148:ASN:ND2	3:B4:251:SER:O	2.24	0.70
5:BA:885:G:O2'	5:BA:1458:A:N7	2.24	0.69
5:AA:222:G:OP1	10:AF:131:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1167:C:OP1	7:AC:172:LYS:NZ	2.24	0.69
5:AA:473:A:H62	5:AA:482:G:H21	1.38	0.69
5:AA:1228:A:N3	5:AA:1286:C:O2'	2.25	0.69
13:AI:151:ASP:OD2	30:AZ:43:ARG:NE	2.25	0.69
5:BA:1031:G:O2'	5:BA:1032:A:O4'	2.08	0.69
11:BG:221:TYR:OH	14:BJ:97:PHE:O	2.09	0.69
3:A4:164:LEU:O	3:A4:167:GLN:NE2	2.26	0.69
5:AA:1079:G:N2	5:AA:1106:A:H62	1.89	0.69
5:AA:1295:C:O3'	13:AI:175:ARG:NH1	2.25	0.69
6:AB:55:ALA:O	6:AB:59:LEU:HD12	1.93	0.69
3:B4:12:TYR:O	3:B4:78:ARG:NH2	2.25	0.69
5:BA:615:G:O6	5:BA:698:A:N1	2.25	0.69
5:BA:1266:A:N7	5:BA:1291:G:O2'	2.26	0.69
5:AA:1169:C:O2'	5:AA:1174:A:N6	2.26	0.69
5:AA:1272:G:OP1	25:AU:33:ARG:NH1	2.25	0.69
5:BA:640:U:O2'	5:BA:641:A:O5'	2.08	0.69
5:BA:936:A:N6	5:BA:1184:U:OP1	2.22	0.69
17:BM:30:THR:O	17:BM:80:ARG:NH2	2.25	0.69
5:AA:433:U:OP2	5:AA:434:A:O2'	2.11	0.69
5:AA:532:C:O2'	22:AR:120:ARG:NH2	2.24	0.69
5:AA:1205:G:N2	26:AV:10:ASP:OD1	2.26	0.69
19:AO:70:ARG:NH2	19:AO:118:ASP:OD2	2.26	0.69
5:AA:431:U:O2'	5:AA:432:G:OP1	2.11	0.69
3:B4:173:ILE:O	3:B4:177:SER:OG	2.10	0.69
6:BB:73:ARG:NH1	6:BB:158:ASN:O	2.26	0.69
5:AA:902:U:C4	5:AA:903:G:O6	2.46	0.69
14:AJ:8:ALA:O	14:AJ:12:SER:OG	2.10	0.69
5:BA:462:A:O2'	5:BA:463:G:O4'	2.11	0.69
3:A4:196:LYS:NZ	3:A4:221:GLY:O	2.24	0.68
5:BA:222:G:OP1	10:BF:131:ARG:NH2	2.26	0.68
5:BA:604:C:OP1	22:BR:74:ARG:NE	2.26	0.68
2:A2:15:ARG:NE	5:AA:1465:C:OP2	2.19	0.68
5:AA:1141:G:O2'	5:AA:1142:G:O4'	2.10	0.68
5:AA:1306:A:O2'	5:AA:1307:G:OP2	2.10	0.68
5:BA:313:G:N2	5:BA:1424:G:OP1	2.26	0.68
5:BA:920:U:OP1	5:BA:1183:C:O2'	2.11	0.68
9:BE:52:ARG:NH2	11:BG:161:ARG:O	2.26	0.68
12:AH:28:LYS:NZ	12:AH:42:GLU:O	2.19	0.68
22:BR:4:MET:SD	22:BR:131:ARG:NH2	2.66	0.68
3:B3:68:THR:OG1	3:B3:70:SER:OG	2.12	0.68
5:BA:369:A:N6	5:BA:387:G:N3	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:198:ARG:NH2	10:BF:236:ASP:OD1	2.25	0.68
15:BK:43:ARG:NH1	15:BK:118:GLY:O	2.27	0.68
5:BA:6:G:O6	11:BG:192:ARG:NH2	2.26	0.68
5:AA:655:A:O2'	5:AA:656:U:OP2	2.12	0.68
5:AA:1120:G:O6	5:AA:1142:G:O6	2.10	0.68
5:BA:1120:G:O6	5:BA:1142:G:N2	2.27	0.68
2:A2:10:LYS:NZ	5:AA:1464:C:OP1	2.16	0.68
11:AG:146:GLU:OE1	11:AG:146:GLU:N	2.27	0.68
5:BA:298:C:OP1	23:BS:59:LYS:NZ	2.20	0.68
19:BO:103:VAL:HG12	19:BO:129:VAL:HG12	1.76	0.68
3:B4:113:GLU:OE1	3:B4:113:GLU:N	2.27	0.68
5:AA:238:G:OP2	19:AO:21:LYS:NZ	2.26	0.68
5:AA:1477:U:OP1	18:AN:136:ARG:NH2	2.27	0.68
5:BA:497:C:OP1	9:BE:27:ARG:NH2	2.28	0.67
4:A5:15:LEU:HG	4:A5:78:ILE:HD11	1.75	0.67
8:AD:11:ASP:O	8:AD:14:LYS:NZ	2.26	0.67
27:AW:37:LYS:NZ	27:AW:51:THR:O	2.27	0.67
5:AA:332:C:O2	5:AA:1423:A:O2'	2.10	0.67
5:BA:824:G:O2'	5:BA:877:A:OP1	2.07	0.67
5:BA:63:G:O2'	5:BA:157:A:N3	2.19	0.67
5:BA:97:C:O2'	5:BA:349:A:O2'	2.11	0.67
5:BA:935:G:N2	5:BA:1323:A:OP1	2.27	0.67
25:AU:55:LYS:NZ	25:AU:75:GLU:O	2.22	0.67
5:AA:656:U:O4	3:B4:27:ARG:NH2	2.27	0.67
14:AJ:116:ALA:O	14:AJ:120:GLY:N	2.28	0.67
5:BA:123:U:OP1	10:BF:76:ARG:NH1	2.28	0.67
5:BA:432:G:O2'	5:BA:437:A:N6	2.27	0.67
14:AJ:87:GLU:OE2	14:AJ:91:LYS:NZ	2.28	0.67
8:BD:97:ARG:O	8:BD:100:THR:OG1	2.12	0.67
5:AA:46:A:N1	5:AA:356:G:O2'	2.26	0.66
5:AA:192:G:O2'	15:AK:64:ASN:OD1	2.09	0.66
5:AA:1182:G:OP2	5:AA:1282:C:N4	2.27	0.66
3:B3:14:GLN:OE1	3:B3:207:TYR:OH	2.13	0.66
5:AA:346:C:N4	5:AA:347:G:O6	2.29	0.66
5:AA:1283:G:O6	25:AU:31:ARG:NH1	2.28	0.66
10:AF:70:LYS:NZ	27:AW:13:LEU:O	2.27	0.66
5:BA:1307:G:O2'	5:BA:1333:G:N1	2.25	0.66
5:AA:6:G:O6	11:AG:192:ARG:NH2	2.28	0.66
5:AA:1275:U:OP2	25:AU:34:ARG:NH2	2.28	0.66
5:BA:1359:C:O2	5:BA:1457:A:N6	2.28	0.66
5:AA:616:G:O2'	5:AA:790:G:OP1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AN:88:GLY:O	18:AN:92:LYS:NZ	2.22	0.66
5:BA:786:G:O2'	5:BA:787:U:O4'	2.08	0.66
6:BB:60:ALA:HB1	6:BB:179:ARG:HG3	1.78	0.66
3:A3:168:ARG:NH2	3:A3:171:SER:OG	2.29	0.66
16:AL:19:ILE:HG22	16:AL:62:ILE:HG23	1.78	0.66
5:AA:607:U:OP1	14:AJ:57:ARG:NE	2.28	0.66
5:AA:1185:A:OP1	20:AP:131:THR:N	2.28	0.66
5:BA:422:U:O2'	5:BA:447:A:N6	2.29	0.66
5:BA:483:G:N2	5:BA:483:G:OP2	2.29	0.66
5:BA:1460:G:O2'	5:BA:1461:U:OP2	2.12	0.66
6:BB:144:GLU:OE2	6:BB:145:ASN:ND2	2.28	0.66
3:A3:143:TYR:O	3:A3:146:THR:OG1	2.12	0.65
5:BA:836:G:OP2	19:BO:4:LYS:NZ	2.29	0.65
3:A3:258:GLU:OE1	3:A3:262:ASN:ND2	2.30	0.65
5:AA:557:G:C2	5:AA:589:U:O2	2.49	0.65
18:BN:25:ASN:OD1	18:BN:26:THR:N	2.29	0.65
5:BA:1205:G:OP1	26:BV:54:ARG:NH2	2.29	0.65
5:BA:1281:U:O2'	25:BU:110:ARG:NH2	2.30	0.65
5:AA:61:A:O2'	5:AA:62:G:OP2	2.14	0.65
11:AG:166:VAL:O	11:AG:185:SER:OG	2.10	0.65
13:AI:176:ASN:OD1	13:AI:177:LYS:N	2.30	0.65
5:AA:400:G:N7	9:AE:36:LYS:NZ	2.45	0.65
5:BA:332:C:O2'	5:BA:1424:G:O2'	2.15	0.65
5:AA:274:G:OP2	23:AS:69:LYS:NZ	2.29	0.65
5:AA:61:A:H62	5:AA:377:A:H62	1.45	0.65
5:BA:934:G:N2	5:BA:1317:G:N3	2.44	0.65
3:B3:58:TYR:OH	3:B3:93:ASP:OD2	2.14	0.65
5:BA:924:U:O2'	5:BA:925:U:OP2	2.14	0.65
16:BL:25:ARG:N	16:BL:61:ASP:OD1	2.29	0.65
18:BN:47:VAL:HG23	18:BN:48:VAL:HG13	1.77	0.65
5:AA:904:G:N2	5:AA:1294:G:O2'	2.29	0.64
12:AH:85:ARG:NH2	12:AH:104:LYS:O	2.29	0.64
2:B2:28:ARG:NH2	5:BA:859:A:O3'	2.30	0.64
5:BA:922:G:N2	17:BM:56:GLU:OE2	2.31	0.64
5:BA:1199:A:O2'	5:BA:1258:C:N4	2.28	0.64
27:AW:4:ARG:NH1	27:AW:5:ILE:O	2.30	0.64
3:B3:267:LYS:NZ	3:B3:269:ILE:O	2.26	0.64
5:BA:1332:C:OP2	16:BL:11:LYS:NZ	2.28	0.64
15:BK:98:GLY:O	15:BK:109:LYS:NZ	2.30	0.64
4:A5:6:TYR:O	4:A5:79:TYR:OH	2.13	0.64
5:BA:1118:C:H42	5:BA:1141:G:H22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:1260:G:O2'	5:BA:1261:U:OP2	2.15	0.64
28:BX:22:CYS:SG	28:BX:42:LYS:NZ	2.69	0.64
5:AA:181:G:O6	10:AF:208:GLY:N	2.30	0.64
5:BA:777:G:O3'	22:BR:3:ARG:NH1	2.31	0.64
2:A2:21:LYS:NZ	5:AA:1470:G:O6	2.29	0.64
21:AQ:37:MET:N	21:AQ:37:MET:SD	2.70	0.64
5:AA:880:G:H21	5:AA:1358:A:H8	1.46	0.64
3:B3:268:THR:O	3:B3:270:PHE:N	2.30	0.64
3:A4:168:ARG:NE	3:A4:168:ARG:O	2.30	0.64
3:A4:237:GLU:OE2	3:A4:237:GLU:N	2.31	0.64
5:AA:252:U:OP1	23:AS:45:LYS:NZ	2.24	0.64
5:AA:340:A:OP2	5:AA:341:C:N4	2.28	0.64
5:AA:447:A:O2'	5:AA:449:U:OP1	2.04	0.64
5:BA:207:G:N2	5:BA:210:A:OP2	2.27	0.64
15:BK:95:ILE:HD11	15:BK:110:VAL:HG21	1.80	0.64
5:AA:397:C:O2'	5:AA:574:A:N3	2.28	0.64
15:AK:35:THR:HG21	15:AK:114:PRO:HB2	1.80	0.64
1:B1:21:ARG:NH1	11:BG:121:ILE:O	2.31	0.64
5:BA:1169:C:O2'	5:BA:1174:A:N6	2.31	0.64
5:AA:974:G:N3	25:AU:66:HIS:ND1	2.46	0.63
20:AP:10:VAL:HG22	20:AP:59:VAL:HG13	1.78	0.63
6:BB:83:PHE:O	6:BB:87:THR:HG22	1.97	0.63
18:AN:61:MET:HE2	18:AN:104:ALA:HB2	1.80	0.63
12:BH:30:ILE:O	12:BH:32:LYS:NZ	2.31	0.63
5:AA:1029:G:O2'	5:AA:1031:G:O6	2.16	0.63
5:BA:540:G:N1	5:BA:708:C:OP2	2.30	0.63
20:BP:125:PRO:HB3	20:BP:129:GLN:HB2	1.80	0.63
5:AA:843:G:O6	19:AO:112:LYS:NZ	2.31	0.63
29:AY:3:LYS:NZ	29:AY:4:PRO:O	2.24	0.63
14:BJ:64:GLN:OE1	14:BJ:65:LEU:N	2.31	0.63
22:BR:111:GLN:OE1	22:BR:112:HIS:NE2	2.32	0.63
5:AA:1079:G:H21	5:AA:1106:A:N6	1.97	0.63
13:AI:76:GLY:N	13:AI:86:MET:O	2.29	0.63
7:AC:64:GLU:OE1	7:AC:67:ARG:NH1	2.32	0.63
20:AP:112:ILE:HG22	25:AU:98:MET:HE2	1.81	0.63
4:B5:33:ARG:NH2	4:B5:38:GLU:OE1	2.32	0.63
13:BI:70:LYS:NZ	13:BI:159:ASP:OD1	2.29	0.63
19:BO:136:GLU:O	19:BO:140:GLY:N	2.31	0.63
20:BP:115:TYR:OH	25:BU:110:ARG:NH1	2.31	0.63
26:BV:16:VAL:HG22	26:BV:132:ILE:HD13	1.79	0.63
5:AA:821:G:N2	5:AA:824:G:OP2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1177:C:OP1	21:AQ:9:ARG:NE	2.32	0.63
26:AV:112:GLU:OE1	26:AV:112:GLU:N	2.32	0.63
5:BA:830:A:O2'	5:BA:831:A:OP2	2.15	0.63
5:BA:430:G:OP1	27:BW:34:LYS:NZ	2.31	0.63
5:AA:104:A:OP1	15:AK:11:LYS:NZ	2.22	0.62
5:BA:143:G:N2	5:BA:148:C:O2	2.26	0.62
5:AA:511:C:OP2	5:AA:512:U:O2'	2.11	0.62
10:AF:185:VAL:HG21	10:AF:199:ILE:HD11	1.82	0.62
5:BA:324:C:OP1	10:BF:4:LYS:NZ	2.23	0.62
5:BA:960:A:N6	5:BA:989:C:OP2	2.32	0.62
5:BA:1047:U:OP1	5:BA:1060:G:N2	2.31	0.62
5:BA:201:G:N2	5:BA:202:G:O6	2.32	0.62
5:BA:1310:C:O2'	13:BI:94:ASN:ND2	2.31	0.62
22:BR:104:ASN:OD1	22:BR:105:LEU:N	2.32	0.62
3:B4:281:VAL:O	3:B4:285:ASN:ND2	2.32	0.62
5:BA:704:C:OP2	22:BR:16:ARG:NH2	2.32	0.62
5:BA:672:G:O2'	5:BA:673:C:OP1	2.16	0.62
5:BA:718:G:H4'	22:BR:116:LEU:HD22	1.82	0.62
5:AA:242:A:N7	5:AA:277:G:N2	2.47	0.62
2:A2:3:ARG:NH1	5:AA:768:A:OP1	2.33	0.62
5:AA:23:G:O2'	5:AA:292:U:OP1	2.18	0.62
5:AA:1251:C:O2'	16:AL:37:GLU:OE2	2.08	0.62
4:B5:69:LEU:HD13	28:BX:15:VAL:HG21	1.81	0.62
5:BA:101:G:N2	5:BA:309:A:O2'	2.33	0.62
5:BA:1149:C:O2'	7:BC:155:GLY:N	2.32	0.62
5:BA:1269:G:N1	5:BA:1289:G:O6	2.32	0.62
5:AA:421:U:C2	5:AA:448:A:N6	2.68	0.62
6:AB:127:MET:O	6:AB:131:VAL:HG23	2.00	0.62
5:AA:891:A:O2'	5:AA:894:A:N7	2.32	0.62
5:AA:910:G:O2'	5:AA:929:C:O2'	2.16	0.62
5:BA:400:G:H5'	9:BE:126:VAL:HG21	1.82	0.62
5:AA:1211:A:O2'	5:AA:1212:U:O4'	2.11	0.61
5:BA:257:U:N3	5:BA:260:C:OP2	2.32	0.61
5:BA:1198:A:O2'	13:BI:90:HIS:ND1	2.32	0.61
19:BO:54:VAL:HG21	19:BO:97:ILE:HD11	1.82	0.61
5:AA:885:G:O2'	5:AA:1487:U:O4'	2.12	0.61
5:AA:1116:G:OP1	24:AT:32:LYS:NZ	2.19	0.61
18:BN:81:ILE:HB	18:BN:115:VAL:HG12	1.82	0.61
5:AA:1264:G:N2	5:AA:1294:G:O6	2.33	0.61
6:AB:131:VAL:HG22	6:AB:149:TYR:CE2	2.35	0.61
10:AF:127:ILE:HD12	10:AF:162:TYR:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:422:U:O2'	5:BA:424:U:O4	2.18	0.61
19:BO:39:GLU:OE1	19:BO:39:GLU:N	2.34	0.61
3:A3:112:LEU:HD21	3:A3:131:GLY:HA3	1.83	0.61
5:AA:977:G:N2	5:AA:980:C:OP2	2.32	0.61
14:AJ:6:PRO:HB2	14:AJ:34:ILE:HD11	1.83	0.61
15:AK:43:ARG:NH1	15:AK:118:GLY:O	2.34	0.61
5:BA:103:A:OP2	5:BA:284:A:N6	2.31	0.61
5:BA:362:C:O2'	5:BA:390:G:N2	2.32	0.61
5:BA:1309:A:N3	5:BA:1334:A:N6	2.48	0.61
8:AD:119:VAL:HG22	8:AD:188:ILE:HG12	1.83	0.61
5:BA:926:C:OP2	5:BA:927:A:O2'	2.06	0.61
5:AA:1198:A:OP1	5:AA:1295:C:O2'	2.18	0.61
4:B5:15:LEU:HG	4:B5:78:ILE:HD11	1.82	0.61
5:AA:408:C:O2'	5:AA:409:C:OP1	2.16	0.61
5:BA:581:G:O2'	9:BE:65:GLN:OE1	2.17	0.61
15:BK:40:GLN:N	15:BK:40:GLN:OE1	2.32	0.61
5:AA:1090:C:O2'	26:AV:130:ASP:OD2	2.18	0.61
5:AA:1247:A:H61	5:AA:1330:G:H21	1.48	0.61
13:AI:215:ARG:NE	30:AZ:59:GLU:OE2	2.34	0.61
5:BA:400:G:N2	5:BA:450:A:N7	2.48	0.61
10:AF:181:LYS:NZ	10:AF:201:GLU:OE1	2.28	0.61
7:BC:21:LEU:HD12	7:BC:33:LEU:HD11	1.82	0.61
5:BA:431:U:O2'	5:BA:432:G:OP1	2.17	0.60
5:AA:473:A:N6	5:AA:482:G:H21	1.99	0.60
5:BA:176:U:HO2'	5:BA:177:A:P	2.23	0.60
5:AA:334:G:H22	5:AA:347:G:H1	1.48	0.60
5:AA:474:G:O2'	5:AA:489:C:O2'	2.15	0.60
3:B4:39:ILE:O	3:B4:105:LYS:NZ	2.25	0.60
5:BA:400:G:N7	9:BE:36:LYS:NZ	2.49	0.60
16:AL:10:ARG:O	16:AL:13:ALA:N	2.34	0.60
9:BE:86:ASP:OD1	9:BE:86:ASP:N	2.34	0.60
6:AB:22:GLN:NE2	6:AB:38:ASP:OD2	2.32	0.60
5:BA:584:C:O2'	5:BA:585:U:OP1	2.14	0.60
20:AP:106:ILE:HG22	20:AP:110:ARG:HE	1.66	0.60
14:AJ:115:GLU:OE2	14:AJ:119:LYS:NZ	2.28	0.60
5:BA:462:A:O2'	5:BA:463:G:O5'	2.20	0.60
5:AA:640:U:O2'	5:AA:641:A:O5'	2.20	0.60
23:AS:84:ASP:OD1	23:AS:109:ALA:N	2.35	0.60
5:BA:139:C:N4	5:BA:153:G:O6	2.34	0.60
5:BA:1171:G:O2'	5:BA:1173:A:N6	2.34	0.60
8:BD:126:MET:N	8:BD:126:MET:SD	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BH:63:ILE:HG21	12:BH:112:ILE:HD11	1.84	0.60
3:A4:10:VAL:HG11	3:A4:196:LYS:O	2.02	0.59
5:AA:701:G:O2'	22:AR:55:ARG:NH1	2.35	0.59
5:BA:1327:C:OP1	16:BL:120:ASN:N	2.35	0.59
6:BB:113:ASP:OD1	11:BG:21:LYS:NZ	2.32	0.59
10:BF:99:HIS:NE2	10:BF:117:GLU:OE1	2.35	0.59
5:AA:1273:G:OP2	25:AU:33:ARG:NH2	2.34	0.59
13:AI:138:SER:O	30:AZ:20:THR:OG1	2.18	0.59
5:BA:1335:A:HO2'	13:BI:73:ARG:NH2	2.00	0.59
5:AA:1275:U:N3	5:AA:1279:A:N6	2.50	0.59
20:AP:21:LEU:HD13	20:AP:54:LEU:HD11	1.85	0.59
5:AA:621:G:OP1	5:AA:686:C:O2'	2.19	0.59
3:B3:143:TYR:O	3:B3:146:THR:OG1	2.20	0.59
6:AB:183:GLN:OE1	6:AB:183:GLN:N	2.35	0.59
13:AI:153:SER:OG	13:AI:155:MET:SD	2.59	0.59
14:AJ:28:LYS:O	14:AJ:28:LYS:NZ	2.31	0.59
14:AJ:41:MET:O	14:AJ:45:GLY:N	2.35	0.59
26:AV:96:SER:OG	26:AV:99:ARG:NH1	2.35	0.59
5:AA:442:C:OP1	27:AW:61:GLY:N	2.36	0.59
5:BA:1327:C:O2'	17:BM:48:THR:HG21	2.03	0.59
5:AA:433:U:N3	5:AA:435:A:OP2	2.36	0.59
11:AG:123:GLU:O	11:AG:209:ASN:ND2	2.35	0.59
20:AP:20:GLN:O	20:AP:24:ALA:N	2.33	0.59
21:AQ:20:ARG:NE	21:AQ:21:CYS:O	2.33	0.59
22:AR:18:PRO:HG3	29:AY:6:ILE:HD11	1.83	0.59
5:BA:182:A:O2'	23:BS:4:ASP:O	2.17	0.59
13:BI:178:MET:N	13:BI:178:MET:SD	2.76	0.59
5:AA:1265:G:N2	5:AA:1292:A:OP2	2.33	0.59
22:AR:68:ASP:OD2	22:AR:80:ARG:NH1	2.36	0.59
5:BA:1019:A:O2'	5:BA:1046:G:OP1	2.18	0.59
3:A3:148:ASN:ND2	3:A3:251:SER:O	2.35	0.59
5:AA:777:G:O2'	22:AR:3:ARG:NH2	2.36	0.59
11:AG:25:MET:SD	11:AG:25:MET:N	2.75	0.59
14:AJ:23:ARG:NH2	14:AJ:65:LEU:O	2.35	0.59
20:AP:55:THR:OG1	20:AP:58:GLN:OE1	2.16	0.59
5:BA:340:A:N6	12:BH:70:ASP:OD1	2.34	0.59
6:BB:6:LEU:O	6:BB:173:ARG:NH2	2.36	0.59
5:AA:1202:G:O2'	26:AV:43:ARG:NH1	2.36	0.58
11:AG:126:ARG:NH2	11:AG:226:GLY:O	2.35	0.58
5:BA:114:A:N3	23:BS:28:LYS:NZ	2.42	0.58
8:BD:111:THR:OG1	8:BD:113:ASP:OD1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BL:7:THR:OG1	16:BL:84:ARG:NH1	2.35	0.58
23:BS:61:GLU:N	23:BS:61:GLU:OE2	2.36	0.58
26:BV:74:ARG:NE	26:BV:93:ALA:O	2.35	0.58
5:AA:765:U:O2'	5:AA:859:A:N1	2.33	0.58
5:AA:974:G:OP2	25:AU:64:ARG:NH1	2.36	0.58
5:BA:557:G:N1	5:BA:589:U:C2	2.70	0.58
8:BD:124:ILE:O	8:BD:181:ARG:N	2.36	0.58
20:BP:114:ALA:O	20:BP:118:ILE:N	2.35	0.58
23:BS:50:GLU:OE2	23:BS:52:GLN:NE2	2.36	0.58
5:AA:1275:U:O4	5:AA:1279:A:N7	2.36	0.58
5:AA:1296:U:O2'	13:AI:85:PHE:N	2.36	0.58
19:AO:102:GLU:OE2	19:AO:131:ARG:NH1	2.35	0.58
10:BF:196:LYS:NZ	10:BF:242:LEU:O	2.23	0.58
13:BI:129:ASN:ND2	13:BI:192:ALA:O	2.37	0.58
3:B4:13:LEU:HD13	3:B4:16:LEU:HD11	1.84	0.58
5:BA:1019:A:O2'	5:BA:1020:G:OP2	2.21	0.58
5:BA:1340:U:O2'	5:BA:1341:C:O5'	2.20	0.58
3:A3:34:LEU:HB3	3:A3:82:ILE:HD13	1.86	0.58
5:AA:135:U:H3	5:AA:156:A:H62	1.51	0.58
14:AJ:28:LYS:HA	14:AJ:60:VAL:HG22	1.85	0.58
19:AO:42:ASP:OD2	19:AO:46:GLY:N	2.36	0.58
5:BA:568:C:OP1	9:BE:79:ARG:NH1	2.36	0.58
3:A4:143:TYR:O	3:A4:146:THR:OG1	2.18	0.58
5:AA:118:U:O2'	5:AA:119:A:N7	2.37	0.58
5:AA:199:A:N1	5:AA:216:G:O2'	2.36	0.58
5:AA:1153:G:OP2	7:AC:131:ARG:NH2	2.35	0.58
17:AM:50:ARG:NH2	17:AM:58:SER:O	2.36	0.58
29:AY:48:THR:OG1	29:AY:51:LYS:O	2.22	0.58
5:BA:640:U:HO2'	5:BA:641:A:P	2.26	0.58
16:BL:6:THR:HG21	16:BL:85:ALA:HA	1.84	0.58
28:BX:15:VAL:O	28:BX:17:ARG:NH1	2.36	0.58
5:AA:135:U:O2'	5:AA:136:A:O5'	2.18	0.58
3:B4:19:LEU:O	3:B4:126:LYS:NZ	2.30	0.58
5:BA:96:G:O2'	5:BA:350:G:O2'	2.22	0.58
5:BA:557:G:C2	5:BA:589:U:O2	2.57	0.58
5:BA:1265:G:N2	5:BA:1292:A:OP2	2.37	0.58
5:AA:706:G:O2'	5:AA:707:A:OP2	2.18	0.58
5:AA:1271:G:OP1	25:AU:9:ARG:NH2	2.36	0.58
1:A1:34:GLU:OE2	1:A1:54:ASN:ND2	2.36	0.58
6:AB:6:LEU:O	6:AB:173:ARG:NH2	2.36	0.58
16:AL:25:ARG:N	16:AL:61:ASP:OD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1256:C:O2'	5:AA:1262:U:N3	2.37	0.57
10:AF:89:ASP:OD1	10:AF:123:LYS:NZ	2.24	0.57
13:BI:132:PRO:O	13:BI:157:ARG:NE	2.37	0.57
5:BA:1276:G:N2	5:BA:1279:A:OP2	2.36	0.57
5:AA:112:G:O2'	23:AS:30:HIS:ND1	2.35	0.57
5:AA:201:G:N2	5:AA:202:G:O6	2.37	0.57
5:AA:1019:A:O2'	5:AA:1020:G:OP2	2.19	0.57
6:AB:115:LEU:HD12	6:AB:116:ILE:N	2.18	0.57
26:AV:37:THR:OG1	26:AV:54:ARG:NH2	2.37	0.57
5:BA:305:C:OP1	10:BF:27:LYS:NZ	2.37	0.57
5:AA:14:C:OP1	11:AG:151:SER:OG	2.22	0.57
5:AA:262:G:O2'	5:AA:263:C:OP2	2.21	0.57
5:AA:1267:U:O4	5:AA:1291:G:N2	2.37	0.57
8:AD:56:THR:HG23	8:AD:58:ASP:H	1.70	0.57
5:BA:1079:G:O2'	16:BL:16:ARG:NH1	2.38	0.57
11:BG:116:TYR:O	11:BG:120:ASN:ND2	2.37	0.57
4:A5:69:LEU:HG	28:AX:10:ILE:HD11	1.86	0.57
13:AI:209:ARG:O	13:AI:211:ALA:N	2.38	0.57
5:BA:532:C:O2'	22:BR:120:ARG:NH2	2.36	0.57
5:BA:982:U:N3	5:BA:983:G:O6	2.38	0.57
26:BV:140:LEU:HD12	26:BV:143:ILE:HG21	1.85	0.57
5:AA:432:G:O2'	5:AA:437:A:N6	2.38	0.57
15:AK:67:ASP:HA	15:AK:124:LEU:HD21	1.86	0.57
3:B3:118:ASP:OD1	3:B3:118:ASP:N	2.35	0.57
19:BO:10:GLU:OE2	19:BO:10:GLU:N	2.34	0.57
23:BS:21:CYS:SG	23:BS:24:HIS:N	2.78	0.57
3:A3:231:GLU:OE1	3:A3:266:ARG:NH2	2.38	0.57
5:AA:111:G:O2'	5:AA:112:G:OP1	2.21	0.57
5:AA:318:C:OP2	5:AA:324:C:N4	2.37	0.57
3:B3:193:SER:OG	3:B3:195:LYS:O	2.22	0.57
2:B2:1:MET:N	5:BA:862:C:OP2	2.24	0.57
11:BG:25:MET:SD	11:BG:25:MET:N	2.75	0.57
23:BS:48:THR:O	23:BS:48:THR:OG1	2.23	0.57
29:BY:8:MET:N	29:BY:8:MET:SD	2.78	0.57
5:AA:368:C:N4	5:AA:384:G:OP2	2.38	0.57
5:AA:557:G:N1	5:AA:589:U:C2	2.73	0.57
5:AA:1245:C:O2'	5:AA:1246:U:OP2	2.23	0.57
9:AE:85:GLU:OE1	9:AE:85:GLU:N	2.38	0.57
20:AP:41:ARG:NH2	26:AV:47:GLN:O	2.38	0.57
5:BA:1166:G:O2'	7:BC:172:LYS:O	2.20	0.57
5:BA:1361:G:O6	5:BA:1459:G:N2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BR:68:ASP:OD2	22:BR:80:ARG:NH1	2.37	0.57
3:A4:148:ASN:ND2	3:A4:251:SER:O	2.37	0.57
5:AA:226:G:OP1	10:AF:31:ARG:NH2	2.38	0.57
19:BO:57:LYS:NZ	19:BO:97:ILE:O	2.27	0.57
22:BR:19:ARG:NH2	29:BY:63:GLU:O	2.38	0.57
5:AA:150:G:OP2	12:AH:95:ARG:NH2	2.38	0.56
6:AB:33:TYR:N	6:AB:42:VAL:O	2.37	0.56
7:AC:35:ILE:HD11	7:AC:42:THR:HB	1.86	0.56
5:BA:106:A:N6	5:BA:235:G:N2	2.39	0.56
14:BJ:72:ALA:HB2	14:BJ:129:VAL:HG23	1.86	0.56
5:BA:557:G:C6	5:BA:589:U:N3	2.73	0.56
11:BG:66:LEU:HD12	11:BG:86:LEU:HG	1.86	0.56
5:AA:926:C:OP2	5:AA:927:A:O2'	2.20	0.56
5:AA:1260:G:O2'	5:AA:1263:C:N4	2.38	0.56
19:AO:10:GLU:O	23:AS:63:TYR:N	2.34	0.56
3:B3:247:ASP:OD2	3:B3:250:LEU:N	2.35	0.56
3:B4:162:GLY:O	3:B4:165:SER:OG	2.22	0.56
5:BA:1022:U:O4	5:BA:1046:G:N2	2.39	0.56
5:BA:1275:U:N3	5:BA:1279:A:N6	2.54	0.56
4:A5:78:ILE:HD12	4:A5:114:ILE:HG23	1.87	0.56
5:AA:260:C:O2'	23:AS:92:ARG:NH1	2.38	0.56
5:AA:1272:G:OP2	25:AU:30:ALA:N	2.38	0.56
5:AA:1412:A:O2'	12:AH:75:ARG:NH2	2.38	0.56
12:AH:58:ASP:OD1	12:AH:58:ASP:N	2.38	0.56
5:BA:368:C:O2'	5:BA:369:A:OP2	2.16	0.56
5:BA:458:G:O2'	5:BA:459:G:OP1	2.21	0.56
9:BE:109:VAL:HG11	9:BE:125:ILE:HD11	1.86	0.56
26:BV:37:THR:OG1	26:BV:54:ARG:NH2	2.38	0.56
7:AC:31:GLY:HA3	7:AC:85:ILE:HD11	1.86	0.56
5:BA:156:A:O2'	5:BA:157:A:O4'	2.15	0.56
5:BA:1162:G:N2	21:BQ:41:HIS:O	2.38	0.56
9:BE:116:ARG:HG3	9:BE:171:ILE:HD13	1.86	0.56
5:BA:1275:U:O2'	5:BA:1320:A:N3	2.36	0.56
6:BB:60:ALA:HB3	6:BB:178:ASN:OD1	2.06	0.56
5:AA:464:G:O2'	5:AA:465:C:OP2	2.13	0.56
7:AC:118:ARG:NH2	7:AC:122:ASN:OD1	2.39	0.56
12:AH:3:THR:O	12:AH:3:THR:OG1	2.20	0.56
5:BA:1202:G:N2	26:BV:46:GLU:OE2	2.39	0.56
5:AA:191:A:O2'	15:AK:72:GLY:N	2.38	0.56
5:AA:933:G:OP2	21:AQ:40:ARG:NH1	2.39	0.56
9:AE:155:ALA:O	9:AE:158:SER:OG	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AV:140:LEU:HG	26:AV:144:ILE:HD13	1.88	0.56
30:AZ:10:GLU:HB2	30:AZ:32:LEU:HD11	1.88	0.56
5:BA:116:C:O2'	5:BA:258:A:N3	2.26	0.56
5:BA:1053:A:N7	6:BB:125:GLN:NE2	2.52	0.56
12:AH:63:ILE:HG21	12:AH:112:ILE:HD11	1.87	0.56
5:BA:257:U:OP1	15:BK:30:ARG:NE	2.32	0.56
5:BA:775:G:O6	19:BO:3:GLY:N	2.39	0.56
11:BG:140:SER:HA	11:BG:180:VAL:HG13	1.88	0.56
5:AA:699:C:N4	5:AA:700:G:O6	2.38	0.55
13:AI:212:GLU:O	13:AI:215:ARG:NH1	2.40	0.55
3:B3:161:LEU:O	3:B3:165:SER:OG	2.20	0.55
5:BA:1329:C:OP2	16:BL:117:HIS:N	2.39	0.55
14:BJ:23:ARG:O	14:BJ:65:LEU:HD12	2.06	0.55
3:A3:152:ASP:N	3:A3:152:ASP:OD1	2.36	0.55
30:AZ:18:THR:HB	30:AZ:67:ILE:HD12	1.89	0.55
1:B1:58:GLU:OE2	1:B1:59:GLY:N	2.39	0.55
5:BA:322:G:OP2	15:BK:47:ARG:NH2	2.39	0.55
5:BA:720:A:N6	5:BA:767:U:C2	2.74	0.55
6:BB:161:ARG:NH1	6:BB:196:GLU:OE1	2.39	0.55
9:BE:59:LEU:O	9:BE:62:ARG:NH2	2.40	0.55
10:BF:192:ASN:ND2	10:BF:224:ASP:O	2.39	0.55
23:AS:5:ILE:HD11	23:AS:29:ILE:HD11	1.87	0.55
5:BA:610:G:OP2	22:BR:2:ALA:N	2.40	0.55
5:BA:1063:A:OP2	5:BA:1064:C:N4	2.36	0.55
5:BA:1340:U:HO2'	5:BA:1341:C:P	2.28	0.55
16:BL:117:HIS:ND1	16:BL:122:SER:O	2.38	0.55
20:BP:105:ASP:OD1	20:BP:108:ARG:NH1	2.40	0.55
21:BQ:21:CYS:SG	21:BQ:22:ILE:N	2.78	0.55
3:A4:36:ASP:N	3:A4:36:ASP:OD1	2.38	0.55
10:AF:116:SER:OG	10:AF:118:ASP:OD1	2.23	0.55
5:BA:111:G:O2'	5:BA:112:G:OP1	2.24	0.55
5:BA:1140:A:OP1	16:BL:104:ARG:NH2	2.39	0.55
11:AG:51:ASP:OD1	11:AG:51:ASP:N	2.35	0.55
17:AM:28:GLU:OE1	17:AM:28:GLU:N	2.37	0.55
22:AR:125:ILE:O	22:AR:129:ILE:HD12	2.07	0.55
3:B4:231:GLU:OE1	3:B4:231:GLU:N	2.38	0.55
3:B3:52:GLU:OE2	3:B3:56:LYS:NZ	2.37	0.55
5:BA:1082:A:H4'	16:BL:18:VAL:HG11	1.89	0.55
10:BF:105:ASN:OD1	10:BF:106:ARG:N	2.39	0.55
3:B3:235:LEU:HA	3:B3:238:ILE:HD12	1.88	0.55
5:BA:314:G:N2	5:BA:1423:A:O2'	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BW:11:ASN:O	27:BW:15:GLY:N	2.39	0.55
5:AA:27:C:O2	19:AO:49:GLN:NE2	2.39	0.55
5:AA:563:U:P	10:AF:24:LYS:HZ2	2.30	0.55
9:AE:86:ASP:OD1	9:AE:86:ASP:N	2.36	0.55
13:AI:179:SER:N	13:AI:182:GLU:OE1	2.37	0.55
5:BA:674:C:O2'	8:BD:100:THR:O	2.21	0.55
5:BA:702:G:N2	5:BA:705:C:H41	2.04	0.55
11:BG:166:VAL:O	11:BG:185:SER:OG	2.16	0.55
19:BO:30:TYR:CE1	19:BO:34:VAL:HG11	2.41	0.55
3:A4:150:VAL:HG23	3:A4:155:GLY:HA3	1.88	0.55
5:AA:1138:G:N2	5:AA:1141:G:OP2	2.38	0.55
3:B4:9:SER:O	3:B4:9:SER:OG	2.22	0.55
18:BN:99:GLN:N	18:BN:99:GLN:OE1	2.39	0.55
28:BX:32:ALA:N	28:BX:39:ALA:O	2.38	0.55
5:AA:1079:G:N2	5:AA:1106:A:N6	2.51	0.55
5:AA:1080:C:O2'	5:AA:1082:A:OP2	2.18	0.55
19:AO:14:ARG:O	19:AO:18:LEU:HD12	2.06	0.55
3:B3:7:LYS:NZ	5:BA:858:A:OP1	2.40	0.55
5:BA:23:G:O2'	5:BA:292:U:OP1	2.23	0.55
5:BA:358:G:N2	5:BA:361:A:OP2	2.38	0.55
5:AA:432:G:HO2'	5:AA:437:A:N6	2.05	0.54
5:AA:568:C:OP1	9:AE:79:ARG:NH1	2.40	0.54
5:BA:621:G:OP1	5:BA:686:C:O2'	2.24	0.54
5:BA:747:U:O2	5:BA:1471:G:O2'	2.25	0.54
5:AA:432:G:HO2'	5:AA:437:A:H62	1.55	0.54
12:AH:8:ILE:HG23	12:AH:61:LEU:HD11	1.89	0.54
13:AI:156:ARG:O	13:AI:160:VAL:HG13	2.08	0.54
5:BA:442:C:O2'	27:BW:28:GLU:O	2.26	0.54
14:BJ:82:LYS:N	14:BJ:85:GLU:OE2	2.38	0.54
5:AA:587:G:OP2	5:AA:587:G:N2	2.39	0.54
5:AA:615:G:O6	5:AA:698:A:C6	2.59	0.54
4:B5:19:ALA:HB2	4:B5:78:ILE:HD13	1.89	0.54
5:BA:563:U:OP1	10:BF:24:LYS:NZ	2.21	0.54
5:BA:681:G:N2	5:BA:684:G:OP2	2.33	0.54
5:BA:1258:C:OP2	13:BI:177:LYS:NZ	2.27	0.54
5:AA:906:G:H21	26:AV:85:HIS:CG	2.25	0.54
5:BA:848:G:O2'	5:BA:864:G:O6	2.25	0.54
5:BA:1005:G:N2	5:BA:1010:G:O6	2.40	0.54
5:BA:1281:U:OP1	20:BP:128:GLY:N	2.40	0.54
8:BD:48:VAL:HG22	18:BN:34:THR:HG22	1.89	0.54
4:A5:65:HIS:HB2	28:AX:10:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1036:G:OP2	5:AA:1037:U:O2'	2.23	0.54
5:AA:1480:G:N7	18:AN:132:ARG:NH1	2.56	0.54
9:AE:52:ARG:NH2	11:AG:161:ARG:O	2.40	0.54
5:BA:408:C:O2'	5:BA:409:C:OP1	2.22	0.54
5:BA:429:A:O3'	27:BW:32:SER:OG	2.26	0.54
5:BA:916:U:N3	5:BA:919:U:OP2	2.40	0.54
10:BF:116:SER:OG	10:BF:119:GLU:OE1	2.26	0.54
11:BG:25:MET:HG2	11:BG:31:ILE:HD12	1.90	0.54
12:AH:67:THR:HG22	12:AH:73:PRO:HD3	1.90	0.54
5:BA:777:G:O2'	14:BJ:2:THR:N	2.32	0.54
20:BP:10:VAL:HG12	20:BP:59:VAL:HG13	1.90	0.54
4:A5:27:ARG:NH1	4:A5:89:ALA:O	2.41	0.54
5:AA:5:C:O2'	5:AA:459:G:O3'	2.25	0.54
5:AA:1361:G:O6	5:AA:1459:G:N2	2.41	0.54
19:AO:71:LYS:HG2	19:AO:94:ILE:HG21	1.89	0.54
3:B3:23:LYS:NZ	5:BA:244:G:N7	2.56	0.54
6:BB:119:ASP:OD2	6:BB:122:ALA:N	2.40	0.54
20:BP:21:LEU:HD13	20:BP:54:LEU:HD11	1.90	0.54
3:B3:51:ILE:HD11	3:B4:185:PHE:O	2.06	0.54
3:B3:134:LEU:O	3:B3:140:ARG:NH1	2.41	0.54
5:BA:63:G:H1	5:BA:86:C:H42	1.55	0.54
6:BB:27:ASP:HB3	6:BB:147:LEU:HD23	1.88	0.54
5:AA:617:A:OP1	8:AD:132:SER:OG	2.22	0.54
14:AJ:55:ASP:HA	29:AY:6:ILE:HD12	1.90	0.54
5:BA:1080:C:O2'	5:BA:1082:A:OP2	2.16	0.54
10:AF:74:ASP:HB3	10:AF:168:VAL:HG21	1.89	0.54
10:AF:105:ASN:N	10:AF:109:LYS:O	2.39	0.54
20:AP:32:GLY:O	20:AP:36:ALA:N	2.40	0.54
5:BA:684:G:N2	5:BA:719:G:O3'	2.41	0.54
5:BA:783:G:OP1	6:BB:26:LYS:NZ	2.24	0.54
11:BG:68:ILE:HG23	11:BG:85:VAL:HG22	1.90	0.54
15:BK:67:ASP:OD1	15:BK:68:LYS:N	2.40	0.54
3:A3:271:SER:OG	3:A3:273:GLU:OE1	2.26	0.53
6:AB:70:VAL:HG22	6:AB:92:ILE:HB	1.90	0.53
25:AU:51:ILE:HG12	25:AU:76:MET:HE3	1.90	0.53
5:BA:143:G:O2'	12:BH:68:ASP:O	2.24	0.53
5:BA:708:C:O5'	22:BR:138:ARG:NH2	2.41	0.53
7:BC:19:GLU:OE2	7:BC:23:LYS:NZ	2.29	0.53
20:BP:25:LEU:HB3	20:BP:31:ILE:HG21	1.90	0.53
1:A1:21:ARG:NH1	11:AG:121:ILE:O	2.37	0.53
5:AA:1248:A:N6	5:AA:1331:G:O2'	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:72:VAL:HG22	6:AB:94:GLY:O	2.08	0.53
9:AE:96:THR:N	9:AE:99:ASP:OD2	2.39	0.53
11:BG:43:GLN:OE1	11:BG:43:GLN:N	2.38	0.53
3:A4:183:ILE:HD11	3:A4:202:VAL:HG21	1.90	0.53
10:AF:105:ASN:OD1	10:AF:106:ARG:N	2.40	0.53
17:AM:12:ASN:ND2	17:AM:15:SER:OG	2.41	0.53
17:AM:29:ARG:NH2	17:AM:84:GLN:OE1	2.41	0.53
19:BO:97:ILE:HD12	19:BO:101:ASP:OD2	2.07	0.53
24:BT:61:LYS:O	24:BT:61:LYS:NZ	2.35	0.53
5:AA:475:C:H41	19:AO:70:ARG:HH22	1.55	0.53
5:BA:1185:A:H2'	25:BU:113:VAL:HG21	1.90	0.53
5:BA:1226:G:N7	26:BV:99:ARG:NH2	2.56	0.53
14:AJ:90:GLU:OE1	14:AJ:94:LEU:HD12	2.09	0.53
19:AO:35:LEU:O	19:AO:40:LYS:NZ	2.31	0.53
3:B3:96:ILE:O	3:B4:3:VAL:N	2.41	0.53
3:B4:8:GLY:O	3:B4:10:VAL:HG22	2.08	0.53
5:BA:534:G:OP1	22:BR:131:ARG:NH1	2.41	0.53
5:BA:557:G:N1	5:BA:589:U:N3	2.56	0.53
6:BB:97:LEU:O	6:BB:100:THR:OG1	2.26	0.53
5:AA:1338:C:O2'	30:AZ:17:ARG:NH2	2.41	0.53
11:AG:24:MET:O	11:AG:28:GLU:N	2.35	0.53
11:AG:167:ILE:HD11	11:AG:197:PHE:HZ	1.74	0.53
5:AA:1285:C:O2'	26:AV:39:ARG:NH2	2.42	0.53
19:AO:136:GLU:O	19:AO:140:GLY:N	2.39	0.53
28:AX:22:CYS:SG	28:AX:24:ARG:NH2	2.82	0.53
3:A4:76:SER:HA	3:A4:79:ILE:HD12	1.89	0.53
5:AA:765:U:H4'	5:AA:859:A:H61	1.74	0.53
5:AA:1205:G:P	26:AV:37:THR:HG21	2.49	0.53
15:AK:80:VAL:HA	15:AK:101:ILE:HG22	1.91	0.53
5:BA:398:C:OP1	9:BE:43:LYS:NZ	2.22	0.53
17:BM:63:ARG:O	21:BQ:54:LYS:NZ	2.42	0.53
5:AA:1173:A:O2'	5:AA:1174:A:O5'	2.26	0.53
5:AA:1252:C:N4	5:AA:1253:G:O6	2.42	0.53
8:AD:156:ASP:OD1	8:AD:156:ASP:N	2.42	0.53
5:BA:29:G:O6	5:BA:502:U:O2	2.27	0.53
5:BA:1261:U:OP2	5:BA:1263:C:N4	2.38	0.53
6:BB:62:PHE:HB2	6:BB:67:ILE:HD11	1.90	0.53
1:A1:16:ARG:NH2	11:AG:210:ARG:O	2.42	0.52
15:AK:124:LEU:H	15:AK:124:LEU:HD23	1.74	0.52
5:BA:101:G:O2'	5:BA:102:U:O4'	2.27	0.52
5:BA:699:C:OP1	5:BA:809:C:O2'	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AC:15:MET:CE	21:AQ:50:LEU:HD22	2.39	0.52
14:AJ:94:LEU:HD13	14:AJ:99:PHE:O	2.08	0.52
5:BA:1307:G:O2'	5:BA:1308:U:OP2	2.27	0.52
6:BB:48:THR:HG22	6:BB:155:PRO:HG2	1.90	0.52
5:AA:258:A:OP1	15:AK:30:ARG:NH2	2.41	0.52
5:AA:441:U:O2'	27:AW:58:SER:OG	2.05	0.52
5:AA:548:A:O2'	5:AA:595:U:O4	2.22	0.52
5:AA:46:A:O2'	5:AA:356:G:N2	2.42	0.52
5:AA:693:C:HO2'	22:AR:108:HIS:HD1	1.54	0.52
5:BA:720:A:N7	5:BA:767:U:O4	2.43	0.52
8:BD:118:ARG:HB2	8:BD:191:LEU:HD21	1.92	0.52
11:BG:163:LEU:N	11:BG:182:ASP:OD1	2.43	0.52
13:BI:214:SER:O	13:BI:214:SER:OG	2.25	0.52
27:BW:78:MET:SD	27:BW:78:MET:N	2.76	0.52
3:A3:247:ASP:OD2	3:A3:250:LEU:N	2.38	0.52
3:A4:10:VAL:HG12	3:A4:199:ILE:HG12	1.90	0.52
3:A4:244:THR:HG21	3:A4:286:ALA:HB1	1.91	0.52
5:AA:803:C:O3'	8:AD:127:ARG:NH2	2.40	0.52
5:AA:962:G:N2	5:AA:988:A:N7	2.57	0.52
8:AD:119:VAL:HG13	8:AD:185:ILE:HD11	1.90	0.52
15:AK:35:THR:HG22	15:AK:57:LEU:O	2.09	0.52
5:BA:431:U:HO2'	5:BA:432:G:P	2.32	0.52
5:BA:646:U:O2'	5:BA:648:A:N7	2.32	0.52
5:BA:1198:A:HO2'	13:BI:90:HIS:CE1	2.27	0.52
5:BA:1306:A:O2'	5:BA:1307:G:OP2	2.21	0.52
20:BP:115:TYR:N	25:BU:105:GLU:O	2.43	0.52
5:AA:61:A:N6	5:AA:377:A:H62	2.05	0.52
6:AB:193:GLU:N	6:AB:193:GLU:OE1	2.42	0.52
7:AC:189:LEU:N	7:AC:192:GLU:OE1	2.41	0.52
5:BA:511:C:OP2	5:BA:512:U:O2'	2.18	0.52
5:BA:525:A:HO2'	5:BA:874:G:HO2'	1.55	0.52
5:BA:918:A:N6	25:BU:109:THR:O	2.42	0.52
5:BA:1182:G:OP2	5:BA:1282:C:N4	2.41	0.52
18:BN:69:GLU:HA	18:BN:72:LEU:HD12	1.92	0.52
12:AH:27:GLU:OE1	12:AH:27:GLU:N	2.43	0.52
30:AZ:6:GLY:HA3	30:AZ:56:ILE:HD11	1.92	0.52
5:BA:242:A:N7	5:BA:277:G:N2	2.58	0.52
3:A3:32:GLU:OE1	3:A3:33:LYS:N	2.43	0.52
5:AA:1079:G:O2'	16:AL:16:ARG:NH1	2.43	0.52
12:AH:23:GLY:O	12:AH:26:THR:OG1	2.27	0.52
5:BA:1152:C:OP1	7:BC:131:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:310:G:OP2	15:AK:24:ARG:NH2	2.41	0.52
9:AE:36:LYS:N	9:AE:40:GLU:OE2	2.42	0.52
9:AE:109:VAL:HG11	9:AE:125:ILE:HD11	1.91	0.52
22:AR:93:GLU:O	22:AR:96:MET:N	2.43	0.52
5:BA:181:G:H21	23:BS:6:GLY:HA3	1.75	0.52
5:AA:1407:U:OP2	5:AA:1408:C:N4	2.43	0.52
11:AG:140:SER:HA	11:AG:180:VAL:HG13	1.91	0.52
5:BA:16:G:H21	5:BA:872:A:H62	1.57	0.52
5:BA:352:A:O2'	5:BA:363:C:O2'	2.28	0.52
5:BA:883:G:N2	5:BA:1458:A:OP1	2.43	0.52
18:BN:135:ARG:O	18:BN:137:VAL:N	2.43	0.52
5:AA:107:C:O2'	5:AA:286:G:N3	2.42	0.51
5:AA:1250:C:OP1	13:AI:91:ARG:NE	2.43	0.51
8:AD:93:ARG:NH2	8:AD:96:VAL:O	2.42	0.51
30:AZ:18:THR:OG1	30:AZ:19:GLY:N	2.43	0.51
3:B4:98:GLU:OE1	3:B4:98:GLU:N	2.41	0.51
3:B4:174:ILE:O	3:B4:178:ASN:ND2	2.40	0.51
13:BI:38:ASN:ND2	13:BI:60:ASN:O	2.43	0.51
16:BL:5:GLN:HG2	16:BL:18:VAL:HG12	1.92	0.51
19:BO:80:ASN:OD1	19:BO:81:GLY:N	2.43	0.51
5:AA:702:G:O4'	22:AR:14:SER:OG	2.27	0.51
5:AA:1112:G:OP1	17:AM:69:HIS:ND1	2.44	0.51
20:AP:41:ARG:NH2	26:AV:45:PRO:O	2.43	0.51
5:BA:699:C:N4	5:BA:700:G:O6	2.44	0.51
5:AA:1298:G:OP2	13:AI:80:LYS:NZ	2.33	0.51
16:AL:28:ILE:HD11	16:AL:33:VAL:HG23	1.91	0.51
5:BA:772:G:O2'	5:BA:774:U:OP2	2.16	0.51
10:BF:207:MET:SD	10:BF:207:MET:N	2.83	0.51
13:BI:140:MET:SD	13:BI:145:ARG:NE	2.81	0.51
22:BR:93:GLU:OE1	22:BR:93:GLU:N	2.43	0.51
29:BY:48:THR:OG1	29:BY:51:LYS:O	2.28	0.51
16:AL:19:ILE:HD11	16:AL:89:TRP:HB2	1.92	0.51
5:BA:5:C:OP2	11:BG:191:THR:OG1	2.28	0.51
5:BA:1004:U:C2	5:BA:1166:G:O6	2.63	0.51
5:BA:1209:C:O2'	16:BL:69:GLY:O	2.26	0.51
7:BC:65:LEU:HA	7:BC:68:ILE:HD12	1.93	0.51
5:BA:1116:G:HO2'	5:BA:1140:A:H61	1.56	0.51
13:BI:91:ARG:O	13:BI:99:LYS:NZ	2.43	0.51
22:BR:64:LYS:O	22:BR:75:ASN:ND2	2.43	0.51
3:A3:214:LEU:HD12	3:A3:226:LYS:O	2.10	0.51
5:AA:470:G:H21	5:AA:483:G:P	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1019:A:O2'	5:AA:1045:A:O2'	2.24	0.51
5:BA:1016:G:O3'	5:BA:1150:G:N2	2.44	0.51
5:BA:1238:G:OP2	5:BA:1238:G:N2	2.39	0.51
20:BP:85:TYR:O	25:BU:9:ARG:N	2.38	0.51
27:BW:87:LEU:O	27:BW:92:LEU:N	2.44	0.51
5:AA:557:G:H4'	10:AF:226:LEU:HD11	1.92	0.51
5:AA:998:A:N6	5:AA:1171:G:O2'	2.43	0.51
13:AI:70:LYS:O	13:AI:163:ARG:NH1	2.44	0.51
5:BA:1007:A:N6	5:BA:1160:C:C2	2.79	0.51
15:BK:41:ASP:OD1	15:BK:61:ALA:N	2.43	0.51
26:BV:140:LEU:HD12	26:BV:143:ILE:CG2	2.40	0.51
3:A3:112:LEU:HD23	3:A3:128:TYR:HA	1.93	0.51
5:AA:1112:G:O5'	17:AM:71:ARG:NH2	2.44	0.51
29:AY:10:ARG:O	29:AY:12:ARG:NH1	2.41	0.51
19:BO:36:ARG:O	19:BO:39:GLU:N	2.43	0.51
25:BU:68:ARG:NH2	25:BU:104:GLY:O	2.43	0.51
3:A4:161:LEU:O	3:A4:165:SER:OG	2.28	0.51
5:AA:222:G:O2'	10:AF:141:ASN:OD1	2.29	0.51
5:AA:352:A:O4'	5:AA:384:G:N2	2.43	0.51
5:AA:1131:G:OP1	24:AT:4:ILE:HD12	2.11	0.51
19:BO:30:TYR:CZ	19:BO:34:VAL:HG11	2.46	0.51
5:AA:534:G:OP1	22:AR:131:ARG:NH1	2.42	0.51
5:BA:661:C:OP1	18:BN:84:ARG:NH1	2.44	0.51
5:BA:1107:C:O2'	16:BL:7:THR:HG22	2.11	0.51
13:AI:48:HIS:O	16:AL:112:ARG:NH2	2.39	0.50
20:AP:14:ASP:OD1	20:AP:15:LEU:N	2.44	0.50
27:BW:23:ILE:HG21	27:BW:31:PRO:HG3	1.93	0.50
5:AA:421:U:O4	5:AA:448:A:N7	2.43	0.50
8:AD:126:MET:N	8:AD:126:MET:SD	2.84	0.50
5:BA:323:A:O2'	5:BA:324:C:O4'	2.30	0.50
10:BF:167:LYS:NZ	10:BF:170:GLU:OE2	2.32	0.50
3:A3:94:VAL:HG23	3:A4:2:LYS:NZ	2.27	0.50
5:AA:344:G:OP1	12:AH:106:THR:OG1	2.22	0.50
12:AH:88:LEU:HD13	12:AH:94:PHE:HB2	1.93	0.50
14:AJ:106:THR:HG22	14:AJ:122:GLY:O	2.11	0.50
20:AP:100:MET:SD	20:AP:101:ALA:N	2.84	0.50
3:B3:214:LEU:HD21	3:B3:225:VAL:CG1	2.41	0.50
8:BD:107:PHE:HD1	8:BD:146:TYR:HH	1.60	0.50
8:BD:119:VAL:HG22	8:BD:188:ILE:HG12	1.92	0.50
5:AA:639:G:O2'	18:AN:41:ARG:NH2	2.45	0.50
5:AA:1226:G:N2	5:AA:1229:A:OP2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1238:G:O3'	7:AC:2:ALA:N	2.45	0.50
5:AA:1340:U:O2'	5:AA:1341:C:OP2	2.26	0.50
10:AF:167:LYS:HB2	10:AF:174:LEU:HD21	1.93	0.50
5:BA:19:G:O2'	5:BA:477:G:N3	2.44	0.50
5:BA:45:U:N3	5:BA:360:A:N7	2.59	0.50
5:BA:45:U:O2	5:BA:358:G:O2'	2.20	0.50
5:BA:1249:A:H61	16:BL:71:PHE:HD1	1.58	0.50
3:A3:125:LEU:HD23	3:A3:129:LEU:HD11	1.93	0.50
3:A4:256:ILE:H	3:A4:256:ILE:HD12	1.76	0.50
5:AA:221:A:O3'	10:AF:131:ARG:NH1	2.44	0.50
9:AE:50:ASN:N	9:AE:50:ASN:OD1	2.43	0.50
23:AS:5:ILE:HD11	23:AS:29:ILE:CD1	2.40	0.50
27:AW:32:SER:OG	27:AW:33:ARG:N	2.45	0.50
10:BF:70:LYS:NZ	27:BW:13:LEU:O	2.42	0.50
5:AA:642:G:N7	3:B4:217:LYS:NZ	2.37	0.50
6:AB:77:GLN:O	6:AB:81:LYS:NZ	2.41	0.50
17:AM:2:GLN:NE2	17:AM:101:ILE:O	2.45	0.50
23:AS:35:GLU:OE2	23:AS:36:GLY:N	2.44	0.50
10:BF:129:ASN:OD1	10:BF:130:LYS:N	2.45	0.50
19:BO:49:GLN:NE2	19:BO:106:GLU:OE1	2.45	0.50
3:A3:192:TYR:O	3:A3:193:SER:OG	2.24	0.50
5:AA:783:G:OP1	6:AB:26:LYS:NZ	2.25	0.50
5:AA:922:G:N2	17:AM:56:GLU:OE2	2.41	0.50
5:AA:1011:C:O3'	21:AQ:44:ARG:NH2	2.40	0.50
16:AL:33:VAL:HG22	16:AL:46:LEU:HD21	1.94	0.50
23:AS:20:LYS:HE3	23:AS:27:LEU:HD23	1.94	0.50
5:BA:458:G:H3'	5:BA:459:G:H21	1.77	0.50
3:A4:294:GLN:O	3:A4:298:GLY:N	2.45	0.50
5:AA:89:G:N2	5:AA:375:G:O3'	2.45	0.50
5:AA:604:C:OP1	22:AR:74:ARG:NH1	2.42	0.50
26:AV:143:ILE:H	26:AV:143:ILE:HD12	1.76	0.50
5:BA:1252:C:H4'	13:BI:5:LEU:HD11	1.93	0.50
17:BM:10:SER:OG	17:BM:93:ASP:OD1	2.29	0.50
5:AA:151:G:O2'	12:AH:64:ARG:NH1	2.45	0.50
5:AA:242:A:N1	5:AA:274:G:O2'	2.38	0.50
5:AA:559:G:H21	5:AA:587:G:N2	2.10	0.50
15:AK:35:THR:OG1	15:AK:95:ILE:O	2.30	0.50
27:AW:70:LYS:NZ	27:AW:82:GLU:OE1	2.40	0.50
3:B3:137:THR:HG22	3:B3:138:PRO:HD2	1.94	0.50
5:BA:718:G:O3'	22:BR:116:LEU:HD13	2.11	0.50
26:BV:59:LEU:HG	26:BV:129:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:26:GLU:OE1	9:AE:38:LYS:NZ	2.31	0.49
11:AG:61:GLU:OE1	11:AG:61:GLU:N	2.40	0.49
5:BA:528:G:O2'	5:BA:529:C:OP2	2.26	0.49
20:BP:29:LYS:O	20:BP:95:THR:N	2.45	0.49
27:BW:73:ASP:OD1	27:BW:74:SER:N	2.45	0.49
5:AA:699:C:OP1	5:AA:809:C:O2'	2.26	0.49
14:AJ:93:PHE:O	14:AJ:94:LEU:HD23	2.12	0.49
18:AN:99:GLN:HA	18:AN:102:ILE:HD12	1.93	0.49
27:AW:19:ILE:HD11	27:AW:40:LEU:HD21	1.94	0.49
3:B4:143:TYR:O	3:B4:146:THR:OG1	2.27	0.49
5:BA:807:C:OP1	6:BB:24:LYS:NZ	2.31	0.49
5:AA:432:G:OP1	27:AW:57:ARG:NH2	2.43	0.49
13:AI:112:GLU:O	13:AI:116:GLY:N	2.44	0.49
5:BA:966:G:N2	28:BX:41:GLY:O	2.44	0.49
6:BB:59:LEU:HD23	6:BB:175:ILE:HD11	1.93	0.49
12:BH:63:ILE:HA	12:BH:121:VAL:HG12	1.93	0.49
22:BR:136:TYR:O	22:BR:140:GLY:N	2.39	0.49
5:AA:540:G:N2	5:AA:708:C:OP2	2.40	0.49
8:AD:117:LEU:HD12	8:AD:190:VAL:HA	1.95	0.49
14:AJ:16:ASN:OD1	14:AJ:19:ARG:NH2	2.41	0.49
23:AS:39:VAL:HA	23:AS:82:VAL:HG13	1.95	0.49
5:BA:983:G:O2'	5:BA:984:C:O4'	2.20	0.49
5:BA:1044:A:N7	24:BT:2:GLY:N	2.61	0.49
5:BA:1110:U:O2'	17:BM:39:PRO:O	2.12	0.49
10:BF:127:ILE:HD12	10:BF:162:TYR:HB2	1.94	0.49
11:BG:67:ASP:OD1	11:BG:194:THR:OG1	2.30	0.49
5:AA:183:A:H3'	5:AA:184:G:C8	2.48	0.49
16:AL:110:ASP:OD2	16:AL:112:ARG:NH2	2.42	0.49
3:B4:214:LEU:HD21	3:B4:225:VAL:HG13	1.94	0.49
4:B5:43:VAL:HG13	4:B5:75:ILE:HD12	1.95	0.49
14:BJ:23:ARG:NH2	14:BJ:65:LEU:O	2.44	0.49
5:AA:61:A:N6	5:AA:377:A:N7	2.60	0.49
8:AD:111:THR:OG1	8:AD:115:TYR:N	2.46	0.49
28:AX:19:ASN:ND2	28:AX:31:MET:O	2.45	0.49
5:BA:1214:G:N2	5:BA:1219:C:O2'	2.45	0.49
3:A4:20:LYS:NZ	3:A4:214:LEU:O	2.46	0.49
5:AA:672:G:HO2'	5:AA:673:C:P	2.34	0.49
5:AA:1049:U:O2'	5:AA:1129:A:N3	2.44	0.49
5:AA:1247:A:H2	5:AA:1313:G:HO2'	1.59	0.49
18:AN:32:ASP:OD2	18:AN:34:THR:N	2.42	0.49
5:BA:1045:A:O2'	5:BA:1060:G:N2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:1079:G:N2	5:BA:1106:A:H62	2.11	0.49
3:A4:262:ASN:O	3:A4:262:ASN:ND2	2.45	0.49
19:AO:27:ASP:OD1	19:AO:28:ILE:N	2.46	0.49
22:AR:46:SER:OG	22:AR:49:MET:SD	2.48	0.49
18:BN:47:VAL:HB	18:BN:62:LEU:HD22	1.95	0.49
3:A3:43:PRO:O	3:A3:105:LYS:N	2.43	0.49
3:A3:125:LEU:HD23	3:A3:129:LEU:CD1	2.43	0.49
3:A4:213:TYR:CE2	3:A4:232:LEU:HD12	2.47	0.49
5:AA:90:C:O2'	5:AA:375:G:OP1	2.31	0.49
8:AD:117:LEU:HD11	8:AD:188:ILE:CG2	2.42	0.49
12:AH:6:LEU:HD23	12:AH:6:LEU:H	1.78	0.49
5:BA:896:A:O2'	30:BZ:23:ASP:OD1	2.25	0.49
5:BA:908:G:HO2'	5:BA:930:G:H1	1.60	0.49
5:BA:1272:G:OP2	25:BU:30:ALA:N	2.46	0.49
14:BJ:41:MET:N	14:BJ:41:MET:SD	2.80	0.49
18:BN:62:LEU:HD21	18:BN:66:ARG:HH21	1.78	0.49
19:BO:27:ASP:OD1	19:BO:28:ILE:N	2.46	0.49
3:A3:187:GLU:O	3:A3:191:ALA:N	2.46	0.49
3:A4:57:ASN:OD1	3:A4:57:ASN:N	2.45	0.49
5:AA:112:G:HO2'	5:AA:113:U:H5'	1.78	0.49
6:AB:131:VAL:HG22	6:AB:149:TYR:CD2	2.47	0.49
9:AE:112:LYS:NZ	9:AE:152:ILE:O	2.42	0.49
22:AR:27:GLU:OE1	22:AR:27:GLU:N	2.45	0.49
4:B5:32:ILE:HG22	4:B5:101:ILE:HG22	1.95	0.49
5:BA:29:G:O6	5:BA:502:U:C2	2.66	0.49
5:BA:480:G:O2'	5:BA:488:A:N1	2.43	0.49
12:BH:34:ILE:HD11	12:BH:74:MET:HB3	1.93	0.49
5:AA:314:G:N2	5:AA:1423:A:O2'	2.46	0.48
8:AD:17:GLN:NE2	8:AD:38:ASP:O	2.41	0.48
12:AH:61:LEU:HD12	12:AH:121:VAL:HB	1.95	0.48
17:AM:14:ARG:NE	17:AM:17:ASP:OD2	2.45	0.48
11:BG:131:TRP:O	11:BG:134:ARG:NH2	2.45	0.48
25:BU:68:ARG:O	25:BU:104:GLY:N	2.41	0.48
5:AA:96:G:H21	5:AA:350:G:C4'	2.25	0.48
7:AC:79:GLN:OE1	7:AC:79:GLN:N	2.46	0.48
5:AA:400:G:OP1	9:AE:122:ARG:NE	2.42	0.48
6:AB:137:ILE:N	6:AB:151:ASP:OD2	2.45	0.48
6:AB:194:GLU:N	6:AB:194:GLU:OE1	2.46	0.48
11:AG:214:SER:OG	11:AG:217:MET:SD	2.61	0.48
30:AZ:31:ILE:HD12	30:AZ:39:ARG:HB3	1.95	0.48
3:B4:87:TRP:O	3:B4:297:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:1338:C:O2'	30:BZ:17:ARG:NE	2.46	0.48
17:AM:9:ALA:HB3	17:AM:95:THR:HG23	1.96	0.48
3:B3:136:ASP:O	3:B3:293:LEU:HD23	2.13	0.48
6:BB:17:VAL:HG22	6:BB:163:ALA:HB1	1.95	0.48
12:BH:6:LEU:HD11	12:BH:121:VAL:HG13	1.94	0.48
30:BZ:59:GLU:OE1	30:BZ:62:ARG:NH2	2.43	0.48
6:AB:147:LEU:O	6:AB:150:VAL:HG22	2.13	0.48
15:AK:31:GLU:O	15:AK:56:ARG:NH1	2.46	0.48
8:BD:20:ILE:N	8:BD:76:GLN:O	2.40	0.48
5:AA:207:G:N2	5:AA:210:A:OP2	2.46	0.48
5:AA:960:A:O4'	5:AA:988:A:N6	2.46	0.48
9:AE:175:LYS:O	9:AE:175:LYS:NZ	2.29	0.48
14:AJ:33:LEU:HD12	14:AJ:33:LEU:O	2.13	0.48
27:AW:8:ILE:HG23	27:AW:19:ILE:HG22	1.95	0.48
27:AW:8:ILE:HG12	27:AW:19:ILE:HG22	1.95	0.48
8:BD:117:LEU:HD12	8:BD:190:VAL:HA	1.94	0.48
11:BG:33:ASP:OD2	11:BG:39:ARG:NH2	2.45	0.48
12:BH:110:ASN:OD1	12:BH:111:THR:N	2.47	0.48
10:AF:184:TYR:N	10:AF:234:GLY:O	2.46	0.48
26:AV:37:THR:HG23	26:AV:41:LYS:HG3	1.96	0.48
7:BC:196:ILE:O	24:BT:20:TYR:OH	2.32	0.48
15:BK:75:VAL:HG11	15:BK:105:ILE:HD11	1.95	0.48
4:A5:6:TYR:CE1	4:A5:63:VAL:HG23	2.49	0.48
5:AA:563:U:OP1	10:AF:24:LYS:NZ	2.47	0.48
5:AA:606:U:O4	5:AA:707:A:N7	2.47	0.48
20:AP:29:LYS:NZ	20:AP:98:LEU:HD23	2.29	0.48
5:BA:1097:G:H21	26:BV:3:THR:HG22	1.79	0.48
7:BC:151:LEU:HD12	7:BC:183:MET:HE3	1.96	0.48
7:BC:185:PRO:O	7:BC:188:ARG:NH2	2.47	0.48
8:AD:165:LYS:O	8:AD:165:LYS:NZ	2.44	0.48
15:AK:81:ILE:HD12	15:AK:100:ILE:HG22	1.95	0.48
16:AL:119:PRO:O	16:AL:129:LYS:NZ	2.47	0.48
19:AO:98:ASP:N	19:AO:101:ASP:OD2	2.39	0.48
5:BA:177:A:O2'	10:BF:155:LYS:NZ	2.37	0.48
5:BA:1194:C:O2'	26:BV:85:HIS:O	2.19	0.48
26:BV:26:ILE:O	26:BV:52:TYR:OH	2.27	0.48
5:AA:1011:C:O2'	21:AQ:44:ARG:NH1	2.47	0.48
17:AM:96:ILE:HD11	17:AM:98:ILE:HD11	1.94	0.48
5:BA:45:U:O2	5:BA:360:A:N6	2.46	0.48
6:BB:70:VAL:HG22	6:BB:92:ILE:HB	1.96	0.48
6:BB:101:MET:SD	6:BB:101:MET:N	2.85	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:94:VAL:O	3:A4:2:LYS:NZ	2.47	0.47
13:AI:104:VAL:HG22	13:AI:108:PHE:CZ	2.49	0.47
27:AW:49:GLU:N	27:AW:49:GLU:OE1	2.47	0.47
3:B4:150:VAL:HG21	3:B4:156:VAL:HG23	1.95	0.47
5:BA:56:A:N6	5:BA:91:G:O2'	2.45	0.47
5:BA:148:C:O3'	12:BH:105:LYS:NZ	2.43	0.47
5:BA:769:A:N3	5:BA:1482:C:O2'	2.40	0.47
9:BE:132:VAL:HG11	9:BE:137:ILE:HD12	1.96	0.47
2:A2:23:ILE:HD11	5:AA:849:U:H5'	1.96	0.47
3:A3:19:LEU:O	3:A3:126:LYS:NZ	2.43	0.47
3:A3:125:LEU:O	3:A3:129:LEU:HD12	2.14	0.47
20:AP:112:ILE:HG22	25:AU:98:MET:CE	2.43	0.47
5:BA:618:G:H22	5:BA:695:G:H1	1.61	0.47
6:AB:21:THR:OG1	6:AB:22:GLN:N	2.47	0.47
8:AD:133:GLN:NE2	8:AD:177:ILE:O	2.46	0.47
12:AH:33:ARG:N	12:AH:36:ASP:OD2	2.47	0.47
27:AW:11:ASN:O	27:AW:15:GLY:N	2.47	0.47
3:A3:36:ASP:O	3:A3:40:THR:OG1	2.19	0.47
5:AA:533:C:OP1	22:AR:7:ARG:NH1	2.47	0.47
5:BA:370:A:H5'	5:BA:434:A:H61	1.80	0.47
8:BD:20:ILE:O	8:BD:78:ALA:N	2.44	0.47
3:A3:268:THR:OG1	3:A3:272:GLU:OE2	2.26	0.47
5:AA:143:G:H21	12:AH:71:GLY:HA3	1.80	0.47
8:AD:133:GLN:CG	8:AD:177:ILE:HG22	2.44	0.47
10:AF:203:LYS:NZ	10:AF:224:ASP:OD2	2.29	0.47
11:AG:33:ASP:OD2	11:AG:36:GLU:N	2.48	0.47
23:AS:21:CYS:HG	23:AS:24:HIS:CG	2.27	0.47
5:BA:1077:U:OP1	5:BA:1105:C:N4	2.47	0.47
5:BA:1182:G:OP1	5:BA:1281:U:O2'	2.13	0.47
7:BC:129:GLU:HB3	7:BC:181:ALA:HB3	1.96	0.47
18:BN:61:MET:HB2	18:BN:104:ALA:HB2	1.96	0.47
3:A3:94:VAL:HG23	3:A4:2:LYS:HZ1	1.79	0.47
5:AA:402:G:H21	9:AE:123:GLN:HE22	1.63	0.47
18:AN:48:VAL:HG12	18:AN:50:ALA:H	1.80	0.47
3:B4:119:LEU:HD13	3:B4:123:GLU:HG3	1.95	0.47
5:BA:139:C:N3	5:BA:153:G:C6	2.83	0.47
5:BA:435:A:OP1	27:BW:89:ARG:NH1	2.48	0.47
9:BE:26:GLU:OE1	9:BE:38:LYS:NZ	2.30	0.47
10:BF:87:ILE:HG22	10:BF:88:MET:HG3	1.96	0.47
11:BG:75:THR:OG1	11:BG:76:ASP:N	2.48	0.47
18:BN:15:GLY:O	18:BN:16:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BO:64:GLN:OE1	19:BO:64:GLN:N	2.48	0.47
28:BX:19:ASN:ND2	28:BX:31:MET:O	2.43	0.47
3:A4:55:ARG:O	3:A4:55:ARG:HD3	2.15	0.47
5:AA:31:U:C2	5:AA:501:G:N1	2.83	0.47
5:AA:661:C:OP1	18:AN:84:ARG:NH1	2.48	0.47
20:AP:80:ASN:OD1	20:AP:93:LEU:N	2.43	0.47
23:AS:35:GLU:OE1	23:AS:85:LYS:NZ	2.38	0.47
20:BP:109:LEU:HD23	20:BP:112:ILE:HD11	1.97	0.47
27:BW:76:GLU:N	27:BW:76:GLU:OE1	2.48	0.47
5:AA:400:G:O2'	5:AA:423:U:O2	2.28	0.47
5:AA:896:A:O2'	30:AZ:46:ARG:NH2	2.48	0.47
5:AA:985:C:H4'	28:AX:29:VAL:HG13	1.96	0.47
11:AG:86:LEU:HD12	11:AG:99:GLY:O	2.15	0.47
14:AJ:5:ASP:OD1	14:AJ:8:ALA:N	2.40	0.47
23:AS:20:LYS:O	23:AS:27:LEU:HD21	2.15	0.47
29:AY:14:LEU:HB3	29:AY:58:ILE:HD13	1.97	0.47
5:BA:257:U:OP2	15:BK:116:GLN:NE2	2.46	0.47
11:BG:19:LYS:N	11:BG:46:GLU:OE2	2.46	0.47
3:B4:57:ASN:N	3:B4:57:ASN:OD1	2.47	0.47
3:B4:233:ARG:NH1	3:B4:260:LEU:O	2.48	0.47
4:B5:114:ILE:O	4:B5:118:VAL:N	2.48	0.47
5:BA:966:G:H21	28:BX:42:LYS:HA	1.79	0.47
5:BA:1368:A:N1	5:BA:1448:A:N6	2.62	0.47
3:A3:43:PRO:HD3	3:A3:59:ALA:HB2	1.97	0.46
3:A3:84:LEU:HD22	3:A3:204:VAL:HG11	1.96	0.46
5:BA:471:G:H21	19:BO:66:ASN:HA	1.80	0.46
5:BA:530:G:H22	5:BA:718:G:H22	1.62	0.46
5:BA:1272:G:OP1	25:BU:33:ARG:NH1	2.48	0.46
5:BA:1295:C:O2'	13:BI:175:ARG:NH1	2.48	0.46
17:BM:5:ARG:HE	17:BM:72:LEU:HD21	1.80	0.46
3:A4:269:ILE:HG23	3:A4:270:PHE:CD2	2.50	0.46
10:AF:74:ASP:OD1	10:AF:90:VAL:N	2.46	0.46
11:AG:44:ILE:HD13	11:AG:50:ILE:HD11	1.96	0.46
19:AO:143:GLU:OE2	19:AO:144:LYS:N	2.47	0.46
20:AP:85:TYR:O	25:AU:9:ARG:N	2.48	0.46
25:AU:53:LEU:HD22	25:AU:58:LYS:HD2	1.97	0.46
10:BF:185:VAL:HG21	10:BF:215:ILE:HD12	1.96	0.46
3:A3:267:LYS:NZ	3:A3:268:THR:O	2.46	0.46
4:A5:60:GLU:O	4:A5:64:ALA:N	2.49	0.46
5:AA:1009:G:O3'	7:AC:166:TYR:OH	2.32	0.46
8:AD:111:THR:OG1	8:AD:113:ASP:OD1	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AG:128:CYS:SG	11:AG:139:HIS:NE2	2.86	0.46
5:BA:1204:C:O2'	26:BV:47:GLN:NE2	2.42	0.46
20:BP:13:VAL:HG21	20:BP:28:ILE:HG23	1.98	0.46
5:AA:247:G:N1	5:AA:262:G:O6	2.48	0.46
23:AS:88:ILE:HD12	23:AS:101:VAL:O	2.15	0.46
14:BJ:25:VAL:HG12	14:BJ:65:LEU:HD11	1.97	0.46
14:BJ:76:LYS:O	14:BJ:78:ARG:N	2.48	0.46
19:BO:14:ARG:NH2	23:BS:65:LEU:O	2.49	0.46
19:BO:15:LYS:NZ	19:BO:18:LEU:HD22	2.30	0.46
21:BQ:52:PHE:O	21:BQ:53:ARG:NE	2.48	0.46
2:A2:29:GLN:OE1	2:A2:30:ARG:N	2.49	0.46
7:AC:15:MET:HE1	21:AQ:50:LEU:HD22	1.98	0.46
23:AS:21:CYS:O	23:AS:25:GLY:N	2.49	0.46
3:B4:20:LYS:NZ	3:B4:210:SER:O	2.40	0.46
3:B4:268:THR:HG21	3:B4:272:GLU:OE2	2.15	0.46
5:BA:262:G:O2'	5:BA:263:C:OP2	2.34	0.46
5:BA:1139:A:H4'	16:BL:108:VAL:HG13	1.98	0.46
7:BC:161:LEU:HD13	7:BC:187:ALA:HB1	1.96	0.46
12:BH:23:GLY:O	12:BH:26:THR:OG1	2.23	0.46
17:BM:75:ILE:HG23	17:BM:82:MET:HE1	1.98	0.46
7:AC:185:PRO:O	7:AC:188:ARG:NH1	2.45	0.46
25:AU:72:ILE:HG21	25:AU:98:MET:CB	2.45	0.46
5:BA:91:G:H3'	5:BA:92:G:H21	1.81	0.46
5:BA:802:G:OP1	8:BD:133:GLN:NE2	2.43	0.46
6:BB:176:LEU:HD13	6:BB:182:ILE:HD12	1.98	0.46
5:AA:172:G:N2	15:AK:70:GLY:O	2.49	0.46
6:AB:63:GLU:OE1	6:AB:65:GLN:N	2.47	0.46
17:AM:9:ALA:HB3	17:AM:95:THR:CG2	2.46	0.46
22:AR:41:ARG:NH1	22:AR:41:ARG:O	2.48	0.46
25:BU:41:THR:HB	25:BU:42:PRO:HD2	1.97	0.46
5:AA:623:C:OP1	22:AR:114:LYS:NZ	2.48	0.46
5:AA:778:G:O4'	14:AJ:2:THR:N	2.48	0.46
12:AH:110:ASN:OD1	12:AH:111:THR:N	2.48	0.46
14:AJ:46:TYR:HB3	14:AJ:69:ILE:HD11	1.98	0.46
18:AN:90:LYS:O	18:AN:92:LYS:NZ	2.43	0.46
3:B3:148:ASN:O	3:B3:148:ASN:ND2	2.49	0.46
5:BA:745:G:N2	5:BA:1453:U:OP1	2.49	0.46
5:BA:985:C:O2'	5:BA:986:G:N3	2.29	0.46
3:A4:174:ILE:HD11	3:A4:297:TYR:HA	1.98	0.46
5:AA:30:C:H41	5:AA:393:A:H62	1.63	0.46
8:AD:140:ILE:HG13	8:AD:177:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:242:VAL:HG13	3:A3:283:LYS:HG3	1.98	0.46
3:A3:260:LEU:O	3:A3:263:THR:OG1	2.33	0.46
3:B3:113:GLU:OE1	3:B3:114:GLU:N	2.49	0.46
5:BA:43:A:HO2'	5:BA:44:C:P	2.39	0.46
5:BA:530:G:H22	5:BA:718:G:N2	2.14	0.46
11:BG:16:TRP:O	11:BG:27:LYS:NZ	2.39	0.46
10:AF:117:GLU:OE1	10:AF:117:GLU:N	2.48	0.45
13:AI:150:VAL:HG12	13:AI:151:ASP:O	2.16	0.45
6:BB:150:VAL:HG11	6:BB:153:ALA:HB2	1.97	0.45
12:BH:32:LYS:HB2	12:BH:112:ILE:HD12	1.97	0.45
12:BH:67:THR:OG1	12:BH:118:GLN:OE1	2.26	0.45
15:BK:42:LYS:HB3	15:BK:59:ALA:HB3	1.98	0.45
29:BY:44:LEU:O	29:BY:55:LYS:N	2.46	0.45
5:AA:1205:G:OP1	26:AV:54:ARG:NH2	2.49	0.45
5:AA:1270:C:O2'	20:AP:82:PRO:O	2.34	0.45
7:AC:194:GLU:OE1	7:AC:194:GLU:N	2.50	0.45
13:AI:155:MET:SD	13:AI:155:MET:N	2.77	0.45
12:BH:65:GLY:O	12:BH:120:ASN:N	2.46	0.45
5:AA:140:C:N4	5:AA:152:G:O6	2.50	0.45
5:AA:320:G:N1	5:AA:323:A:OP2	2.50	0.45
16:AL:6:THR:HG21	16:AL:81:ALA:O	2.17	0.45
22:AR:92:PRO:HD3	22:AR:142:LEU:HD21	1.98	0.45
8:BD:17:GLN:OE1	8:BD:17:GLN:N	2.49	0.45
5:AA:700:G:O3'	29:AY:10:ARG:NH2	2.50	0.45
5:AA:730:G:N2	5:AA:756:A:OP2	2.49	0.45
6:AB:28:MET:N	6:AB:28:MET:SD	2.90	0.45
5:BA:117:C:HO2'	15:BK:49:TYR:HE1	1.62	0.45
5:BA:764:C:H1'	5:BA:857:C:H41	1.81	0.45
17:BM:6:ILE:HG23	17:BM:98:ILE:HG12	1.99	0.45
5:AA:43:A:O2'	5:AA:44:C:OP2	2.27	0.45
5:AA:143:G:O2'	12:AH:69:LYS:O	2.34	0.45
9:AE:34:GLU:OE1	9:AE:119:ARG:NH1	2.49	0.45
10:AF:198:ARG:NH2	10:AF:236:ASP:O	2.48	0.45
5:BA:474:G:OP2	19:BO:71:LYS:NZ	2.36	0.45
5:BA:1335:A:HO2'	13:BI:73:ARG:HH21	1.64	0.45
18:BN:90:LYS:O	18:BN:92:LYS:NZ	2.49	0.45
22:BR:98:LEU:HD22	22:BR:125:ILE:HD11	1.99	0.45
4:A5:57:VAL:HG12	4:A5:59:PRO:HD2	1.98	0.45
5:AA:904:G:H21	5:AA:1294:G:H4'	1.80	0.45
5:AA:1037:U:OP1	5:AA:1046:G:N2	2.50	0.45
13:AI:11:ILE:HG23	13:AI:12:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:3:ARG:NH2	23:AS:25:GLY:O	2.48	0.45
8:BD:43:VAL:HG12	8:BD:70:VAL:HG11	1.99	0.45
4:A5:15:LEU:CG	4:A5:78:ILE:HD11	2.44	0.45
5:AA:359:A:N7	19:AO:79:LYS:NZ	2.53	0.45
5:AA:517:U:O2'	23:AS:62:ARG:NH2	2.50	0.45
5:AA:550:G:H21	14:AJ:124:ARG:NH2	2.14	0.45
5:AA:903:G:N2	5:AA:1298:G:N7	2.65	0.45
5:AA:1196:A:O2'	5:AA:1294:G:N2	2.49	0.45
5:AA:1487:U:H2'	5:AA:1488:C:C2	2.52	0.45
9:AE:44:HIS:HA	9:AE:47:GLN:OE1	2.17	0.45
14:AJ:33:LEU:O	14:AJ:37:VAL:HG23	2.17	0.45
5:BA:903:G:H21	5:BA:1299:A:H62	1.65	0.45
5:BA:1268:C:N4	5:BA:1290:U:O2	2.50	0.45
5:AA:960:A:N6	5:AA:989:C:OP2	2.49	0.45
5:AA:977:G:O2'	5:AA:978:G:OP2	2.27	0.45
5:AA:1241:U:O4	17:AM:5:ARG:NH2	2.44	0.45
6:AB:97:LEU:O	6:AB:100:THR:OG1	2.34	0.45
3:B4:116:PHE:HB3	3:B4:119:LEU:HD12	1.98	0.45
11:BG:17:GLU:O	11:BG:19:LYS:NZ	2.36	0.45
29:BY:18:CYS:SG	29:BY:19:ILE:N	2.90	0.45
5:AA:50:C:H2'	5:AA:348:C:H41	1.82	0.45
9:AE:170:MET:N	9:AE:170:MET:SD	2.90	0.45
15:AK:107:LYS:O	15:AK:125:LEU:HD12	2.17	0.45
24:AT:14:ARG:NH1	24:AT:53:TYR:OH	2.49	0.45
25:AU:55:LYS:HD2	25:AU:79:LEU:HD11	1.98	0.45
5:BA:963:A:O2'	5:BA:965:G:N7	2.50	0.45
13:BI:51:HIS:ND1	13:BI:57:GLY:O	2.49	0.45
3:A3:86:LEU:HD23	3:A3:91:LEU:HD12	1.99	0.45
5:AA:1085:C:H41	5:AA:1102:A:H2	1.65	0.45
11:AG:160:PRO:HD2	11:AG:163:LEU:HD22	1.99	0.45
19:AO:7:PRO:HD2	19:AO:16:LEU:HD12	1.99	0.45
15:BK:39:GLU:OE1	15:BK:39:GLU:N	2.44	0.45
5:AA:181:G:H21	23:AS:6:GLY:HA3	1.81	0.44
20:BP:15:LEU:HD22	20:BP:27:ALA:HB3	1.98	0.44
5:AA:95:G:OP1	10:AF:3:ARG:NH1	2.49	0.44
5:AA:331:C:O2'	5:AA:1393:A:N3	2.43	0.44
11:AG:43:GLN:N	11:AG:43:GLN:OE1	2.49	0.44
3:B4:31:ILE:HD11	3:B4:78:ARG:NH2	2.32	0.44
5:BA:1262:U:O2'	5:BA:1263:C:OP1	2.27	0.44
8:BD:89:ARG:NH2	18:BN:117:ASP:O	2.51	0.44
11:BG:51:ASP:N	11:BG:51:ASP:OD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:176:U:H2'	5:AA:177:A:C8	2.52	0.44
5:AA:597:C:O2'	14:AJ:78:ARG:NH1	2.47	0.44
5:AA:935:G:N1	5:AA:1323:A:OP1	2.42	0.44
16:AL:86:LEU:HD11	16:AL:95:LEU:HD21	1.97	0.44
23:AS:51:ARG:O	23:AS:68:SER:N	2.50	0.44
5:BA:237:C:P	19:BO:21:LYS:HZ2	2.39	0.44
22:BR:142:LEU:HD13	22:BR:146:TRP:CD1	2.53	0.44
10:AF:87:ILE:HG22	10:AF:88:MET:HG2	1.99	0.44
13:AI:87:ARG:HE	13:AI:89:GLU:HG3	1.81	0.44
3:B3:35:VAL:HB	3:B3:82:ILE:HD11	1.99	0.44
4:B5:57:VAL:HG21	4:B5:63:VAL:HG11	2.00	0.44
5:BA:58:U:O2	5:BA:375:G:O2'	2.34	0.44
5:BA:534:G:N2	5:BA:714:G:N7	2.65	0.44
5:BA:1271:G:OP1	25:BU:9:ARG:NH2	2.46	0.44
10:BF:43:ILE:HB	10:BF:110:LEU:HD21	2.00	0.44
20:BP:77:TRP:HZ2	26:BV:35:VAL:HG22	1.83	0.44
1:A1:39:ARG:NH2	1:A1:48:LYS:O	2.51	0.44
5:AA:1126:G:N1	5:AA:1129:A:OP2	2.45	0.44
8:AD:58:ASP:OD2	8:AD:60:THR:OG1	2.33	0.44
9:AE:172:GLU:O	9:AE:176:GLN:NE2	2.50	0.44
13:AI:47:THR:HG22	13:AI:65:GLU:OE2	2.16	0.44
5:BA:91:G:OP1	5:BA:321:A:N6	2.50	0.44
24:BT:6:GLN:H	24:BT:9:ILE:HD11	1.82	0.44
3:A3:179:MET:HA	3:A3:201:LEU:HD12	1.99	0.44
4:A5:68:PRO:HG2	28:AX:10:ILE:HD13	1.98	0.44
5:AA:112:G:HO2'	23:AS:30:HIS:HD1	1.52	0.44
5:AA:916:U:N3	5:AA:919:U:OP2	2.51	0.44
8:AD:93:ARG:NE	8:AD:93:ARG:O	2.51	0.44
5:BA:329:G:O2'	12:BH:102:ARG:O	2.36	0.44
5:AA:238:G:P	19:AO:21:LYS:HZ1	2.40	0.44
5:AA:528:G:H1	5:AA:838:C:H42	1.65	0.44
5:AA:606:U:H3	5:AA:707:A:H62	1.65	0.44
5:AA:1403:U:O3'	12:AH:33:ARG:NH2	2.50	0.44
5:BA:1006:C:O4'	5:BA:1156:A:O2'	2.28	0.44
30:BZ:9:ALA:HB1	30:BZ:29:VAL:HG22	1.98	0.44
5:AA:693:C:O2'	22:AR:108:HIS:ND1	2.44	0.44
5:AA:936:A:O2'	5:AA:938:C:OP2	2.36	0.44
5:AA:975:A:O2'	5:AA:976:A:OP1	2.33	0.44
9:AE:31:ASP:OD1	9:AE:32:LYS:N	2.51	0.44
9:AE:59:LEU:O	9:AE:62:ARG:NH1	2.48	0.44
17:AM:53:PRO:O	21:AQ:41:HIS:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:146:A:N1	5:BA:343:G:O2'	2.43	0.44
5:BA:699:C:OP2	22:BR:12:SER:N	2.51	0.44
5:BA:746:A:O2'	5:BA:747:U:OP2	2.25	0.44
5:BA:932:C:H3'	5:BA:933:G:H5"	2.00	0.44
5:BA:1120:G:C6	5:BA:1142:G:N2	2.83	0.44
6:BB:10:ASP:OD1	6:BB:10:ASP:N	2.50	0.44
6:AB:49:ASP:O	6:AB:52:LEU:HD12	2.18	0.44
8:AD:116:LYS:HG2	8:AD:191:LEU:HD12	2.00	0.44
19:AO:44:LEU:CD2	19:AO:50:ALA:HB2	2.48	0.44
22:AR:24:ILE:H	22:AR:24:ILE:HD12	1.82	0.44
5:BA:365:C:OP2	5:BA:384:G:N1	2.45	0.44
5:BA:401:U:O2'	5:BA:450:A:O5'	2.36	0.44
5:BA:525:A:O2'	5:BA:874:G:O2'	2.27	0.44
5:BA:1016:G:H1'	5:BA:1150:G:H21	1.82	0.44
5:AA:1276:G:O6	25:AU:38:ARG:NH1	2.51	0.43
5:BA:56:A:H62	5:BA:92:G:H4'	1.82	0.43
5:BA:911:C:H5"	5:BA:923:A:H61	1.83	0.43
5:BA:1317:G:H5"	21:BQ:33:ILE:HD11	2.00	0.43
13:BI:176:ASN:OD1	13:BI:177:LYS:N	2.50	0.43
5:BA:276:A:O2'	5:BA:277:G:OP1	2.35	0.43
5:BA:935:G:O2'	5:BA:1322:C:N4	2.51	0.43
5:BA:1200:U:HO2'	5:BA:1201:G:C4'	2.31	0.43
26:BV:140:LEU:HA	26:BV:143:ILE:HG22	2.00	0.43
4:A5:19:ALA:HB2	4:A5:78:ILE:HD13	2.00	0.43
6:AB:41:TYR:HB2	6:AB:143:THR:HG21	2.00	0.43
23:AS:21:CYS:SG	23:AS:24:HIS:N	2.90	0.43
5:BA:1210:A:OP1	16:BL:68:GLY:N	2.48	0.43
30:BZ:45:VAL:HG11	30:BZ:49:VAL:HB	2.00	0.43
5:AA:142:G:H21	12:AH:67:THR:HG21	1.82	0.43
18:AN:15:GLY:C	18:AN:79:VAL:HG23	2.39	0.43
3:B3:138:PRO:O	3:B3:142:VAL:HG23	2.18	0.43
3:B4:152:ASP:OD2	3:B4:222:LYS:NZ	2.27	0.43
13:BI:129:ASN:O	13:BI:204:LYS:NZ	2.28	0.43
19:BO:53:ILE:HG12	19:BO:78:ILE:HD11	1.99	0.43
3:A3:68:THR:OG1	3:A3:70:SER:OG	2.34	0.43
3:A4:137:THR:HG23	3:A4:140:ARG:H	1.83	0.43
5:AA:615:G:H22	5:AA:790:G:H4'	1.83	0.43
5:AA:618:G:H22	5:AA:695:G:H1	1.65	0.43
10:AF:22:GLU:OE1	10:AF:25:ALA:N	2.52	0.43
10:AF:62:ALA:HA	10:AF:65:ILE:HG22	2.00	0.43
13:AI:44:LEU:HD11	16:AL:40:ILE:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:530:G:H1	5:BA:718:G:H22	1.66	0.43
5:BA:1213:G:OP1	17:BM:46:ARG:NH2	2.51	0.43
13:BI:2:ALA:HB1	13:BI:5:LEU:HD12	2.01	0.43
13:BI:108:PHE:HA	13:BI:111:ILE:HG12	1.99	0.43
20:BP:5:ARG:N	20:BP:52:GLY:O	2.50	0.43
26:BV:146:GLU:OE1	26:BV:146:GLU:N	2.43	0.43
5:AA:3:U:O4	9:AE:22:ARG:NH2	2.48	0.43
5:AA:91:G:H3'	5:AA:92:G:H21	1.84	0.43
5:AA:1105:C:O2	5:AA:1106:A:N7	2.52	0.43
24:AT:17:VAL:HG13	24:AT:61:LYS:HE2	2.00	0.43
5:BA:34:G:N7	5:BA:450:A:N6	2.66	0.43
5:BA:557:G:C2	5:BA:589:U:C2	3.06	0.43
17:BM:32:VAL:HG23	17:BM:78:ASP:OD1	2.19	0.43
5:AA:30:C:H41	5:AA:393:A:N6	2.17	0.43
5:AA:376:G:N2	5:AA:379:A:OP2	2.51	0.43
18:AN:47:VAL:HG23	18:AN:48:VAL:HG23	2.00	0.43
19:AO:56:GLU:OE2	19:AO:57:LYS:N	2.51	0.43
20:AP:45:LEU:HD11	20:AP:58:GLN:HG2	2.01	0.43
3:B4:36:ASP:OD1	3:B4:37:THR:N	2.50	0.43
3:B4:219:GLU:OE1	3:B4:219:GLU:N	2.52	0.43
4:B5:43:VAL:HG11	4:B5:69:LEU:HG	2.01	0.43
5:BA:422:U:O2'	5:BA:446:G:N2	2.52	0.43
5:BA:475:C:H41	19:BO:70:ARG:HH22	1.65	0.43
5:BA:684:G:H21	5:BA:720:A:P	2.41	0.43
21:BQ:43:PHE:HA	21:BQ:46:VAL:HG22	1.99	0.43
3:A3:150:VAL:HG13	3:A3:155:GLY:HA3	2.00	0.43
5:BA:1119:U:O5'	24:BT:5:ARG:NH2	2.51	0.43
5:BA:1447:A:O2'	5:BA:1448:A:O4'	2.25	0.43
13:BI:68:ILE:HG23	13:BI:100:ALA:HB1	2.01	0.43
23:BS:84:ASP:OD1	23:BS:84:ASP:N	2.50	0.43
8:AD:69:GLN:OE1	8:AD:70:VAL:N	2.51	0.43
3:B3:4:VAL:HG23	3:B3:4:VAL:O	2.19	0.43
5:BA:411:C:O2'	5:BA:412:U:OP2	2.30	0.43
3:A4:206:PHE:HD2	3:A4:223:LEU:HD23	1.83	0.43
7:AC:35:ILE:HD13	7:AC:44:VAL:HG12	2.01	0.43
11:AG:43:GLN:HG3	11:AG:45:LYS:HZ2	1.83	0.43
15:AK:40:GLN:OE1	15:AK:40:GLN:N	2.52	0.43
3:B3:249:GLY:O	3:B3:250:LEU:HD22	2.18	0.43
14:BJ:11:LEU:HD12	14:BJ:74:ALA:HB2	2.00	0.43
18:BN:107:ARG:NH1	30:BZ:61:GLU:OE1	2.52	0.43
3:A3:215:ASP:N	3:A3:215:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A4:260:LEU:HA	3:A4:260:LEU:HD23	1.85	0.42
5:AA:616:G:H22	5:AA:697:A:H2	1.67	0.42
5:AA:1076:G:H4'	17:AM:38:ILE:HD11	2.01	0.42
8:AD:133:GLN:HG3	8:AD:177:ILE:HG22	2.00	0.42
28:AX:32:ALA:HB3	28:AX:39:ALA:O	2.19	0.42
3:B4:109:ALA:O	3:B4:110:SER:OG	2.29	0.42
9:BE:169:MET:SD	9:BE:169:MET:N	2.92	0.42
13:BI:193:ASN:ND2	13:BI:195:ASP:OD2	2.52	0.42
30:BZ:23:ASP:OD1	30:BZ:23:ASP:N	2.52	0.42
5:AA:38:G:H21	9:AE:7:GLN:CD	2.23	0.42
5:AA:718:G:H4'	22:AR:116:LEU:HD22	2.01	0.42
5:AA:1079:G:N2	5:AA:1107:C:N3	2.67	0.42
27:AW:37:LYS:HB2	27:AW:53:ILE:HD11	2.01	0.42
30:AZ:41:ILE:HG23	30:AZ:63:GLU:HG2	2.00	0.42
5:BA:1414:G:H4'	12:BH:78:ILE:HG23	2.00	0.42
5:AA:849:U:OP2	5:AA:864:G:N1	2.44	0.42
6:AB:19:ILE:O	6:AB:157:ASN:ND2	2.52	0.42
11:AG:90:GLY:HA3	11:AG:96:VAL:HG23	2.01	0.42
16:AL:47:GLU:OE2	16:AL:102:TYR:OH	2.31	0.42
18:AN:135:ARG:O	18:AN:137:VAL:N	2.51	0.42
19:AO:94:ILE:HG22	19:AO:95:LYS:HZ2	1.84	0.42
5:BA:553:C:OP2	14:BJ:82:LYS:NZ	2.50	0.42
6:BB:172:ALA:HA	6:BB:175:ILE:HD12	2.00	0.42
10:BF:180:GLU:N	10:BF:180:GLU:OE1	2.53	0.42
20:BP:45:LEU:HD11	20:BP:58:GLN:HG2	2.00	0.42
20:BP:68:ASP:O	20:BP:72:HIS:ND1	2.50	0.42
4:A5:50:LEU:HD12	4:A5:76:PRO:HG2	2.00	0.42
5:AA:334:G:N2	5:AA:347:G:H22	2.16	0.42
15:AK:41:ASP:OD1	15:AK:61:ALA:N	2.52	0.42
25:AU:55:LYS:NZ	25:AU:77:VAL:O	2.28	0.42
3:B4:71:ARG:NH2	5:BA:736:A:N1	2.68	0.42
5:BA:232:G:H5"	23:BS:70:ILE:HD11	2.00	0.42
5:BA:937:A:O2'	5:BA:1282:C:N3	2.52	0.42
7:BC:90:LEU:HD22	7:BC:184:PRO:HA	2.01	0.42
30:BZ:42:ARG:NE	30:BZ:64:ALA:O	2.52	0.42
5:AA:434:A:OP1	5:AA:435:A:N6	2.28	0.42
12:AH:87:LEU:HD11	12:AH:102:ARG:HB3	2.00	0.42
3:B4:16:LEU:H	3:B4:16:LEU:HD12	1.83	0.42
3:B4:31:ILE:HD11	3:B4:78:ARG:HH22	1.84	0.42
5:BA:242:A:O2'	5:BA:243:G:OP2	2.28	0.42
8:BD:69:GLN:NE2	8:BD:70:VAL:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BJ:3:LEU:O	14:BJ:4:LEU:HD23	2.19	0.42
22:BR:109:LEU:HD13	22:BR:119:MET:CE	2.50	0.42
3:A4:6:ILE:HD11	3:A4:84:LEU:HD12	2.01	0.42
5:AA:181:G:N2	23:AS:6:GLY:O	2.53	0.42
5:AA:267:C:OP1	15:AK:87:ARG:NH2	2.51	0.42
5:AA:321:A:O5'	15:AK:47:ARG:NH2	2.53	0.42
5:AA:985:C:H2'	5:AA:986:G:C4	2.54	0.42
11:AG:58:ASN:OD1	11:AG:58:ASN:N	2.53	0.42
16:AL:93:MET:SD	16:AL:94:SER:N	2.92	0.42
5:BA:766:G:O2'	5:BA:767:U:OP2	2.30	0.42
5:BA:1412:A:O2'	12:BH:90:LYS:O	2.38	0.42
3:A3:84:LEU:HD21	3:A3:201:LEU:HD22	2.01	0.42
4:A5:50:LEU:HD13	4:A5:111:VAL:HG13	2.02	0.42
5:AA:19:G:O2'	5:AA:477:G:N3	2.44	0.42
5:AA:594:A:N6	5:AA:595:U:O4	2.52	0.42
5:AA:911:C:H5"	5:AA:923:A:H61	1.85	0.42
10:AF:106:ARG:NH1	10:AF:194:ALA:O	2.52	0.42
10:AF:126:ARG:HE	10:AF:161:SER:HA	1.83	0.42
13:AI:203:LYS:HA	13:AI:206:GLU:HG2	2.02	0.42
15:AK:48:THR:HG21	15:AK:54:LYS:HG3	2.02	0.42
22:AR:19:ARG:NH2	29:AY:63:GLU:O	2.48	0.42
23:AS:78:ILE:O	23:AS:108:ARG:NH2	2.53	0.42
27:AW:19:ILE:HD11	27:AW:69:ALA:HB3	2.02	0.42
27:AW:43:MET:SD	27:AW:43:MET:N	2.91	0.42
28:AX:29:VAL:HG11	28:AX:42:LYS:HZ2	1.85	0.42
3:B3:188:GLU:OE1	3:B4:55:ARG:NH1	2.52	0.42
5:BA:439:G:H21	5:BA:440:C:N4	2.18	0.42
5:BA:627:G:OP1	8:BD:108:ASN:ND2	2.53	0.42
9:BE:102:GLU:HA	9:BE:107:THR:HG21	2.02	0.42
9:BE:164:GLN:OE1	9:BE:164:GLN:N	2.51	0.42
1:A1:22:GLU:OE1	1:A1:41:GLU:N	2.43	0.42
5:AA:433:U:H3'	5:AA:434:A:H4'	2.01	0.42
8:AD:25:ASP:N	8:AD:79:TYR:OH	2.52	0.42
11:AG:218:ILE:O	11:AG:223:ILE:N	2.48	0.42
15:AK:86:ASN:OD1	15:AK:87:ARG:N	2.53	0.42
26:AV:26:ILE:HG22	26:AV:104:GLN:HB3	2.02	0.42
5:BA:142:G:H21	12:BH:67:THR:HG21	1.84	0.42
5:BA:172:G:H5"	15:BK:123:ILE:HD11	2.01	0.42
5:BA:1029:G:O2'	5:BA:1031:G:O6	2.37	0.42
5:AA:627:G:OP1	8:AD:118:ARG:NH2	2.53	0.42
5:AA:1276:G:N7	25:AU:38:ARG:NH2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AB:124:HIS:HA	6:AB:127:MET:HE2	2.01	0.42
17:AM:83:ARG:O	17:AM:87:ARG:NH1	2.52	0.42
8:BD:117:LEU:HD11	8:BD:188:ILE:CG2	2.50	0.42
16:BL:97:GLU:OE1	16:BL:101:LYS:HG3	2.19	0.42
22:BR:68:ASP:CG	22:BR:84:LYS:HZ1	2.22	0.42
29:BY:3:LYS:NZ	29:BY:4:PRO:O	2.47	0.42
5:AA:530:G:C4	5:AA:770:A:C2	3.07	0.42
5:AA:643:G:OP1	18:AN:25:ASN:ND2	2.48	0.42
26:AV:74:ARG:HG3	26:AV:98:ILE:HD11	2.01	0.42
3:B3:276:GLU:O	3:B3:280:ASN:ND2	2.53	0.42
5:BA:1269:G:O2'	20:BP:81:ARG:NH1	2.45	0.42
6:BB:29:LYS:HA	6:BB:32:ILE:HD12	2.02	0.42
6:BB:118:THR:HA	6:BB:140:LEU:HD12	2.02	0.42
9:BE:68:ILE:HG22	9:BE:72:GLN:OE1	2.20	0.42
3:A3:87:TRP:CD1	3:A3:94:VAL:HG22	2.54	0.41
6:AB:118:THR:HA	6:AB:140:LEU:HD12	2.02	0.41
3:B4:242:VAL:HG22	3:B4:279:VAL:HG13	2.02	0.41
5:BA:646:U:OP2	18:BN:24:ASN:ND2	2.52	0.41
5:BA:1246:U:O2'	26:BV:75:THR:O	2.37	0.41
11:BG:89:VAL:HG11	11:BG:114:ILE:HG23	2.02	0.41
11:BG:140:SER:OG	11:BG:182:ASP:O	2.27	0.41
12:BH:33:ARG:NE	12:BH:111:THR:OG1	2.53	0.41
23:BS:41:ASP:N	23:BS:41:ASP:OD1	2.49	0.41
3:A4:247:ASP:OD1	3:A4:249:GLY:N	2.54	0.41
5:AA:839:G:H2'	5:AA:840:C:O4'	2.20	0.41
5:AA:1204:C:O2'	26:AV:47:GLN:NE2	2.52	0.41
5:AA:1256:C:HO2'	5:AA:1262:U:H3	1.63	0.41
5:AA:1378:A:H61	5:AA:1437:G:C2'	2.33	0.41
7:AC:4:GLU:OE1	7:AC:4:GLU:N	2.46	0.41
9:AE:91:ASP:OD1	9:AE:91:ASP:N	2.49	0.41
5:BA:320:G:N1	5:BA:323:A:OP2	2.53	0.41
5:BA:453:G:O2'	5:BA:502:U:O2'	2.12	0.41
5:BA:535:U:H3	5:BA:713:A:H62	1.68	0.41
5:BA:1275:U:OP2	25:BU:38:ARG:NH2	2.53	0.41
7:BC:8:ILE:HD13	17:BM:66:LEU:HD11	2.02	0.41
5:AA:615:G:C6	5:AA:698:A:N1	2.86	0.41
6:AB:182:ILE:HG23	6:AB:187:ASP:HB2	2.02	0.41
7:AC:58:GLY:O	7:AC:63:ARG:NH2	2.48	0.41
8:AD:192:GLU:HG2	8:AD:193:GLU:H	1.84	0.41
14:AJ:37:VAL:HG12	14:AJ:41:MET:HE1	2.01	0.41
25:AU:63:ILE:HG23	25:AU:81:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:235:LEU:HA	3:B4:238:ILE:HD12	2.02	0.41
3:B4:294:GLN:OE1	3:B4:295:ASN:N	2.53	0.41
5:BA:178:C:H2'	5:BA:179:U:C6	2.55	0.41
5:BA:331:C:O2'	5:BA:1393:A:N3	2.39	0.41
5:BA:1070:C:H1'	5:BA:1139:A:C5	2.55	0.41
23:BS:17:ASP:OD1	23:BS:17:ASP:N	2.41	0.41
3:A3:171:SER:HB2	3:A3:172:LEU:HD12	2.03	0.41
5:AA:924:U:O2'	5:AA:925:U:OP2	2.25	0.41
13:AI:132:PRO:O	13:AI:157:ARG:NE	2.43	0.41
27:AW:92:LEU:HD12	27:AW:92:LEU:N	2.35	0.41
3:B3:69:VAL:HG22	3:B3:69:VAL:O	2.20	0.41
4:B5:42:ALA:O	4:B5:46:GLY:N	2.52	0.41
4:B5:57:VAL:HG12	4:B5:59:PRO:HD2	2.03	0.41
5:BA:104:A:OP1	15:BK:11:LYS:NZ	2.23	0.41
5:BA:960:A:H5"	5:BA:961:U:H2'	2.02	0.41
5:BA:1227:A:H62	20:BP:77:TRP:HB2	1.84	0.41
5:BA:1436:U:HO2'	5:BA:1437:G:P	2.43	0.41
6:BB:182:ILE:HG23	6:BB:187:ASP:HB3	2.02	0.41
10:BF:45:LEU:HA	10:BF:48:ILE:HD12	2.03	0.41
13:BI:13:HIS:CE1	16:BL:46:LEU:HD21	2.55	0.41
5:AA:96:G:N2	5:AA:350:G:O4'	2.44	0.41
5:AA:1406:U:O2'	5:AA:1409:G:O6	2.15	0.41
10:AF:116:SER:N	10:AF:119:GLU:OE1	2.46	0.41
5:BA:5:C:O2'	5:BA:459:G:O3'	2.34	0.41
6:BB:198:LYS:HD3	6:BB:198:LYS:N	2.36	0.41
10:BF:128:ARG:N	10:BF:141:ASN:O	2.53	0.41
2:A2:19:ILE:O	2:A2:23:ILE:HG22	2.20	0.41
5:AA:997:G:O6	5:AA:1171:G:O2'	2.38	0.41
5:BA:934:G:N1	17:BM:48:THR:O	2.54	0.41
5:AA:984:C:O2'	28:AX:30:PHE:O	2.39	0.41
6:AB:59:LEU:HD12	6:AB:59:LEU:H	1.85	0.41
12:AH:68:ASP:N	12:AH:72:PHE:O	2.47	0.41
13:AI:47:THR:HG23	13:AI:49:GLY:H	1.86	0.41
5:BA:587:G:H3'	5:BA:588:C:H5'	2.03	0.41
5:BA:1096:G:O3'	16:BL:25:ARG:NH1	2.54	0.41
7:BC:15:MET:HE1	21:BQ:50:LEU:HA	2.03	0.41
1:A1:45:VAL:HG23	1:A1:46:LEU:HD12	2.02	0.41
5:AA:1143:G:HO2'	5:AA:1144:G:P	2.43	0.41
20:AP:81:ARG:HB3	20:AP:93:LEU:HD13	2.03	0.41
26:AV:139:GLU:O	26:AV:143:ILE:HD12	2.20	0.41
5:BA:1116:G:O2'	5:BA:1140:A:N6	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:59:LEU:HD13	11:BG:132:GLU:O	2.21	0.41
11:BG:123:GLU:O	11:BG:209:ASN:ND2	2.48	0.41
19:BO:77:LEU:HD23	19:BO:80:ASN:OD1	2.20	0.41
3:A3:257:LEU:HA	3:A3:260:LEU:HD12	2.02	0.41
3:A4:82:ILE:O	3:A4:86:LEU:HD23	2.20	0.41
5:AA:144:G:O2'	5:AA:145:A:N7	2.52	0.41
5:AA:958:G:N3	5:AA:990:G:N2	2.69	0.41
5:AA:963:A:H62	5:AA:988:A:H1'	1.86	0.41
5:AA:1298:G:P	13:AI:80:LYS:HZ3	2.41	0.41
15:AK:110:VAL:HG12	15:AK:112:SER:H	1.85	0.41
20:AP:38:MET:CE	20:AP:39:VAL:HG13	2.50	0.41
24:AT:17:VAL:HG21	24:AT:57:LEU:HD13	2.03	0.41
26:AV:12:LEU:HD22	26:AV:60:ARG:HE	1.86	0.41
29:AY:3:LYS:HZ3	29:AY:4:PRO:HG2	1.85	0.41
30:AZ:21:THR:O	30:AZ:21:THR:HG22	2.21	0.41
4:B5:39:THR:HG23	4:B5:100:ALA:HB2	2.03	0.41
5:BA:615:G:N2	5:BA:790:G:O3'	2.54	0.41
6:BB:63:GLU:OE1	6:BB:65:GLN:NE2	2.49	0.41
14:BJ:22:LYS:O	14:BJ:23:ARG:NH1	2.53	0.41
18:BN:133:ARG:HE	18:BN:136:ARG:HD3	1.86	0.41
5:AA:1216:A:OP1	7:AC:5:ARG:NH2	2.54	0.41
5:AA:1275:U:C4	5:AA:1279:A:N7	2.89	0.41
7:AC:21:LEU:O	7:AC:25:LEU:N	2.43	0.41
7:AC:185:PRO:O	7:AC:188:ARG:NH2	2.51	0.41
20:AP:109:LEU:HD22	20:AP:116:ARG:HB2	2.02	0.41
23:AS:51:ARG:O	23:AS:68:SER:OG	2.31	0.41
3:B3:54:ILE:O	3:B3:55:ARG:HG2	2.20	0.41
4:B5:78:ILE:HD12	4:B5:114:ILE:HG23	2.02	0.41
20:BP:119:ARG:HB2	20:BP:126:VAL:HG22	2.03	0.41
3:A4:187:GLU:O	3:A4:191:ALA:N	2.51	0.40
5:AA:436:A:H2'	5:AA:437:A:O4'	2.20	0.40
5:AA:1228:A:OP1	26:AV:96:SER:N	2.48	0.40
14:AJ:90:GLU:OE2	14:AJ:113:HIS:NE2	2.53	0.40
18:AN:117:ASP:OD1	18:AN:118:VAL:N	2.54	0.40
3:B3:160:ILE:HD11	3:B3:176:LEU:HD13	2.03	0.40
5:BA:151:G:H2'	5:BA:152:G:C8	2.55	0.40
5:BA:473:A:N6	5:BA:482:G:C2	2.89	0.40
5:BA:1491:C:H2'	5:BA:1492:U:O4'	2.21	0.40
13:BI:111:ILE:CD1	13:BI:188:ILE:HD11	2.51	0.40
22:BR:111:GLN:O	22:BR:111:GLN:NE2	2.53	0.40
5:AA:1093:C:H41	26:AV:138:LYS:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AG:24:MET:SD	11:AG:24:MET:N	2.77	0.40
12:AH:32:LYS:HB2	12:AH:112:ILE:HD12	2.02	0.40
21:AQ:38:LEU:HD21	21:AQ:43:PHE:HA	2.03	0.40
25:AU:72:ILE:HG21	25:AU:98:MET:HB3	2.03	0.40
5:BA:461:A:O3'	5:BA:462:A:H3'	2.20	0.40
5:BA:778:G:O4'	14:BJ:2:THR:N	2.55	0.40
5:BA:1032:A:O3'	11:BG:71:THR:OG1	2.38	0.40
14:BJ:50:PHE:HB2	14:BJ:63:VAL:HG22	2.03	0.40
3:A3:94:VAL:HG12	3:A3:103:VAL:HG12	2.03	0.40
3:A3:140:ARG:NH2	3:A3:239:ASP:OD1	2.54	0.40
5:AA:101:G:H22	5:AA:309:A:H4'	1.87	0.40
5:AA:789:G:C6	5:AA:810:G:C6	3.10	0.40
5:AA:960:A:O2'	5:AA:961:U:OP1	2.28	0.40
5:AA:1247:A:H61	5:AA:1330:G:N2	2.17	0.40
5:AA:1436:U:H2'	5:AA:1437:G:O4'	2.21	0.40
10:AF:186:PHE:CD1	10:AF:242:LEU:HD22	2.56	0.40
3:B4:176:LEU:HA	3:B4:179:MET:SD	2.62	0.40
5:BA:262:G:O2'	5:BA:263:C:P	2.80	0.40
5:BA:975:A:H2'	5:BA:976:A:C8	2.57	0.40
10:BF:168:VAL:N	10:BF:169:PRO:HD2	2.36	0.40
21:BQ:20:ARG:NH2	21:BQ:21:CYS:O	2.53	0.40
26:BV:102:LEU:HD13	26:BV:119:ARG:HD2	2.02	0.40
2:A2:16:TRP:HA	2:A2:19:ILE:HD12	2.04	0.40
4:A5:37:ASN:ND2	5:AA:962:G:OP1	2.55	0.40
5:AA:207:G:H1'	5:AA:210:A:H62	1.87	0.40
5:AA:262:G:O2'	5:AA:263:C:P	2.79	0.40
5:AA:376:G:H3'	5:AA:377:A:C5'	2.52	0.40
10:AF:12:ARG:NH1	10:AF:28:TRP:O	2.55	0.40
18:AN:25:ASN:OD1	18:AN:26:THR:N	2.50	0.40
20:AP:111:ARG:NH1	25:AU:97:GLU:OE1	2.55	0.40
3:B3:232:LEU:HG	3:B3:260:LEU:HD21	2.04	0.40
3:B4:20:LYS:NZ	3:B4:214:LEU:O	2.54	0.40
3:B4:97:ILE:HG22	3:B4:98:GLU:H	1.86	0.40
5:BA:950:C:H41	5:BA:1172:A:H1'	1.86	0.40
5:BA:1307:G:O2'	5:BA:1308:U:P	2.79	0.40
10:BF:105:ASN:N	10:BF:109:LYS:O	2.43	0.40
3:A4:183:ILE:HD11	3:A4:202:VAL:HG11	2.04	0.40
5:AA:702:G:OP1	29:AY:11:SER:OG	2.39	0.40
5:AA:975:A:HO2'	5:AA:976:A:P	2.43	0.40
5:AA:990:G:O2'	5:AA:991:C:O4'	2.37	0.40
10:AF:175:GLU:N	10:AF:175:GLU:OE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AR:92:PRO:CD	22:AR:142:LEU:HD21	2.50	0.40
3:B3:184:LYS:NZ	3:B4:298:GLY:O	2.54	0.40
5:BA:39:U:H3	5:BA:394:C:H42	1.70	0.40
5:BA:1105:C:O2'	5:BA:1106:A:O5'	2.38	0.40
14:BJ:13:HIS:O	14:BJ:17:SER:OG	2.25	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	A1	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
1	B1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
2	A2	33/37 (89%)	33 (100%)	0	0	100	100
2	B2	33/37 (89%)	31 (94%)	2 (6%)	0	100	100
3	A3	294/306 (96%)	268 (91%)	26 (9%)	0	100	100
3	A4	288/306 (94%)	265 (92%)	23 (8%)	0	100	100
3	B3	291/306 (95%)	265 (91%)	25 (9%)	1 (0%)	37	69
3	B4	286/306 (94%)	263 (92%)	23 (8%)	0	100	100
4	A5	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
4	B5	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
6	AB	195/202 (96%)	182 (93%)	13 (7%)	0	100	100
6	BB	195/202 (96%)	188 (96%)	7 (4%)	0	100	100
7	AC	193/210 (92%)	186 (96%)	7 (4%)	0	100	100
7	BC	193/210 (92%)	188 (97%)	4 (2%)	1 (0%)	25	60
8	AD	182/198 (92%)	181 (100%)	1 (0%)	0	100	100
8	BD	182/198 (92%)	180 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AE	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
9	BE	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
10	AF	240/243 (99%)	226 (94%)	14 (6%)	0	100	100
10	BF	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
11	AG	225/236 (95%)	217 (96%)	8 (4%)	0	100	100
11	BG	225/236 (95%)	215 (96%)	10 (4%)	0	100	100
12	AH	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
12	BH	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
13	AI	212/215 (99%)	193 (91%)	18 (8%)	1 (0%)	25	60
13	BI	212/215 (99%)	192 (91%)	20 (9%)	0	100	100
14	AJ	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
14	BJ	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
15	AK	122/127 (96%)	116 (95%)	6 (5%)	0	100	100
15	BK	122/127 (96%)	118 (97%)	4 (3%)	0	100	100
16	AL	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
16	BL	126/135 (93%)	120 (95%)	5 (4%)	1 (1%)	16	51
17	AM	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
17	BM	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
18	AN	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
18	BN	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
19	AO	141/147 (96%)	131 (93%)	10 (7%)	0	100	100
19	BO	141/147 (96%)	139 (99%)	2 (1%)	0	100	100
20	AP	129/148 (87%)	124 (96%)	5 (4%)	0	100	100
20	BP	129/148 (87%)	123 (95%)	6 (5%)	0	100	100
21	AQ	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
21	BQ	48/56 (86%)	44 (92%)	4 (8%)	0	100	100
22	AR	153/158 (97%)	146 (95%)	7 (5%)	0	100	100
22	BR	153/158 (97%)	149 (97%)	4 (3%)	0	100	100
23	AS	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
23	BS	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
24	AT	61/67 (91%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BT	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
25	AU	113/132 (86%)	110 (97%)	3 (3%)	0	100	100
25	BU	113/132 (86%)	108 (96%)	5 (4%)	0	100	100
26	AV	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
26	BV	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
27	AW	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
27	BW	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
28	AX	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
28	BX	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
29	AY	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
29	BY	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
30	AZ	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
30	BZ	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
All	All	8173/8652 (94%)	7767 (95%)	402 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B3	269	ILE
13	AI	15	ILE
16	BL	119	PRO
7	BC	78	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	53/53 (100%)	52 (98%)	1 (2%)	52	76
1	B1	53/53 (100%)	52 (98%)	1 (2%)	52	76
2	A2	33/35 (94%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B2	33/35 (94%)	33 (100%)	0	100	100
3	A3	265/273 (97%)	260 (98%)	5 (2%)	52	76
3	A4	260/273 (95%)	254 (98%)	6 (2%)	45	72
3	B3	263/273 (96%)	259 (98%)	4 (2%)	60	81
3	B4	258/273 (94%)	246 (95%)	12 (5%)	22	55
4	A5	99/99 (100%)	99 (100%)	0	100	100
4	B5	99/99 (100%)	98 (99%)	1 (1%)	73	87
6	AB	169/173 (98%)	163 (96%)	6 (4%)	30	62
6	BB	169/173 (98%)	168 (99%)	1 (1%)	84	92
7	AC	153/167 (92%)	150 (98%)	3 (2%)	50	75
7	BC	153/167 (92%)	151 (99%)	2 (1%)	65	83
8	AD	161/171 (94%)	156 (97%)	5 (3%)	35	66
8	BD	161/171 (94%)	157 (98%)	4 (2%)	42	71
9	AE	156/160 (98%)	154 (99%)	2 (1%)	65	83
9	BE	156/160 (98%)	153 (98%)	3 (2%)	52	76
10	AF	212/213 (100%)	205 (97%)	7 (3%)	33	64
10	BF	212/213 (100%)	208 (98%)	4 (2%)	52	76
11	AG	188/197 (95%)	179 (95%)	9 (5%)	21	55
11	BG	188/197 (95%)	185 (98%)	3 (2%)	58	79
12	AH	107/108 (99%)	104 (97%)	3 (3%)	38	68
12	BH	107/108 (99%)	106 (99%)	1 (1%)	75	89
13	AI	183/184 (100%)	175 (96%)	8 (4%)	24	57
13	BI	183/184 (100%)	181 (99%)	2 (1%)	70	86
14	AJ	107/108 (99%)	105 (98%)	2 (2%)	52	76
14	BJ	107/108 (99%)	106 (99%)	1 (1%)	75	89
15	AK	100/103 (97%)	96 (96%)	4 (4%)	27	59
15	BK	100/103 (97%)	98 (98%)	2 (2%)	50	75
16	AL	104/111 (94%)	104 (100%)	0	100	100
16	BL	104/111 (94%)	100 (96%)	4 (4%)	28	60
17	AM	91/91 (100%)	87 (96%)	4 (4%)	24	57
17	BM	91/91 (100%)	87 (96%)	4 (4%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AN	94/104 (90%)	94 (100%)	0	100 100
18	BN	94/104 (90%)	92 (98%)	2 (2%)	48 74
19	AO	117/121 (97%)	117 (100%)	0	100 100
19	BO	117/121 (97%)	114 (97%)	3 (3%)	41 70
20	AP	108/122 (88%)	105 (97%)	3 (3%)	38 68
20	BP	108/122 (88%)	106 (98%)	2 (2%)	52 76
21	AQ	42/46 (91%)	38 (90%)	4 (10%)	7 28
21	BQ	42/46 (91%)	39 (93%)	3 (7%)	12 42
22	AR	140/143 (98%)	138 (99%)	2 (1%)	62 82
22	BR	140/143 (98%)	139 (99%)	1 (1%)	81 92
23	AS	99/102 (97%)	97 (98%)	2 (2%)	50 75
23	BS	99/102 (97%)	98 (99%)	1 (1%)	73 87
24	AT	57/61 (93%)	57 (100%)	0	100 100
24	BT	57/61 (93%)	55 (96%)	2 (4%)	31 63
25	AU	101/114 (89%)	96 (95%)	5 (5%)	20 54
25	BU	101/114 (89%)	100 (99%)	1 (1%)	73 87
26	AV	125/127 (98%)	123 (98%)	2 (2%)	58 79
26	BV	125/127 (98%)	120 (96%)	5 (4%)	27 59
27	AW	84/89 (94%)	79 (94%)	5 (6%)	16 48
27	BW	84/89 (94%)	82 (98%)	2 (2%)	44 71
28	AX	37/41 (90%)	36 (97%)	1 (3%)	40 69
28	BX	37/41 (90%)	37 (100%)	0	100 100
29	AY	53/54 (98%)	52 (98%)	1 (2%)	52 76
29	BY	53/54 (98%)	52 (98%)	1 (2%)	52 76
30	AZ	56/60 (93%)	56 (100%)	0	100 100
30	BZ	56/60 (93%)	56 (100%)	0	100 100
All	All	7104/7406 (96%)	6942 (98%)	162 (2%)	46 72

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	32	CYS
3	A3	76	SER

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Mol	Chain	Res	Type
3	A3	88	ASN
3	A3	167	GLN
3	A3	203	ASP
3	A3	218	ARG
3	A4	117	LYS
3	A4	143	TYR
3	A4	152	ASP
3	A4	253	SER
3	A4	262	ASN
3	A4	265	ARG
6	AB	38	ASP
6	AB	52	LEU
6	AB	148	SER
6	AB	149	TYR
6	AB	184	SER
6	AB	188	PHE
7	AC	6	TYR
7	AC	27	ARG
7	AC	53	TYR
8	AD	38	ASP
8	AD	59	PHE
8	AD	85	MET
8	AD	104	ASP
8	AD	184	GLU
9	AE	86	ASP
9	AE	169	MET
10	AF	39	MET
10	AF	63	ARG
10	AF	121	PHE
10	AF	128	ARG
10	AF	157	ASN
10	AF	211	ASP
10	AF	231	PHE
11	AG	8	TYR
11	AG	24	MET
11	AG	25	MET
11	AG	33	ASP
11	AG	51	ASP
11	AG	82	ARG
11	AG	143	PHE
11	AG	169	ASP
11	AG	196	ASN

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Mol	Chain	Res	Type
12	AH	44	ASN
12	AH	58	ASP
12	AH	82	ARG
13	AI	9	PHE
13	AI	46	HIS
13	AI	50	ARG
13	AI	92	SER
13	AI	140	MET
13	AI	146	TYR
13	AI	155	MET
13	AI	164	ASN
14	AJ	57	ARG
14	AJ	112	SER
15	AK	25	LYS
15	AK	62	TYR
15	AK	124	LEU
15	AK	125	LEU
17	AM	7	LYS
17	AM	80	ARG
17	AM	82	MET
17	AM	97	GLU
20	AP	38	MET
20	AP	49	MET
20	AP	100	MET
21	AQ	20	ARG
21	AQ	24	CYS
21	AQ	36	LEU
21	AQ	39	CYS
22	AR	4	MET
22	AR	57	GLN
23	AS	35	GLU
23	AS	54	TYR
25	AU	17	MET
25	AU	20	SER
25	AU	28	PHE
25	AU	60	LYS
25	AU	95	LYS
26	AV	42	GLU
26	AV	61	ARG
27	AW	20	TYR
27	AW	33	ARG
27	AW	45	ASP

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Mol	Chain	Res	Type
27	AW	57	ARG
27	AW	90	ASP
28	AX	5	TRP
29	AY	36	ARG
1	B1	4	MET
3	B3	143	TYR
3	B3	157	LYS
3	B3	254	LYS
3	B3	292	ASP
3	B4	12	TYR
3	B4	16	LEU
3	B4	23	LYS
3	B4	33	LYS
3	B4	58	TYR
3	B4	120	SER
3	B4	143	TYR
3	B4	152	ASP
3	B4	179	MET
3	B4	223	LEU
3	B4	264	LYS
3	B4	294	GLN
4	B5	77	TYR
6	BB	38	ASP
7	BC	20	PHE
7	BC	72	GLN
8	BD	90	SER
8	BD	120	MET
8	BD	157	PHE
8	BD	172	LYS
9	BE	72	GLN
9	BE	160	PHE
9	BE	170	MET
10	BF	38	ASN
10	BF	128	ARG
10	BF	179	PHE
10	BF	211	ASP
11	BG	42	TYR
11	BG	73	ARG
11	BG	143	PHE
12	BH	4	PHE
13	BI	13	HIS
13	BI	46	HIS

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Mol	Chain	Res	Type
14	BJ	130	TYR
15	BK	62	TYR
15	BK	83	ASN
16	BL	49	LEU
16	BL	51	LEU
16	BL	57	TRP
16	BL	94	SER
17	BM	61	PHE
17	BM	74	ASP
17	BM	84	GLN
17	BM	100	LEU
18	BN	61	MET
18	BN	111	LYS
19	BO	69	MET
19	BO	71	LYS
19	BO	96	PHE
20	BP	46	ASP
20	BP	85	TYR
21	BQ	13	LYS
21	BQ	20	ARG
21	BQ	39	CYS
22	BR	104	ASN
23	BS	84	ASP
24	BT	30	HIS
24	BT	36	GLN
25	BU	11	TYR
26	BV	12	LEU
26	BV	49	ASP
26	BV	50	TRP
26	BV	65	ASP
26	BV	90	PHE
27	BW	78	MET
27	BW	85	TYR
29	BY	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
7	BC	77	ASN
13	BI	94	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	AA	1494/1495 (99%)	295 (19%)	43 (2%)
5	BA	1494/1495 (99%)	290 (19%)	46 (3%)
All	All	2988/2990 (99%)	585 (19%)	89 (2%)

All (585) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AA	2	U
5	AA	3	U
5	AA	4	C
5	AA	20	G
5	AA	32	A
5	AA	35	G
5	AA	40	C
5	AA	42	G
5	AA	43	A
5	AA	44	C
5	AA	47	A
5	AA	50	C
5	AA	57	G
5	AA	59	C
5	AA	61	A
5	AA	62	G
5	AA	64	G
5	AA	73	U
5	AA	74	U
5	AA	76	U
5	AA	100	A
5	AA	104	A
5	AA	105	C
5	AA	106	A
5	AA	112	G
5	AA	114	A
5	AA	115	A
5	AA	116	C
5	AA	129	G
5	AA	151	G
5	AA	155	U
5	AA	158	U
5	AA	175	G
5	AA	177	A

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Mol	Chain	Res	Type
5	AA	197	A
5	AA	199	A
5	AA	222	G
5	AA	229	G
5	AA	240	U
5	AA	241	U
5	AA	243	G
5	AA	247	G
5	AA	248	U
5	AA	254	G
5	AA	255	G
5	AA	262	G
5	AA	263	C
5	AA	278	A
5	AA	285	C
5	AA	297	G
5	AA	299	G
5	AA	321	A
5	AA	324	C
5	AA	325	A
5	AA	326	C
5	AA	328	G
5	AA	340	A
5	AA	341	C
5	AA	342	G
5	AA	343	G
5	AA	344	G
5	AA	347	G
5	AA	348	C
5	AA	349	A
5	AA	350	G
5	AA	363	C
5	AA	369	A
5	AA	370	A
5	AA	377	A
5	AA	378	A
5	AA	379	A
5	AA	384	G
5	AA	393	A
5	AA	394	C
5	AA	400	G
5	AA	402	G

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Mol	Chain	Res	Type
5	AA	409	C
5	AA	410	U
5	AA	413	G
5	AA	422	U
5	AA	423	U
5	AA	424	U
5	AA	432	G
5	AA	434	A
5	AA	436	A
5	AA	438	A
5	AA	439	G
5	AA	440	C
5	AA	445	G
5	AA	448	A
5	AA	450	A
5	AA	460	C
5	AA	461	A
5	AA	462	A
5	AA	463	G
5	AA	464	G
5	AA	465	C
5	AA	471	G
5	AA	472	C
5	AA	474	G
5	AA	480	G
5	AA	484	U
5	AA	485	A
5	AA	486	A
5	AA	487	U
5	AA	500	A
5	AA	509	C
5	AA	516	A
5	AA	517	U
5	AA	525	A
5	AA	529	C
5	AA	530	G
5	AA	531	G
5	AA	540	G
5	AA	541	G
5	AA	564	C
5	AA	585	U
5	AA	586	C

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Mol	Chain	Res	Type
5	AA	587	G
5	AA	588	C
5	AA	596	A
5	AA	606	U
5	AA	607	U
5	AA	610	G
5	AA	615	G
5	AA	619	A
5	AA	640	U
5	AA	641	A
5	AA	642	G
5	AA	649	A
5	AA	655	A
5	AA	656	U
5	AA	657	A
5	AA	673	C
5	AA	675	A
5	AA	676	G
5	AA	677	U
5	AA	678	G
5	AA	685	G
5	AA	702	G
5	AA	707	A
5	AA	709	G
5	AA	713	A
5	AA	735	A
5	AA	746	A
5	AA	747	U
5	AA	748	A
5	AA	767	U
5	AA	769	A
5	AA	771	G
5	AA	775	G
5	AA	782	A
5	AA	799	C
5	AA	800	G
5	AA	801	A
5	AA	802	G
5	AA	804	U
5	AA	860	G
5	AA	872	A
5	AA	884	G

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Mol	Chain	Res	Type
5	AA	885	G
5	AA	892	C
5	AA	893	U
5	AA	901	G
5	AA	903	G
5	AA	904	G
5	AA	917	A
5	AA	918	A
5	AA	919	U
5	AA	920	U
5	AA	924	U
5	AA	925	U
5	AA	928	A
5	AA	930	G
5	AA	933	G
5	AA	934	G
5	AA	935	G
5	AA	936	A
5	AA	937	A
5	AA	941	C
5	AA	951	G
5	AA	954	G
5	AA	960	A
5	AA	961	U
5	AA	962	G
5	AA	964	A
5	AA	965	G
5	AA	970	G
5	AA	972	C
5	AA	973	U
5	AA	976	A
5	AA	977	G
5	AA	978	G
5	AA	983	G
5	AA	987	G
5	AA	989	C
5	AA	990	G
5	AA	995	G
5	AA	997	G
5	AA	998	A
5	AA	1002	G
5	AA	1005	G

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Mol	Chain	Res	Type
5	AA	1006	C
5	AA	1008	U
5	AA	1010	G
5	AA	1017	U
5	AA	1018	C
5	AA	1020	G
5	AA	1040	A
5	AA	1044	A
5	AA	1046	G
5	AA	1047	U
5	AA	1048	G
5	AA	1053	A
5	AA	1054	A
5	AA	1076	G
5	AA	1077	U
5	AA	1081	C
5	AA	1082	A
5	AA	1094	U
5	AA	1096	G
5	AA	1104	G
5	AA	1105	C
5	AA	1112	G
5	AA	1118	C
5	AA	1119	U
5	AA	1128	U
5	AA	1144	G
5	AA	1156	A
5	AA	1157	G
5	AA	1160	C
5	AA	1161	A
5	AA	1162	G
5	AA	1171	G
5	AA	1172	A
5	AA	1173	A
5	AA	1174	A
5	AA	1175	C
5	AA	1184	U
5	AA	1185	A
5	AA	1197	C
5	AA	1198	A
5	AA	1199	A
5	AA	1200	U

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Mol	Chain	Res	Type
5	AA	1205	G
5	AA	1210	A
5	AA	1213	G
5	AA	1214	G
5	AA	1217	C
5	AA	1218	C
5	AA	1220	G
5	AA	1230	G
5	AA	1239	A
5	AA	1240	A
5	AA	1246	U
5	AA	1247	A
5	AA	1258	C
5	AA	1260	G
5	AA	1261	U
5	AA	1262	U
5	AA	1263	C
5	AA	1265	G
5	AA	1296	U
5	AA	1298	G
5	AA	1305	U
5	AA	1307	G
5	AA	1308	U
5	AA	1313	G
5	AA	1323	A
5	AA	1324	U
5	AA	1328	G
5	AA	1332	C
5	AA	1337	A
5	AA	1341	C
5	AA	1354	A
5	AA	1358	A
5	AA	1377	G
5	AA	1407	U
5	AA	1409	G
5	AA	1413	G
5	AA	1422	G
5	AA	1424	G
5	AA	1437	G
5	AA	1445	A
5	AA	1454	A
5	AA	1457	A

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Mol	Chain	Res	Type
5	AA	1459	G
5	AA	1460	G
5	AA	1461	U
5	AA	1475	C
5	AA	1484	C
5	AA	1485	G
5	AA	1487	U
5	AA	1491	C
5	AA	1492	U
5	BA	2	U
5	BA	4	C
5	BA	8	U
5	BA	17	C
5	BA	34	G
5	BA	38	G
5	BA	40	C
5	BA	42	G
5	BA	43	A
5	BA	44	C
5	BA	47	A
5	BA	57	G
5	BA	60	A
5	BA	73	U
5	BA	74	U
5	BA	75	C
5	BA	77	G
5	BA	85	A
5	BA	89	G
5	BA	100	A
5	BA	101	G
5	BA	104	A
5	BA	105	C
5	BA	106	A
5	BA	112	G
5	BA	114	A
5	BA	115	A
5	BA	116	C
5	BA	135	U
5	BA	146	A
5	BA	148	C
5	BA	149	U
5	BA	177	A

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Mol	Chain	Res	Type
5	BA	183	A
5	BA	197	A
5	BA	199	A
5	BA	226	G
5	BA	240	U
5	BA	241	U
5	BA	243	G
5	BA	247	G
5	BA	254	G
5	BA	258	A
5	BA	262	G
5	BA	263	C
5	BA	266	A
5	BA	277	G
5	BA	278	A
5	BA	285	C
5	BA	304	C
5	BA	312	U
5	BA	317	A
5	BA	324	C
5	BA	325	A
5	BA	328	G
5	BA	340	A
5	BA	341	C
5	BA	343	G
5	BA	347	G
5	BA	348	C
5	BA	349	A
5	BA	350	G
5	BA	361	A
5	BA	363	C
5	BA	369	A
5	BA	370	A
5	BA	393	A
5	BA	394	C
5	BA	402	G
5	BA	409	C
5	BA	410	U
5	BA	411	C
5	BA	412	U
5	BA	413	G
5	BA	423	U

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Mol	Chain	Res	Type
5	BA	424	U
5	BA	425	C
5	BA	432	G
5	BA	433	U
5	BA	434	A
5	BA	435	A
5	BA	436	A
5	BA	438	A
5	BA	439	G
5	BA	440	C
5	BA	449	U
5	BA	450	A
5	BA	458	G
5	BA	459	G
5	BA	460	C
5	BA	461	A
5	BA	462	A
5	BA	463	G
5	BA	464	G
5	BA	465	C
5	BA	471	G
5	BA	472	C
5	BA	474	G
5	BA	480	G
5	BA	486	A
5	BA	500	A
5	BA	513	A
5	BA	516	A
5	BA	517	U
5	BA	520	G
5	BA	525	A
5	BA	526	A
5	BA	529	C
5	BA	530	G
5	BA	549	A
5	BA	572	U
5	BA	585	U
5	BA	586	C
5	BA	588	C
5	BA	596	A
5	BA	607	U
5	BA	615	G

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Mol	Chain	Res	Type
5	BA	619	A
5	BA	640	U
5	BA	641	A
5	BA	642	G
5	BA	649	A
5	BA	655	A
5	BA	657	A
5	BA	671	C
5	BA	673	C
5	BA	677	U
5	BA	678	G
5	BA	685	G
5	BA	702	G
5	BA	703	U
5	BA	707	A
5	BA	709	G
5	BA	731	A
5	BA	735	A
5	BA	741	A
5	BA	747	U
5	BA	748	A
5	BA	767	U
5	BA	769	A
5	BA	771	G
5	BA	775	G
5	BA	782	A
5	BA	798	U
5	BA	799	C
5	BA	800	G
5	BA	801	A
5	BA	804	U
5	BA	829	U
5	BA	831	A
5	BA	847	A
5	BA	848	G
5	BA	860	G
5	BA	872	A
5	BA	880	G
5	BA	884	G
5	BA	885	G
5	BA	890	C
5	BA	892	C

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Mol	Chain	Res	Type
5	BA	904	G
5	BA	910	G
5	BA	917	A
5	BA	918	A
5	BA	919	U
5	BA	920	U
5	BA	924	U
5	BA	925	U
5	BA	928	A
5	BA	930	G
5	BA	931	C
5	BA	933	G
5	BA	934	G
5	BA	935	G
5	BA	936	A
5	BA	939	C
5	BA	950	C
5	BA	951	G
5	BA	953	C
5	BA	960	A
5	BA	961	U
5	BA	962	G
5	BA	963	A
5	BA	964	A
5	BA	968	C
5	BA	970	G
5	BA	976	A
5	BA	977	G
5	BA	978	G
5	BA	983	G
5	BA	986	G
5	BA	987	G
5	BA	989	C
5	BA	991	C
5	BA	993	C
5	BA	998	A
5	BA	1002	G
5	BA	1005	G
5	BA	1006	C
5	BA	1007	A
5	BA	1017	U
5	BA	1018	C

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Mol	Chain	Res	Type
5	BA	1020	G
5	BA	1022	U
5	BA	1033	G
5	BA	1038	C
5	BA	1046	G
5	BA	1047	U
5	BA	1053	A
5	BA	1054	A
5	BA	1077	U
5	BA	1081	C
5	BA	1082	A
5	BA	1093	C
5	BA	1096	G
5	BA	1105	C
5	BA	1110	U
5	BA	1112	G
5	BA	1117	A
5	BA	1119	U
5	BA	1128	U
5	BA	1131	G
5	BA	1143	G
5	BA	1144	G
5	BA	1157	G
5	BA	1162	G
5	BA	1171	G
5	BA	1172	A
5	BA	1175	C
5	BA	1184	U
5	BA	1185	A
5	BA	1186	C
5	BA	1187	A
5	BA	1198	A
5	BA	1200	U
5	BA	1201	G
5	BA	1202	G
5	BA	1209	C
5	BA	1210	A
5	BA	1213	G
5	BA	1214	G
5	BA	1218	C
5	BA	1220	G
5	BA	1230	G

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Mol	Chain	Res	Type
5	BA	1239	A
5	BA	1240	A
5	BA	1245	C
5	BA	1246	U
5	BA	1247	A
5	BA	1252	C
5	BA	1253	G
5	BA	1260	G
5	BA	1261	U
5	BA	1262	U
5	BA	1263	C
5	BA	1264	G
5	BA	1265	G
5	BA	1279	A
5	BA	1280	C
5	BA	1281	U
5	BA	1296	U
5	BA	1307	G
5	BA	1308	U
5	BA	1323	A
5	BA	1324	U
5	BA	1325	C
5	BA	1332	C
5	BA	1336	U
5	BA	1337	A
5	BA	1341	C
5	BA	1343	C
5	BA	1354	A
5	BA	1357	C
5	BA	1358	A
5	BA	1410	G
5	BA	1424	G
5	BA	1437	G
5	BA	1445	A
5	BA	1452	G
5	BA	1454	A
5	BA	1457	A
5	BA	1458	A
5	BA	1459	G
5	BA	1461	U
5	BA	1471	G
5	BA	1473	A

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Mol	Chain	Res	Type
5	BA	1475	C
5	BA	1484	C
5	BA	1485	G
5	BA	1487	U
5	BA	1491	C

All (89) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AA	43	A
5	AA	56	A
5	AA	99	C
5	AA	111	G
5	AA	176	U
5	AA	239	A
5	AA	246	A
5	AA	262	G
5	AA	277	G
5	AA	368	C
5	AA	408	C
5	AA	431	U
5	AA	471	G
5	AA	641	A
5	AA	655	A
5	AA	672	G
5	AA	712	G
5	AA	766	G
5	AA	871	A
5	AA	919	U
5	AA	924	U
5	AA	960	A
5	AA	975	A
5	AA	977	G
5	AA	1017	U
5	AA	1019	A
5	AA	1053	A
5	AA	1143	G
5	AA	1161	A
5	AA	1217	C
5	AA	1245	C
5	AA	1260	G
5	AA	1261	U

Continued on next page...

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Mol	Chain	Res	Type
5	AA	1262	U
5	AA	1306	A
5	AA	1307	G
5	AA	1322	C
5	AA	1340	U
5	AA	1436	U
5	AA	1453	U
5	AA	1459	G
5	AA	1460	G
5	AA	1483	U
5	BA	42	G
5	BA	43	A
5	BA	56	A
5	BA	99	C
5	BA	111	G
5	BA	176	U
5	BA	239	A
5	BA	246	A
5	BA	262	G
5	BA	277	G
5	BA	324	C
5	BA	368	C
5	BA	408	C
5	BA	424	U
5	BA	431	U
5	BA	434	A
5	BA	458	G
5	BA	462	A
5	BA	471	G
5	BA	528	G
5	BA	584	C
5	BA	641	A
5	BA	672	G
5	BA	746	A
5	BA	766	G
5	BA	871	A
5	BA	891	A
5	BA	919	U
5	BA	924	U
5	BA	975	A
5	BA	977	G
5	BA	985	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	1019	A
5	BA	1053	A
5	BA	1161	A
5	BA	1245	C
5	BA	1260	G
5	BA	1261	U
5	BA	1262	U
5	BA	1306	A
5	BA	1307	G
5	BA	1340	U
5	BA	1436	U
5	BA	1453	U
5	BA	1460	G
5	BA	1483	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

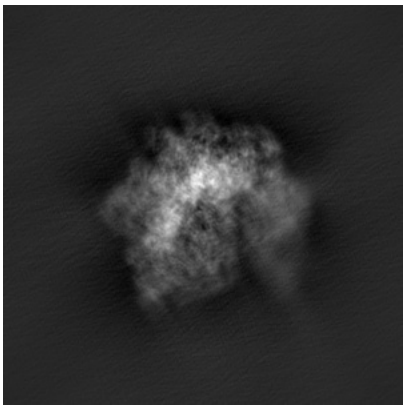
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50611. These allow visual inspection of the internal detail of the map and identification of artifacts.

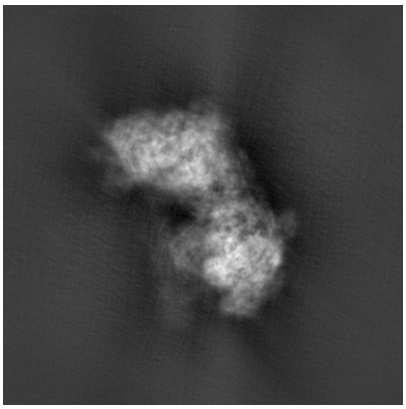
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

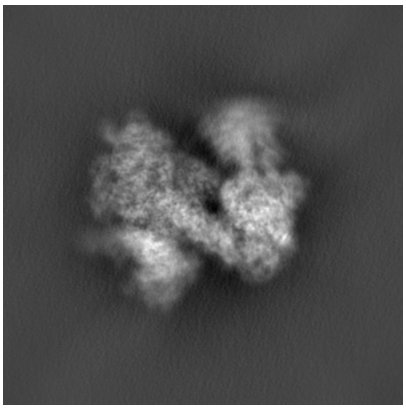
6.1.1 Primary map



X

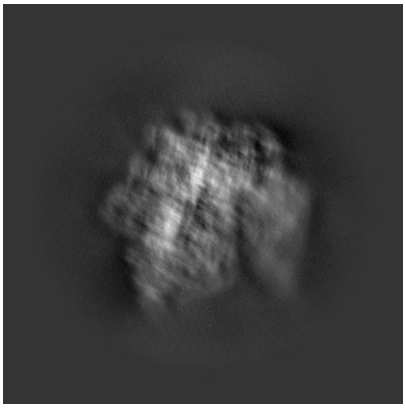


Y

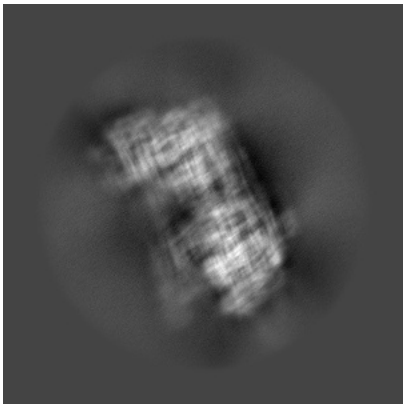


Z

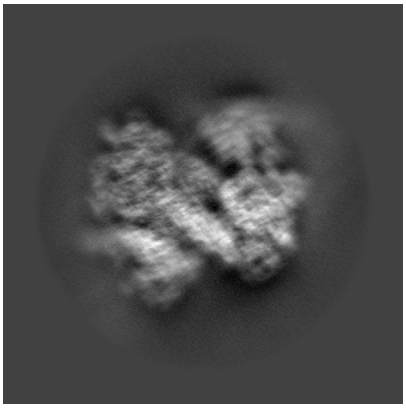
6.1.2 Raw map



X



Y

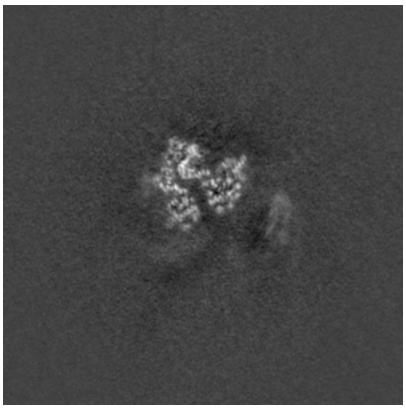


Z

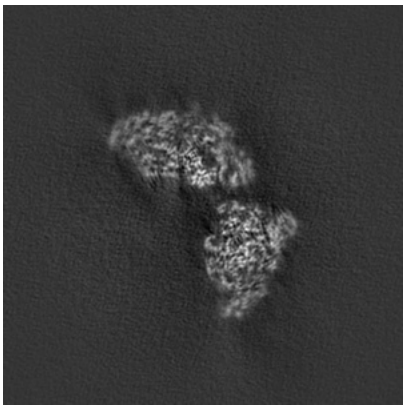
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

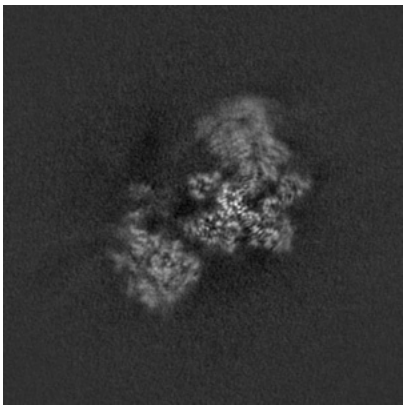
6.2.1 Primary map



X Index: 288

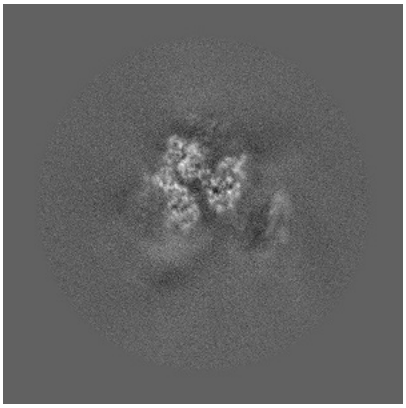


Y Index: 288

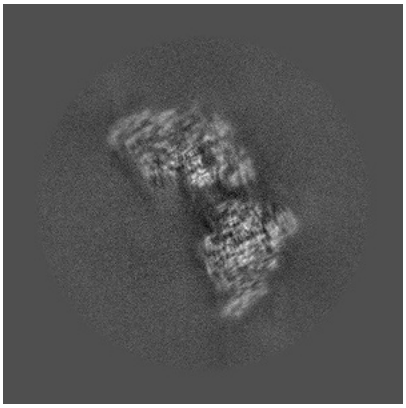


Z Index: 288

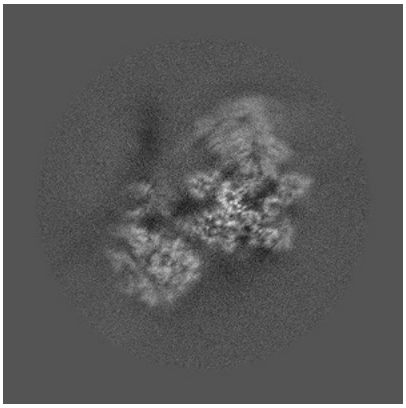
6.2.2 Raw map



X Index: 288



Y Index: 288

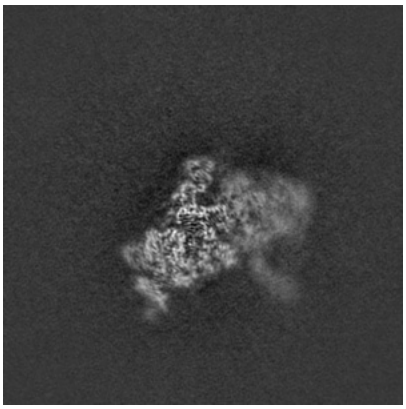


Z Index: 288

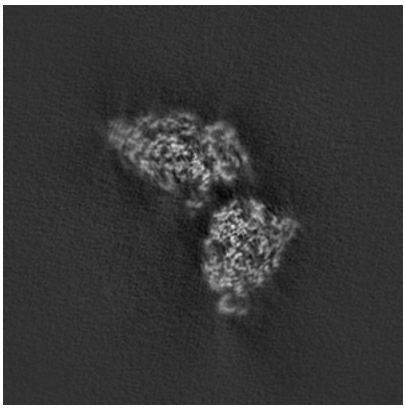
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

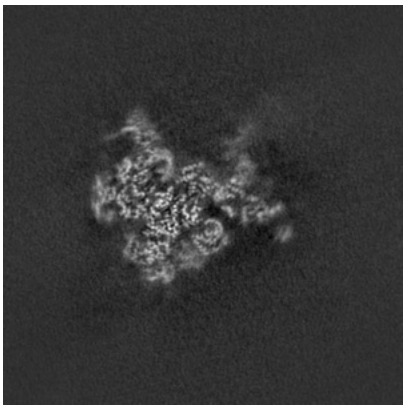
6.3.1 Primary map



X Index: 354

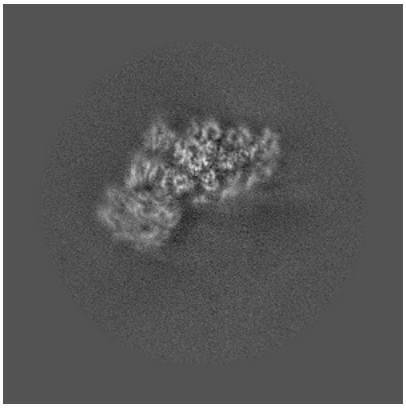


Y Index: 278

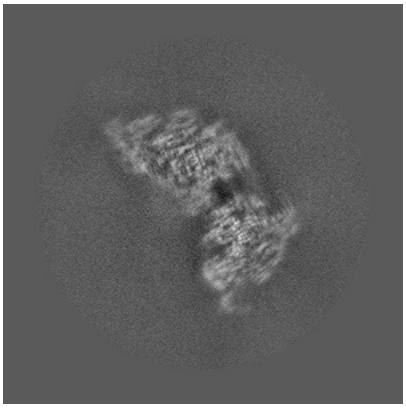


Z Index: 324

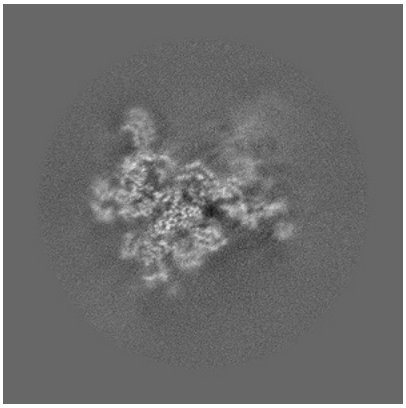
6.3.2 Raw map



X Index: 231



Y Index: 273

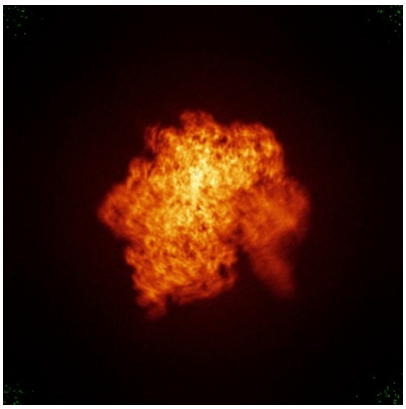


Z Index: 319

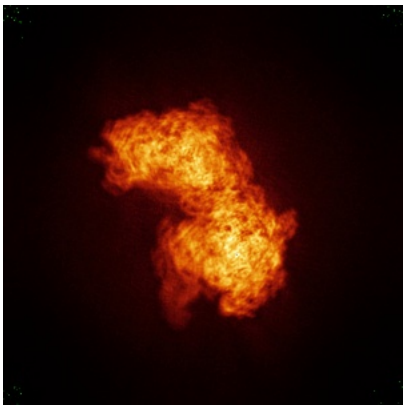
The images above show the largest variance slices of the map in three orthogonal directions.

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

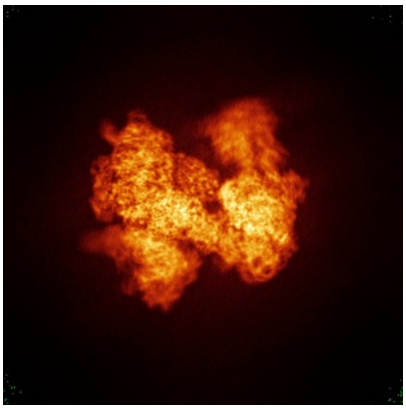
6.4.1 Primary map



X

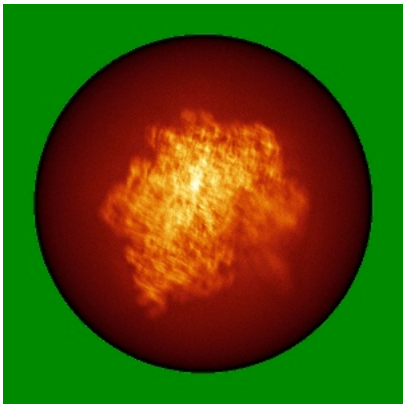


Y

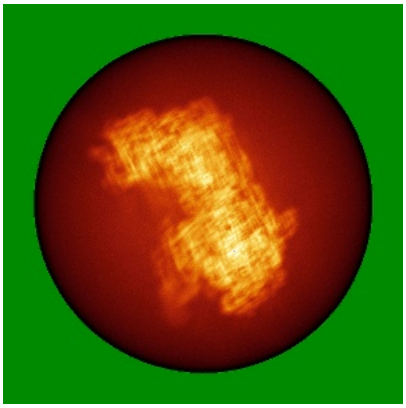


Z

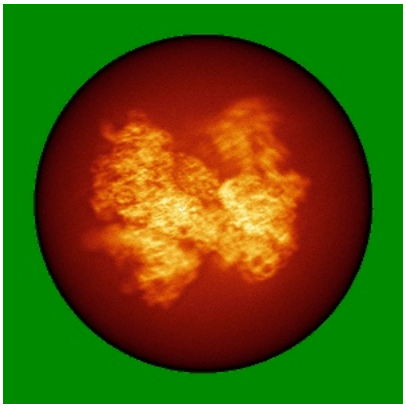
6.4.2 Raw map



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.

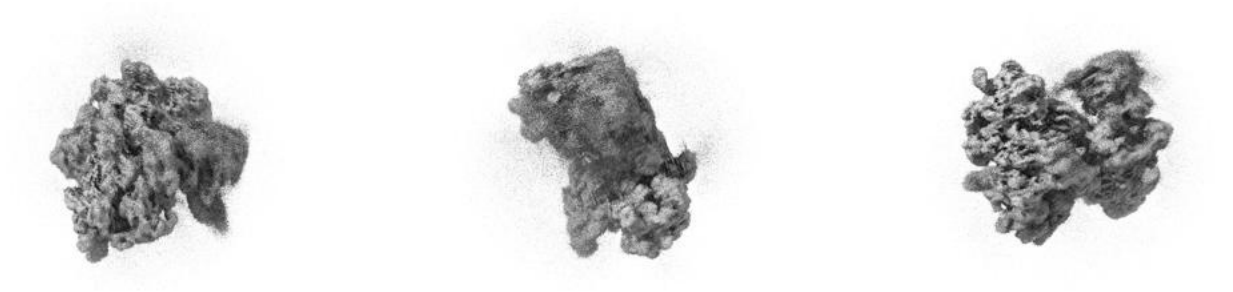
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

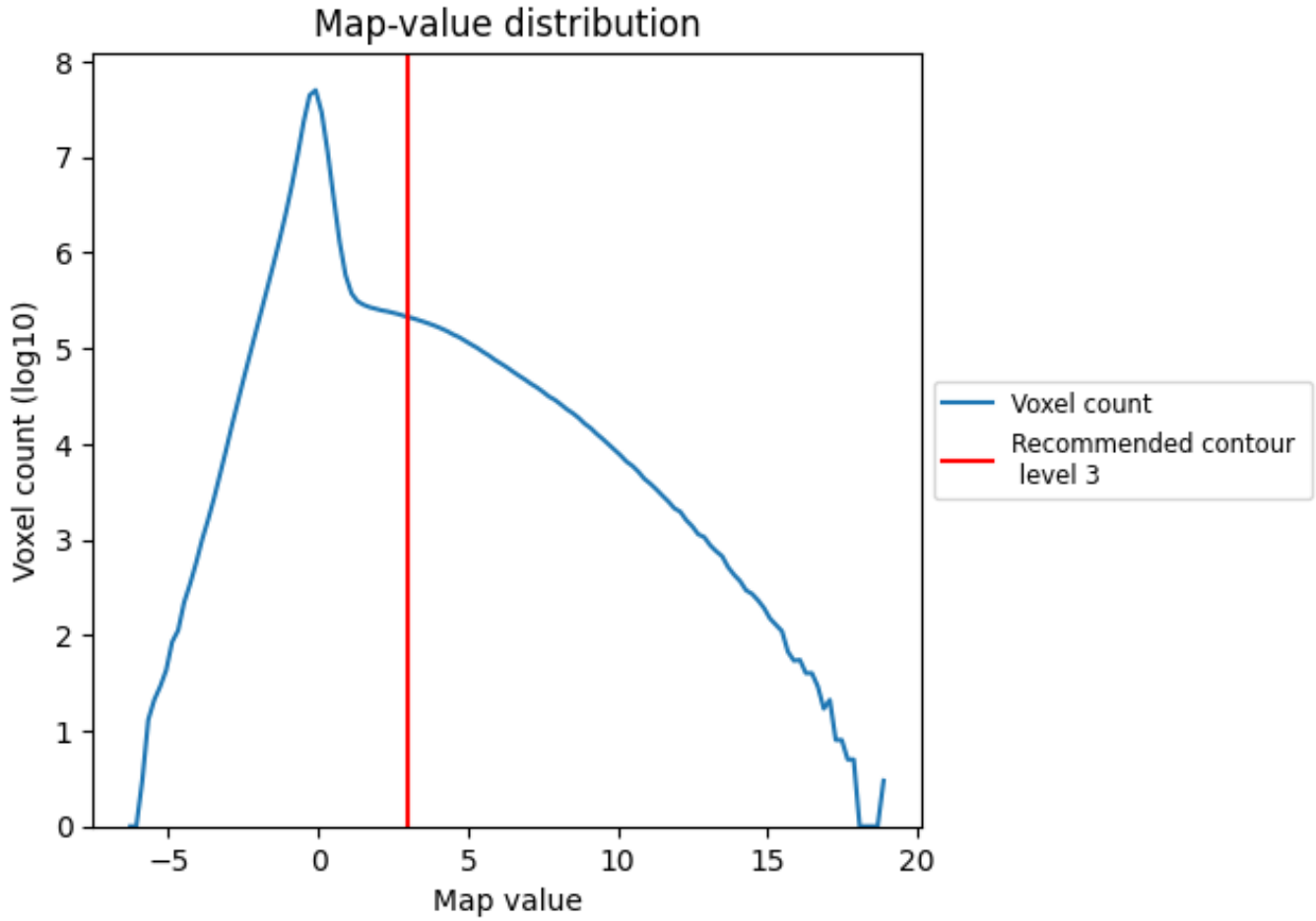
6.6 Mask visualisation (i)

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

7 Map analysis

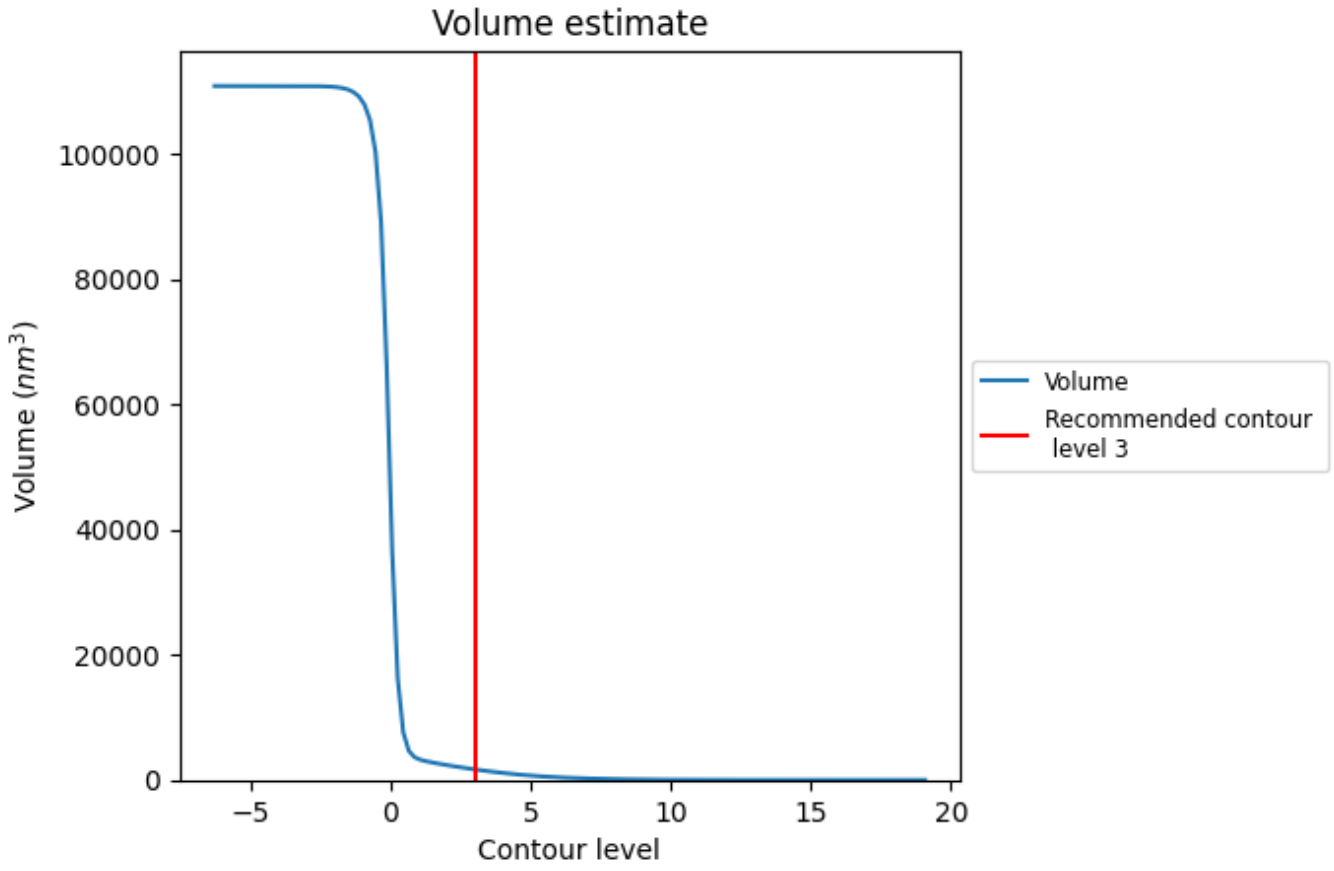
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

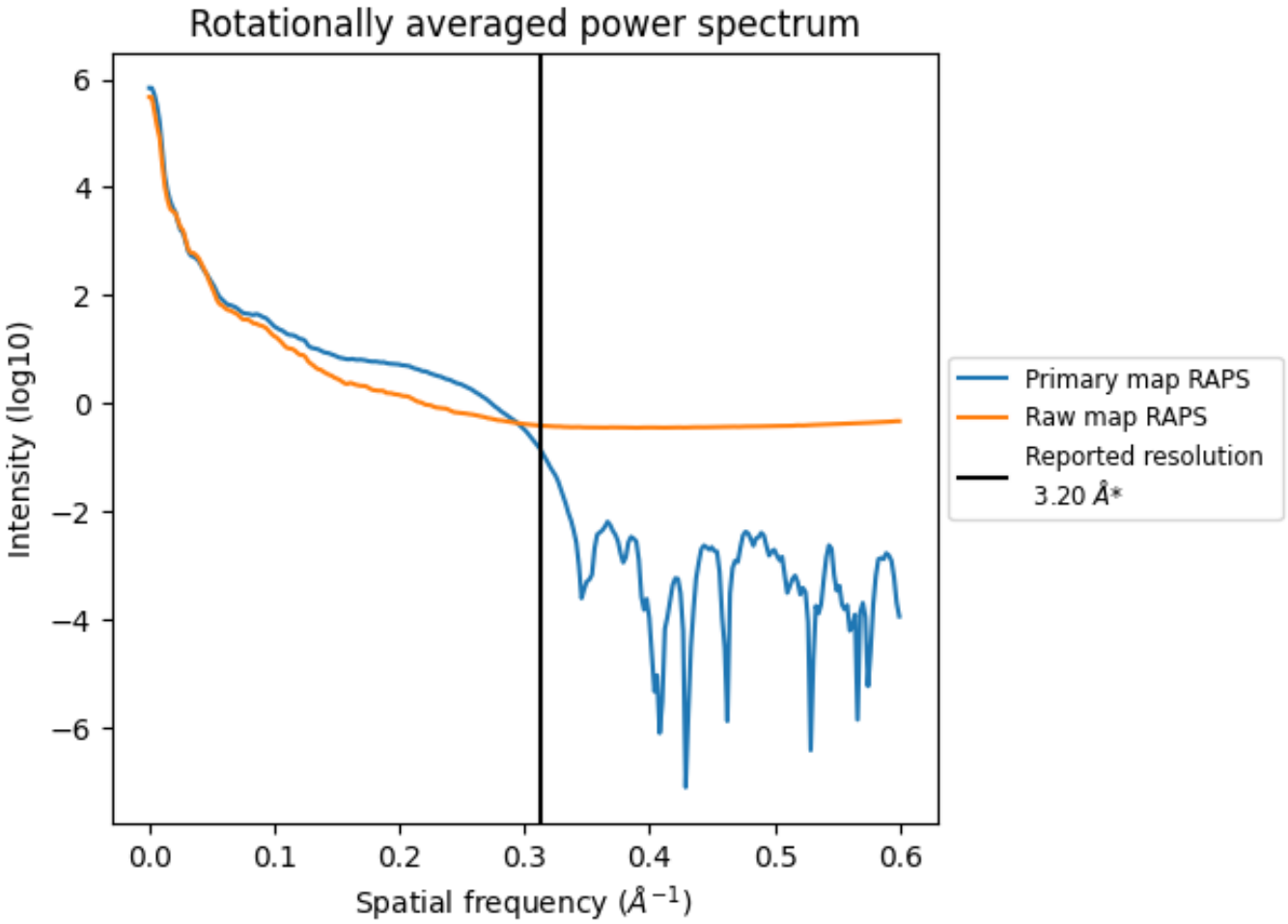
7.2 Volume estimate



The volume at the recommended contour level is 1689 nm^3; this corresponds to an approximate mass of 1525 kDa.

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

7.3 Rotationally averaged power spectrum (i)

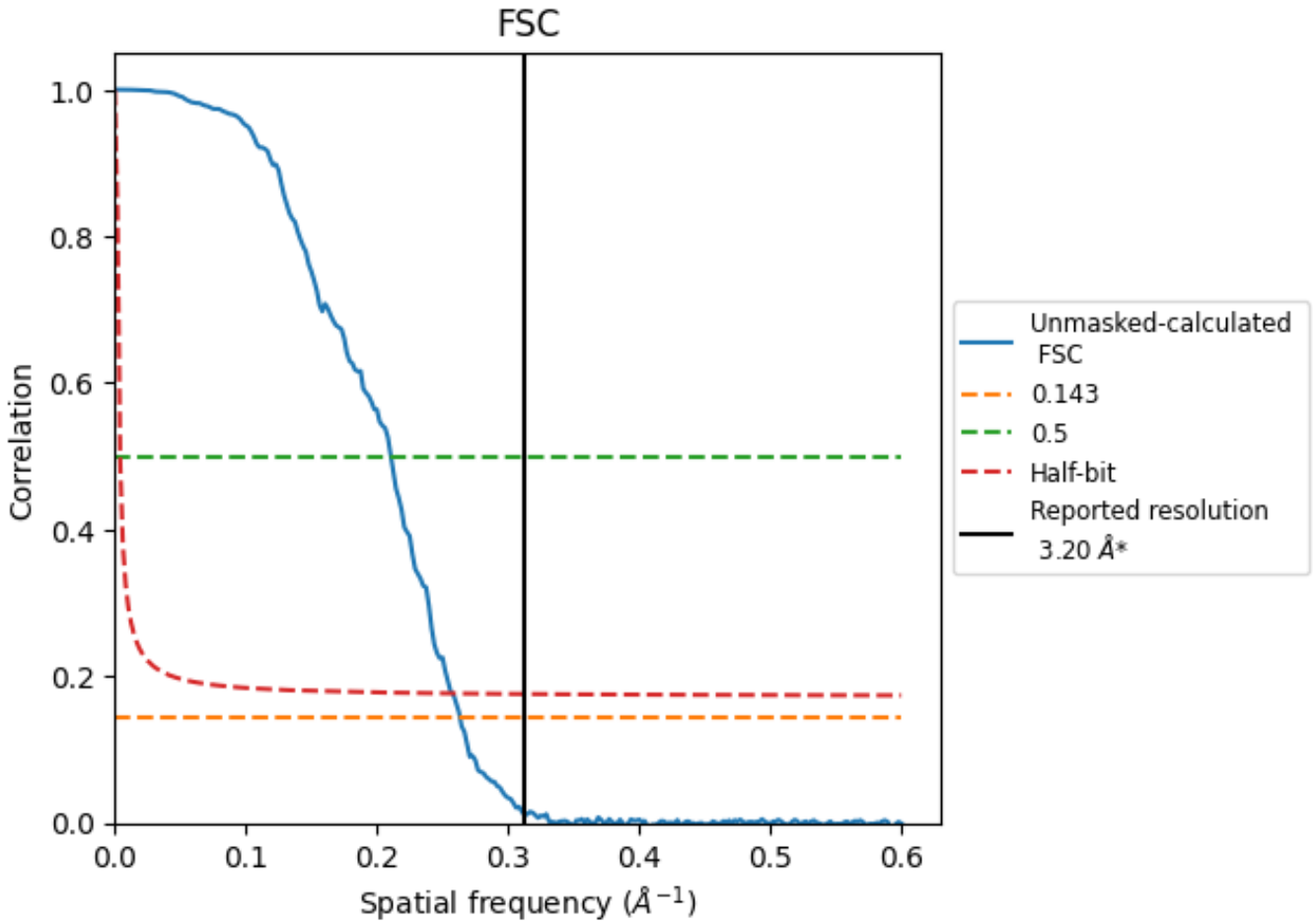


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

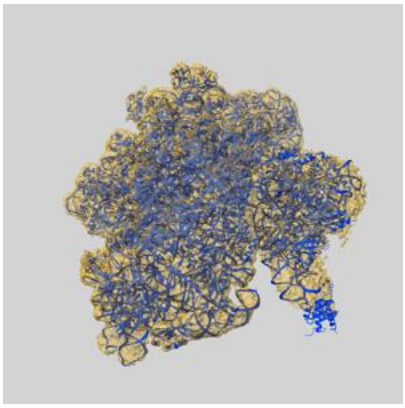
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.75	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.2 by more than 10 %

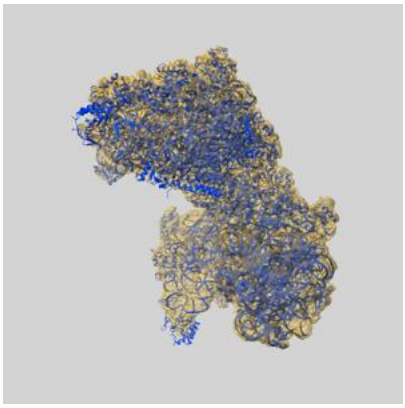
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50611 and PDB model 9FNY. Per-residue inclusion information can be found in section 3 on page 13.

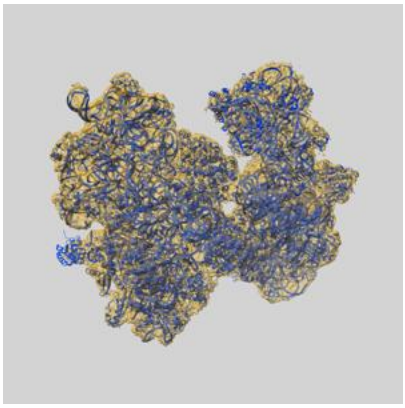
9.1 Map-model overlay



X



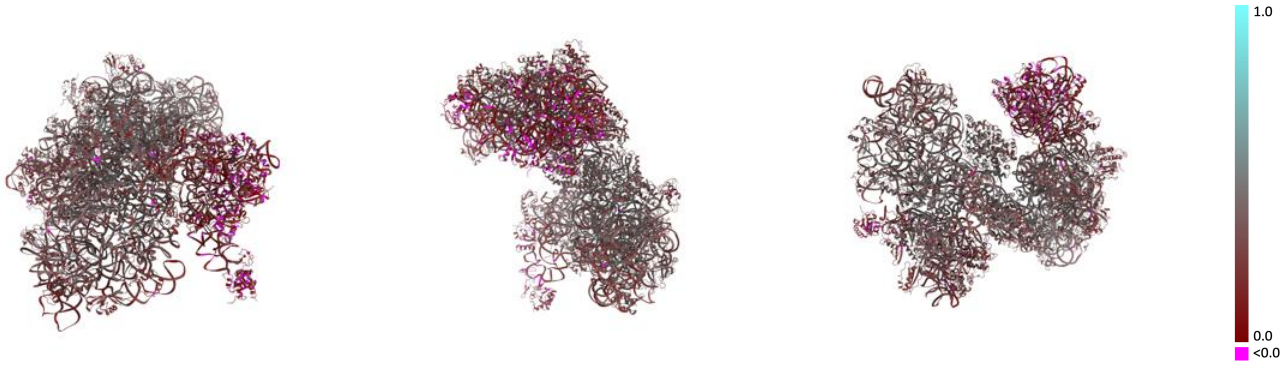
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

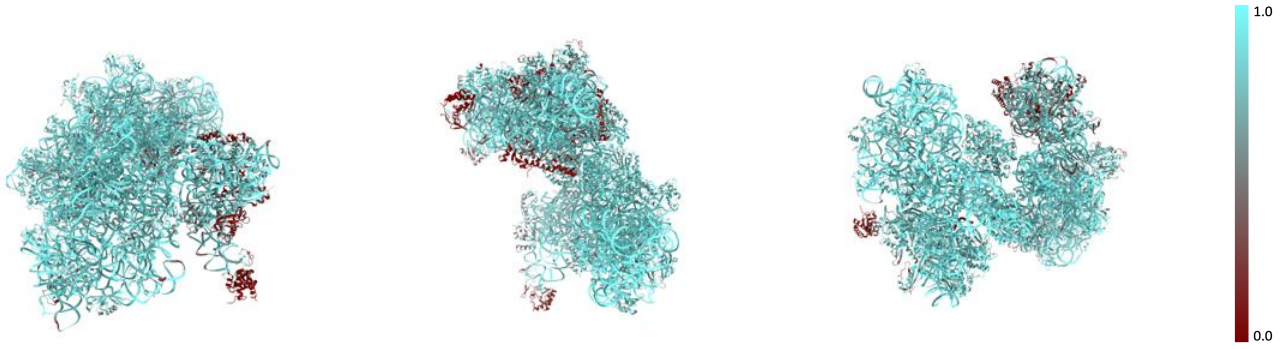
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

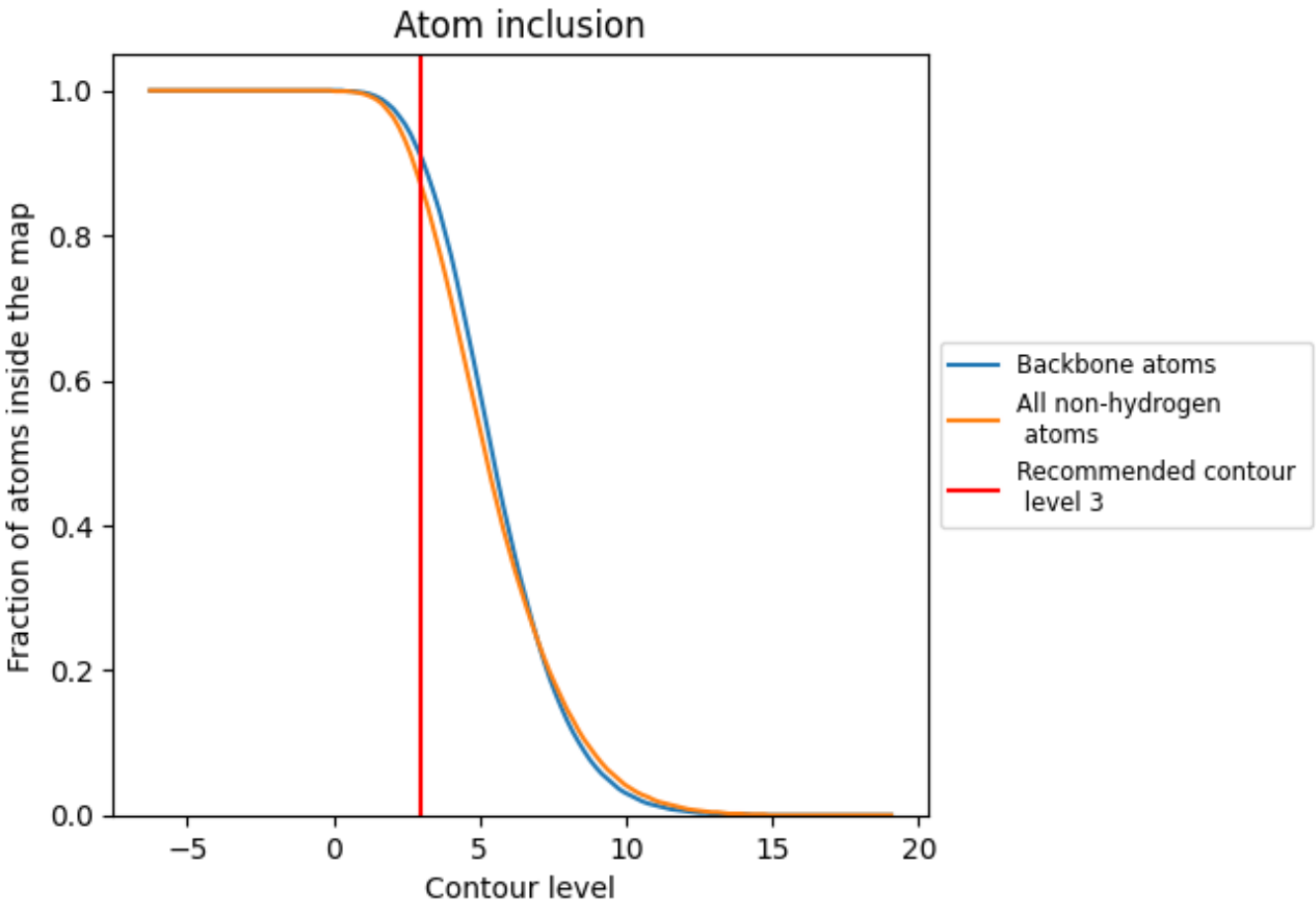
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.3130
A1	0.8700	0.3900
A2	0.9580	0.4570
A3	0.8810	0.3920
A4	0.8820	0.3870
A5	0.1450	0.1510
AA	0.9750	0.3500
AB	0.8250	0.3460
AC	0.7740	0.3160
AD	0.9250	0.3460
AE	0.8940	0.3740
AF	0.8420	0.3770
AG	0.8630	0.4060
AH	0.8250	0.3020
AI	0.8680	0.2500
AJ	0.9050	0.3920
AK	0.9240	0.3720
AL	0.9070	0.2910
AM	0.6750	0.2800
AN	0.9700	0.4050
AO	0.9300	0.3960
AP	0.7720	0.1890
AQ	0.8910	0.3140
AR	0.8730	0.3390
AS	0.8840	0.3630
AT	0.9000	0.3190
AU	0.6120	0.1680
AV	0.8690	0.2130
AW	0.8180	0.3480
AX	0.4970	0.1410
AY	0.8560	0.2790
AZ	0.9300	0.3010
B1	0.7800	0.3050
B2	0.8810	0.4250
B3	0.8520	0.3770

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Continued from previous page...

Chain	Atom inclusion	Q-score
B4	0.8620	0.3840
B5	0.1230	0.1200
BA	0.9310	0.2920
BB	0.7250	0.2830
BC	0.5020	0.1980
BD	0.8500	0.3290
BE	0.8560	0.3110
BF	0.8240	0.3400
BG	0.8400	0.3500
BH	0.6420	0.2590
BI	0.5970	0.1750
BJ	0.8580	0.3690
BK	0.8820	0.3410
BL	0.7530	0.1740
BM	0.6560	0.1500
BN	0.9460	0.3670
BO	0.9170	0.3500
BP	0.3020	0.1240
BQ	0.8430	0.1720
BR	0.8670	0.3220
BS	0.8840	0.3840
BT	0.7280	0.2000
BU	0.2350	0.0990
BV	0.6890	0.1210
BW	0.7660	0.2770
BX	0.4470	0.1250
BY	0.7590	0.2620
BZ	0.7720	0.2160