



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 09:56 am BST

PDB ID : 6ZTJ / pdb_00006ztj
EMDB ID : EMD-11418
Title : E. coli 70S-RNAP expressome complex in NusG-coupled state (38 nt intervening mRNA)
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on : 2020-07-20
Resolution : 3.40 Å (reported)
Based on initial models : 4YBB, 6ALH

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

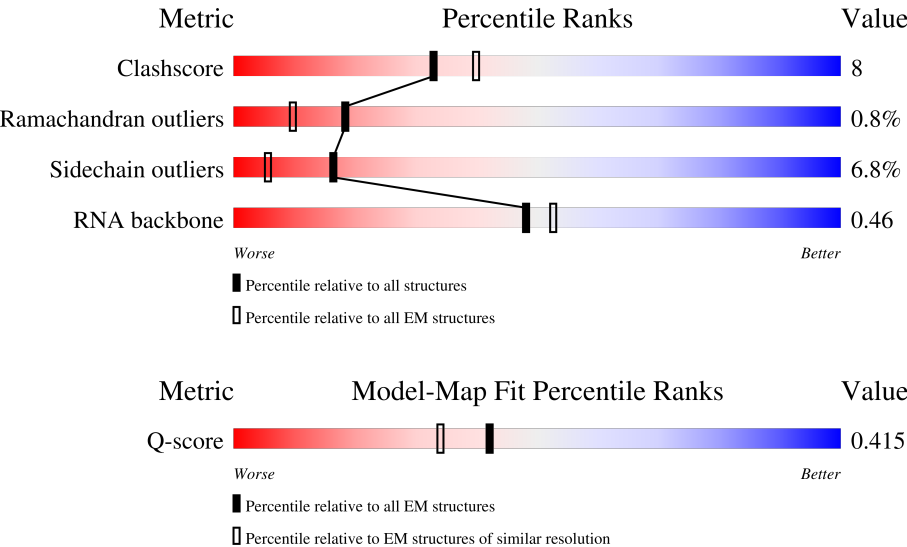
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	6% 60% 32% 7% ..
2	AB	241	76% 62% 29% 6% .
3	AC	233	20% 61% 26% 9% .

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Mol	Chain	Length	Quality of chain
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	53	
23	AW	77	
24	AX	76	
25	AY	557	
26	BA	2904	
27	BB	120	
28	BC	273	

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Mol	Chain	Length	Quality of chain
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	149	
34	BI	165	
35	BJ	142	
36	BK	142	
37	BL	123	
38	BM	144	
39	BN	136	
40	BO	127	
41	BP	117	
42	BQ	115	
43	BR	118	
44	BS	103	
45	BT	110	
46	BU	100	
47	BV	104	
48	BW	94	
49	BX	85	
50	BY	78	
51	BZ	63	
52	B1	59	
53	B2	57	

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Mol	Chain	Length	Quality of chain
54	B3	55	
55	B4	46	
56	B5	65	
57	B6	50	
58	B7	70	
59	CN	39	
60	CT	39	
61	CA	329	
61	CB	329	
62	CC	1342	
63	CD	1407	
64	CE	91	
65	CF	181	

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 176970 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32909	14684	6037	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	101	Total	C	N	O	S	0	0
			808	504	155	148	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	60	Total	C	N	O	0	0
			494	310	93	91		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	40	Total	C	N	O	P	0	0
			849	381	154	274	40		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 25 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AY	89	Total	C	N	O	0	0
			677	423	112	142		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2900	Total	C	N	O	P	0	0
			62270	27786	11456	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 35 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BO	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BS	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BU	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	BV	103	Total	C	N	O		
			789	498	148	143	0	0

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BX	76	Total	C	N	O	S		
			582	360	117	104	1	0	0

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BZ	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B1	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 59 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 60 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 61 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
61	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 62 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 63 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 64 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	CE	51	Total	C	N	O	S	0	0
			399	246	77	75	1		

- Molecule 65 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	CF	161	Total	C	N	O	S	0	0
			1283	818	221	237	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	121	ALA	LYS	conflict	UNP P0AFG1

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

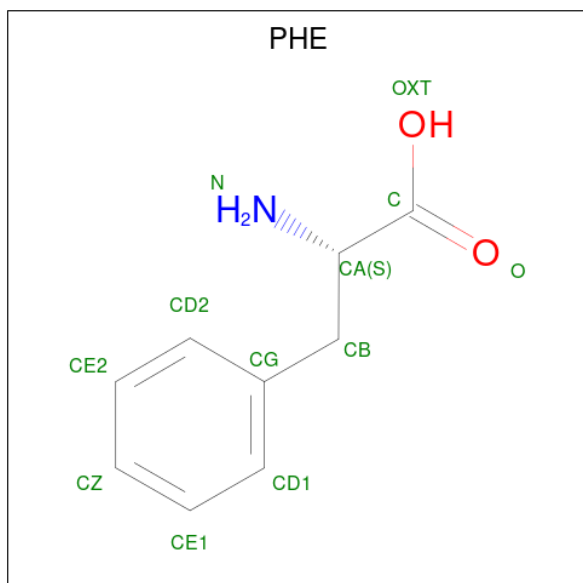
Mol	Chain	Residues	Atoms		AltConf
66	AA	148	Total	Mg	0
			148	148	
66	AI	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
66	AW	1	Total	Mg	0
			1	1	
66	AX	1	Total	Mg	0
			1	1	
66	BA	314	Total	Mg	0
			314	314	
66	BB	6	Total	Mg	0
			6	6	
66	BC	3	Total	Mg	0
			3	3	
66	BD	1	Total	Mg	0
			1	1	
66	BE	1	Total	Mg	0
			1	1	
66	BQ	1	Total	Mg	0
			1	1	
66	BT	1	Total	Mg	0
			1	1	
66	CD	1	Total	Mg	0
			1	1	

- Molecule 67 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
67	AX	1	Total	C	N	O	0
			11	9	1	1	

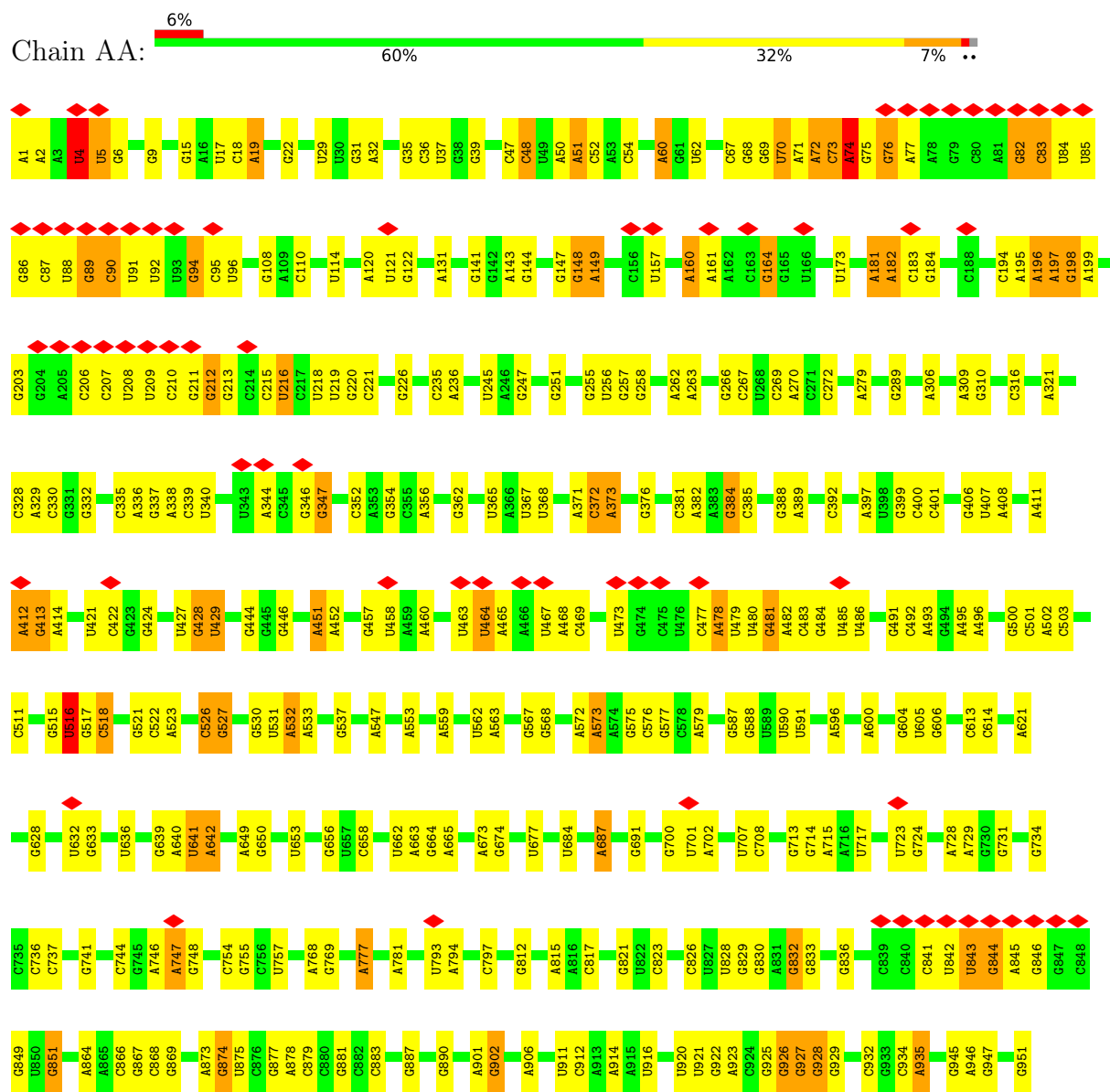
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

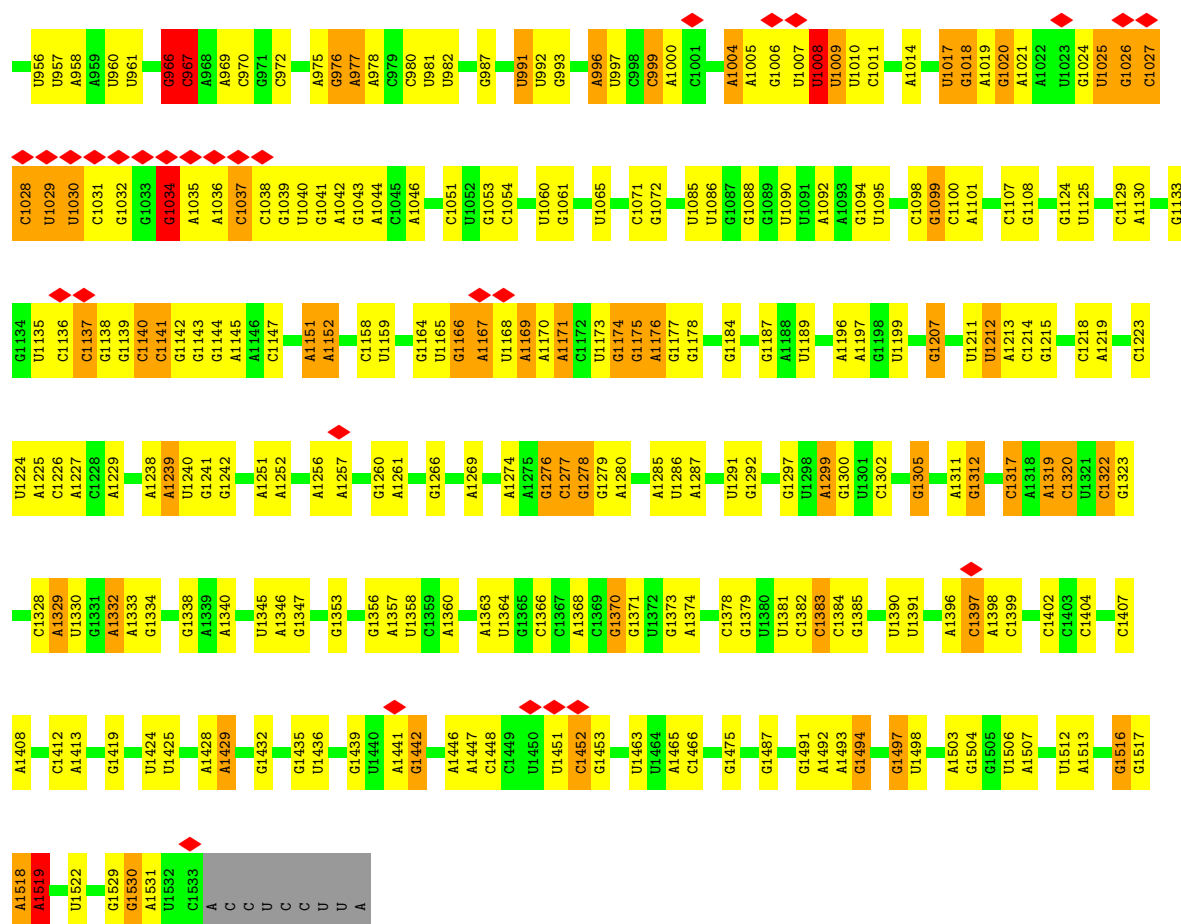
Mol	Chain	Residues	Atoms		AltConf
68	B6	1	Total 1	Zn 1	0
68	B7	1	Total 1	Zn 1	0
68	CD	2	Total 2	Zn 2	0

3 Residue-property plots

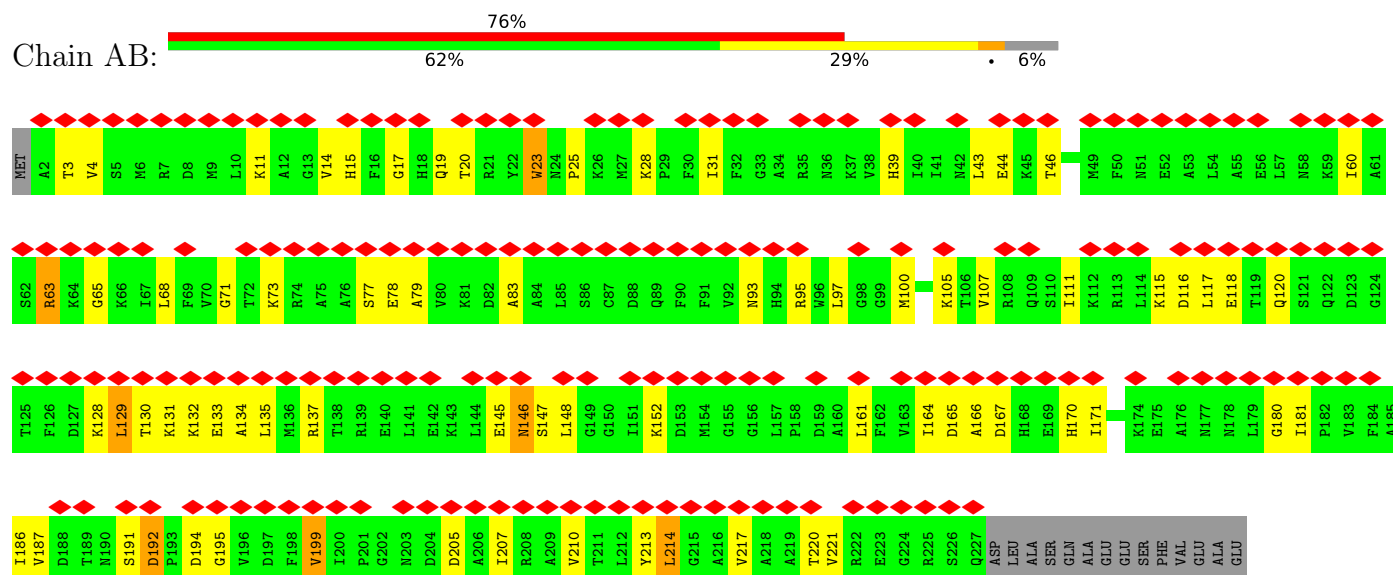
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA



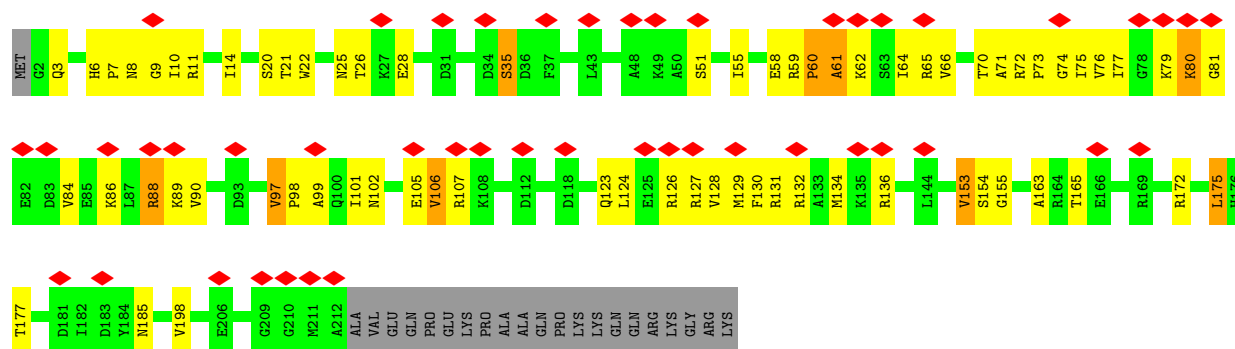


• Molecule 2: 30S ribosomal protein S2

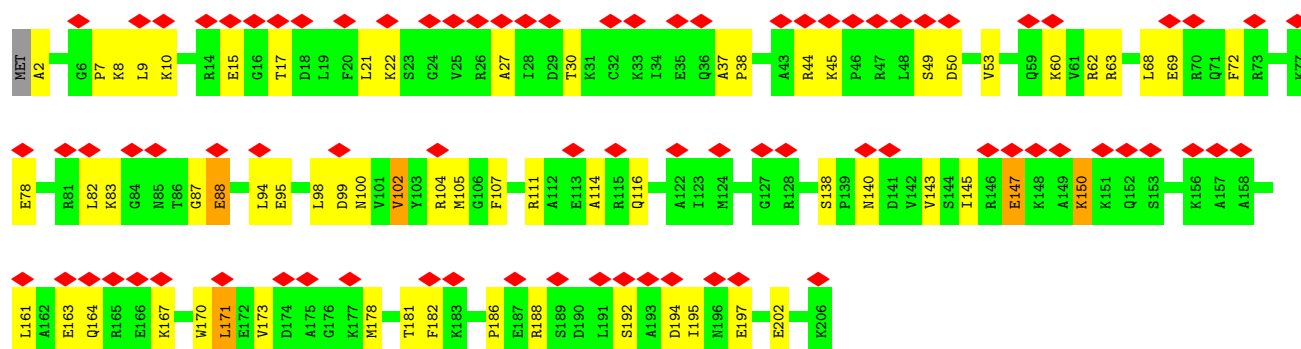


• Molecule 3: 30S ribosomal protein S3

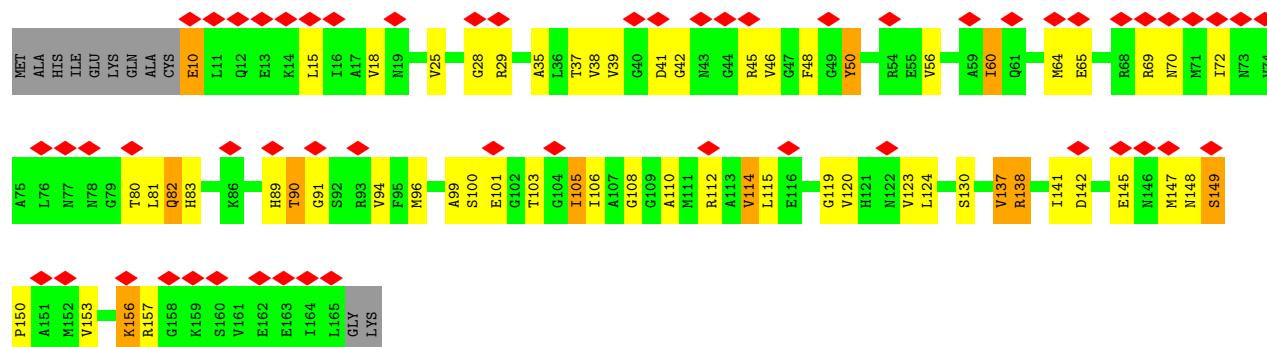




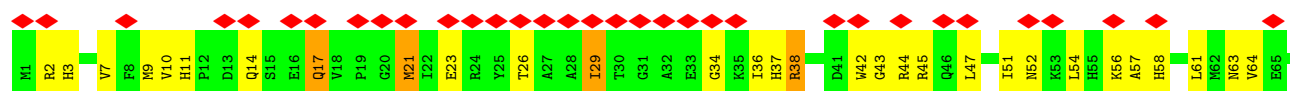
• Molecule 4: 30S ribosomal protein S4

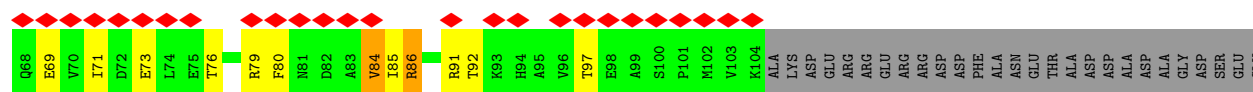


• Molecule 5: 30S ribosomal protein S5

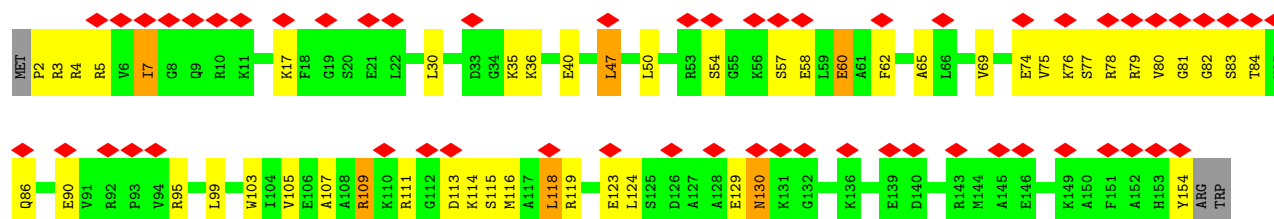
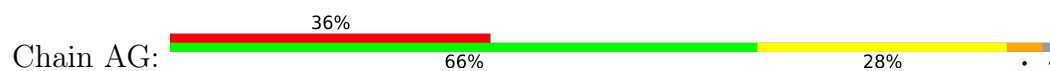


• Molecule 6: 30S ribosomal protein S6

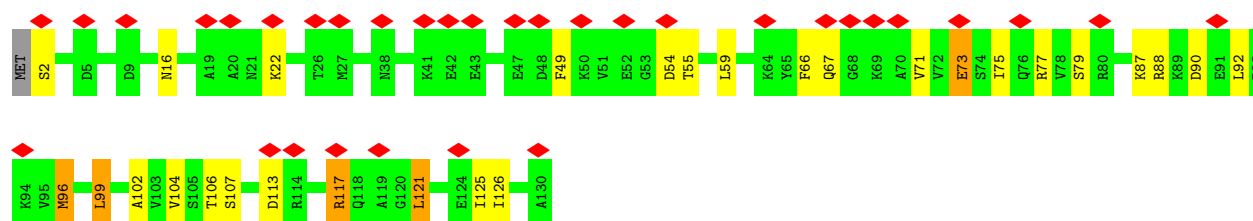
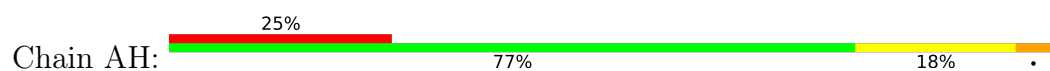




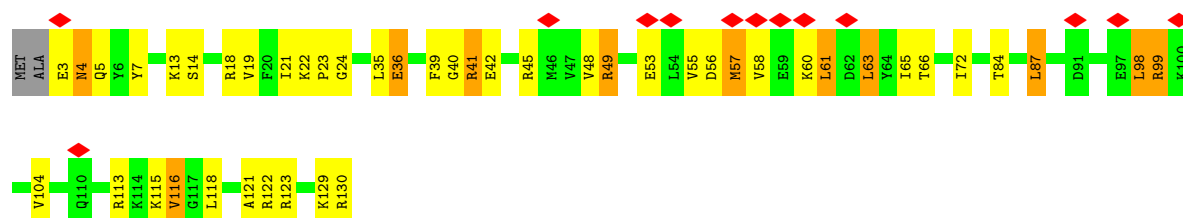
• Molecule 7: 30S ribosomal protein S7



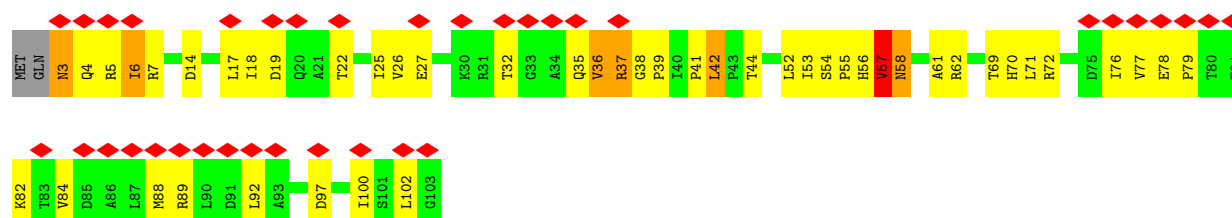
• Molecule 8: 30S ribosomal protein S8



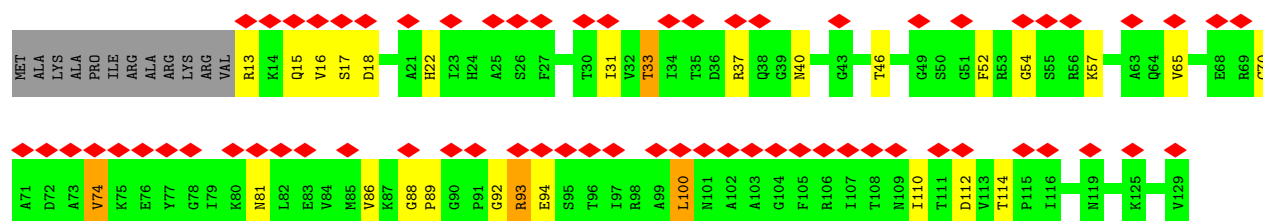
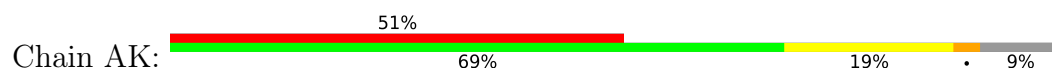
• Molecule 9: 30S ribosomal protein S9



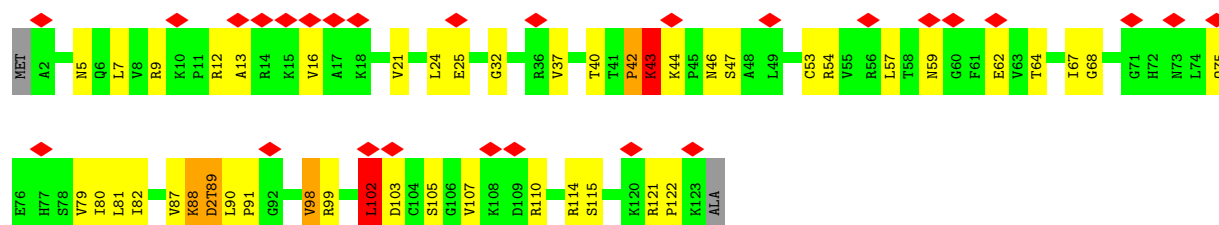
• Molecule 10: 30S ribosomal protein S10



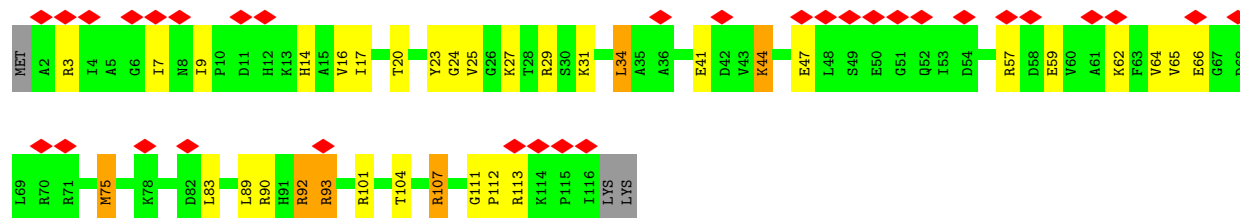
• Molecule 11: 30S ribosomal protein S11



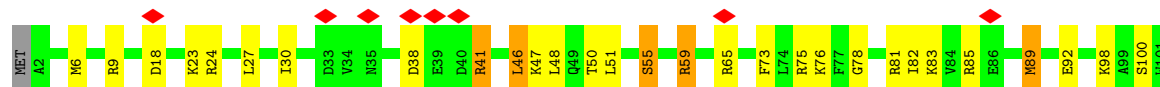
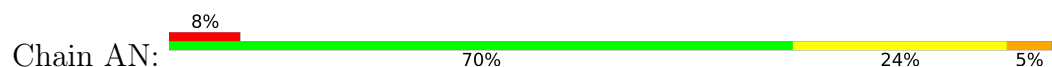
• Molecule 12: 30S ribosomal protein S12



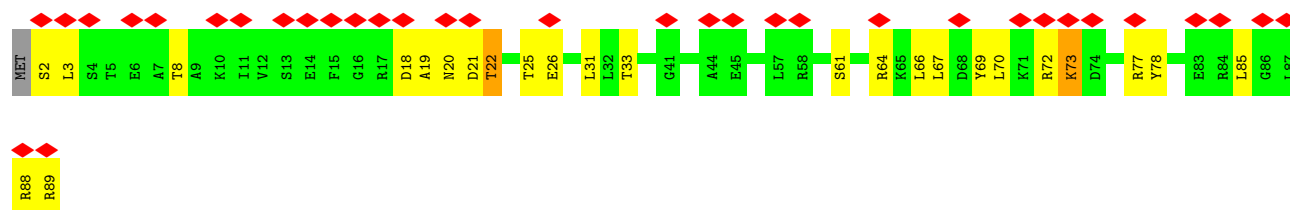
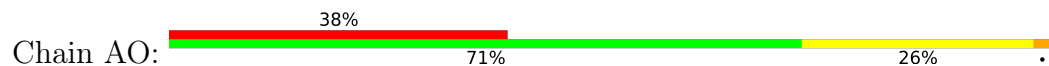
• Molecule 13: 30S ribosomal protein S13



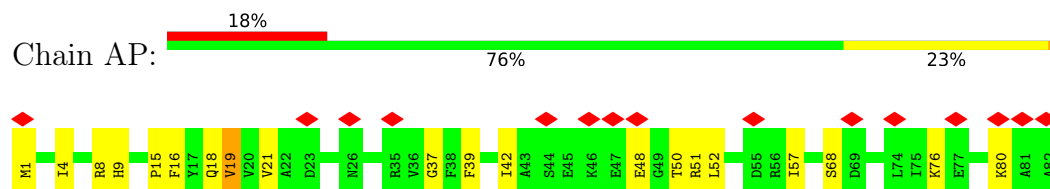
• Molecule 14: 30S ribosomal protein S14



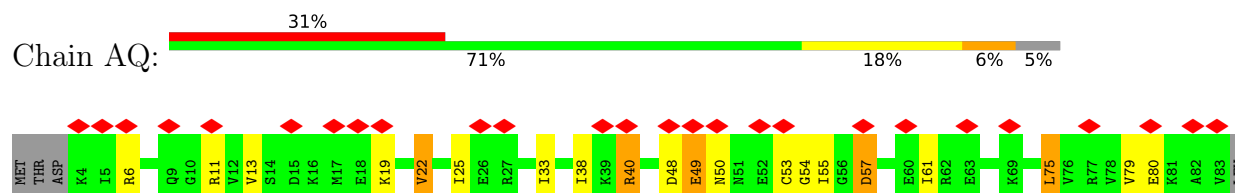
• Molecule 15: 30S ribosomal protein S15



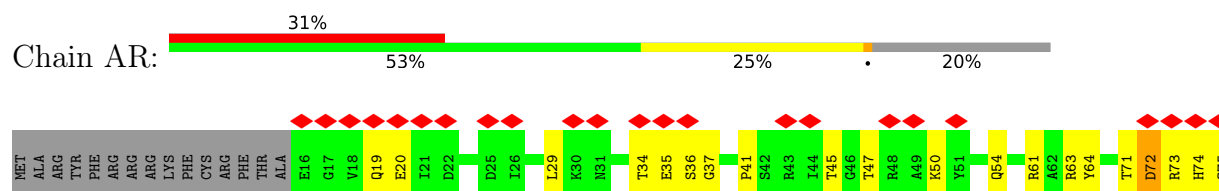
- Molecule 16: 30S ribosomal protein S16



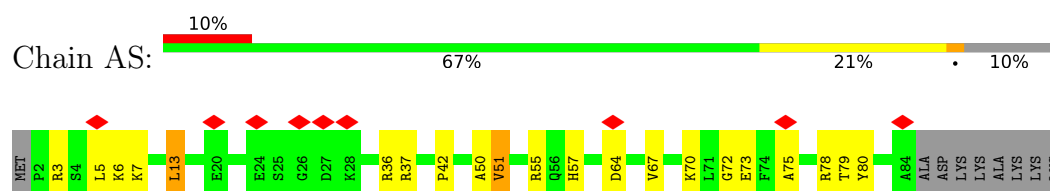
- Molecule 17: 30S ribosomal protein S17



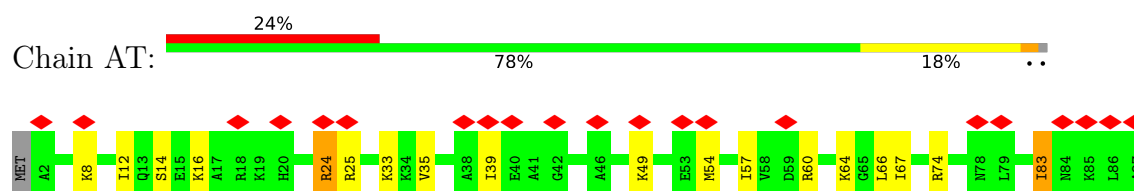
- Molecule 18: 30S ribosomal protein S18



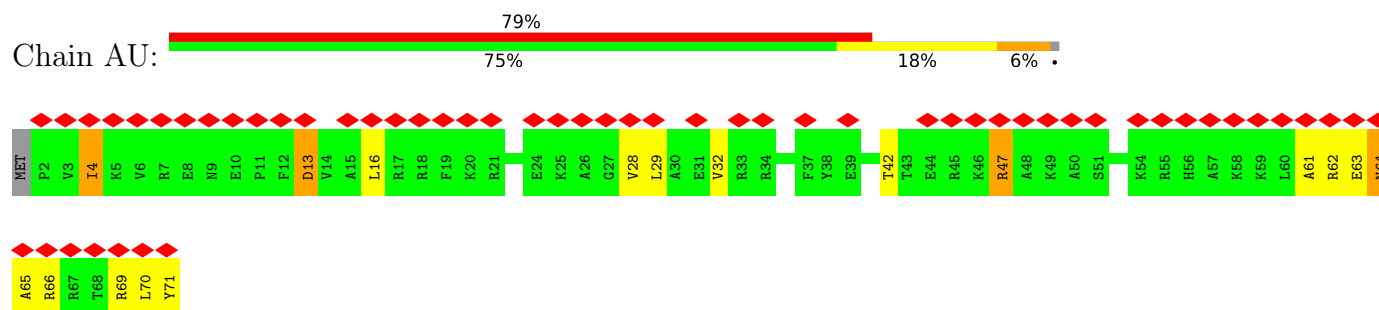
- Molecule 19: 30S ribosomal protein S19



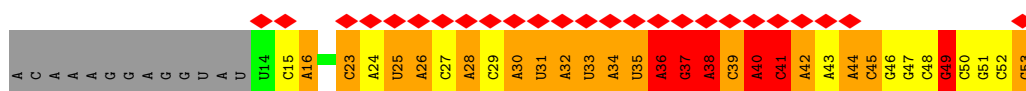
- Molecule 20: 30S ribosomal protein S20



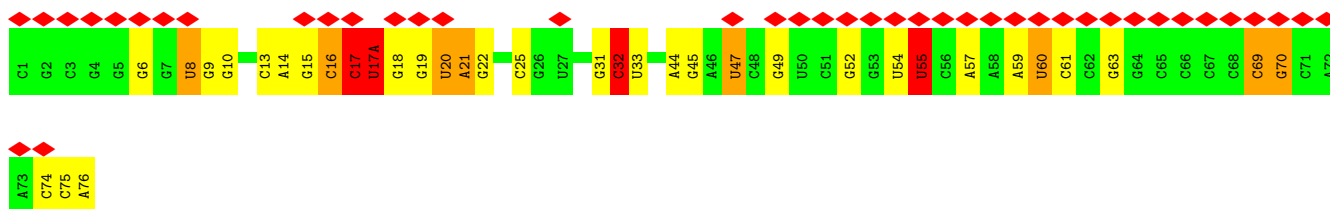
- Molecule 21: 30S ribosomal protein S21



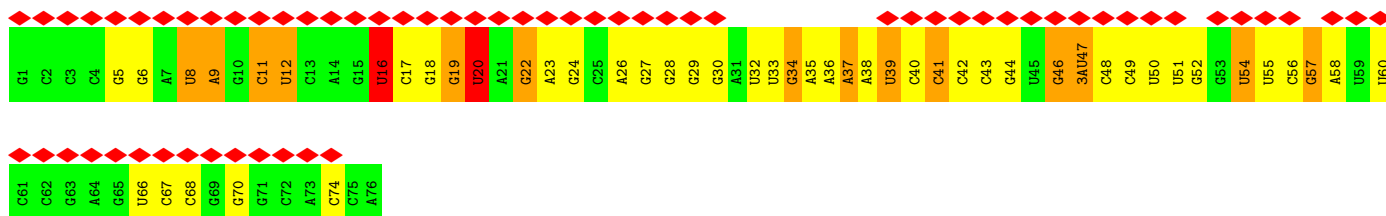
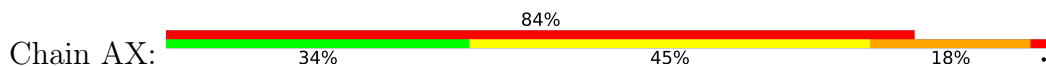
- Molecule 22: mRNA



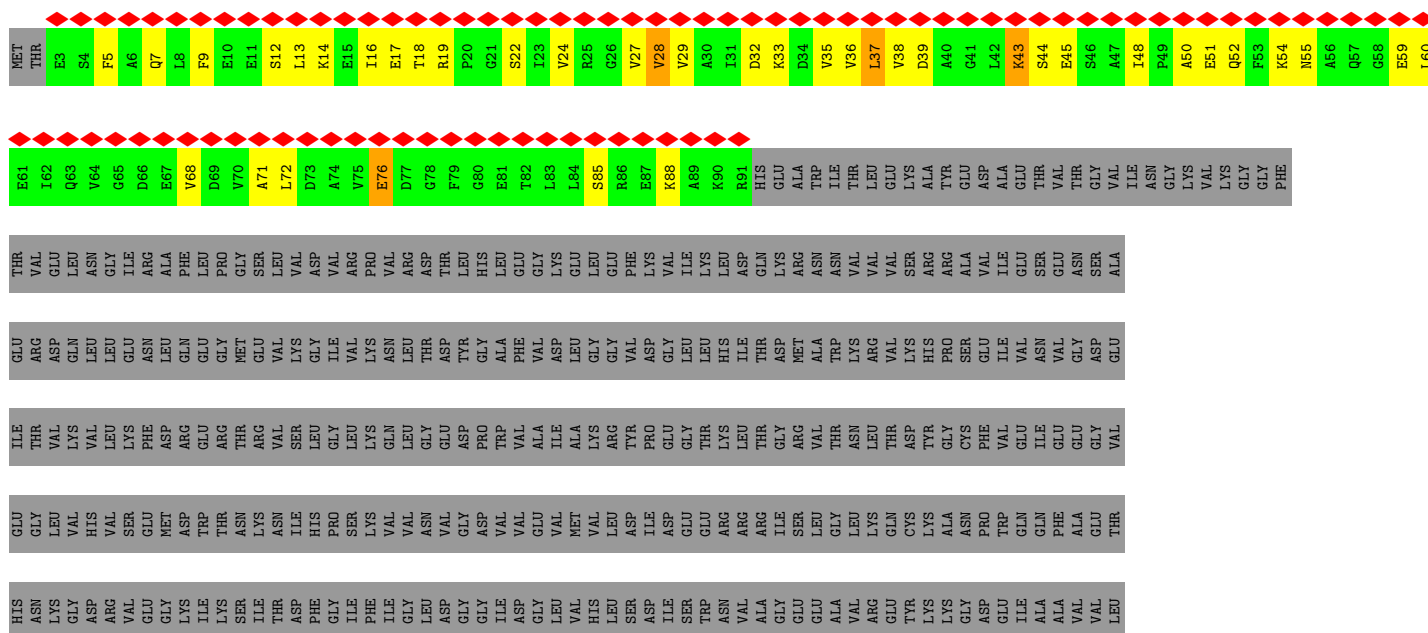
• Molecule 23: tRNA(fmet) P-site



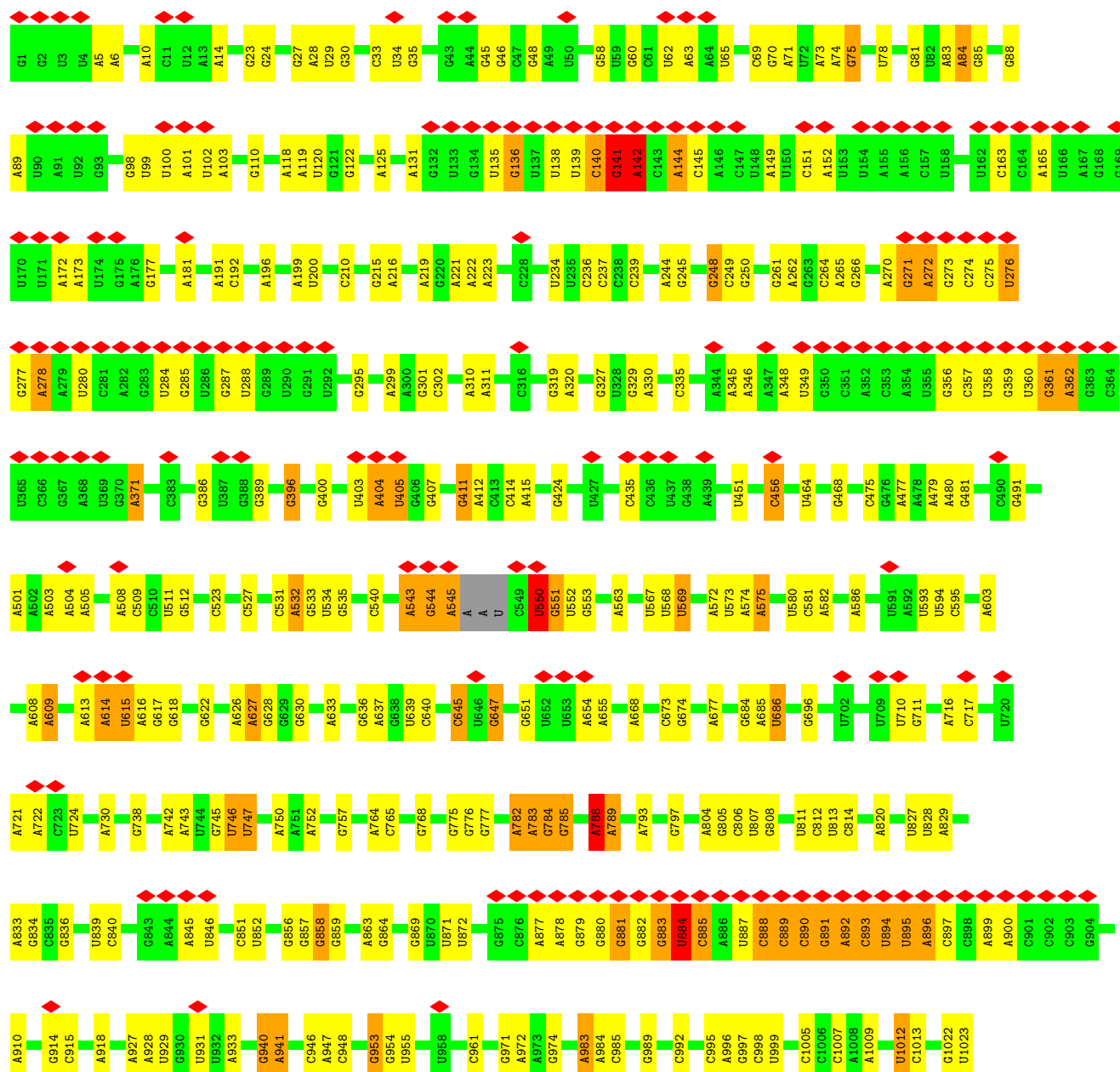
• Molecule 24: Phe-NH-tRNA(Phe) A-site

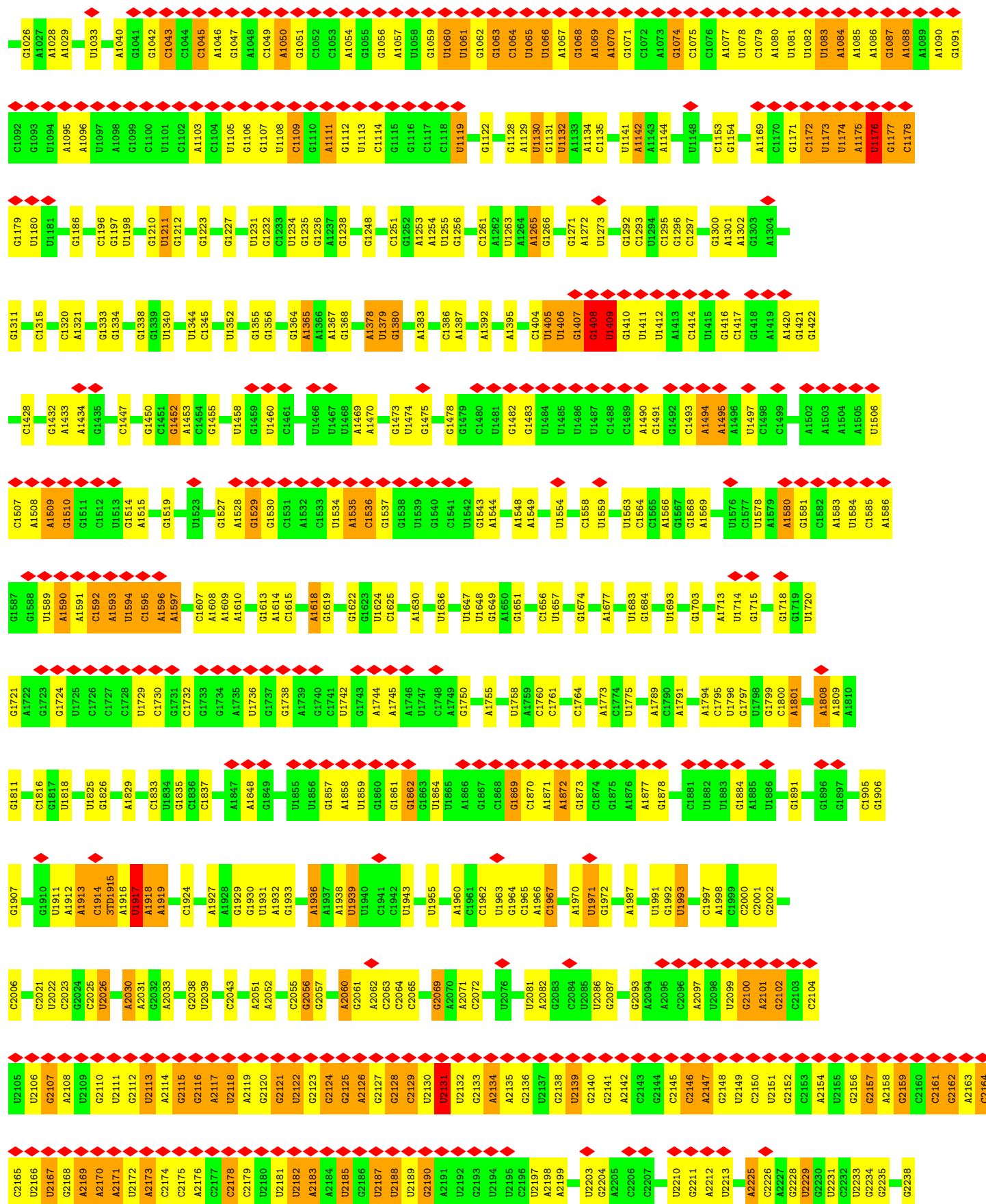


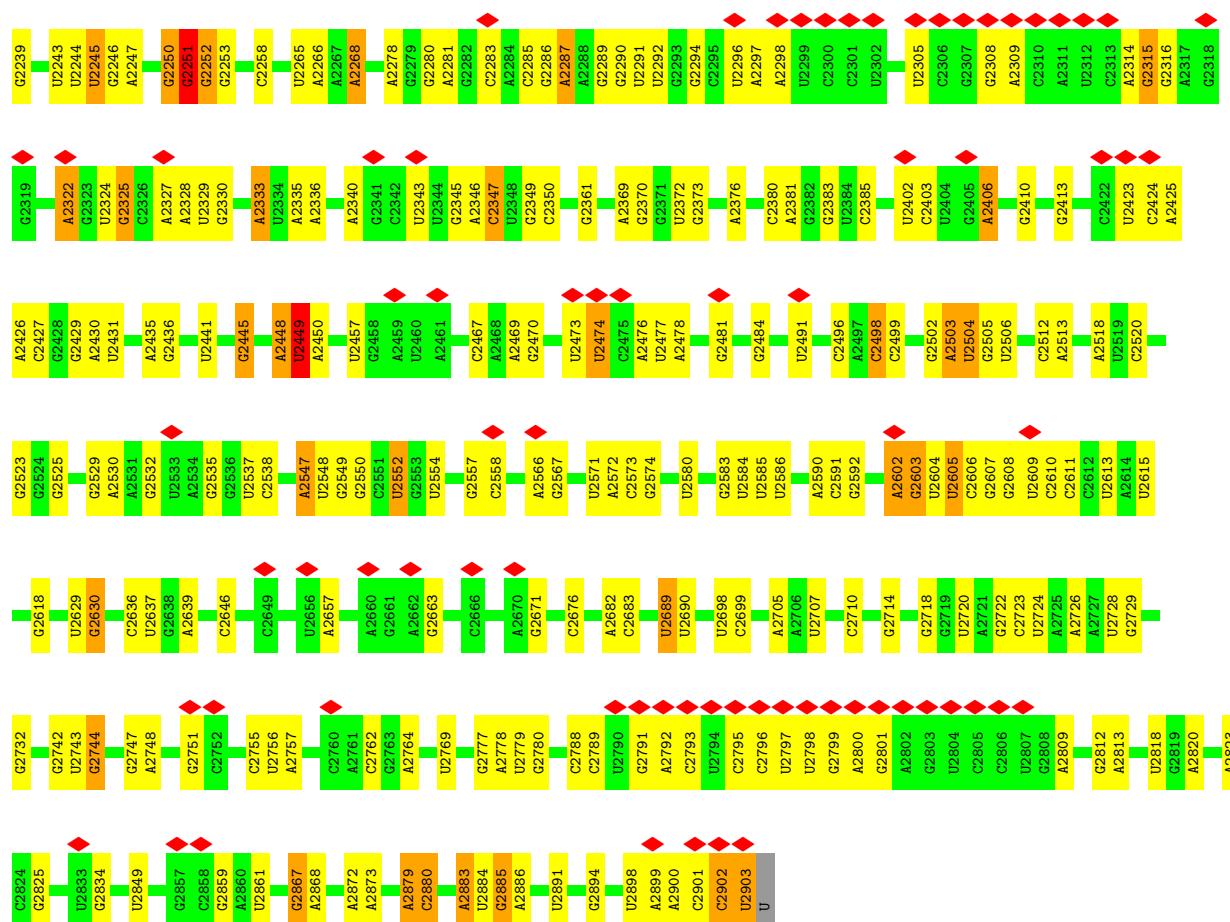
• Molecule 25: 30S ribosomal protein S1



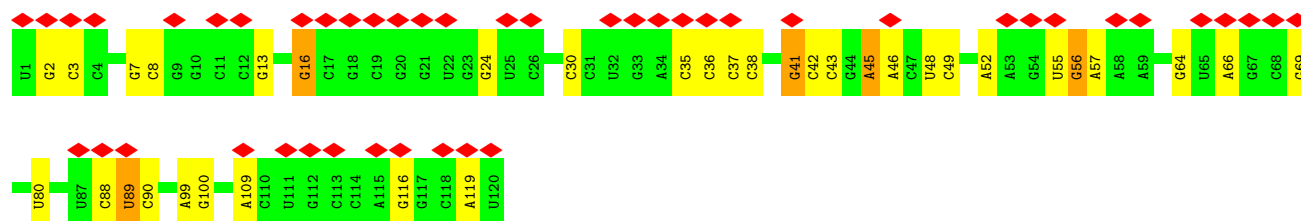
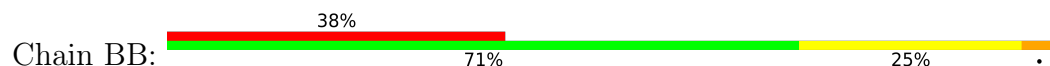
- Molecule 26: 23S ribosomal RNA



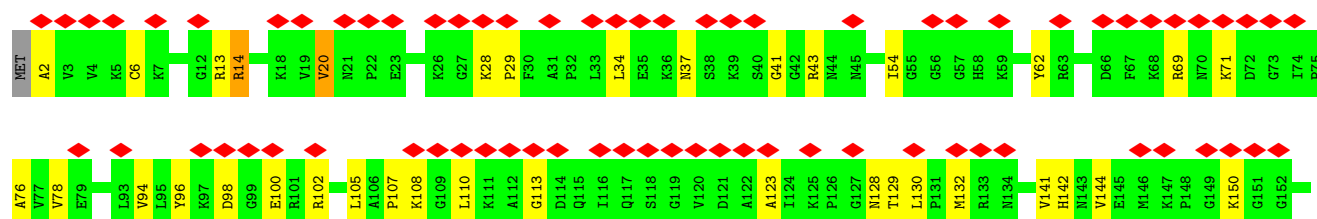
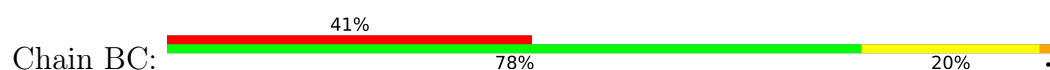


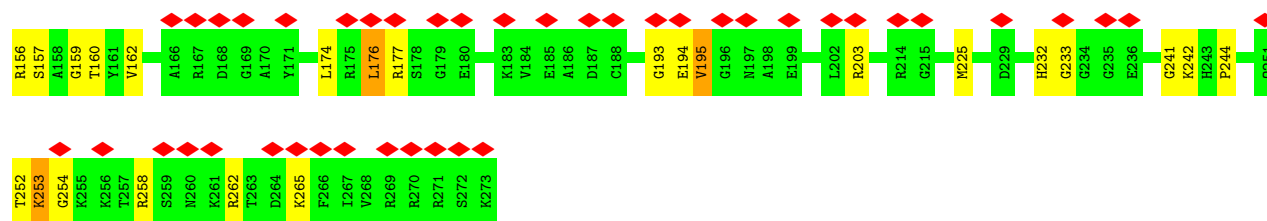


• Molecule 27: 5S ribosomal RNA

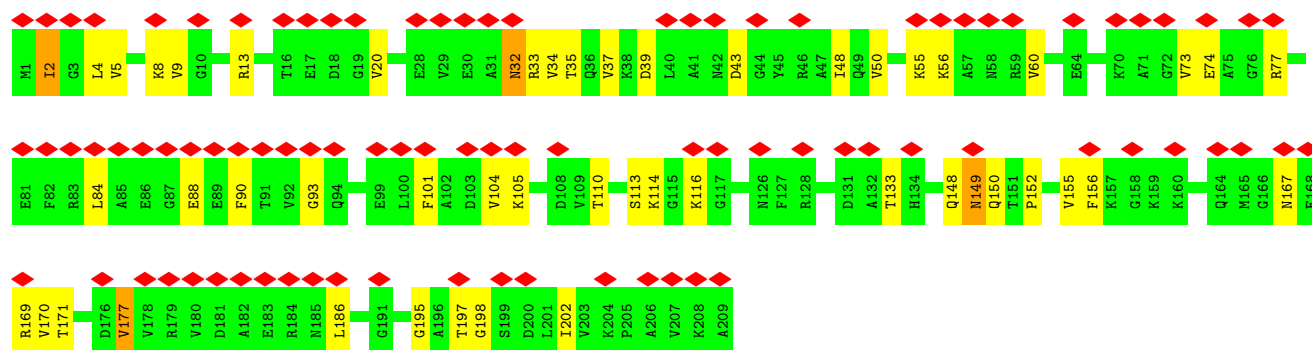
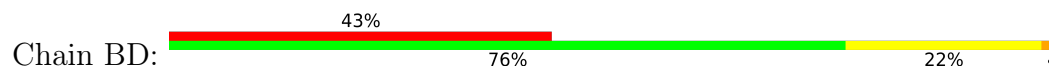


• Molecule 28: 50S ribosomal protein L2

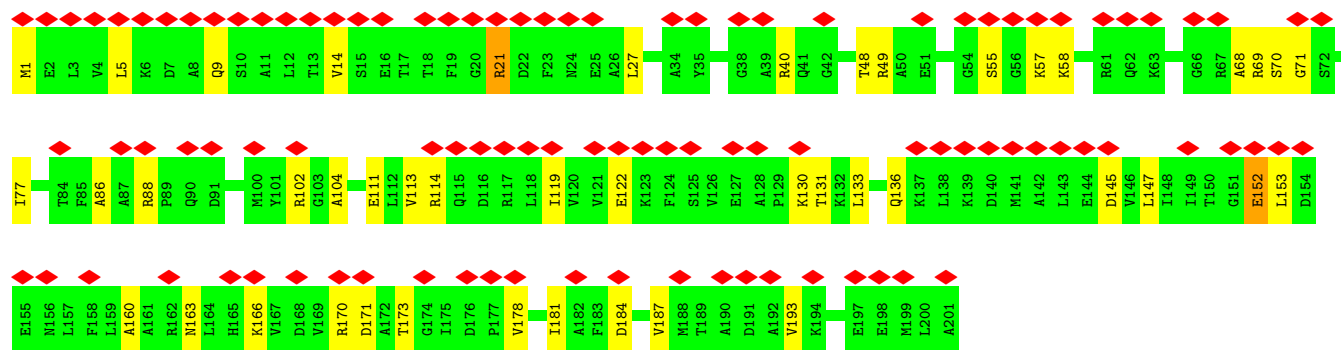
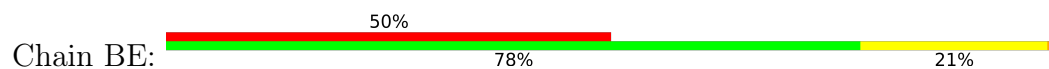




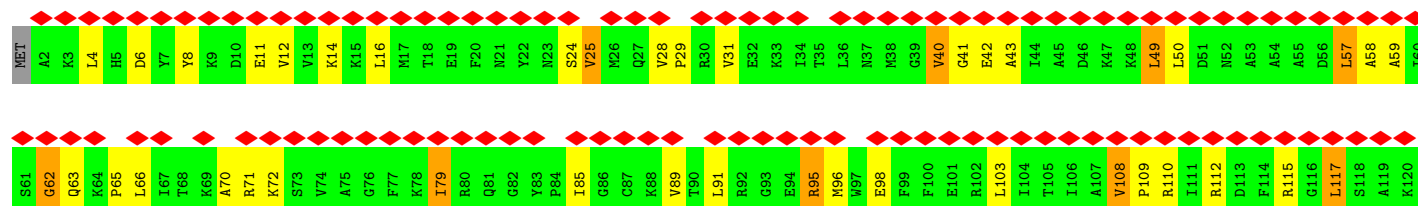
• Molecule 29: 50S ribosomal protein L3

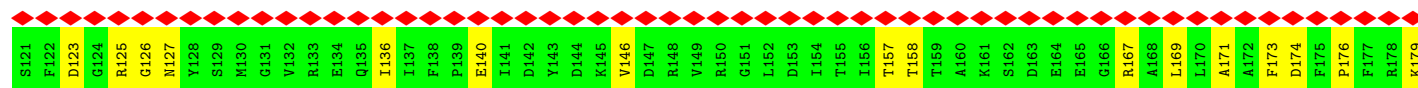


• Molecule 30: 50S ribosomal protein L4

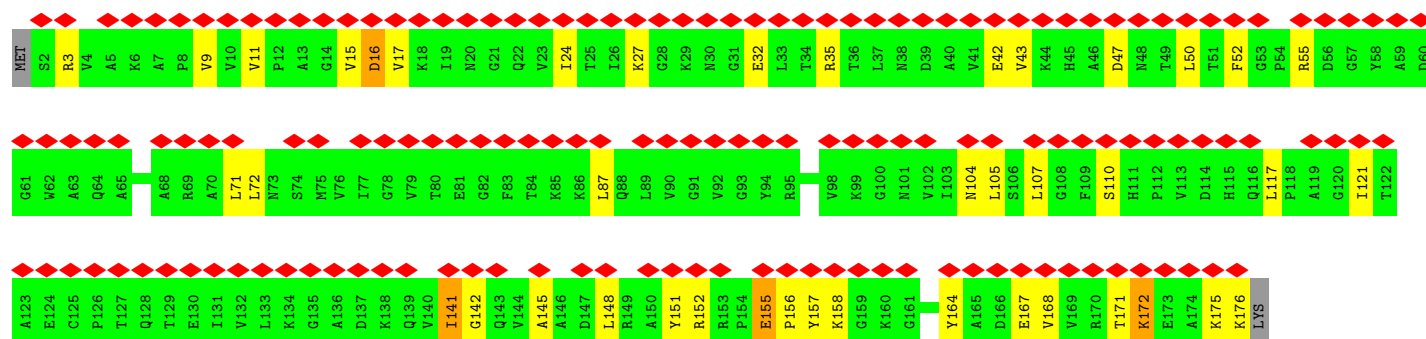
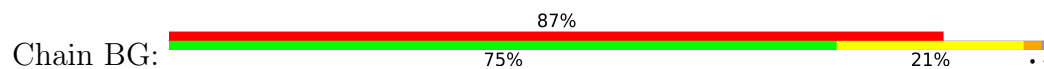


• Molecule 31: 50S ribosomal protein L5

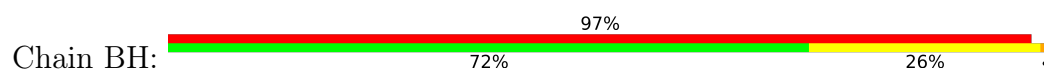




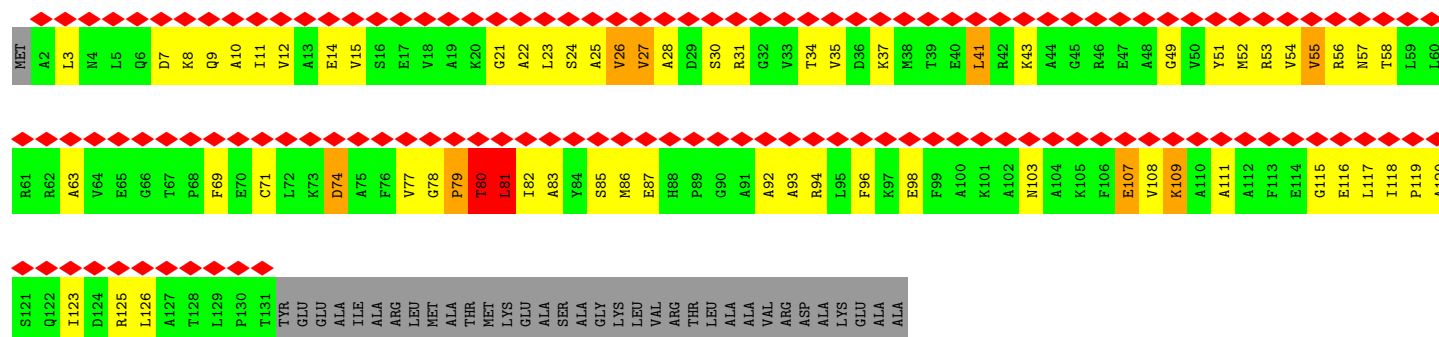
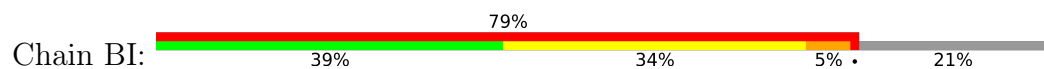
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9

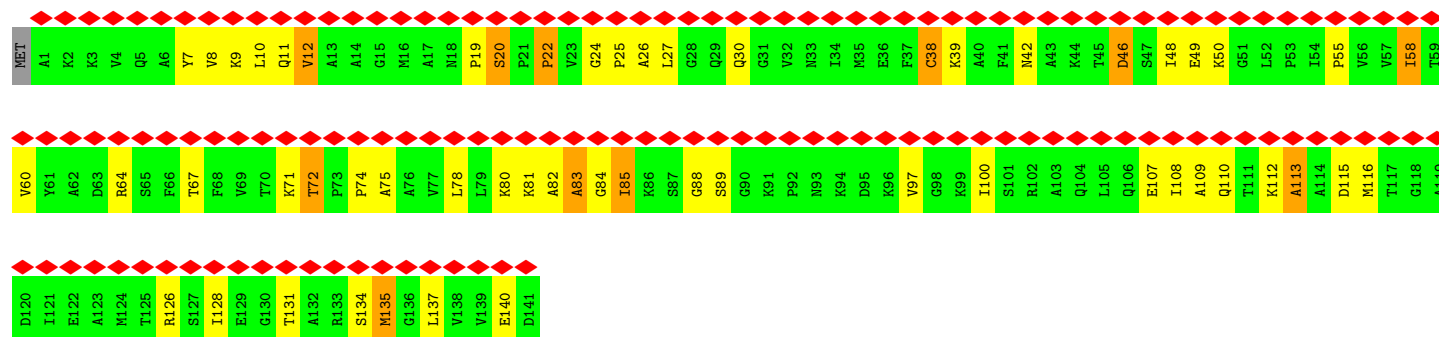


• Molecule 34: 50S ribosomal protein L10

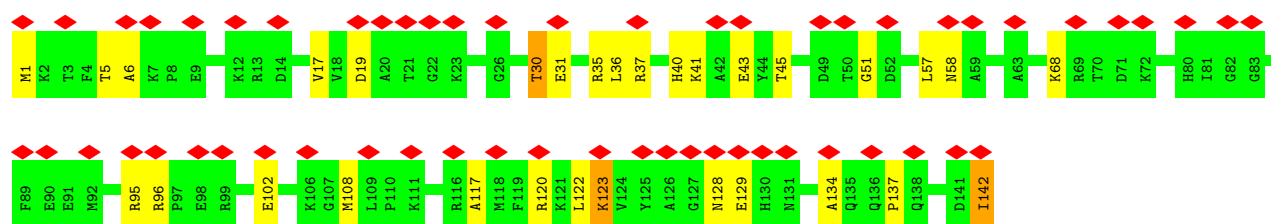
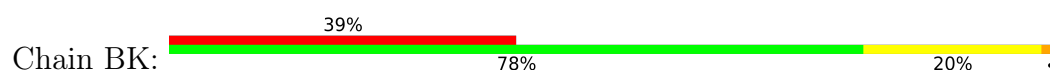


• Molecule 35: 50S ribosomal protein L11

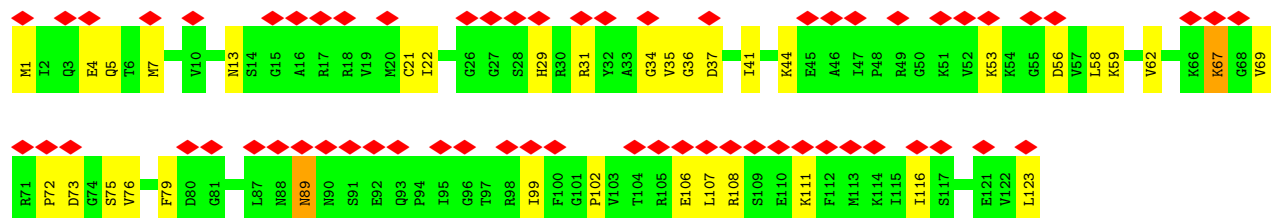
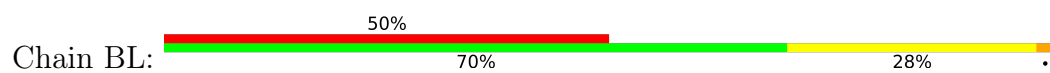




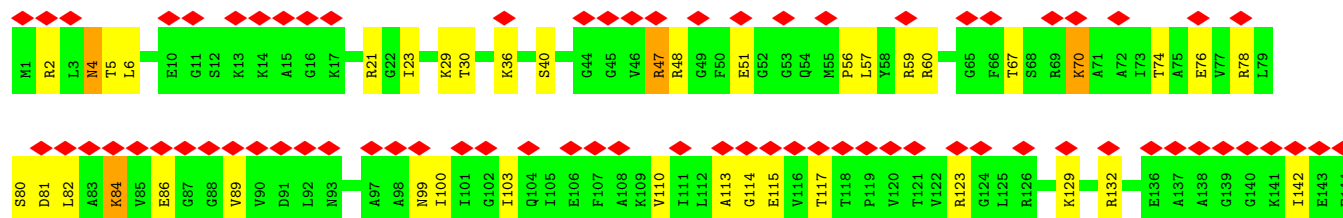
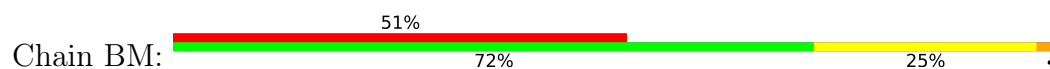
• Molecule 36: 50S ribosomal protein L13



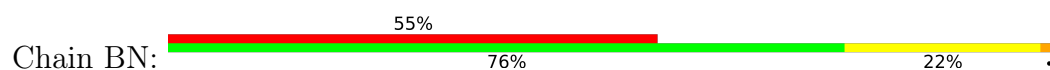
• Molecule 37: 50S ribosomal protein L14

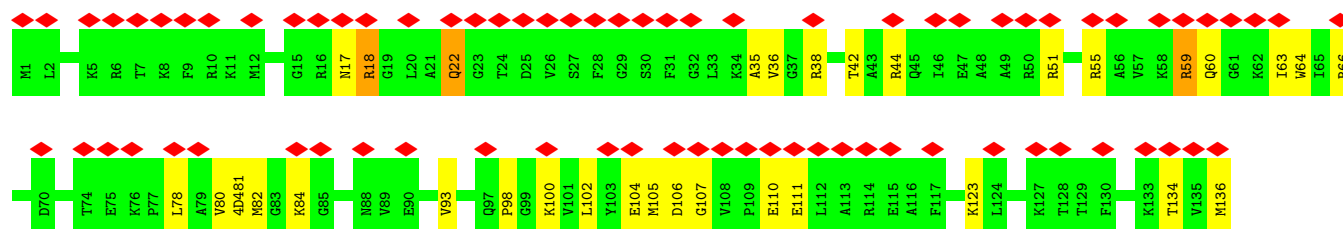


• Molecule 38: 50S ribosomal protein L15

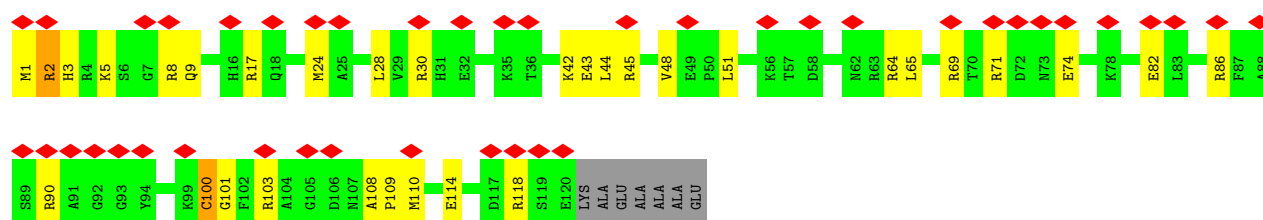


• Molecule 39: 50S ribosomal protein L16

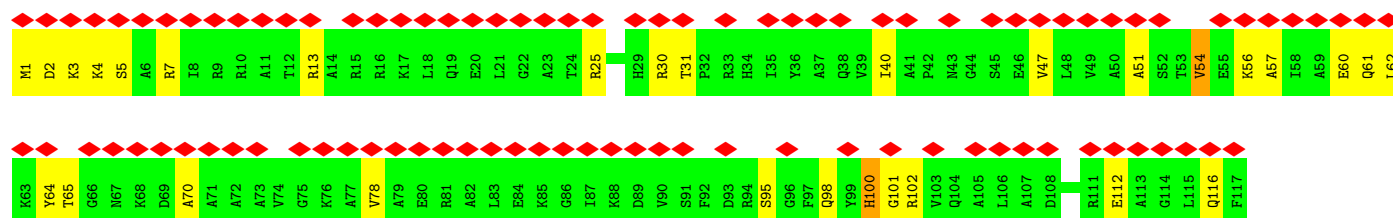
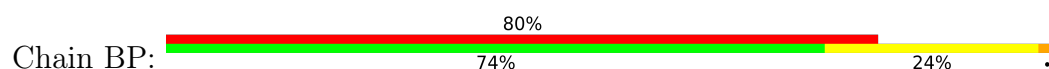




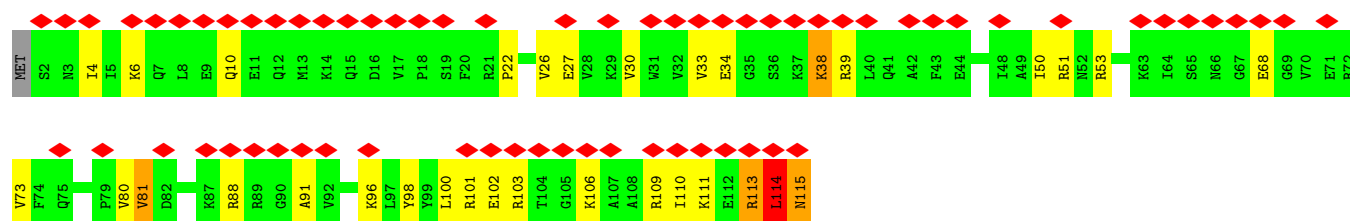
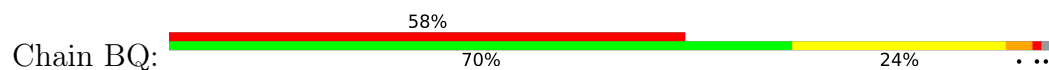
• Molecule 40: 50S ribosomal protein L17



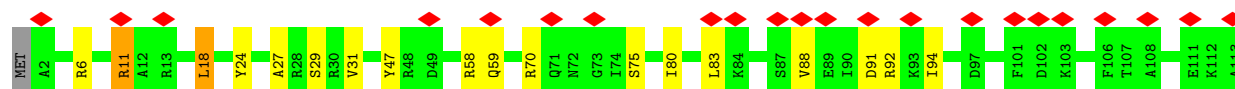
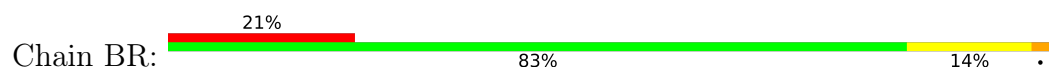
• Molecule 41: 50S ribosomal protein L18



• Molecule 42: 50S ribosomal protein L19

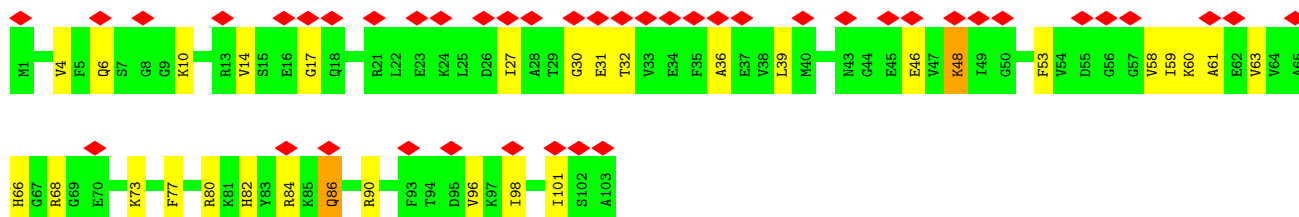
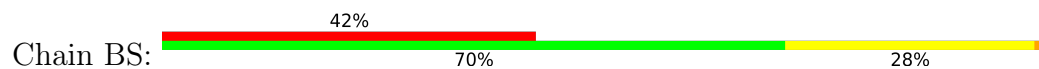


• Molecule 43: 50S ribosomal protein L20

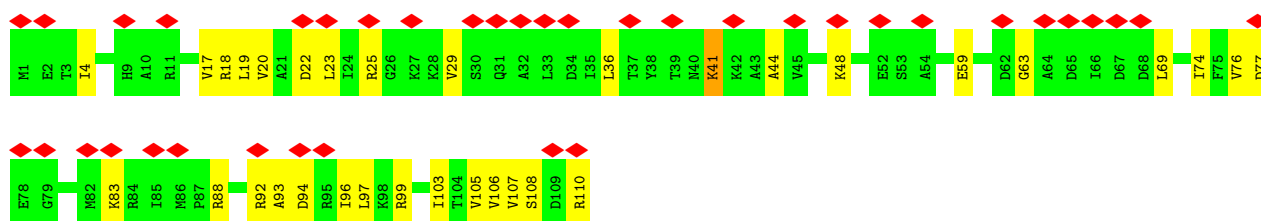
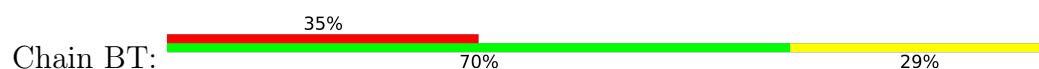




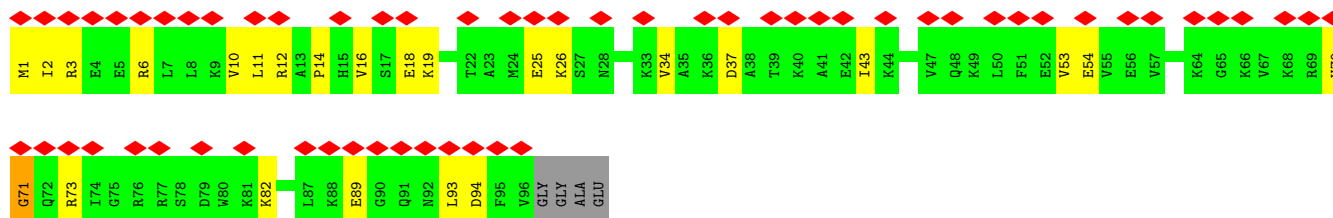
- Molecule 44: 50S ribosomal protein L21



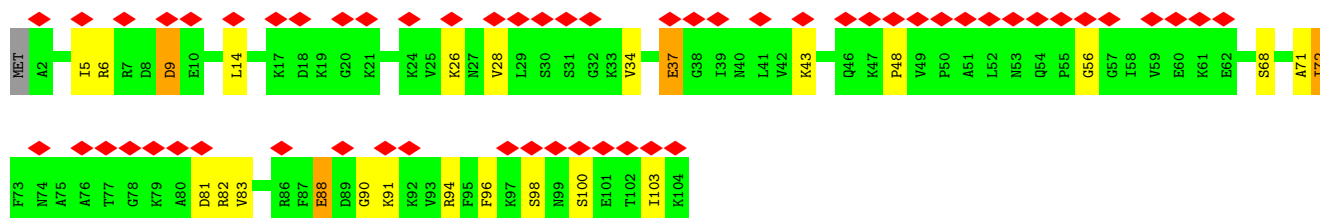
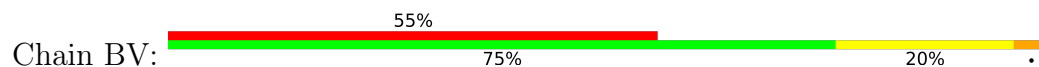
- Molecule 45: 50S ribosomal protein L22



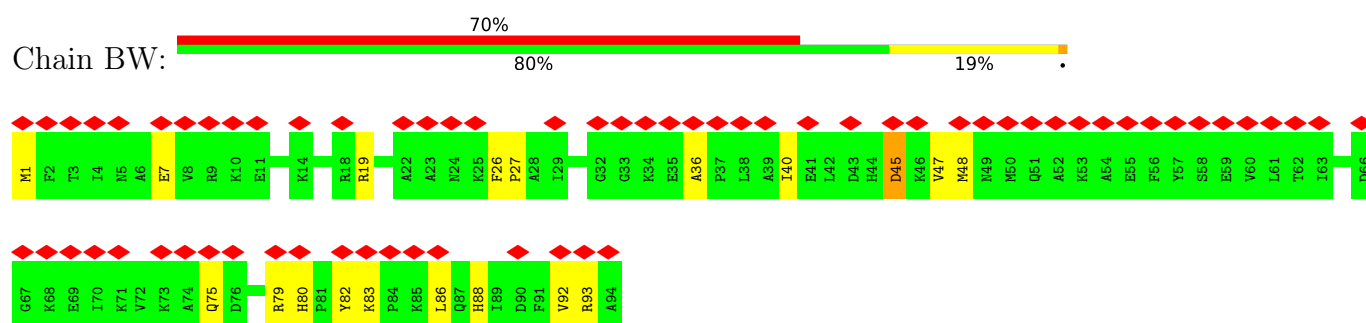
- Molecule 46: 50S ribosomal protein L23



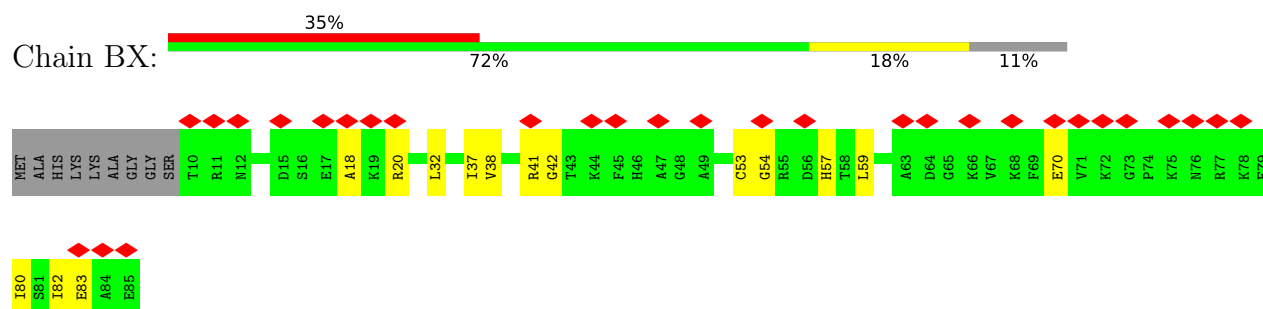
- Molecule 47: 50S ribosomal protein L24



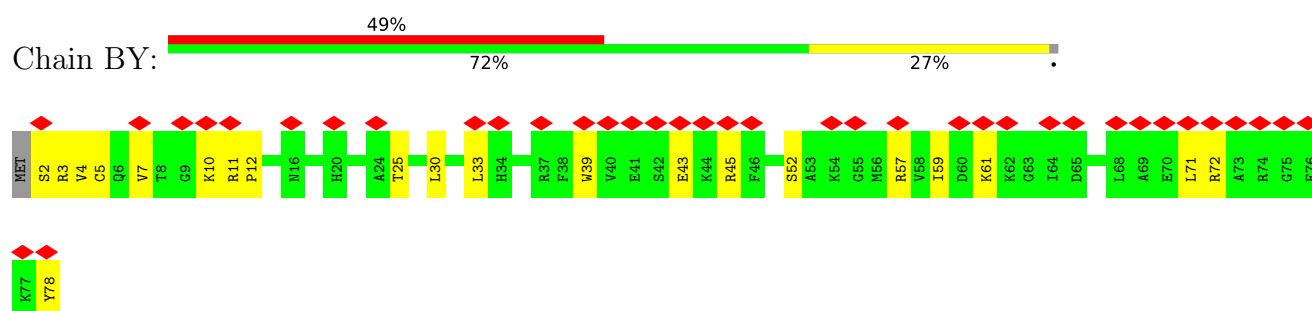
- Molecule 48: 50S ribosomal protein L25



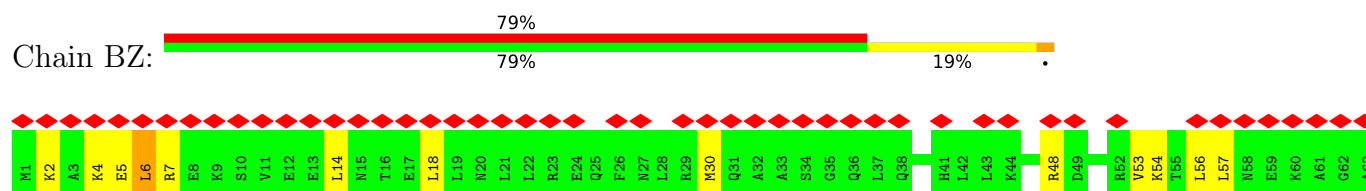
- Molecule 49: 50S ribosomal protein L27



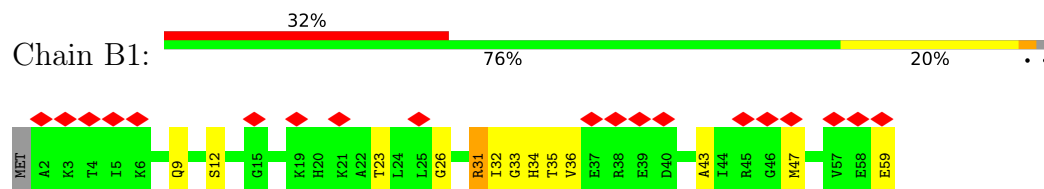
- Molecule 50: 50S ribosomal protein L28



- Molecule 51: 50S ribosomal protein L29

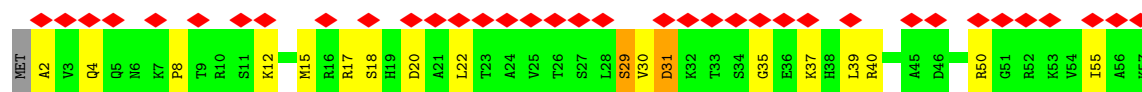


- Molecule 52: 50S ribosomal protein L30



- Molecule 53: 50S ribosomal protein L32

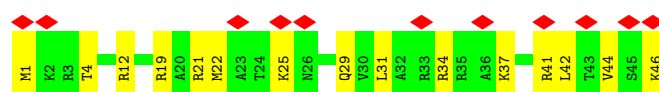




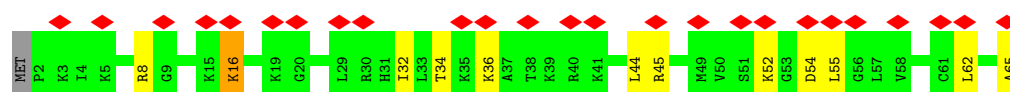
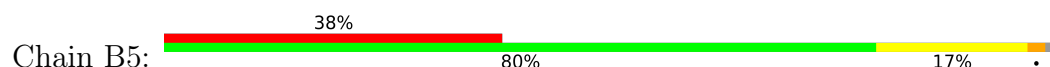
- Molecule 54: 50S ribosomal protein L33



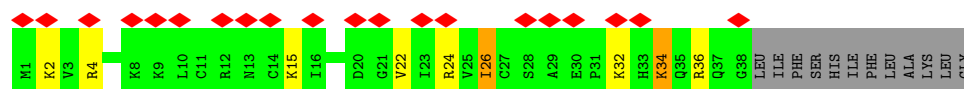
- Molecule 55: 50S ribosomal protein L34



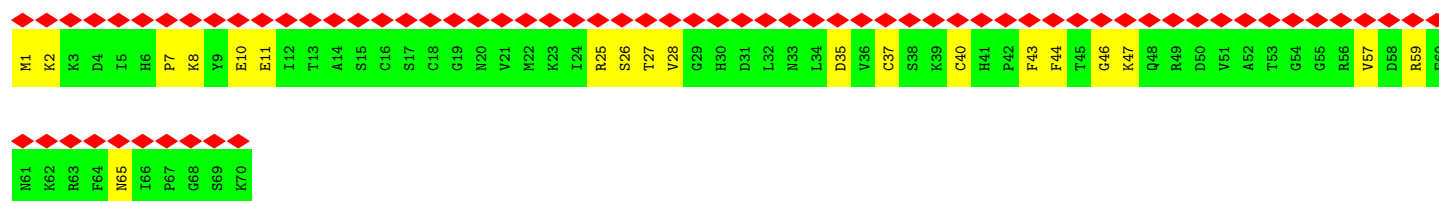
- Molecule 56: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L36

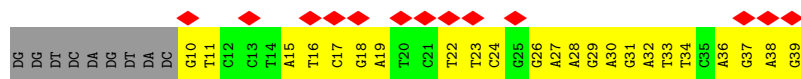


- Molecule 58: 50S ribosomal protein L31

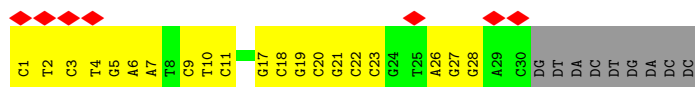


- Molecule 59: Non-template DNA strand

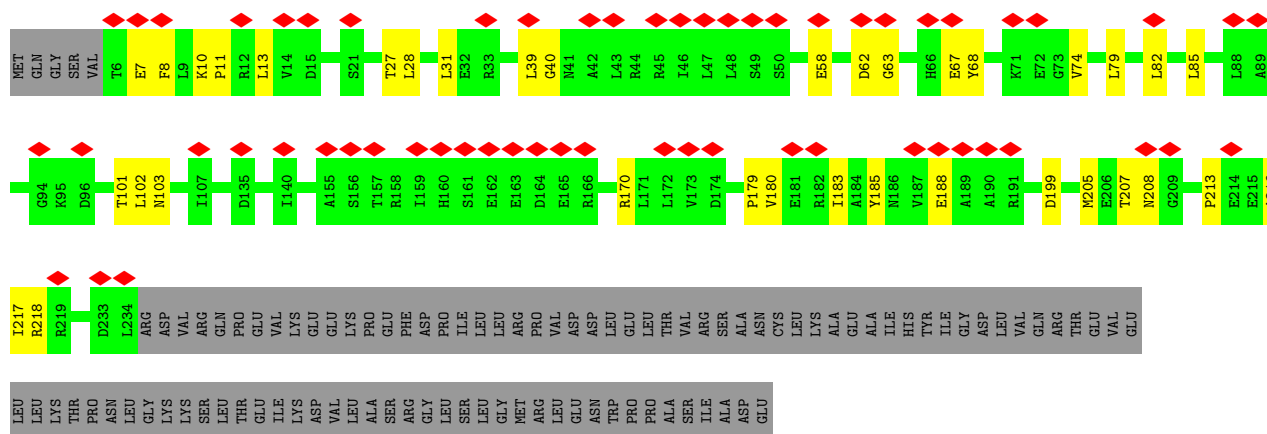




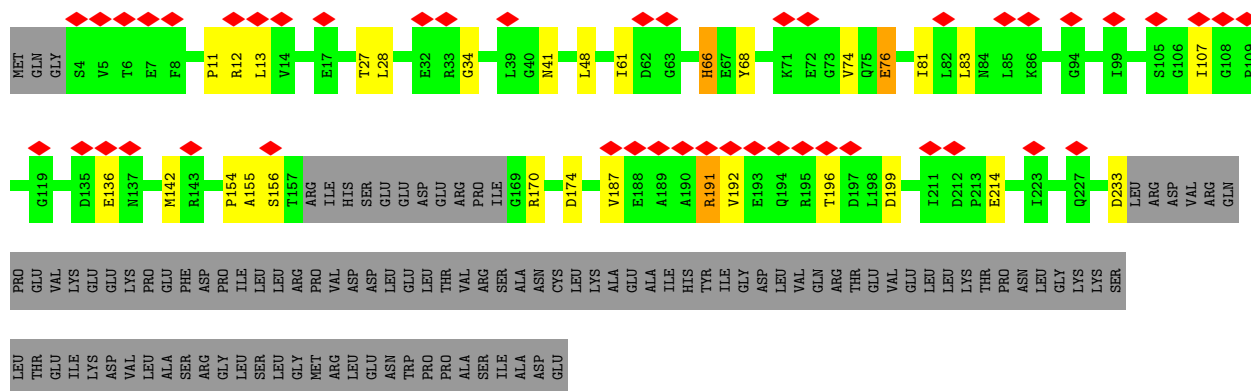
- Molecule 60: Template DNA strand



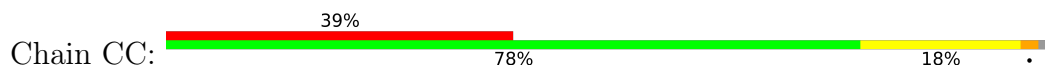
- Molecule 61: DNA-directed RNA polymerase subunit alpha

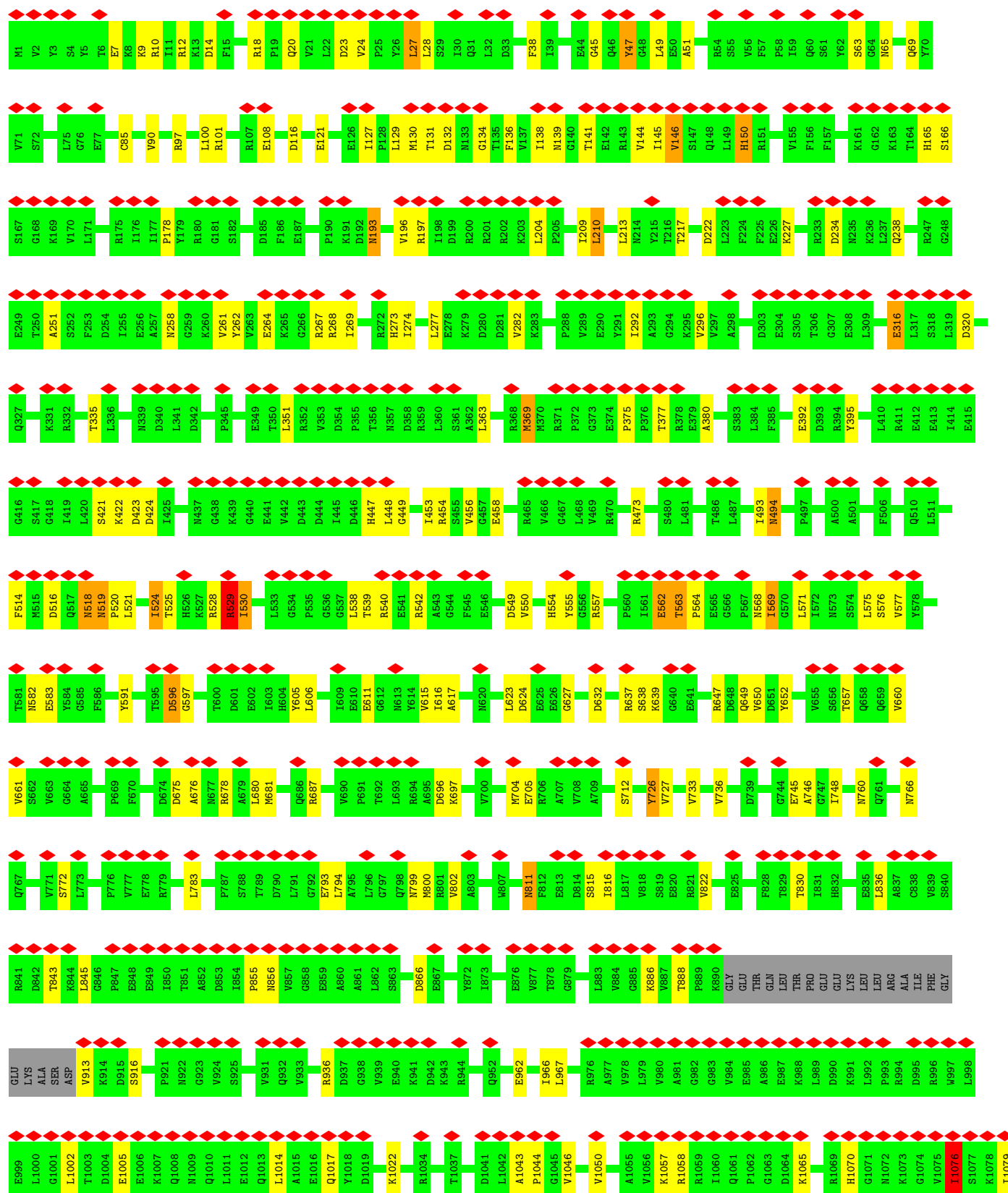


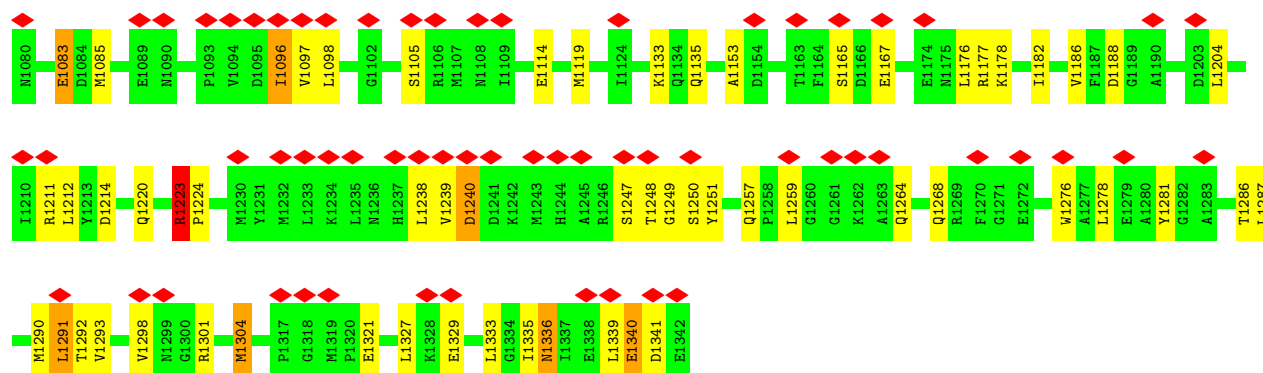
- Molecule 61: DNA-directed RNA polymerase subunit alpha



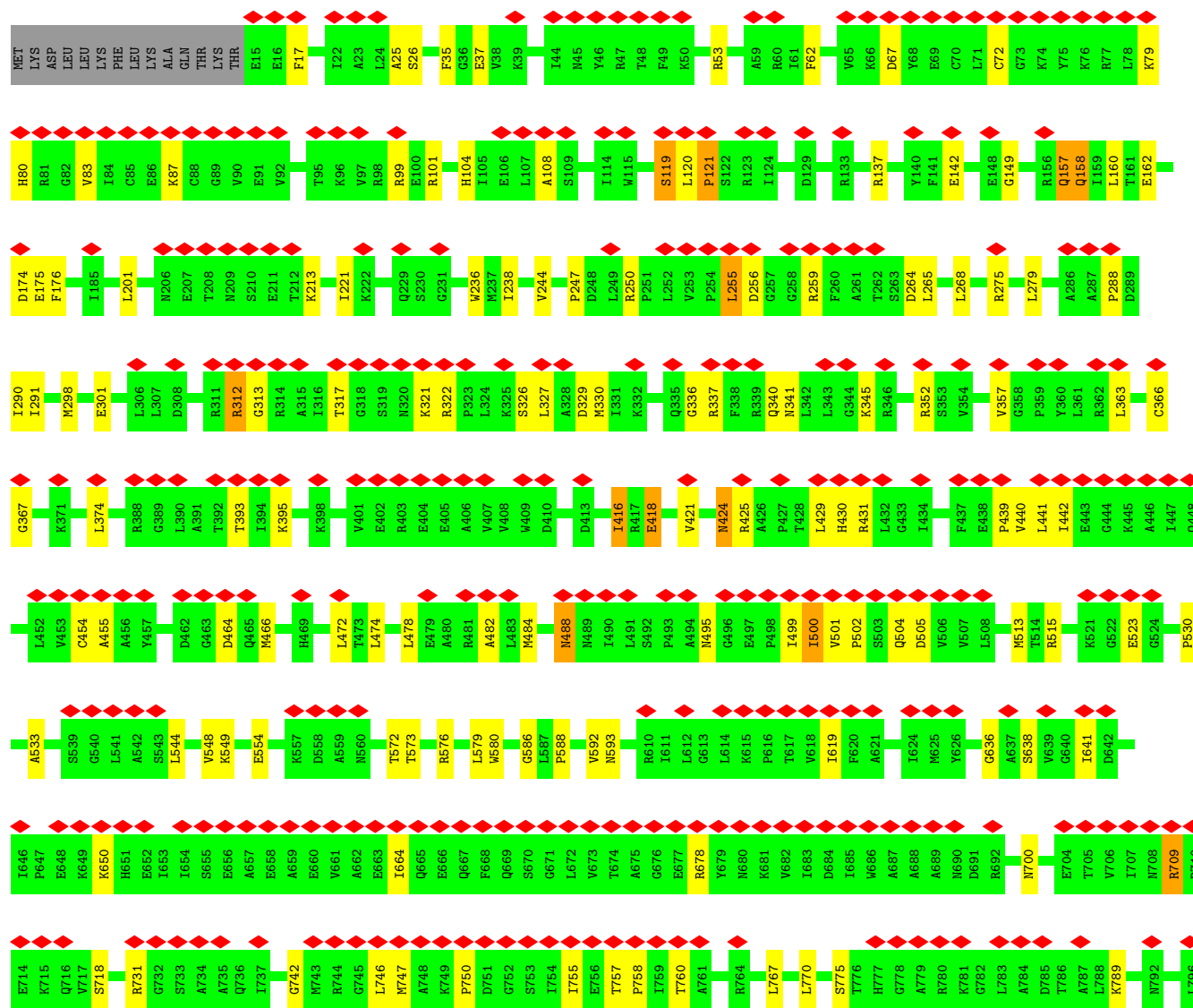
- Molecule 62: DNA-directed RNA polymerase subunit beta

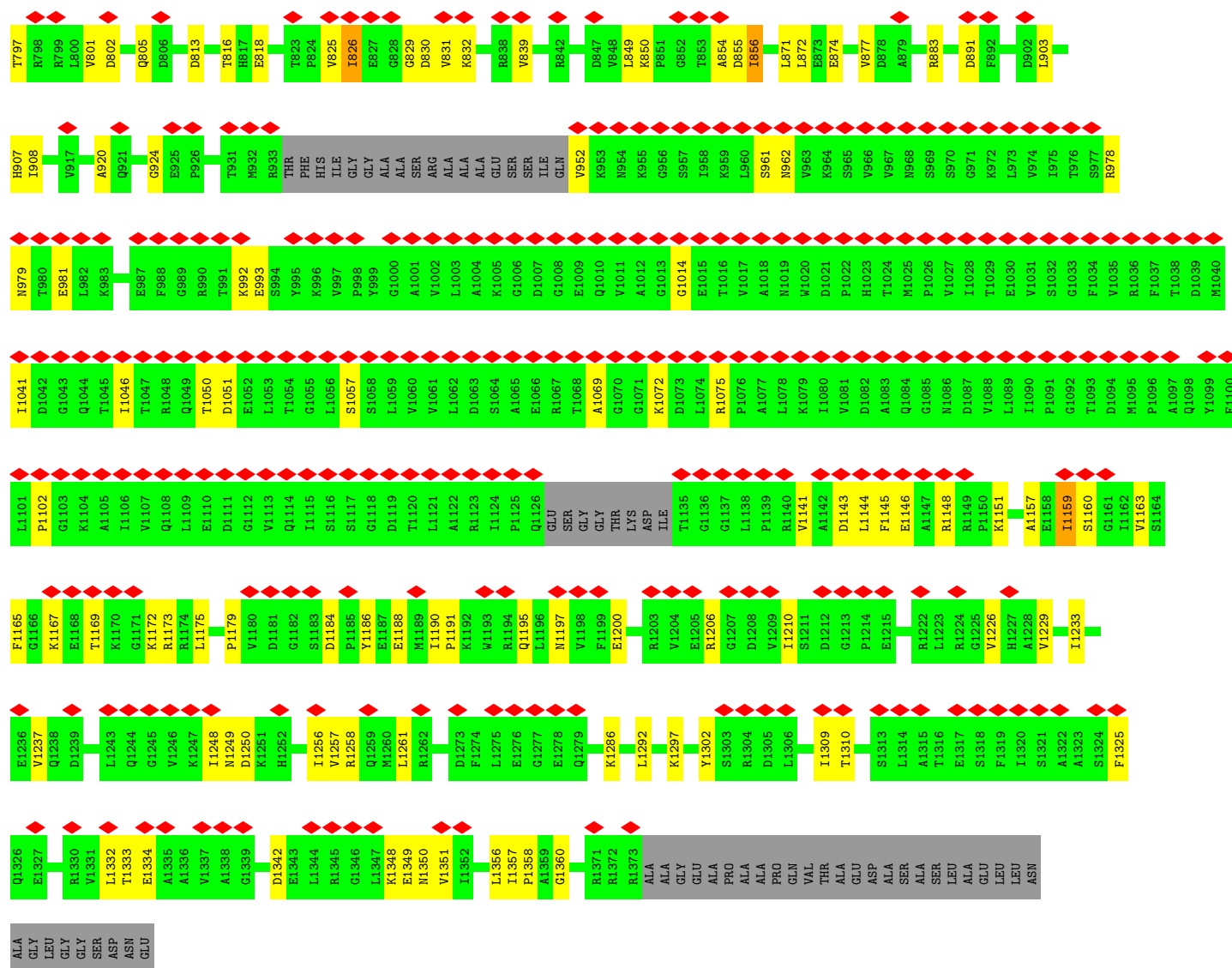




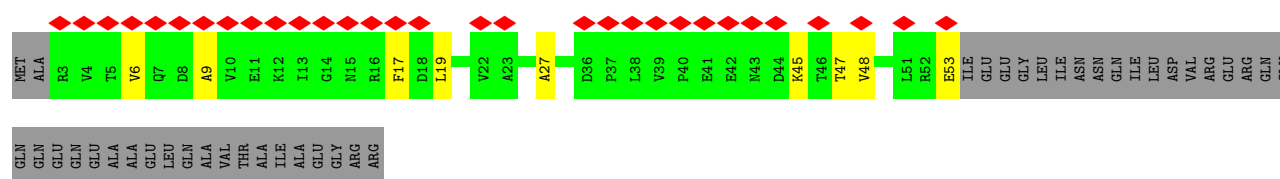


• Molecule 63: DNA-directed RNA polymerase subunit beta'

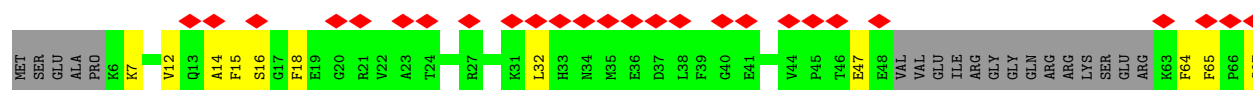




- Molecule 64: DNA-directed RNA polymerase subunit omega



- Molecule 65: Transcription termination/antitermination protein NusG



Y68	V69	L70	V71	Q72	M73	V74	M75	N76	D77	A78	S79	W80	H81	S85	V86	P87	R88	V89	M90	G91	F92	I93	G94	G95	T96	S97	D98	R99	P100	I103	S104	D105	K106	E107	V108	D109	A110	I111	M112	N113	R114	L115	Q116	Q117	V118	G119	D120	A121	P122	R123	P124	K125	T126	L127	F128	E129	P130
G131	E132	M133	V134	R135	V136	N137	D138	G139	P140	F141	A142	D143	F144	N145	G146	V147	V148	E149	E150	V151	D152	Y153	E154	K155	S156	R157	L158	K159	V160	S161	V162	S163	I164	F165	G166	R167	A168	T169	P170	V171	E172	L173	D174	F175	S176	Q177	V178	E179	K180	ALA							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.415	Depositor
Minimum map value	-0.341	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	673.28, 673.28, 673.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 7MG, 6MZ, 5MC, 3TD, D2T, OMC, MG, 4SU, UR3, MEQ, OMU, 5MU, 3AU, 2MA, H2U, PSU, MA6, OMG, ZN, 1MG, 4OC, G7M, 2MG, 4D4

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	AA	0.38	0/36569	0.58	9/57044 (0.0%)
2	AB	0.28	0/1796	0.68	0/2420
3	AC	0.37	0/1680	0.71	2/2263 (0.1%)
4	AD	0.32	0/1665	0.64	0/2227
5	AE	0.33	0/1161	0.77	2/1563 (0.1%)
6	AF	0.32	0/867	0.68	0/1171
7	AG	0.32	0/1219	0.75	0/1635
8	AH	0.30	0/989	0.58	0/1326
9	AI	0.40	0/1043	0.79	0/1387
10	AJ	0.39	0/818	0.85	3/1105 (0.3%)
11	AK	0.27	0/893	0.58	0/1205
12	AL	0.40	0/954	0.94	7/1279 (0.5%)
13	AM	0.35	0/900	0.68	0/1204
14	AN	0.39	0/817	0.61	0/1088
15	AO	0.29	0/722	0.63	0/964
16	AP	0.32	0/659	0.66	0/884
17	AQ	0.32	0/657	0.65	0/881
18	AR	0.29	0/501	0.60	0/672
19	AS	0.40	0/680	0.72	0/915
20	AT	0.31	0/676	0.54	0/895
21	AU	0.30	0/598	0.74	1/792 (0.1%)
22	AV	0.79	0/949	0.93	7/1475 (0.5%)
23	AW	0.33	0/1725	0.61	2/2687 (0.1%)
24	AX	0.22	0/1584	0.32	0/2463
25	AY	0.14	0/682	0.42	0/918
26	BA	0.32	2/69165 (0.0%)	0.56	13/107893 (0.0%)
27	BB	0.27	0/2872	0.49	0/4478
28	BC	0.30	0/2131	0.67	0/2863
29	BD	0.30	0/1576	0.60	0/2119
30	BE	0.26	0/1571	0.55	0/2113
31	BF	0.24	0/1444	0.63	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BG	0.23	0/1333	0.60	0/1805
33	BH	0.25	0/1122	0.74	0/1515
34	BI	0.25	0/993	0.98	1/1340 (0.1%)
35	BJ	0.25	0/1046	0.70	1/1410 (0.1%)
36	BK	0.28	0/1152	0.52	0/1551
37	BL	0.31	0/956	0.61	0/1279
38	BM	0.30	0/1061	0.64	0/1412
39	BN	0.28	0/1081	0.52	0/1443
40	BO	0.30	0/973	0.60	0/1301
41	BP	0.25	0/910	0.66	0/1219
42	BQ	0.28	0/929	0.69	0/1242
43	BR	0.37	0/960	0.62	0/1278
44	BS	0.32	0/829	0.76	0/1107
45	BT	0.31	0/864	0.60	0/1156
46	BU	0.24	0/771	0.53	0/1031
47	BV	0.24	0/797	0.66	0/1062
48	BW	0.26	0/766	0.58	0/1025
49	BX	0.29	0/589	0.58	0/779
50	BY	0.26	0/635	0.52	0/848
51	BZ	0.25	0/510	0.67	0/677
52	B1	0.31	0/453	0.68	0/605
53	B2	0.35	0/450	0.85	2/599 (0.3%)
54	B3	0.21	0/443	0.70	0/587
55	B4	0.30	0/380	0.68	0/498
56	B5	0.28	0/513	0.61	0/676
57	B6	0.28	0/302	0.53	0/397
58	B7	0.28	0/559	0.86	1/745 (0.1%)
59	CN	0.79	0/693	0.77	0/1068
60	CT	1.19	0/676	0.84	0/1039
61	CA	1.10	0/1797	0.96	0/2436
61	CB	0.81	0/1703	0.90	0/2308
62	CC	1.34	18/10581 (0.2%)	1.05	2/14275 (0.0%)
63	CD	1.10	6/10532 (0.1%)	0.97	1/14219 (0.0%)
64	CE	0.44	0/401	0.83	0/540
65	CF	0.27	0/1312	0.59	0/1771
All	All	0.54	26/188635 (0.0%)	0.66	54/278109 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
2	AB	0	1
10	AJ	0	1
12	AL	0	1
13	AM	0	1
22	AV	0	1
26	BA	0	1
28	BC	0	1
31	BF	0	1
34	BI	0	1
40	BO	0	1
49	BX	0	1
58	B7	0	1
All	All	0	15

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CC	799	ASN	CB-CG	-6.31	1.36	1.52
63	CD	424	ASN	CB-CG	-6.29	1.36	1.52
62	CC	519	ASN	CB-CG	-6.21	1.36	1.52
62	CC	530	ILE	CB-CG2	-6.15	1.32	1.52
63	CD	760	THR	CA-C	-6.09	1.42	1.52
62	CC	1076	ILE	CB-CG1	-6.08	1.41	1.53
62	CC	518	ASN	CB-CG	-5.95	1.37	1.52
26	BA	550	U	C1'-N1	5.67	1.56	1.48
62	CC	146	VAL	CB-CG1	-5.63	1.33	1.52
62	CC	144	VAL	CB-CG1	-5.56	1.34	1.52
63	CD	424	ASN	CA-CB	-5.54	1.42	1.53
26	BA	545	A	C1'-N9	-5.50	1.39	1.48
62	CC	811	ASN	CB-CG	-5.45	1.38	1.52
63	CD	1357	ILE	C-N	-5.44	1.15	1.34
62	CC	146	VAL	CB-CG2	-5.37	1.34	1.52
62	CC	136	PHE	CB-CG	-5.33	1.38	1.50
63	CD	1333	THR	CB-CG2	-5.33	1.34	1.52
63	CD	1145	PHE	CB-CG	-5.33	1.38	1.50
62	CC	453	ILE	CB-CG2	-5.32	1.34	1.52
62	CC	816	ILE	CB-CG2	-5.24	1.35	1.52
62	CC	802	VAL	CB-CG1	-5.22	1.35	1.52
62	CC	712	SER	CA-C	-5.22	1.31	1.52
62	CC	27	LEU	CG-CD2	-5.20	1.35	1.52
62	CC	520	PRO	CB-CG	-5.19	1.23	1.49
62	CC	1096	ILE	CB-CG2	-5.18	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CC	563	THR	CA-CB	-5.01	1.47	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	1176	U	O4'-C1'-N1	11.17	125.26	108.50
22	AV	38	A	C4'-C3'-O3'	-10.79	93.22	109.40
21	AU	64	ASN	N-CA-C	-9.77	94.72	109.86
34	BI	49	GLY	N-CA-C	9.66	122.74	111.63
5	AE	50	TYR	CA-C-N	8.65	138.36	121.41
5	AE	50	TYR	C-N-CA	8.65	138.36	121.41
22	AV	49	G	O3'-P-O5'	-8.32	91.51	104.00
12	AL	98	VAL	CA-C-N	8.12	133.10	121.50
12	AL	98	VAL	C-N-CA	8.12	133.10	121.50
22	AV	37	G	C4'-C3'-O3'	-7.55	101.68	113.00
1	AA	1494	G	P-O5'-C5'	-6.72	110.82	120.90
26	BA	2131	U	N1-C1'-C2'	6.58	121.87	112.00
62	CC	529	ARG	CA-CB-CG	6.26	126.62	114.10
1	AA	1008	U	O4'-C1'-N1	6.19	117.79	108.50
22	AV	40	A	C2'-C3'-O3'	6.17	118.76	109.50
26	BA	141	G	O3'-P-O5'	6.11	113.17	104.00
3	AC	60	PRO	CA-C-N	6.01	133.03	121.54
3	AC	60	PRO	C-N-CA	6.01	133.03	121.54
35	BJ	113	ALA	N-CA-C	-5.91	105.33	112.54
22	AV	40	A	C4'-C3'-O3'	5.88	118.22	109.40
26	BA	2225	A	P-O3'-C3'	5.87	129.00	120.20
1	AA	1008	U	C2'-C3'-O3'	-5.83	104.95	113.70
1	AA	4	U	P-O3'-C3'	5.80	128.90	120.20
26	BA	1408	G	O3'-P-O5'	-5.78	95.33	104.00
26	BA	884	U	N1-C1'-C2'	-5.76	103.37	112.00
1	AA	74	A	O5'-C5'-C4'	5.69	120.03	111.50
1	AA	1034	G	O3'-P-O5'	-5.66	95.50	104.00
26	BA	1176	U	N1-C1'-C2'	5.66	120.49	112.00
53	B2	31	ASP	CA-C-N	5.60	128.24	120.29
53	B2	31	ASP	C-N-CA	5.60	128.24	120.29
12	AL	42	PRO	CA-C-N	5.59	133.42	121.45
12	AL	42	PRO	C-N-CA	5.59	133.42	121.45
1	AA	1491	G	O3'-P-O5'	5.59	112.38	104.00
26	BA	2117	A	N9-C1'-C2'	5.58	122.37	114.00
10	AJ	38	GLY	CA-C-N	5.56	140.35	127.00
10	AJ	38	GLY	C-N-CA	5.56	140.35	127.00
1	AA	1008	U	O5'-C5'-C4'	5.53	119.80	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	80	ILE	CA-C-N	-5.51	115.40	123.00
12	AL	80	ILE	C-N-CA	-5.51	115.40	123.00
58	B7	46	GLY	N-CA-C	-5.44	105.91	112.49
26	BA	788	A	P-O3'-C3'	5.43	128.35	120.20
1	AA	812	G	O4'-C1'-N9	5.42	116.33	108.20
62	CC	210	LEU	CA-CB-CG	-5.32	97.69	116.30
10	AJ	38	GLY	C-N-CD	-5.25	109.05	120.60
22	AV	41	C	N1-C1'-C2'	5.24	121.86	114.00
23	AW	17(A)	U	O5'-C5'-C4'	5.23	119.54	111.70
22	AV	36	A	C4'-C3'-O3'	5.21	117.21	109.40
23	AW	17	C	P-O3'-C3'	5.19	125.93	119.70
26	BA	788	A	C4'-C3'-O3'	5.17	117.15	109.40
26	BA	1409	U	C5'-C4'-C3'	5.12	123.69	116.00
26	BA	142	A	P-O5'-C5'	5.09	128.54	120.90
26	BA	2117	A	O4'-C1'-N9	5.06	115.79	108.20
12	AL	98	VAL	O-C-N	5.05	130.18	122.76
63	CD	502	PRO	N-CA-C	5.03	119.10	110.95

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	60	A	Sidechain
2	AB	17	GLY	Mainchain
10	AJ	42	LEU	Mainchain
12	AL	43	LYS	Peptide
13	AM	65	VAL	Peptide
22	AV	45	C	Sidechain
58	B7	44	PHE	Mainchain
26	BA	2131	U	Sidechain
28	BC	176	LEU	Mainchain
31	BF	126	GLY	Mainchain
34	BI	81	LEU	Mainchain
40	BO	100	CYS	Mainchain
49	BX	54	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32909	0	16580	337	0
2	AB	1765	0	1792	50	0
3	AC	1653	0	1727	70	0
4	AD	1643	0	1707	40	0
5	AE	1148	0	1195	48	0
6	AF	848	0	846	24	0
7	AG	1203	0	1254	35	0
8	AH	979	0	1031	18	0
9	AI	1031	0	1076	38	0
10	AJ	808	0	845	43	0
11	AK	877	0	887	21	0
12	AL	951	0	1011	38	0
13	AM	891	0	952	26	0
14	AN	805	0	844	26	0
15	AO	714	0	734	16	0
16	AP	649	0	666	11	0
17	AQ	648	0	691	12	0
18	AR	494	0	512	12	0
19	AS	663	0	688	20	0
20	AT	670	0	719	14	0
21	AU	590	0	629	12	0
22	AV	849	0	433	63	0
23	AW	1645	0	842	12	0
24	AX	1624	0	823	33	0
25	AY	677	0	675	22	0
26	BA	62270	0	31337	604	0
27	BB	2569	0	1301	29	0
28	BC	2092	0	2167	37	0
29	BD	1566	0	1618	34	0
30	BE	1552	0	1618	26	0
31	BF	1420	0	1457	46	0
32	BG	1313	0	1358	23	0
33	BH	1111	0	1148	32	0
34	BI	980	0	1013	57	0
35	BJ	1032	0	1088	35	0
36	BK	1129	0	1162	17	0
37	BL	947	0	1023	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BM	1052	0	1127	24	0
39	BN	1075	0	1154	21	0
40	BO	960	0	1000	21	0
41	BP	900	0	935	18	0
42	BQ	917	0	962	26	0
43	BR	947	0	1019	19	0
44	BS	816	0	839	18	0
45	BT	857	0	922	23	0
46	BU	764	0	829	15	0
47	BV	789	0	844	15	0
48	BW	753	0	780	12	0
49	BX	582	0	599	6	0
50	BY	625	0	652	13	0
51	BZ	509	0	543	11	0
52	B1	449	0	488	7	0
53	B2	444	0	458	14	0
54	B3	436	0	477	12	0
55	B4	377	0	418	14	0
56	B5	504	0	572	9	0
57	B6	301	0	340	6	0
58	B7	549	0	549	15	0
59	CN	618	0	338	59	0
60	CT	606	0	338	38	0
61	CA	1775	0	1800	22	0
61	CB	1684	0	1713	18	0
62	CC	10415	0	10428	216	0
63	CD	10375	0	10595	198	0
64	CE	399	0	417	5	0
65	CF	1283	0	1261	102	0
66	AA	148	0	0	0	0
66	AI	1	0	0	0	0
66	AW	1	0	0	0	0
66	AX	1	0	0	0	0
66	BA	314	0	0	0	0
66	BB	6	0	0	0	0
66	BC	3	0	0	0	0
66	BD	1	0	0	0	0
66	BE	1	0	0	0	0
66	BQ	1	0	0	0	0
66	BT	1	0	0	0	0
66	CD	1	0	0	0	0
67	AX	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	B6	1	0	0	0	0
68	B7	1	0	0	0	0
68	CD	2	0	0	0	0
All	All	176970	0	127854	2535	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 8.

All (2535) 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)
3:AC:88:ARG:NH2	63:CD:79:LYS:HD3	1.37	1.36
62:CC:375:PRO:CG	65:CF:80:TRP:CH2	2.08	1.35
3:AC:88:ARG:CZ	63:CD:79:LYS:HD3	1.65	1.26
3:AC:102:ASN:HA	22:AV:36:A:N6	1.49	1.26
59:CN:18:DG:N2	65:CF:12:VAL:O	1.76	1.19
65:CF:47:GLU:HG3	65:CF:64:PHE:CE1	1.80	1.16
65:CF:123:ARG:HB3	65:CF:124:PRO:HD2	1.19	1.15
33:BH:5:LEU:O	33:BH:16:GLY:HA2	1.46	1.15
62:CC:380:ALA:HB2	65:CF:81:HIS:NE2	1.59	1.15
3:AC:88:ARG:NH2	63:CD:79:LYS:CD	2.09	1.15
65:CF:123:ARG:HB3	65:CF:124:PRO:CD	1.74	1.15
62:CC:375:PRO:HG2	65:CF:80:TRP:CZ3	1.81	1.14
21:AU:61:ALA:O	21:AU:65:ALA:HB3	1.47	1.12
59:CN:18:DG:N2	65:CF:68:TYR:HA	1.63	1.11
5:AE:35:ALA:O	5:AE:50:TYR:O	1.70	1.09
62:CC:375:PRO:CD	65:CF:80:TRP:CH2	2.37	1.08
10:AJ:89:ARG:HH22	62:CC:845:LEU:HA	0.94	1.08
65:CF:47:GLU:HG3	65:CF:64:PHE:HE1	1.01	1.07
59:CN:19:DA:H5"	65:CF:89:VAL:H	1.04	1.07
62:CC:63:SER:HB2	65:CF:32:LEU:HD13	1.35	1.07
62:CC:380:ALA:CB	65:CF:81:HIS:NE2	2.17	1.06
62:CC:375:PRO:HG3	65:CF:80:TRP:CH2	1.86	1.05
3:AC:88:ARG:HH21	63:CD:79:LYS:CD	1.68	1.05
62:CC:375:PRO:CG	65:CF:80:TRP:CZ3	2.38	1.04
59:CN:19:DA:H5"	65:CF:89:VAL:N	1.73	1.03
34:BI:26:VAL:HA	34:BI:83:ALA:O	1.56	1.03
62:CC:63:SER:CB	65:CF:32:LEU:CD1	2.34	1.02
62:CC:63:SER:CB	65:CF:32:LEU:HD13	1.88	1.01
62:CC:375:PRO:CD	65:CF:80:TRP:HH2	1.72	1.01
62:CC:375:PRO:HD2	65:CF:80:TRP:HH2	1.23	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:89:ARG:NH2	62:CC:845:LEU:HA	1.75	0.99
65:CF:47:GLU:CG	65:CF:64:PHE:HE1	1.76	0.98
22:AV:44:A:C6	62:CC:1264:GLN:NE2	2.29	0.98
59:CN:16:DT:H5'	65:CF:15:PHE:HD1	1.28	0.98
3:AC:88:ARG:HH21	63:CD:79:LYS:HD3	1.19	0.97
34:BI:24:SER:HA	34:BI:85:SER:O	1.63	0.97
1:AA:1239:A:H62	1:AA:1299:A:H62	1.06	0.97
59:CN:19:DA:C5'	65:CF:89:VAL:H	1.77	0.96
34:BI:28:ALA:HB2	34:BI:81:LEU:O	1.66	0.94
26:BA:2118:U:O4	26:BA:2148:G:N2	2.01	0.93
63:CD:162:GLU:HG3	65:CF:95:GLY:HA3	1.48	0.92
3:AC:102:ASN:HA	22:AV:36:A:H61	1.34	0.92
3:AC:77:ILE:HD13	22:AV:36:A:H5''	1.51	0.92
26:BA:2119:A:H2'	26:BA:2168:G:H1	1.35	0.91
26:BA:1724:G:H1	26:BA:1736:U:H3	0.92	0.91
24:AX:26:A:N6	24:AX:44:G:H1	1.69	0.91
3:AC:88:ARG:NE	63:CD:79:LYS:HD3	1.86	0.90
3:AC:88:ARG:HH21	63:CD:79:LYS:CG	1.84	0.90
62:CC:380:ALA:HB2	65:CF:81:HIS:CD2	2.06	0.90
1:AA:60:A:H62	1:AA:110:C:N4	1.68	0.90
24:AX:26:A:H61	24:AX:44:G:H1	1.09	0.90
26:BA:1407:G:H2'	26:BA:1408:G:H8	1.37	0.89
10:AJ:3:ASN:N	10:AJ:3:ASN:HD22	1.64	0.89
30:BE:5:LEU:O	30:BE:9:GLN:HA	1.72	0.89
59:CN:19:DA:C2'	65:CF:87:PRO:HA	2.00	0.88
1:AA:411:A:H4'	1:AA:412:A:H5'	1.54	0.88
62:CC:375:PRO:HG2	65:CF:80:TRP:CH2	1.94	0.88
1:AA:481:G:O2'	1:AA:483:C:N4	2.05	0.88
13:AM:107:ARG:NH1	13:AM:111:GLY:O	2.07	0.88
4:AD:105:MET:HG3	4:AD:171:LEU:HD12	1.56	0.87
59:CN:17:DC:O5'	65:CF:15:PHE:CE1	2.26	0.86
26:BA:29:U:H3	26:BA:511:U:H3	0.89	0.86
26:BA:2880:C:O2'	40:BO:90:ARG:NH1	2.09	0.86
59:CN:18:DG:H22	65:CF:69:VAL:N	1.73	0.85
33:BH:47:PHE:HA	33:BH:51:ARG:HB2	1.56	0.85
14:AN:41:ARG:NH1	19:AS:6:LYS:O	2.10	0.84
34:BI:27:VAL:HG23	34:BI:83:ALA:HB3	1.58	0.84
13:AM:23:TYR:HB3	13:AM:66:GLU:HG2	1.59	0.83
26:BA:572:A:OP2	44:BS:80:ARG:NH2	2.11	0.83
26:BA:2171:A:O2'	26:BA:2173:A:OP1	1.95	0.83
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:CD:829:GLY:O	63:CD:993:GLU:HA	1.79	0.83
1:AA:1167:A:O2'	1:AA:1169:A:N7	2.12	0.82
62:CC:375:PRO:HD2	65:CF:80:TRP:CH2	2.10	0.82
1:AA:83:C:O2	1:AA:87:C:N4	2.12	0.82
22:AV:50:C:H2'	22:AV:51:G:H8	1.43	0.82
3:AC:102:ASN:CA	22:AV:36:A:N6	2.40	0.82
26:BA:2100:G:H2'	26:BA:2101:A:H8	1.44	0.82
26:BA:475:C:O2	26:BA:479:A:N6	2.11	0.82
26:BA:1918:A:O2'	26:BA:1919:A:N7	2.12	0.82
34:BI:24:SER:OG	34:BI:85:SER:N	2.11	0.82
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.13	0.81
63:CD:87:LYS:O	65:CF:133:MET:HE3	1.80	0.81
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.80	0.81
1:AA:6:G:H1	5:AE:103:THR:HG21	1.46	0.81
26:BA:404:A:O2'	26:BA:405:U:OP2	1.98	0.81
47:BV:48:PRO:HG3	47:BV:56:GLY:HA3	1.62	0.81
26:BA:1086:A:H5''	26:BA:1087:G:H5'	1.62	0.81
31:BF:70:ALA:HB2	31:BF:79:ILE:HD11	1.62	0.81
42:BQ:100:LEU:HA	42:BQ:103:ARG:HG2	1.63	0.81
22:AV:51:G:H2'	22:AV:52:C:H6	1.44	0.80
61:CB:191:ARG:HB3	61:CB:196:THR:HG23	1.64	0.80
26:BA:1069:A:O2'	26:BA:1074:G:O6	1.99	0.80
18:AR:36:SER:HA	18:AR:72:ASP:HB2	1.62	0.80
22:AV:38:A:H4'	22:AV:39:C:H5''	1.63	0.80
59:CN:18:DG:N2	65:CF:68:TYR:CA	2.45	0.80
63:CD:830:ASP:HA	63:CD:992:LYS:O	1.80	0.79
13:AM:16:VAL:HG13	13:AM:17:ILE:HD12	1.65	0.79
1:AA:736:C:OP1	18:AR:61:ARG:NH1	2.16	0.79
10:AJ:89:ARG:HH22	62:CC:845:LEU:CA	1.86	0.79
26:BA:2286:G:OP2	54:B3:6:ARG:NH2	2.15	0.79
59:CN:19:DA:C5'	65:CF:89:VAL:N	2.35	0.79
1:AA:843:U:OP1	1:AA:844:G:N2	2.15	0.79
26:BA:2885:G:H2'	26:BA:2886:A:O4'	1.83	0.78
63:CD:291:ILE:HD11	65:CF:65:PHE:CE2	2.18	0.78
1:AA:600:A:OP2	8:AH:88:ARG:NH1	2.16	0.78
22:AV:38:A:OP1	22:AV:38:A:H2'	1.82	0.78
26:BA:2467:C:O2	39:BN:123:LYS:NZ	2.16	0.78
34:BI:103:ASN:HA	34:BI:107:GLU:HB3	1.65	0.78
26:BA:2145:C:H5''	26:BA:2146:C:H5	1.48	0.78
7:AG:76:LYS:HD2	7:AG:78:ARG:HH21	1.48	0.78
26:BA:1535:A:H3'	26:BA:1536:C:H5''	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:CD:291:ILE:CD1	65:CF:65:PHE:CE2	2.67	0.78
63:CD:1186:TYR:OH	63:CD:1188:GLU:OE1	2.01	0.78
26:BA:1084:A:N3	26:BA:1105:U:O2'	2.17	0.77
59:CN:18:DG:C2	65:CF:68:TYR:HA	2.18	0.77
60:CT:18:DC:H2'	60:CT:19:DG:C8	2.19	0.77
1:AA:1006:G:H2'	1:AA:1007:U:H6	1.50	0.77
42:BQ:113:ARG:O	42:BQ:115:ASN:ND2	2.17	0.77
63:CD:429:LEU:H	63:CD:429:LEU:HD22	1.47	0.77
1:AA:1051:C:O2	1:AA:1207:2MG:N2	2.17	0.76
37:BL:36:GLY:N	37:BL:62:VAL:O	2.17	0.76
35:BJ:7:TYR:HA	35:BJ:58:ILE:HG23	1.66	0.76
59:CN:17:DC:O5'	65:CF:15:PHE:HE1	1.64	0.76
61:CB:74:VAL:HG21	61:CB:81:ILE:HD11	1.66	0.76
1:AA:1029:U:H5'	1:AA:1030:U:C4	2.21	0.76
5:AE:115:LEU:HD13	5:AE:123:VAL:HG11	1.67	0.76
26:BA:239:C:HO2'	26:BA:622:G:HO2'	1.24	0.76
26:BA:1407:G:H2'	26:BA:1408:G:C8	2.20	0.76
61:CA:62:ASP:OD1	61:CA:63:GLY:N	2.19	0.76
2:AB:129:LEU:HB2	2:AB:133:GLU:HB2	1.68	0.76
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.16	0.76
22:AV:38:A:H4'	22:AV:39:C:C5'	2.16	0.76
29:BD:34:VAL:O	29:BD:93:GLY:N	2.17	0.76
33:BH:5:LEU:O	33:BH:16:GLY:CA	2.31	0.76
26:BA:1068:G:N2	26:BA:1095:A:O2'	2.19	0.75
34:BI:26:VAL:HB	34:BI:82:ILE:HG23	1.68	0.75
26:BA:864:G:OP2	39:BN:22:GLN:NE2	2.19	0.75
22:AV:50:C:H2'	22:AV:51:G:C8	2.21	0.75
34:BI:25:ALA:O	34:BI:83:ALA:O	2.04	0.75
63:CD:829:GLY:HA2	63:CD:993:GLU:HB3	1.68	0.75
14:AN:27:LEU:HD11	14:AN:47:LYS:HD3	1.69	0.75
21:AU:61:ALA:O	21:AU:64:ASN:O	2.04	0.75
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.19	0.75
26:BA:783:A:H2'	26:BA:783:A:N3	2.00	0.75
46:BU:1:MET:SD	46:BU:2:ILE:N	2.59	0.75
59:CN:18:DG:O6	65:CF:67:GLY:HA2	1.85	0.75
65:CF:123:ARG:CB	65:CF:124:PRO:CD	2.57	0.75
23:AW:17:C:H2'	23:AW:17(A):U:H6	1.52	0.74
26:BA:2298:A:OP1	31:BF:71:ARG:NH2	2.20	0.74
1:AA:1261:A:N6	1:AA:1274:A:O2'	2.20	0.74
26:BA:1084:A:H2'	26:BA:1085:A:C8	2.21	0.74
44:BS:17:GLY:N	44:BS:98:ILE:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:375:PRO:HG3	65:CF:80:TRP:CZ3	2.16	0.74
26:BA:1084:A:H62	34:BI:56:ARG:HH22	1.33	0.74
26:BA:2243:U:H2'	26:BA:2244:U:C6	2.23	0.74
1:AA:4:U:O2'	1:AA:5:U:O5'	2.04	0.74
39:BN:136:MET:OXT	48:BW:79:ARG:NH2	2.20	0.74
63:CD:87:LYS:O	65:CF:133:MET:CE	2.36	0.74
26:BA:1590:A:H2'	26:BA:1591:A:C8	2.23	0.74
55:B4:34:ARG:NE	55:B4:42:LEU:O	2.21	0.74
59:CN:18:DG:H22	65:CF:68:TYR:HA	1.53	0.74
26:BA:2182:U:O2'	26:BA:2183:A:N7	2.18	0.73
1:AA:1035:A:H2'	1:AA:1036:A:H8	1.53	0.73
26:BA:100:U:O2'	47:BV:91:LYS:NZ	2.21	0.73
63:CD:1179:PRO:HD2	63:CD:1184:ASP:HA	1.69	0.73
1:AA:522:C:O2	1:AA:527:G7M:N2	2.18	0.73
26:BA:1869:G:N2	26:BA:1871:A:O2'	2.21	0.73
63:CD:816:THR:OG1	63:CD:818:GLU:OE1	2.04	0.73
62:CC:10:ARG:NH2	62:CC:793:GLU:OE1	2.21	0.73
1:AA:60:A:N6	1:AA:110:C:N4	2.37	0.73
1:AA:339:C:OP1	37:BL:13:ASN:ND2	2.19	0.73
3:AC:101:ILE:O	22:AV:36:A:N1	2.22	0.73
26:BA:2100:G:O6	26:BA:2189:U:O4	2.07	0.73
26:BA:1494:A:O2'	26:BA:1495:A:OP1	2.04	0.73
7:AG:79:ARG:NH1	7:AG:82:GLY:O	2.22	0.73
5:AE:105:ILE:HD11	5:AE:112:ARG:HA	1.69	0.73
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.70	0.73
26:BA:1084:A:OP1	34:BI:55:VAL:N	2.22	0.73
26:BA:2100:G:H2'	26:BA:2101:A:C8	2.23	0.72
35:BJ:46:ASP:OD1	35:BJ:50:LYS:NZ	2.21	0.72
1:AA:1239:A:H62	1:AA:1299:A:N6	1.86	0.72
59:CN:18:DG:H21	65:CF:12:VAL:C	1.94	0.72
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.25	0.72
26:BA:1083:U:H5'	34:BI:53:ARG:HH11	1.55	0.72
24:AX:26:A:N1	24:AX:44:G:N2	2.37	0.72
33:BH:38:PRO:O	33:BH:43:ASN:ND2	2.21	0.72
41:BP:31:THR:O	41:BP:102:ARG:NH1	2.22	0.72
1:AA:663:A:H5''	18:AR:50:LYS:HE3	1.69	0.72
26:BA:1406:U:C2'	26:BA:1407:G:H5''	2.19	0.72
1:AA:1008:U:H2'	1:AA:1009:U:C6	2.25	0.72
54:B3:10:LYS:NZ	54:B3:55:LYS:O	2.22	0.72
26:BA:210:C:OP1	55:B4:29:GLN:NE2	2.22	0.72
1:AA:1178:G:N7	9:AI:99:ARG:NH1	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:17:C:H2'	23:AW:17(A):U:C6	2.24	0.72
26:BA:276:U:O2'	26:BA:278:A:N7	2.23	0.72
1:AA:1061:G:OP2	3:AC:3:GLN:NE2	2.23	0.71
26:BA:1528:A:H2'	26:BA:1529:G:O4'	1.89	0.71
1:AA:60:A:N6	1:AA:110:C:C4	2.58	0.71
26:BA:389:G:C8	26:BA:2413:G:H4'	2.25	0.71
40:BO:101:GLY:O	40:BO:110:MET:N	2.24	0.71
65:CF:123:ARG:CB	65:CF:124:PRO:HD2	2.11	0.71
30:BE:147:LEU:HD11	30:BE:170:ARG:HD2	1.71	0.71
2:AB:129:LEU:HD11	2:AB:134:ALA:HB2	1.73	0.71
13:AM:57:ARG:NH2	58:B7:35:ASP:OD1	2.24	0.71
26:BA:1494:A:HO2'	26:BA:1495:A:P	2.14	0.71
63:CD:454:CYS:SG	63:CD:455:ALA:N	2.64	0.71
11:AK:88:GLY:O	11:AK:93:ARG:NH1	2.24	0.70
24:AX:20:H2U:O4	26:BA:882:G:O2'	2.08	0.70
26:BA:550:U:H2'	26:BA:551:G:H5''	1.72	0.70
62:CC:375:PRO:HG2	65:CF:80:TRP:HZ3	1.55	0.70
14:AN:38:ASP:OD2	58:B7:65:ASN:ND2	2.24	0.70
62:CC:27:LEU:O	62:CC:528:ARG:NH1	2.24	0.70
1:AA:573:A:N3	1:AA:883:C:O2'	2.24	0.70
35:BJ:110:GLN:HA	35:BJ:113:ALA:HB2	1.73	0.70
22:AV:51:G:H2'	22:AV:52:C:C6	2.25	0.70
26:BA:1171:G:C2'	26:BA:1172:C:H5'	2.21	0.70
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.25	0.70
26:BA:2530:A:N7	32:BG:172:LYS:NZ	2.38	0.70
17:AQ:49:GLU:OE1	17:AQ:50:ASN:N	2.25	0.70
4:AD:102:VAL:HG23	4:AD:107:PHE:HB2	1.73	0.70
24:AX:54:5MU:H4'	39:BN:51:ARG:HE	1.56	0.70
26:BA:1592:C:H2'	26:BA:1593:A:H8	1.54	0.70
34:BI:24:SER:CA	34:BI:85:SER:O	2.40	0.70
41:BP:1:MET:O	41:BP:5:SER:CB	2.40	0.70
63:CD:290:ILE:HD13	65:CF:103:ILE:HG22	1.73	0.70
35:BJ:55:PRO:HD3	35:BJ:74:PRO:HD3	1.73	0.70
2:AB:19:GLN:NE2	25:AY:76:GLU:O	2.25	0.70
59:CN:18:DG:N2	65:CF:69:VAL:H	1.90	0.70
63:CD:1157:ALA:HB2	63:CD:1210:ILE:HD11	1.74	0.70
26:BA:2245:U:O2'	26:BA:2436:G:OP2	2.10	0.69
18:AR:73:ARG:HG2	18:AR:74:HIS:H	1.57	0.69
26:BA:1311:G:OP2	26:BA:1311:G:N2	2.24	0.69
31:BF:140:GLU:OE1	58:B7:26:SER:OG	2.10	0.69
26:BA:543:A:C6	26:BA:544:G:C6	2.80	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2139:U:O2	26:BA:2152:G:O6	2.10	0.69
26:BA:2285:C:OP2	54:B3:6:ARG:NH1	2.25	0.69
26:BA:2718:G:O4'	26:BA:2718:G:O2'	2.04	0.69
1:AA:970:C:N4	9:AI:130:ARG:O	2.25	0.69
3:AC:97:VAL:HG22	3:AC:98:PRO:HD2	1.73	0.69
21:AU:13:ASP:N	21:AU:13:ASP:OD1	2.26	0.69
65:CF:159:LYS:HA	65:CF:172:GLU:HA	1.74	0.69
36:BK:5:THR:HG23	36:BK:45:THR:HG21	1.74	0.69
62:CC:63:SER:CB	65:CF:32:LEU:HD11	2.15	0.69
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.75	0.69
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.25	0.69
26:BA:1693:U:O2'	28:BC:14:ARG:NH2	2.24	0.69
26:BA:2901:C:H2'	26:BA:2902:C:C6	2.27	0.69
28:BC:107:PRO:HD2	28:BC:110:LEU:HD22	1.75	0.69
39:BN:106:ASP:OD1	39:BN:107:GLY:N	2.26	0.69
50:BY:72:ARG:NH1	50:BY:78:TYR:OH	2.24	0.69
51:BZ:2:LYS:HB2	51:BZ:5:GLU:HG2	1.73	0.69
59:CN:18:DG:H22	65:CF:68:TYR:C	2.00	0.69
26:BA:219:A:N3	26:BA:234:U:O2'	2.26	0.69
26:BA:1064:C:OP1	35:BJ:89:SER:N	2.26	0.69
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.26	0.69
26:BA:797:G:OP1	30:BE:55:SER:OG	2.10	0.69
38:BM:78:ARG:HG2	38:BM:113:ALA:HB3	1.74	0.68
28:BC:76:ALA:HB2	28:BC:96:TYR:CD1	2.28	0.68
59:CN:18:DG:H22	65:CF:68:TYR:CA	2.04	0.68
1:AA:1017:U:O2'	1:AA:1018:G:O4'	2.12	0.68
58:B7:43:PHE:O	58:B7:47:LYS:HB2	1.93	0.68
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.20	0.68
15:AO:18:ASP:O	15:AO:21:ASP:N	2.21	0.68
26:BA:78:U:OP1	51:BZ:7:ARG:NH2	2.26	0.68
60:CT:19:DG:H2'	60:CT:20:DC:C6	2.29	0.68
1:AA:927:G:O2'	1:AA:928:G:H5'	1.94	0.68
3:AC:102:ASN:OD1	22:AV:36:A:N6	2.26	0.68
26:BA:2349:G:OP1	56:B5:45:ARG:NH2	2.27	0.68
26:BA:2788:C:O2'	26:BA:2809:A:N3	2.25	0.68
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.26	0.68
26:BA:807:U:O2	30:BE:69:ARG:NH2	2.26	0.68
53:B2:15:MET:O	53:B2:18:SER:HB3	1.93	0.68
3:AC:9:GLY:HA3	14:AN:89:MET:HE3	1.75	0.68
10:AJ:79:PRO:HB2	65:CF:140:PRO:HB3	1.75	0.68
26:BA:927:A:H2'	26:BA:928:A:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CN:18:DG:O6	65:CF:67:GLY:CA	2.42	0.68
1:AA:1317:C:O2	19:AS:37:ARG:NH2	2.27	0.68
41:BP:7:ARG:NH1	41:BP:95:SER:O	2.27	0.68
3:AC:71:ALA:HA	3:AC:106:VAL:HG22	1.75	0.68
26:BA:1916:A:H2'	26:BA:1917:PSU:C6	2.27	0.68
59:CN:18:DG:N2	65:CF:69:VAL:N	2.40	0.68
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.76	0.67
5:AE:91:GLY:HA3	5:AE:130:SER:HB3	1.75	0.67
26:BA:1108:U:H2'	26:BA:1109:C:C6	2.28	0.67
34:BI:63:ALA:HB3	34:BI:78:GLY:HA2	1.75	0.67
55:B4:12:ARG:HD3	55:B4:44:VAL:HG21	1.76	0.67
62:CC:624:ASP:OD1	62:CC:627:GLY:N	2.25	0.67
1:AA:195:A:O2'	1:AA:196:A:H5'	1.94	0.67
1:AA:413:G:O2'	1:AA:428:G:N2	2.27	0.67
3:AC:129:MET:HG3	3:AC:132:ARG:HH21	1.58	0.67
5:AE:156:LYS:HG3	8:AH:71:VAL:HG13	1.75	0.67
26:BA:284:U:O2	26:BA:356:G:O6	2.10	0.67
41:BP:40:ILE:HG12	41:BP:47:VAL:HG22	1.74	0.67
37:BL:59:LYS:NZ	37:BL:89:ASN:O	2.28	0.67
26:BA:568:U:H1'	26:BA:2030:6MZ:H9C1	1.76	0.67
14:AN:46:LEU:HD12	19:AS:13:LEU:HD23	1.77	0.67
44:BS:61:ALA:HB2	44:BS:98:ILE:HD13	1.75	0.67
26:BA:1404:C:H2'	26:BA:1405:U:H5'	1.77	0.67
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.29	0.67
10:AJ:3:ASN:N	10:AJ:3:ASN:ND2	2.37	0.67
1:AA:1240:U:O4	7:AG:109:ARG:NH1	2.27	0.67
3:AC:126:ARG:HH12	22:AV:30:A:H4'	1.60	0.67
26:BA:1056:G:O2'	26:BA:1103:A:N6	2.28	0.67
1:AA:35:G:N3	12:AL:115:SER:OG	2.27	0.66
1:AA:746:A:H2'	1:AA:747:A:C8	2.30	0.66
11:AK:17:SER:O	11:AK:81:ASN:N	2.28	0.66
1:AA:1124:G:N2	1:AA:1125:U:O4	2.28	0.66
10:AJ:5:ARG:HB2	10:AJ:77:VAL:HA	1.78	0.66
22:AV:49:G:H5''	62:CC:540:ARG:NH2	2.10	0.66
34:BI:58:THR:OG1	34:BI:79:PRO:O	2.13	0.66
26:BA:371:A:O2'	50:BY:61:LYS:NZ	2.26	0.66
1:AA:198:G:H2'	1:AA:199:A:H8	1.61	0.66
29:BD:48:ILE:HG23	29:BD:84:LEU:HD11	1.76	0.66
31:BF:62:GLY:HA2	58:B7:7:PRO:HG2	1.78	0.66
34:BI:24:SER:HB3	34:BI:116:GLU:HG2	1.77	0.66
3:AC:75:ILE:HD11	22:AV:33:U:H4'	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:107:VAL:HG11	12:AL:110:ARG:HH11	1.60	0.66
40:BO:24:MET:HG2	40:BO:44:LEU:HD22	1.76	0.66
14:AN:24:ARG:NH1	14:AN:55:SER:OG	2.29	0.66
4:AD:100:ASN:OD1	4:AD:111:ARG:NH2	2.28	0.66
31:BF:110:ARG:NH1	31:BF:136:ILE:O	2.27	0.66
26:BA:1410:G:H2'	26:BA:1411:U:C6	2.31	0.66
61:CB:27:THR:C	61:CB:28:LEU:HD22	2.20	0.66
1:AA:1439:G:OP1	20:AT:33:LYS:NZ	2.29	0.66
26:BA:335:C:OP2	47:BV:82:ARG:NH2	2.28	0.66
28:BC:78:VAL:O	28:BC:113:GLY:N	2.25	0.66
62:CC:377:THR:HG21	65:CF:81:HIS:CE1	2.31	0.66
40:BO:82:GLU:OE2	40:BO:86:ARG:NH2	2.29	0.65
1:AA:1018:G:H2'	1:AA:1019:A:C8	2.32	0.65
26:BA:2116:G:N2	26:BA:2161:C:OP2	2.30	0.65
60:CT:17:DG:C5	60:CT:18:DC:C5	2.84	0.65
1:AA:4:U:HO2'	1:AA:5:U:C5'	2.09	0.65
1:AA:829:G:O3'	2:AB:23:TRP:HH2	1.79	0.65
12:AL:90:LEU:HD12	12:AL:91:PRO:HD2	1.78	0.65
24:AX:5:G:H2'	24:AX:6:G:H8	1.61	0.65
26:BA:1693:U:O2	28:BC:14:ARG:NH1	2.30	0.65
5:AE:65:GLU:OE2	5:AE:69:ARG:NH2	2.30	0.65
28:BC:252:THR:HG23	28:BC:253:LYS:HG3	1.79	0.65
59:CN:32:DA:H5'	59:CN:32:DA:C8	2.32	0.65
26:BA:2683:C:O2	37:BL:70:ARG:NH2	2.30	0.65
40:BO:114:GLU:OE1	40:BO:118:ARG:NH2	2.30	0.65
5:AE:82:GLN:NE2	5:AE:149:SER:OG	2.29	0.65
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.29	0.65
35:BJ:110:GLN:O	35:BJ:113:ALA:N	2.28	0.65
59:CN:16:DT:P	65:CF:16:SER:OG	2.55	0.65
63:CD:504:GLN:NE2	63:CD:505:ASP:OD1	2.18	0.65
1:AA:196:A:OP1	20:AT:64:LYS:NZ	2.28	0.65
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.31	0.65
22:AV:44:A:N6	62:CC:1264:GLN:NE2	2.45	0.65
26:BA:2071:A:H2'	26:BA:2072:C:C6	2.32	0.65
33:BH:75:LEU:HD22	33:BH:106:ALA:HB1	1.78	0.65
42:BQ:113:ARG:O	42:BQ:114:LEU:HD12	1.97	0.65
5:AE:29:ARG:HB2	5:AE:29:ARG:HH11	1.62	0.65
26:BA:2370:G:O2'	54:B3:44:ARG:NH1	2.29	0.65
27:BB:55:U:H2'	27:BB:56:G:H5'	1.78	0.65
33:BH:64:ALA:O	33:BH:68:ARG:HG2	1.95	0.65
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1936:A:H2	26:BA:1943:U:H3	1.43	0.64
29:BD:34:VAL:O	29:BD:93:GLY:CA	2.44	0.64
34:BI:43:LYS:HZ1	34:BI:98:GLU:HG2	1.60	0.64
3:AC:102:ASN:CA	22:AV:36:A:H61	2.04	0.64
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.61	0.64
14:AN:48:LEU:HD12	14:AN:51:LEU:HD12	1.80	0.64
1:AA:1174:G:H2'	1:AA:1175:G:H5'	1.80	0.64
28:BC:6:CYS:SG	28:BC:13:ARG:NH2	2.70	0.64
30:BE:5:LEU:O	30:BE:9:GLN:CA	2.43	0.64
33:BH:84:ALA:HB3	33:BH:148:ALA:HA	1.79	0.64
62:CC:380:ALA:HB2	65:CF:81:HIS:CE1	2.30	0.64
4:AD:63:ARG:HG2	4:AD:63:ARG:HH11	1.63	0.64
24:AX:23:A:H2'	24:AX:24:G:C8	2.32	0.64
26:BA:1068:G:O2'	26:BA:1070:A:N7	2.30	0.64
26:BA:1404:C:C2'	26:BA:1405:U:H5'	2.27	0.64
34:BI:30:SER:HB2	34:BI:109:LYS:NZ	2.12	0.64
13:AM:14:HIS:HA	13:AM:44:LYS:HA	1.78	0.64
63:CD:429:LEU:HD22	63:CD:429:LEU:N	2.12	0.64
63:CD:474:LEU:HD21	64:CE:27:ALA:HB3	1.79	0.64
14:AN:6:MET:SD	14:AN:9:ARG:NH2	2.71	0.64
31:BF:79:ILE:HD12	31:BF:85:ILE:HD13	1.77	0.64
34:BI:116:GLU:OE1	34:BI:117:LEU:N	2.27	0.64
62:CC:582:ASN:OD1	62:CC:583:GLU:N	2.31	0.64
11:AK:92:GLY:C	11:AK:94:GLU:H	2.06	0.64
19:AS:3:ARG:HE	19:AS:7:LYS:HB3	1.63	0.64
26:BA:1196:C:HO2'	26:BA:1227:G:HO2'	1.45	0.64
26:BA:1568:G:N7	28:BC:28:LYS:NZ	2.46	0.64
26:BA:1826:G:O2'	26:BA:1971:U:OP2	2.15	0.64
60:CT:19:DG:H2'	60:CT:20:DC:H6	1.63	0.64
62:CC:251:ALA:HB2	62:CC:269:ILE:HD11	1.80	0.64
63:CD:256:ASP:O	63:CD:259:ARG:NH2	2.22	0.64
13:AM:92:ARG:HH21	26:BA:888:C:H5'	1.62	0.64
26:BA:768:G:N2	26:BA:1379:U:O2'	2.31	0.64
33:BH:14:SER:HB2	33:BH:17:ASP:HB2	1.79	0.64
59:CN:19:DA:H2'	65:CF:87:PRO:HA	1.78	0.64
62:CC:18:ARG:NH1	62:CC:1188:ASP:OD1	2.31	0.64
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.30	0.63
21:AU:61:ALA:O	21:AU:65:ALA:CB	2.36	0.63
26:BA:1592:C:H2'	26:BA:1593:A:C8	2.32	0.63
26:BA:2244:U:H2'	26:BA:2245:U:C6	2.33	0.63
26:BA:411:G:OP2	26:BA:2406:A:O2'	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1166:G:O2'	1:AA:1167:A:OP1	2.13	0.63
26:BA:141:G:H2'	26:BA:142:A:O4'	1.98	0.63
26:BA:2885:G:O6	53:B2:29:SER:OG	2.16	0.63
59:CN:16:DT:OP2	65:CF:16:SER:OG	2.16	0.63
62:CC:696:ASP:CG	62:CC:697:LYS:H	2.06	0.63
1:AA:926:G:N2	22:AV:16:A:OP1	2.30	0.63
3:AC:88:ARG:NH2	63:CD:79:LYS:NZ	2.47	0.63
26:BA:2115:G:O5'	26:BA:2166:U:O2'	2.17	0.63
60:CT:19:DG:C6	60:CT:20:DC:C4	2.86	0.63
2:AB:100:MET:HA	2:AB:107:VAL:HG21	1.80	0.63
12:AL:37:VAL:HG22	12:AL:53:CYS:SG	2.39	0.63
29:BD:35:THR:HG22	29:BD:73:VAL:HG21	1.81	0.63
32:BG:42:GLU:OE2	32:BG:55:ARG:NH2	2.32	0.63
1:AA:781:A:O2'	1:AA:1522:U:O2	2.17	0.63
1:AA:851:G:OP1	1:AA:851:G:H4'	1.99	0.63
9:AI:53:GLU:OE1	9:AI:53:GLU:N	2.32	0.63
26:BA:1386:C:H2'	26:BA:1387:A:C8	2.33	0.63
27:BB:8:C:O3'	41:BP:25:ARG:NH1	2.32	0.63
34:BI:80:THR:O	34:BI:82:ILE:HG12	1.99	0.63
15:AO:26:GLU:OE2	15:AO:77:ARG:NE	2.24	0.63
22:AV:44:A:H2'	22:AV:44:A:OP2	1.99	0.63
26:BA:888:C:O4'	26:BA:889:C:H5'	1.98	0.63
26:BA:1064:C:H4'	35:BJ:89:SER:O	1.98	0.63
29:BD:8:LYS:O	29:BD:198:GLY:N	2.31	0.63
34:BI:117:LEU:HB2	34:BI:120:ALA:HA	1.79	0.63
50:BY:43:GLU:OE2	50:BY:45:ARG:NH1	2.31	0.63
17:AQ:79:VAL:HG22	17:AQ:80:GLU:HG3	1.80	0.63
22:AV:38:A:C4'	22:AV:39:C:H5''	2.29	0.63
26:BA:1594:U:H2'	26:BA:1595:C:C6	2.33	0.63
26:BA:2291:U:H2'	26:BA:2292:U:C6	2.34	0.63
9:AI:18:ARG:NH1	9:AI:66:THR:OG1	2.31	0.62
12:AL:81:LEU:HB3	12:AL:98:VAL:HB	1.79	0.62
26:BA:1171:G:H2'	26:BA:1172:C:H5'	1.81	0.62
26:BA:29:U:O4	26:BA:511:U:O4	2.17	0.62
17:AQ:40:ARG:HA	17:AQ:40:ARG:HE	1.62	0.62
26:BA:2127:G:N7	26:BA:2162:G:N1	2.47	0.62
26:BA:2175:C:H2'	26:BA:2176:A:C8	2.34	0.62
44:BS:14:VAL:HG21	44:BS:98:ILE:HG13	1.79	0.62
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.80	0.62
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.65	0.62
4:AD:98:LEU:O	4:AD:102:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:35:VAL:HG21	20:AT:54:MET:HG2	1.81	0.62
60:CT:19:DG:C5	60:CT:20:DC:C5	2.87	0.62
25:AY:43:LYS:HD2	25:AY:76:GLU:HG2	1.80	0.62
63:CD:523:GLU:CD	63:CD:709:ARG:HH22	2.07	0.62
3:AC:35:SER:HG	3:AC:59:ARG:HH22	1.45	0.62
35:BJ:78:LEU:HD23	35:BJ:108:ILE:HG23	1.80	0.62
38:BM:4:ASN:C	38:BM:4:ASN:HD22	2.07	0.62
56:B5:32:ILE:O	56:B5:36:LYS:NZ	2.28	0.62
63:CD:504:GLN:HG3	63:CD:505:ASP:H	1.65	0.62
63:CD:978:ARG:HG3	63:CD:1197:ASN:ND2	2.15	0.62
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.34	0.62
26:BA:2100:G:O2'	26:BA:2101:A:H5'	2.00	0.62
26:BA:464:U:O3'	55:B4:12:ARG:NH1	2.33	0.62
26:BA:1450:G:N2	26:BA:1452:G:O6	2.19	0.62
60:CT:9:DC:H2'	60:CT:10:DT:C6	2.34	0.62
62:CC:12:ARG:HH21	62:CC:793:GLU:CD	2.07	0.62
4:AD:145:ILE:HG22	4:AD:150:LYS:HG2	1.81	0.62
6:AF:69:GLU:OE1	6:AF:69:GLU:N	2.24	0.62
26:BA:2720:U:OP1	42:BQ:53:ARG:NH2	2.32	0.62
26:BA:2780:G:N1	36:BK:102:GLU:OE2	2.27	0.62
63:CD:576:ARG:NH1	63:CD:593:ASN:O	2.32	0.62
1:AA:373:A:O2'	1:AA:451:A:N7	2.33	0.62
1:AA:1305:G:H21	1:AA:1332:A:H2	1.46	0.62
31:BF:40:VAL:HG23	31:BF:42:GLU:CD	2.25	0.62
35:BJ:71:LYS:HE3	35:BJ:72:THR:H	1.64	0.62
63:CD:429:LEU:H	63:CD:429:LEU:CD2	2.13	0.62
1:AA:1008:U:OP2	1:AA:1008:U:H6	1.82	0.61
2:AB:60:ILE:HA	2:AB:63:ARG:HD2	1.82	0.61
41:BP:1:MET:O	41:BP:5:SER:HB3	2.00	0.61
1:AA:31:G:O2'	1:AA:48:C:N4	2.33	0.61
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.33	0.61
1:AA:1276:G:O2'	1:AA:1277:C:H5'	2.00	0.61
7:AG:77:SER:OG	7:AG:86:GLN:OE1	2.18	0.61
10:AJ:44:THR:HA	10:AJ:69:THR:O	2.01	0.61
11:AK:22:HIS:HB2	11:AK:33:THR:HG23	1.82	0.61
19:AS:67:VAL:HG21	58:B7:57:VAL:HG22	1.82	0.61
26:BA:1340:U:OP2	46:BU:82:LYS:NZ	2.30	0.61
46:BU:34:VAL:HG21	46:BU:43:ILE:HD11	1.82	0.61
57:B6:22:VAL:HG11	57:B6:36:ARG:HH11	1.65	0.61
1:AA:356:A:N3	1:AA:368:U:O2'	2.31	0.61
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:156:LYS:NZ	8:AH:73:GLU:OE1	2.32	0.61
9:AI:19:VAL:HG22	9:AI:65:ILE:HG12	1.81	0.61
26:BA:2129:C:OP1	26:BA:2129:C:H4'	2.01	0.61
59:CN:38:DA:H2''	59:CN:39:DG:N7	2.14	0.61
1:AA:1175:G:HO2'	1:AA:1176:A:H8	1.48	0.61
4:AD:140:ASN:N	4:AD:182:PHE:O	2.32	0.61
26:BA:569:U:O2'	26:BA:983:A:N1	2.32	0.61
26:BA:888:C:C1'	26:BA:889:C:H5'	2.31	0.61
26:BA:888:C:H4'	26:BA:889:C:OP1	1.99	0.61
63:CD:291:ILE:CD1	65:CF:65:PHE:CD2	2.84	0.61
28:BC:141:VAL:HG23	28:BC:162:VAL:HG23	1.82	0.61
33:BH:50:ARG:HH22	33:BH:51:ARG:HH21	1.46	0.61
47:BV:28:VAL:HG22	47:BV:34:VAL:HG12	1.82	0.61
61:CA:8:PHE:O	61:CA:10:LYS:NZ	2.26	0.61
7:AG:111:ARG:NH2	7:AG:113:ASP:OD1	2.33	0.61
22:AV:41:C:O2	22:AV:41:C:H2'	1.99	0.61
26:BA:1071:G:N2	26:BA:1091:G:OP2	2.33	0.61
26:BA:1506:U:H2'	26:BA:1507:C:C6	2.36	0.61
42:BQ:100:LEU:HD23	42:BQ:103:ARG:HD2	1.82	0.61
10:AJ:79:PRO:HG2	65:CF:140:PRO:HG3	1.83	0.61
28:BC:232:HIS:HA	28:BC:242:LYS:HD3	1.82	0.61
26:BA:1915:3TD:H2'	26:BA:1916:A:C8	2.36	0.61
26:BA:1916:A:H2'	26:BA:1917:PSU:H6	1.66	0.61
26:BA:2547:A:H2'	26:BA:2548:U:C6	2.36	0.61
59:CN:16:DT:H5'	65:CF:15:PHE:CD1	2.21	0.61
1:AA:73:C:C2'	1:AA:74:A:H5'	2.31	0.61
26:BA:639:U:H2'	26:BA:640:C:C6	2.36	0.61
26:BA:2243:U:H2'	26:BA:2244:U:H6	1.66	0.61
4:AD:62:ARG:NH1	4:AD:69:GLU:OE1	2.34	0.60
9:AI:4:ASN:OD1	9:AI:4:ASN:N	2.34	0.60
26:BA:125:A:OP2	55:B4:19:ARG:NH2	2.29	0.60
32:BG:16:ASP:N	32:BG:16:ASP:OD1	2.32	0.60
26:BA:135:U:H2'	26:BA:136:G:O4'	2.01	0.60
3:AC:20:SER:OG	3:AC:22:TRP:NE1	2.35	0.60
9:AI:21:ILE:HD13	9:AI:63:LEU:HB3	1.82	0.60
26:BA:1265:A:H4'	26:BA:1266:G:H4'	1.84	0.60
1:AA:830:G:H5'	2:AB:23:TRP:HZ3	1.66	0.60
1:AA:1451:U:OP2	1:AA:1452:C:N4	2.33	0.60
26:BA:2167:U:H3	26:BA:2170:A:H5''	1.66	0.60
45:BT:4:ILE:HG12	45:BT:106:VAL:HG22	1.82	0.60
61:CB:76:GLU:H	61:CB:76:GLU:CD	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:203:G:O2'	1:AA:465:A:N1	2.35	0.60
3:AC:153:VAL:HG13	3:AC:198:VAL:HG22	1.83	0.60
4:AD:88:GLU:OE1	4:AD:88:GLU:N	2.35	0.60
5:AE:110:ALA:HB1	5:AE:137:VAL:HG23	1.83	0.60
16:AP:19:VAL:HG13	16:AP:37:GLY:C	2.27	0.60
63:CD:1360:GLY:HA2	64:CE:17:PHE:CZ	2.35	0.60
26:BA:278:A:OP2	26:BA:361:G:N1	2.33	0.60
26:BA:1607:C:N4	26:BA:1622:G:OP2	2.32	0.60
62:CC:423:ASP:N	62:CC:423:ASP:OD1	2.33	0.60
12:AL:53:CYS:SG	12:AL:67:ILE:HD11	2.41	0.60
24:AX:51:U:H2'	24:AX:52:G:H8	1.66	0.60
63:CD:291:ILE:HD11	65:CF:65:PHE:CD2	2.37	0.60
1:AA:1137:C:O2	1:AA:1138:G:N1	2.35	0.60
63:CD:650:LYS:HE3	63:CD:742:GLY:O	2.02	0.60
1:AA:526:C:OP1	12:AL:88:LYS:NZ	2.30	0.60
26:BA:1378:A:O2'	26:BA:1380:G:OP2	2.18	0.60
26:BA:2252:G:H2'	26:BA:2253:G:H8	1.67	0.60
31:BF:103:LEU:O	31:BF:108:VAL:HG22	2.01	0.60
34:BI:10:ALA:O	34:BI:14:GLU:HG3	2.01	0.60
59:CN:18:DG:C6	65:CF:67:GLY:CA	2.85	0.60
62:CC:638:SER:OG	62:CC:639:LYS:N	2.32	0.60
1:AA:823:C:HO2'	8:AH:2:SER:N	2.00	0.60
10:AJ:37:ARG:HB3	10:AJ:37:ARG:HH11	1.65	0.60
22:AV:37:G:C5'	22:AV:37:G:C8	2.84	0.60
59:CN:27:DA:C4	59:CN:28:DA:C8	2.90	0.60
62:CC:525:THR:HG21	62:CC:687:ARG:HH11	1.67	0.60
25:AY:29:VAL:N	25:AY:37:LEU:O	2.30	0.59
63:CD:441:LEU:HD22	63:CD:441:LEU:N	2.16	0.59
26:BA:1410:G:H2'	26:BA:1411:U:H6	1.66	0.59
26:BA:2134:A:N6	26:BA:2157:G:O2'	2.35	0.59
26:BA:2149:U:H2'	26:BA:2150:C:C6	2.37	0.59
26:BA:2792:A:H2'	26:BA:2793:C:C6	2.37	0.59
29:BD:2:ILE:HD13	29:BD:2:ILE:H	1.68	0.59
30:BE:145:ASP:HB3	30:BE:184:ASP:HB2	1.84	0.59
1:AA:864:A:H4'	5:AE:90:THR:HG23	1.84	0.59
3:AC:58:GLU:OE1	3:AC:65:ARG:NH1	2.35	0.59
4:AD:27:ALA:O	4:AD:30:THR:OG1	2.18	0.59
26:BA:614:A:H8	26:BA:614:A:OP1	1.84	0.59
46:BU:25:GLU:OE2	46:BU:26:LYS:NZ	2.35	0.59
63:CD:1169:THR:OG1	63:CD:1173:ARG:HB3	2.02	0.59
1:AA:641:U:H1'	1:AA:642:A:OP2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1064:C:H42	26:BA:1075:C:H42	1.48	0.59
34:BI:71:CYS:O	34:BI:74:ASP:HB2	2.02	0.59
39:BN:66:ARG:NH1	39:BN:104:GLU:OE1	2.33	0.59
62:CC:705:GLU:HB3	62:CC:794:LEU:H	1.67	0.59
1:AA:411:A:C4'	1:AA:412:A:H5'	2.31	0.59
1:AA:1018:G:H2'	1:AA:1019:A:H8	1.67	0.59
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.20	0.59
26:BA:1177:G:O2'	26:BA:1178:C:O5'	2.15	0.59
10:AJ:6:ILE:HD11	10:AJ:76:ILE:HB	1.85	0.59
26:BA:1057:A:N6	26:BA:1087:G:OP2	2.22	0.59
54:B3:22:THR:HG23	56:B5:34:THR:HG23	1.84	0.59
63:CD:797:THR:HG22	63:CD:924:GLY:HA3	1.83	0.59
1:AA:67:C:H2'	1:AA:68:G:C8	2.38	0.59
9:AI:49:ARG:HB3	9:AI:53:GLU:OE2	2.03	0.59
36:BK:19:ASP:OD1	36:BK:58:ASN:ND2	2.30	0.59
61:CA:67:GLU:OE1	62:CC:1057:LYS:NZ	2.33	0.59
1:AA:212:G:C2	1:AA:213:G:C8	2.90	0.59
15:AO:33:THR:HG21	15:AO:85:LEU:HD22	1.85	0.59
11:AK:54:GLY:N	11:AK:57:LYS:HG2	2.18	0.59
26:BA:2469:A:H4'	39:BN:55:ARG:HD2	1.84	0.59
45:BT:17:VAL:HG11	45:BT:103:ILE:HG12	1.84	0.59
10:AJ:100:ILE:HD11	65:CF:165:PHE:HE2	1.68	0.59
33:BH:104:THR:HA	33:BH:108:VAL:O	2.03	0.59
48:BW:75:GLN:HB2	48:BW:92:VAL:HG23	1.84	0.59
59:CN:26:DG:OP2	62:CC:542:ARG:NH1	2.35	0.59
1:AA:1088:G:H1'	21:AU:71:TYR:HB3	1.85	0.58
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.84	0.58
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.85	0.58
29:BD:37:VAL:HG22	29:BD:48:ILE:HG22	1.85	0.58
1:AA:1345:U:OP1	9:AI:122:ARG:NH1	2.36	0.58
3:AC:102:ASN:HA	22:AV:36:A:H62	1.62	0.58
9:AI:41:ARG:HH21	9:AI:41:ARG:HG3	1.68	0.58
31:BF:8:TYR:OH	31:BF:29:PRO:O	2.19	0.58
32:BG:148:LEU:HA	32:BG:151:TYR:HD2	1.68	0.58
63:CD:1069:ALA:HA	63:CD:1072:LYS:HB2	1.85	0.58
10:AJ:26:VAL:HA	10:AJ:36:VAL:HG11	1.84	0.58
26:BA:1406:U:H2'	26:BA:1407:G:H5''	1.84	0.58
65:CF:134:VAL:N	65:CF:146:GLY:O	2.33	0.58
1:AA:1383:C:H2'	1:AA:1384:C:C6	2.38	0.58
2:AB:129:LEU:HD13	2:AB:134:ALA:H	1.68	0.58
26:BA:2523:G:HO2'	26:BA:2764:A:HO2'	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2532:G:O2'	26:BA:2657:A:N1	2.36	0.58
63:CD:829:GLY:C	63:CD:993:GLU:HA	2.28	0.58
24:AX:51:U:H2'	24:AX:52:G:C8	2.39	0.58
26:BA:1506:U:H2'	26:BA:1507:C:H6	1.67	0.58
26:BA:2116:G:H22	26:BA:2164:C:H42	1.48	0.58
62:CC:525:THR:HG21	62:CC:687:ARG:NH1	2.18	0.58
1:AA:1189:U:OP1	14:AN:98:LYS:NZ	2.37	0.58
24:AX:43:C:H2'	24:AX:44:G:C8	2.39	0.58
30:BE:171:ASP:OD2	30:BE:173:THR:OG1	2.16	0.58
42:BQ:38:LYS:NZ	42:BQ:38:LYS:H	2.02	0.58
9:AI:3:GLU:HB2	9:AI:22:LYS:HE2	1.86	0.58
26:BA:2187:U:H2'	26:BA:2188:U:C5	2.38	0.58
40:BO:1:MET:HE2	40:BO:3:HIS:CE1	2.38	0.58
43:BR:11:ARG:HH11	43:BR:11:ARG:HB2	1.68	0.58
60:CT:17:DG:C6	60:CT:18:DC:C4	2.91	0.58
5:AE:148:ASN:ND2	8:AH:73:GLU:OE1	2.36	0.58
60:CT:20:DC:H2'	60:CT:21:DG:H8	1.68	0.58
60:CT:26:DA:H2''	60:CT:27:DG:C8	2.39	0.58
62:CC:380:ALA:CB	65:CF:81:HIS:CD2	2.79	0.58
1:AA:337:G:H2'	1:AA:338:A:C8	2.39	0.58
26:BA:1174:U:O2'	26:BA:1176:U:O2	2.21	0.58
59:CN:18:DG:H2''	65:CF:91:GLY:H	1.69	0.58
1:AA:532:A:C2	1:AA:1207:2MG:H4'	2.39	0.58
1:AA:673:A:H2'	1:AA:674:G:C8	2.39	0.58
1:AA:1006:G:H2'	1:AA:1007:U:C6	2.37	0.58
26:BA:617:G:OP1	30:BE:102:ARG:NH2	2.36	0.58
26:BA:2646:C:OP2	26:BA:2732:G:O2'	2.17	0.58
63:CD:317:THR:OG1	63:CD:322:ARG:O	2.20	0.58
63:CD:515:ARG:NH2	63:CD:718:SER:O	2.37	0.58
26:BA:1059:G:H2'	26:BA:1060:U:C5	2.39	0.57
26:BA:1131:G:N2	26:BA:1132:U:O4	2.37	0.57
26:BA:1171:G:O2'	26:BA:1172:C:H5'	2.03	0.57
31:BF:127:ASN:HD22	31:BF:157:THR:HG23	1.67	0.57
62:CC:494:ASN:C	62:CC:494:ASN:HD22	2.08	0.57
1:AA:744:C:O2'	1:AA:851:G:N2	2.37	0.57
9:AI:23:PRO:HA	9:AI:61:LEU:HD23	1.87	0.57
37:BL:5:GLN:N	37:BL:21:CYS:O	2.35	0.57
1:AA:198:G:H2'	1:AA:199:A:C8	2.39	0.57
26:BA:2328:A:H2'	26:BA:2329:U:C6	2.40	0.57
26:BA:2769:U:OP1	36:BK:95:ARG:NH2	2.37	0.57
29:BD:37:VAL:HG21	29:BD:90:PHE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BH:5:LEU:HD13	33:BH:13:GLY:HA2	1.85	0.57
47:BV:5:ILE:HG13	47:BV:72:ILE:HG13	1.85	0.57
53:B2:30:VAL:HG22	53:B2:37:LYS:HG2	1.85	0.57
63:CD:495:ASN:OD1	63:CD:495:ASN:N	2.37	0.57
26:BA:829:A:N7	26:BA:2247:A:O2'	2.34	0.57
26:BA:1153:C:OP1	43:BR:92:ARG:NH2	2.37	0.57
26:BA:2676:C:OP1	37:BL:31:ARG:NH2	2.37	0.57
40:BO:9:GLN:O	40:BO:17:ARG:NH2	2.37	0.57
62:CC:392:GLU:CD	62:CC:392:GLU:H	2.12	0.57
62:CC:591:TYR:OH	62:CC:637:ARG:NH2	2.36	0.57
62:CC:726:TYR:HB3	62:CC:733:VAL:CG1	2.34	0.57
26:BA:136:G:H4'	26:BA:136:G:OP1	2.03	0.57
32:BG:141:ILE:HG13	32:BG:142:GLY:N	2.20	0.57
59:CN:28:DA:H2''	59:CN:29:DG:H8	1.70	0.57
62:CC:519:ASN:C	62:CC:519:ASN:OD1	2.46	0.57
2:AB:73:LYS:NZ	2:AB:205:ASP:OD1	2.37	0.57
24:AX:58:A:O2'	24:AX:60:U:OP2	2.15	0.57
40:BO:103:ARG:N	40:BO:108:ALA:O	2.33	0.57
48:BW:27:PRO:O	48:BW:88:HIS:HA	2.05	0.57
15:AO:88:ARG:NH1	26:BA:716:A:OP2	2.38	0.57
38:BM:80:SER:O	38:BM:84:LYS:HD2	2.05	0.57
41:BP:1:MET:O	41:BP:5:SER:HB2	2.04	0.57
1:AA:17:U:H2'	1:AA:18:C:C6	2.40	0.57
24:AX:19:G:O2'	26:BA:896:A:N1	2.34	0.57
26:BA:1063:G:H5''	35:BJ:80:LYS:HE3	1.87	0.57
26:BA:1063:G:H4'	35:BJ:135:MET:HE2	1.87	0.57
26:BA:1340:U:OP1	46:BU:19:LYS:NZ	2.31	0.57
30:BE:181:ILE:HD13	38:BM:6:LEU:HD11	1.87	0.57
59:CN:34:DT:H6	59:CN:34:DT:H5'	1.70	0.57
60:CT:18:DC:H2'	60:CT:19:DG:H8	1.65	0.57
60:CT:19:DG:C4	60:CT:20:DC:C5	2.93	0.57
1:AA:945:G:C2	1:AA:946:A:C8	2.92	0.56
4:AD:147:GLU:HA	4:AD:150:LYS:HB2	1.87	0.56
7:AG:129:GLU:O	7:AG:130:ASN:HB2	2.05	0.56
26:BA:245:G:O6	56:B5:8:ARG:NH1	2.38	0.56
26:BA:1529:G:H2'	26:BA:1530:G:H8	1.70	0.56
26:BA:1936:A:N6	26:BA:1963:U:O2	2.38	0.56
29:BD:20:VAL:HG22	37:BL:72:PRO:HB3	1.86	0.56
13:AM:89:LEU:HA	13:AM:92:ARG:HH11	1.70	0.56
22:AV:48:C:H2'	22:AV:49:G:O4'	2.04	0.56
26:BA:890:C:H2'	26:BA:891:G:H4'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BQ:38:LYS:H	42:BQ:38:LYS:HZ1	1.52	0.56
1:AA:51:A:N7	1:AA:114:U:O2'	2.35	0.56
7:AG:74:GLU:OE2	7:AG:95:ARG:NH2	2.32	0.56
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	1.86	0.56
23:AW:16:C:O2'	23:AW:60:U:O3'	2.23	0.56
24:AX:20:H2U:H61	24:AX:20:H2U:OP1	2.05	0.56
26:BA:1591:A:H2'	26:BA:1592:C:H6	1.69	0.56
26:BA:1591:A:H2'	26:BA:1592:C:C6	2.40	0.56
42:BQ:98:TYR:HA	42:BQ:101:ARG:HG3	1.87	0.56
45:BT:17:VAL:HG12	45:BT:76:VAL:HG21	1.85	0.56
65:CF:123:ARG:HB3	65:CF:124:PRO:HD3	1.83	0.56
1:AA:1130:A:H61	1:AA:1144:G:H1'	1.69	0.56
5:AE:150:PRO:HA	5:AE:153:VAL:HG22	1.87	0.56
6:AF:38:ARG:NH2	6:AF:63:ASN:OD1	2.38	0.56
11:AK:54:GLY:H	11:AK:57:LYS:HG2	1.71	0.56
54:B3:40:ASP:HB3	54:B3:43:VAL:HG22	1.87	0.56
1:AA:496:A:H2'	1:AA:496:A:N3	2.20	0.56
1:AA:1168:U:O2'	1:AA:1169:A:O5'	2.21	0.56
26:BA:2315:G:O2'	26:BA:2316:G:O4'	2.23	0.56
54:B3:17:THR:HG21	54:B3:42:VAL:HG21	1.87	0.56
63:CD:301:GLU:OE1	63:CD:312:ARG:NH1	2.37	0.56
1:AA:714:G:H2'	1:AA:715:A:C8	2.40	0.56
5:AE:56:VAL:O	5:AE:60:ILE:HG23	2.06	0.56
11:AK:18:ASP:HA	11:AK:81:ASN:O	2.06	0.56
26:BA:1386:C:H2'	26:BA:1387:A:H8	1.71	0.56
47:BV:14:LEU:HD11	47:BV:71:ALA:HB2	1.88	0.56
62:CC:267:ARG:NE	62:CC:268:ARG:O	2.37	0.56
62:CC:1083:GLU:CD	62:CC:1083:GLU:H	2.13	0.56
62:CC:1165:SER:O	62:CC:1167:GLU:N	2.37	0.56
13:AM:24:GLY:O	13:AM:29:ARG:NH1	2.39	0.56
16:AP:48:GLU:OE2	16:AP:51:ARG:NH2	2.34	0.56
26:BA:1595:C:O2'	26:BA:1596:A:H5'	2.06	0.56
27:BB:49:C:OP1	41:BP:101:GLY:HA3	2.06	0.56
28:BC:29:PRO:HG2	28:BC:34:LEU:HD11	1.86	0.56
29:BD:116:LYS:HD2	40:BO:1:MET:HE1	1.88	0.56
32:BG:155:GLU:OE2	32:BG:158:LYS:N	2.28	0.56
34:BI:118:ILE:HB	34:BI:119:PRO:HD3	1.88	0.56
59:CN:19:DA:H2'	65:CF:88:ARG:H	1.71	0.56
62:CC:421:SER:H	62:CC:424:ASP:HB2	1.69	0.56
1:AA:492:C:H2'	1:AA:493:A:C8	2.41	0.56
37:BL:34:GLY:N	37:BL:37:ASP:OD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:12:ARG:NE	62:CC:793:GLU:OE2	2.36	0.56
30:BE:1:MET:HB3	30:BE:14:VAL:HG23	1.88	0.55
30:BE:48:THR:HG23	30:BE:86:ALA:HB3	1.86	0.55
31:BF:127:ASN:ND2	31:BF:157:THR:HG23	2.21	0.55
34:BI:22:ALA:HB3	34:BI:87:GLU:O	2.06	0.55
44:BS:77:PHE:HD2	44:BS:84:ARG:HB3	1.70	0.55
1:AA:890:G:O2'	1:AA:906:A:N6	2.39	0.55
2:AB:23:TRP:HB3	2:AB:39:HIS:CE1	2.40	0.55
9:AI:24:GLY:H	9:AI:61:LEU:HA	1.71	0.55
26:BA:274:C:H2'	26:BA:275:C:C6	2.40	0.55
26:BA:1084:A:OP2	34:BI:53:ARG:HB3	2.06	0.55
50:BY:7:VAL:HG21	50:BY:59:ILE:HD11	1.88	0.55
52:B1:31:ARG:HG2	52:B1:34:HIS:HB2	1.88	0.55
56:B5:62:LEU:HB3	56:B5:65:ALA:HB3	1.87	0.55
3:AC:88:ARG:HH21	63:CD:79:LYS:CB	2.19	0.55
27:BB:48:U:P	41:BP:30:ARG:HH22	2.29	0.55
29:BD:9:VAL:O	29:BD:197:THR:HG23	2.07	0.55
62:CC:632:ASP:N	62:CC:632:ASP:OD1	2.39	0.55
6:AF:2:ARG:HB3	6:AF:91:ARG:HD3	1.88	0.55
7:AG:7:ILE:HD13	7:AG:7:ILE:H	1.71	0.55
26:BA:871:U:H2'	26:BA:872:U:C6	2.40	0.55
34:BI:81:LEU:HD23	34:BI:111:ALA:HB2	1.89	0.55
38:BM:51:GLU:OE1	38:BM:60:ARG:NH1	2.40	0.55
4:AD:188:ARG:NE	4:AD:197:GLU:OE1	2.34	0.55
13:AM:7:ILE:HG22	31:BF:112:ARG:HH11	1.70	0.55
15:AO:2:SER:OG	15:AO:3:LEU:N	2.39	0.55
26:BA:81:G:O2'	26:BA:295:G:O2'	2.12	0.55
34:BI:109:LYS:HB3	34:BI:109:LYS:HZ2	1.71	0.55
37:BL:107:LEU:HB3	37:BL:116:ILE:HD11	1.87	0.55
26:BA:1796:U:H2'	26:BA:1797:G:H8	1.70	0.55
27:BB:41:G:H5''	31:BF:66:LEU:HD13	1.88	0.55
35:BJ:48:ILE:HG23	35:BJ:49:GLU:H	1.71	0.55
48:BW:45:ASP:OD1	48:BW:45:ASP:N	2.30	0.55
63:CD:37:GLU:HB2	63:CD:104:HIS:CE1	2.42	0.55
1:AA:451:A:H1'	1:AA:452:A:C2	2.42	0.55
1:AA:1035:A:H2'	1:AA:1036:A:C8	2.40	0.55
26:BA:880:G:C2	26:BA:881:G:C8	2.94	0.55
30:BE:21:ARG:O	30:BE:114:ARG:NH2	2.36	0.55
33:BH:14:SER:HB2	33:BH:17:ASP:CB	2.36	0.55
39:BN:134:THR:OG1	48:BW:79:ARG:NH1	2.39	0.55
62:CC:726:TYR:C	62:CC:726:TYR:CD1	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:980:C:H4'	14:AN:59:ARG:NH2	2.22	0.55
8:AH:66:PHE:CD2	8:AH:67:GLN:HG3	2.41	0.55
19:AS:42:PRO:HB3	58:B7:57:VAL:HG13	1.89	0.55
26:BA:1095:A:H2'	26:BA:1096:A:C8	2.41	0.55
26:BA:2178:C:H2'	26:BA:2179:C:C5	2.41	0.55
45:BT:59:GLU:O	45:BT:63:GLY:HA2	2.06	0.55
62:CC:1176:LEU:O	62:CC:1178:LYS:N	2.39	0.55
26:BA:1993:U:H4'	29:BD:133:THR:HG22	1.89	0.55
63:CD:162:GLU:CG	65:CF:95:GLY:HA3	2.29	0.55
1:AA:411:A:H4'	1:AA:412:A:C5'	2.31	0.55
13:AM:7:ILE:HG22	31:BF:112:ARG:HE	1.72	0.55
1:AA:181:A:O2'	1:AA:194:C:N4	2.40	0.54
1:AA:362:G:N2	1:AA:365:U:OP2	2.39	0.54
1:AA:1397:C:H5'	22:AV:23:C:H41	1.71	0.54
24:AX:41:C:H2'	24:AX:42:C:C6	2.41	0.54
25:AY:71:ALA:H	25:AY:85:SER:HA	1.71	0.54
26:BA:2187:U:H2'	26:BA:2188:U:C6	2.42	0.54
26:BA:2287:A:C8	26:BA:2289:G:C8	2.95	0.54
26:BA:2343:U:HO2'	26:BA:2373:G:HO2'	1.45	0.54
63:CD:175:GLU:CD	63:CD:175:GLU:H	2.15	0.54
65:CF:47:GLU:CG	65:CF:64:PHE:CE1	2.64	0.54
1:AA:866:C:C4	1:AA:867:G:H1'	2.43	0.54
26:BA:144:A:H2'	26:BA:145:C:C6	2.42	0.54
28:BC:2:ALA:N	28:BC:20:VAL:O	2.40	0.54
49:BX:59:LEU:HD12	49:BX:80:ILE:HD12	1.89	0.54
64:CE:9:ALA:HB1	64:CE:19:LEU:HD11	1.89	0.54
1:AA:1:A:H2'	1:AA:2:A:C8	2.42	0.54
1:AA:1004:A:H5'	1:AA:1025:U:O2	2.08	0.54
2:AB:25:PRO:HA	2:AB:28:LYS:HB2	1.90	0.54
4:AD:2:ALA:O	4:AD:68:LEU:HD11	2.08	0.54
26:BA:278:A:N6	26:BA:362:A:N7	2.55	0.54
26:BA:793:A:OP2	26:BA:2071:A:O2'	2.24	0.54
26:BA:1062:G:O6	26:BA:1077:A:N6	2.40	0.54
3:AC:77:ILE:HG12	3:AC:84:VAL:HG21	1.89	0.54
5:AE:89:HIS:HE2	5:AE:138:ARG:HH11	1.55	0.54
7:AG:79:ARG:HD2	7:AG:84:THR:HG22	1.89	0.54
10:AJ:55:PRO:HA	14:AN:82:ILE:HD11	1.89	0.54
26:BA:2166:U:H3'	26:BA:2167:U:H5''	1.88	0.54
26:BA:2723:C:OP1	29:BD:114:LYS:NZ	2.33	0.54
62:CC:524:ILE:HG22	62:CC:525:THR:N	2.22	0.54
63:CD:160:LEU:HD23	63:CD:160:LEU:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:16:VAL:O	13:AM:20:THR:HG23	2.06	0.54
22:AV:40:A:H5''	22:AV:41:C:C4	2.42	0.54
26:BA:2244:U:O2'	26:BA:2245:U:H5'	2.07	0.54
32:BG:105:LEU:HD11	32:BG:148:LEU:HD22	1.90	0.54
53:B2:29:SER:OG	53:B2:40:ARG:NH1	2.38	0.54
15:AO:25:THR:HG23	15:AO:66:LEU:HD22	1.89	0.54
26:BA:400:G:N7	50:BY:57:ARG:NH1	2.53	0.54
37:BL:1:MET:HE3	37:BL:67:LYS:HG3	1.90	0.54
44:BS:30:GLY:N	44:BS:63:VAL:O	2.39	0.54
1:AA:1100:C:OP2	2:AB:95:ARG:HD3	2.08	0.54
2:AB:77:SER:HB2	2:AB:93:ASN:HB2	1.90	0.54
3:AC:79:LYS:O	3:AC:81:GLY:N	2.40	0.54
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.89	0.54
59:CN:31:DG:H2''	59:CN:32:DA:C8	2.42	0.54
62:CC:1079:ILE:HG23	62:CC:1079:ILE:O	2.07	0.54
7:AG:40:GLU:OE2	9:AI:41:ARG:NH2	2.41	0.54
11:AK:18:ASP:HB2	11:AK:37:ARG:HH21	1.73	0.54
22:AV:37:G:C8	22:AV:37:G:H5''	2.42	0.54
26:BA:172:A:H2'	26:BA:173:A:C8	2.43	0.54
26:BA:1084:A:N6	34:BI:56:ARG:HH22	2.04	0.54
26:BA:1392:A:N6	46:BU:18:GLU:OE1	2.33	0.54
48:BW:80:HIS:CE1	48:BW:83:LYS:HD2	2.43	0.54
3:AC:88:ARG:NH2	63:CD:79:LYS:CE	2.69	0.54
26:BA:851:C:H2'	26:BA:852:U:C6	2.43	0.54
26:BA:1447:C:O2'	26:BA:1544:A:N3	2.32	0.54
39:BN:35:ALA:HB2	39:BN:102:LEU:HD11	1.90	0.54
62:CC:1070:HIS:NE2	62:CC:1114:GLU:OE1	2.41	0.54
24:AX:41:C:H2'	24:AX:42:C:H6	1.73	0.54
26:BA:1596:A:O2'	26:BA:1597:A:H5'	2.08	0.54
26:BA:2899:A:H2'	26:BA:2900:A:H8	1.73	0.54
11:AK:92:GLY:O	11:AK:94:GLU:N	2.41	0.53
26:BA:1108:U:H2'	26:BA:1109:C:H6	1.73	0.53
62:CC:320:ASP:N	62:CC:320:ASP:OD1	2.37	0.53
65:CF:147:VAL:HG13	65:CF:161:SER:HB3	1.90	0.53
1:AA:687:A:N1	1:AA:700:G:O2'	2.36	0.53
7:AG:74:GLU:HG2	7:AG:75:VAL:H	1.73	0.53
15:AO:69:TYR:OH	15:AO:73:LYS:HD3	2.08	0.53
1:AA:473:U:H5''	16:AP:76:LYS:NZ	2.24	0.53
1:AA:951:G:OP2	13:AM:101:ARG:NH1	2.42	0.53
26:BA:2071:A:H2'	26:BA:2072:C:H6	1.73	0.53
62:CC:178:PRO:HB3	62:CC:395:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:696:ASP:OD1	62:CC:697:LYS:N	2.39	0.53
10:AJ:54:SER:O	14:AN:81:ARG:NH1	2.37	0.53
26:BA:630:G:N2	26:BA:633:A:OP2	2.34	0.53
26:BA:1096:A:N1	35:BJ:26:ALA:HB2	2.23	0.53
26:BA:2506:U:O2	26:BA:2506:U:H2'	2.09	0.53
62:CC:1321:GLU:OE2	63:CD:99:ARG:NH1	2.41	0.53
6:AF:36:ILE:HG12	6:AF:64:VAL:HG22	1.90	0.53
6:AF:79:ARG:HG3	6:AF:80:PHE:N	2.23	0.53
9:AI:39:PHE:O	9:AI:45:ARG:NE	2.41	0.53
26:BA:2104:C:H42	26:BA:2185:U:H3	1.55	0.53
1:AA:932:C:H3'	7:AG:3:ARG:HD2	1.91	0.53
25:AY:51:GLU:HA	25:AY:54:LYS:HD3	1.90	0.53
29:BD:5:VAL:HG22	29:BD:202:ILE:HD12	1.90	0.53
33:BH:40:THR:C	33:BH:42:LYS:H	2.16	0.53
34:BI:87:GLU:OE1	34:BI:93:ALA:HB3	2.09	0.53
52:B1:23:THR:HG23	52:B1:47:MET:HG2	1.89	0.53
59:CN:26:DG:C6	59:CN:27:DA:N6	2.76	0.53
62:CC:150:HIS:CE1	62:CC:454:ARG:HG3	2.43	0.53
62:CC:538:LEU:HD12	62:CC:539:THR:N	2.23	0.53
63:CD:367:GLY:HA2	63:CD:440:VAL:O	2.08	0.53
1:AA:500:G:H5''	12:AL:121:ARG:HH12	1.74	0.53
1:AA:1277:C:O2'	1:AA:1278:G:O5'	2.27	0.53
3:AC:25:ASN:OD1	3:AC:26:THR:N	2.40	0.53
21:AU:64:ASN:O	21:AU:66:ARG:N	2.42	0.53
26:BA:2228:G:H2'	26:BA:2229:U:C6	2.44	0.53
26:BA:2788:C:H2'	26:BA:2789:C:C6	2.44	0.53
61:CB:13:LEU:HA	61:CB:28:LEU:HD13	1.89	0.53
62:CC:23:ASP:OD1	62:CC:23:ASP:N	2.34	0.53
1:AA:269:C:H2'	1:AA:270:A:C8	2.44	0.53
1:AA:981:U:OP1	14:AN:9:ARG:NH1	2.41	0.53
4:AD:102:VAL:HG13	4:AD:114:ALA:HB1	1.89	0.53
12:AL:32:GLY:O	12:AL:79:VAL:HA	2.09	0.53
30:BE:58:LYS:NZ	30:BE:70:SER:O	2.42	0.53
34:BI:23:LEU:HB2	34:BI:92:ALA:HA	1.91	0.53
60:CT:21:DG:C6	60:CT:22:DC:N4	2.77	0.53
1:AA:1504:G:OP2	1:AA:1507:A:O2'	2.26	0.53
8:AH:106:THR:HB	8:AH:121:LEU:HD13	1.91	0.53
24:AX:33:U:N3	24:AX:36:A:OP2	2.40	0.53
26:BA:1580:A:H3'	26:BA:1581:G:H8	1.74	0.53
26:BA:2120:G:O2'	26:BA:2121:G:O5'	2.25	0.53
34:BI:81:LEU:HD21	34:BI:109:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BU:93:LEU:HD23	46:BU:94:ASP:O	2.09	0.53
61:CB:191:ARG:NH2	61:CB:192:VAL:O	2.42	0.53
63:CD:312:ARG:HG2	63:CD:313:GLY:N	2.24	0.53
63:CD:441:LEU:HD22	63:CD:441:LEU:H	1.73	0.53
1:AA:88:U:H2'	1:AA:89:G:H5'	1.90	0.53
26:BA:1083:U:O2'	26:BA:1085:A:OP2	2.27	0.53
26:BA:1744:A:H3'	26:BA:1745:A:H8	1.72	0.53
28:BC:144:VAL:HG21	28:BC:162:VAL:HG21	1.91	0.53
35:BJ:110:GLN:C	35:BJ:113:ALA:H	2.17	0.53
1:AA:518:C:H1'	12:AL:47:SER:HB3	1.91	0.52
9:AI:115:LYS:NZ	9:AI:121:ALA:O	2.26	0.52
12:AL:79:VAL:O	12:AL:103:ASP:HB2	2.08	0.52
26:BA:1066:U:N3	26:BA:1069:A:OP2	2.30	0.52
26:BA:1818:U:H2'	28:BC:156:ARG:HG3	1.91	0.52
5:AE:157:ARG:NH2	8:AH:99:LEU:O	2.41	0.52
26:BA:742:A:H2'	26:BA:743:A:C8	2.44	0.52
26:BA:1527:G:N1	26:BA:1544:A:OP2	2.43	0.52
31:BF:108:VAL:HG23	31:BF:109:PRO:HD3	1.91	0.52
36:BK:58:ASN:ND2	36:BK:128:ASN:OD1	2.37	0.52
62:CC:85:CYS:SG	62:CC:90:VAL:HG23	2.50	0.52
3:AC:75:ILE:HG12	22:AV:34:A:C8	2.44	0.52
15:AO:8:THR:HG23	15:AO:31:LEU:HD21	1.90	0.52
26:BA:1494:A:H2'	26:BA:1495:A:C8	2.43	0.52
58:B7:11:GLU:HA	58:B7:25:ARG:HA	1.91	0.52
62:CC:193:ASN:HD22	62:CC:193:ASN:N	2.08	0.52
62:CC:726:TYR:CD1	62:CC:727:VAL:N	2.77	0.52
2:AB:210:VAL:O	2:AB:214:LEU:HD22	2.09	0.52
6:AF:14:GLN:O	6:AF:17:GLN:HG3	2.10	0.52
12:AL:102:LEU:H	12:AL:102:LEU:HD13	1.74	0.52
17:AQ:57:ASP:OD1	17:AQ:57:ASP:N	2.43	0.52
20:AT:24:ARG:HH11	20:AT:24:ARG:HA	1.75	0.52
26:BA:511:U:H4'	26:BA:1235:G:H4'	1.90	0.52
47:BV:96:PHE:O	47:BV:100:SER:HA	2.10	0.52
1:AA:197:A:H4'	1:AA:198:G:O5'	2.10	0.52
1:AA:1008:U:OP2	1:AA:1008:U:C6	2.61	0.52
3:AC:88:ARG:CZ	63:CD:79:LYS:CD	2.60	0.52
12:AL:121:ARG:HD2	12:AL:122:PRO:HD2	1.92	0.52
26:BA:543:A:N6	26:BA:544:G:O6	2.42	0.52
26:BA:971:G:O2'	26:BA:983:A:N3	2.31	0.52
26:BA:1054:A:H4'	34:BI:31:ARG:HA	1.91	0.52
40:BO:28:LEU:HD23	40:BO:48:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:CA:218:ARG:NH1	61:CB:233:ASP:OD1	2.42	0.52
62:CC:377:THR:CB	65:CF:81:HIS:HE1	2.23	0.52
1:AA:203:G:N2	1:AA:215:C:C2	2.77	0.52
1:AA:768:A:N3	1:AA:1512:U:O2'	2.42	0.52
1:AA:881:G:P	12:AL:9:ARG:HH22	2.33	0.52
1:AA:1014:A:C2	1:AA:1219:A:H1'	2.45	0.52
1:AA:1137:C:H1'	1:AA:1138:G:N2	2.25	0.52
26:BA:1998:A:HO2'	26:BA:2724:U:HO2'	1.58	0.52
26:BA:2120:G:H2'	26:BA:2121:G:C8	2.44	0.52
29:BD:32:ASN:HD22	29:BD:32:ASN:N	2.08	0.52
37:BL:73:ASP:OD2	37:BL:75:SER:OG	2.26	0.52
62:CC:516:ASP:O	62:CC:518:ASN:N	2.41	0.52
63:CD:35:PHE:CD1	63:CD:101:ARG:HB3	2.44	0.52
63:CD:87:LYS:C	65:CF:133:MET:HE3	2.33	0.52
63:CD:801:VAL:HG12	63:CD:920:ALA:HB3	1.91	0.52
25:AY:28:VAL:HA	25:AY:38:VAL:HA	1.91	0.52
26:BA:151:C:H2'	26:BA:152:A:H8	1.75	0.52
26:BA:1063:G:O2'	26:BA:1064:C:O4'	2.27	0.52
26:BA:1172:C:O2'	26:BA:1173:U:H3'	2.10	0.52
26:BA:2115:G:O2'	26:BA:2166:U:O2	2.21	0.52
28:BC:37:ASN:HB2	28:BC:62:TYR:HB2	1.92	0.52
1:AA:337:G:H2'	1:AA:338:A:H8	1.75	0.52
5:AE:80:THR:HA	5:AE:120:VAL:HG13	1.92	0.52
26:BA:1590:A:H2'	26:BA:1591:A:H8	1.73	0.52
33:BH:5:LEU:HD23	33:BH:36:ALA:HB2	1.92	0.52
45:BT:20:VAL:HG11	45:BT:44:ALA:HA	1.92	0.52
62:CC:1333:LEU:C	62:CC:1335:ILE:H	2.18	0.52
63:CD:978:ARG:HG3	63:CD:1197:ASN:HD21	1.74	0.52
1:AA:1060:U:OP1	14:AN:85:ARG:NH2	2.43	0.52
7:AG:47:LEU:HD11	7:AG:62:PHE:HB2	1.92	0.52
26:BA:1084:A:H2	26:BA:1105:U:O2	1.92	0.52
26:BA:1744:A:H3'	26:BA:1745:A:C8	2.45	0.52
26:BA:2128:G:H3'	26:BA:2129:C:C5'	2.39	0.52
26:BA:2330:G:H21	49:BX:42:GLY:HA2	1.74	0.52
45:BT:36:LEU:HD13	45:BT:48:LYS:HA	1.91	0.52
63:CD:1159:ILE:O	63:CD:1206:ARG:N	2.43	0.52
65:CF:127:LEU:HD23	65:CF:127:LEU:H	1.74	0.52
1:AA:19:A:H5'	5:AE:90:THR:HG22	1.91	0.52
1:AA:713:G:H2'	1:AA:714:G:C8	2.44	0.52
1:AA:1390:U:H2'	1:AA:1391:U:C6	2.45	0.52
22:AV:33:U:H1'	22:AV:34:A:H2'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:27:G:C2	24:AX:44:G:C2	2.97	0.52
26:BA:2167:U:N3	26:BA:2170:A:H5''	2.24	0.52
40:BO:2:ARG:HG2	40:BO:5:LYS:HB2	1.92	0.52
63:CD:825:VAL:HG13	63:CD:825:VAL:O	2.09	0.52
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.46	0.51
12:AL:54:ARG:NH1	12:AL:64:THR:OG1	2.43	0.51
13:AM:89:LEU:O	13:AM:92:ARG:HG3	2.10	0.51
22:AV:37:G:C8	22:AV:37:G:C3'	2.92	0.51
23:AW:9:G:O2'	23:AW:10:G:N7	2.41	0.51
26:BA:550:U:OP2	26:BA:550:U:H6	1.93	0.51
26:BA:1407:G:O6	26:BA:1596:A:N6	2.43	0.51
32:BG:17:VAL:HG11	32:BG:50:LEU:HD21	1.91	0.51
35:BJ:71:LYS:HE2	35:BJ:115:ASP:OD1	2.10	0.51
62:CC:296:VAL:O	62:CC:335:THR:HB	2.10	0.51
1:AA:72:A:C5	1:AA:73:C:C5	2.97	0.51
1:AA:384:G:H2'	1:AA:385:C:C6	2.45	0.51
1:AA:1370:G:C2	1:AA:1371:G:C8	2.99	0.51
3:AC:88:ARG:HE	63:CD:79:LYS:HD3	1.69	0.51
6:AF:2:ARG:HE	6:AF:91:ARG:NE	2.08	0.51
25:AY:19:ARG:HD3	25:AY:24:VAL:HG21	1.91	0.51
26:BA:807:U:O2'	26:BA:2060:A:N1	2.39	0.51
26:BA:856:G:H2'	26:BA:857:G:C8	2.45	0.51
26:BA:1411:U:H2'	26:BA:1412:U:C6	2.45	0.51
26:BA:2618:G:H21	29:BD:155:VAL:HG21	1.75	0.51
44:BS:36:ALA:HA	44:BS:58:VAL:HG23	1.92	0.51
62:CC:766:ASN:CG	62:CC:766:ASN:O	2.53	0.51
5:AE:35:ALA:O	5:AE:50:TYR:C	2.50	0.51
6:AF:47:LEU:HD21	6:AF:57:ALA:HB3	1.93	0.51
9:AI:57:MET:HG3	9:AI:60:LYS:HD2	1.92	0.51
26:BA:396:G:H21	26:BA:2231:U:HO2'	1.57	0.51
26:BA:575:A:OP2	26:BA:2499:C:O2'	2.28	0.51
26:BA:1022:G:O6	36:BK:68:LYS:NZ	2.42	0.51
26:BA:1049:C:C2'	26:BA:1050:A:H5'	2.41	0.51
26:BA:1408:G:O2'	26:BA:1409:U:H5'	2.10	0.51
26:BA:1857:G:O2'	26:BA:1884:G:N2	2.44	0.51
26:BA:2122:U:H2'	26:BA:2123:G:C8	2.45	0.51
26:BA:2258:C:O2'	26:BA:2427:C:OP2	2.21	0.51
32:BG:24:ILE:HD11	32:BG:43:VAL:HG11	1.92	0.51
34:BI:27:VAL:H	34:BI:83:ALA:H	1.57	0.51
38:BM:81:ASP:HB3	38:BM:100:ILE:HD13	1.92	0.51
1:AA:148:G:O2'	1:AA:149:A:O5'	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.43	0.51
5:AE:100:SER:O	5:AE:103:THR:HG23	2.11	0.51
8:AH:77:ARG:NH1	8:AH:126:ILE:HG23	2.25	0.51
23:AW:21:A:H61	23:AW:47:U:H5''	1.75	0.51
26:BA:284:U:C2	26:BA:356:G:O6	2.63	0.51
38:BM:56:PRO:HG2	38:BM:59:ARG:HG3	1.91	0.51
40:BO:30:ARG:NH1	40:BO:74:GLU:OE1	2.43	0.51
63:CD:288:PRO:HD2	63:CD:291:ILE:HD12	1.93	0.51
1:AA:562:U:C2	12:AL:13:ALA:O	2.63	0.51
9:AI:99:ARG:HH21	9:AI:104:VAL:HG23	1.75	0.51
34:BI:30:SER:HB2	34:BI:109:LYS:HZ2	1.76	0.51
43:BR:94:ILE:HG21	44:BS:4:VAL:HG11	1.93	0.51
60:CT:18:DC:O2	60:CT:19:DG:C8	2.64	0.51
62:CC:855:PRO:HG3	62:CC:913:VAL:HG23	1.92	0.51
13:AM:92:ARG:O	26:BA:888:C:N4	2.44	0.51
26:BA:357:C:H2'	26:BA:358:U:H6	1.74	0.51
26:BA:468:G:OP2	55:B4:37:LYS:NZ	2.39	0.51
26:BA:1012:U:OP2	43:BR:70:ARG:NH1	2.44	0.51
26:BA:1154:G:OP2	43:BR:58:ARG:NH2	2.43	0.51
26:BA:1407:G:C6	26:BA:1596:A:C6	2.99	0.51
34:BI:9:GLN:O	34:BI:12:VAL:HG22	2.10	0.51
6:AF:47:LEU:HD13	6:AF:51:ILE:HG13	1.92	0.51
16:AP:1:MET:N	16:AP:1:MET:SD	2.78	0.51
17:AQ:48:ASP:HB3	17:AQ:75:LEU:HD23	1.93	0.51
26:BA:1028:A:H2'	26:BA:1029:A:C8	2.46	0.51
28:BC:41:GLY:O	28:BC:43:ARG:NH1	2.41	0.51
29:BD:105:LYS:O	29:BD:177:VAL:HG12	2.09	0.51
62:CC:7:GLU:O	62:CC:9:LYS:N	2.34	0.51
63:CD:366:CYS:O	63:CD:439:PRO:HA	2.11	0.51
63:CD:504:GLN:HG3	63:CD:505:ASP:N	2.25	0.51
63:CD:1075:ARG:HH21	63:CD:1102:PRO:HA	1.75	0.51
65:CF:115:LEU:O	65:CF:118:VAL:HG13	2.10	0.51
1:AA:925:G:C6	1:AA:927:G:N7	2.79	0.51
5:AE:69:ARG:HG2	5:AE:70:ASN:H	1.76	0.51
5:AE:153:VAL:HA	5:AE:156:LYS:HE3	1.93	0.51
20:AT:25:ARG:HG3	20:AT:66:LEU:HD21	1.93	0.51
26:BA:1223:G:OP1	44:BS:68:ARG:NH2	2.44	0.51
58:B7:37:CYS:N	58:B7:40:CYS:SG	2.74	0.51
1:AA:76:G:C4	1:AA:77:A:C8	2.98	0.51
1:AA:958:A:OP1	19:AS:55:ARG:NH1	2.41	0.51
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:357:C:H2'	26:BA:358:U:C6	2.46	0.51
26:BA:1796:U:O2'	28:BC:254:GLY:N	2.31	0.51
26:BA:2126:A:O2'	26:BA:2162:G:N2	2.31	0.51
60:CT:9:DC:H2'	60:CT:10:DT:H71	1.93	0.51
62:CC:705:GLU:CD	62:CC:705:GLU:H	2.14	0.51
65:CF:71:VAL:HG12	65:CF:73:MET:HB2	1.93	0.51
1:AA:1397:C:H5'	22:AV:23:C:N4	2.25	0.51
13:AM:75:MET:N	13:AM:75:MET:SD	2.84	0.51
26:BA:888:C:H1'	26:BA:889:C:H5'	1.93	0.51
26:BA:1914:C:H2'	26:BA:1915:3TD:O4	2.11	0.51
26:BA:2116:G:N2	26:BA:2164:C:H42	2.08	0.51
31:BF:42:GLU:CG	31:BF:49:LEU:HD23	2.41	0.51
35:BJ:20:SER:HA	35:BJ:24:GLY:HA2	1.93	0.51
45:BT:25:ARG:NH1	45:BT:74:ILE:O	2.44	0.51
61:CA:68:TYR:CD1	61:CA:68:TYR:N	2.79	0.51
1:AA:91:U:H2'	1:AA:92:U:H6	1.76	0.50
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.92	0.50
22:AV:52:C:H2'	22:AV:53:G:C1'	2.41	0.50
26:BA:2343:U:O2'	26:BA:2373:G:O2'	2.23	0.50
49:BX:18:ALA:O	49:BX:20:ARG:NH1	2.44	0.50
22:AV:51:G:C2	22:AV:52:C:C4	3.00	0.50
26:BA:276:U:H2'	26:BA:277:G:C8	2.47	0.50
26:BA:1528:A:OP2	26:BA:1543:G:N2	2.39	0.50
26:BA:1915:3TD:H2'	26:BA:1916:A:H8	1.77	0.50
26:BA:2605:PSU:H2'	26:BA:2606:C:C6	2.46	0.50
51:BZ:18:LEU:HD21	51:BZ:54:LYS:HE3	1.93	0.50
63:CD:907:HIS:ND1	63:CD:908:ILE:O	2.36	0.50
1:AA:658:C:H1'	15:AO:22:THR:HG21	1.92	0.50
1:AA:1169:A:OP2	1:AA:1169:A:H8	1.94	0.50
26:BA:2106:U:H5''	26:BA:2107:G:OP2	2.11	0.50
26:BA:2591:C:H2'	26:BA:2592:G:C8	2.47	0.50
26:BA:2698:U:H2'	26:BA:2699:C:C6	2.46	0.50
28:BC:71:LYS:NZ	28:BC:98:ASP:OD2	2.37	0.50
31:BF:8:TYR:HB2	31:BF:173:PHE:CZ	2.47	0.50
59:CN:23:DT:H1'	59:CN:24:DC:C4	2.47	0.50
1:AA:923:A:O2'	1:AA:1399:C:OP2	2.22	0.50
26:BA:2233:U:H2'	26:BA:2234:G:C8	2.46	0.50
34:BI:8:LYS:O	34:BI:12:VAL:HG13	2.11	0.50
63:CD:326:SER:O	63:CD:329:ASP:N	2.43	0.50
1:AA:1383:C:H2'	1:AA:1384:C:H6	1.77	0.50
4:AD:15:GLU:HG2	4:AD:60:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1066:U:O2'	26:BA:1068:G:N7	2.42	0.50
26:BA:1069:A:H4'	26:BA:1070:A:O5'	2.12	0.50
26:BA:2683:C:OP1	42:BQ:51:ARG:NH1	2.44	0.50
62:CC:375:PRO:HG3	65:CF:80:TRP:CZ2	2.42	0.50
62:CC:617:ALA:HB2	62:CC:650:VAL:HG21	1.93	0.50
1:AA:83:C:O2'	1:AA:85:U:O2	2.28	0.50
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.47	0.50
11:AK:88:GLY:N	11:AK:114:THR:HG22	2.27	0.50
12:AL:57:LEU:HD11	12:AL:82:ILE:HD11	1.93	0.50
15:AO:18:ASP:OD1	15:AO:21:ASP:HB2	2.12	0.50
20:AT:57:ILE:HD13	20:AT:60:ARG:HH12	1.77	0.50
28:BC:162:VAL:HG12	28:BC:176:LEU:HA	1.94	0.50
31:BF:8:TYR:HB2	31:BF:173:PHE:HZ	1.76	0.50
32:BG:15:VAL:HA	32:BG:27:LYS:O	2.11	0.50
44:BS:63:VAL:HG22	44:BS:96:VAL:HG12	1.92	0.50
61:CB:28:LEU:HD22	61:CB:28:LEU:N	2.27	0.50
63:CD:530:PRO:O	63:CD:533:ALA:HB3	2.12	0.50
1:AA:606:G:N2	1:AA:632:U:OP1	2.42	0.50
1:AA:1320:C:N3	19:AS:36:ARG:NH1	2.59	0.50
1:AA:1432:G:OP1	42:BQ:106:LYS:N	2.35	0.50
5:AE:38:VAL:HG12	5:AE:48:PHE:HB2	1.94	0.50
13:AM:107:ARG:HH12	13:AM:112:PRO:C	2.19	0.50
26:BA:1051:G:H1	26:BA:1108:U:H3	1.58	0.50
42:BQ:91:ALA:HB2	42:BQ:113:ARG:HB2	1.94	0.50
43:BR:11:ARG:HB2	43:BR:11:ARG:NH1	2.26	0.50
62:CC:274:ILE:HA	62:CC:277:LEU:HD12	1.93	0.50
1:AA:160:A:H1'	1:AA:344:A:C5	2.47	0.50
1:AA:966:2MG:H5''	1:AA:967:5MC:OP2	2.12	0.50
12:AL:87:VAL:O	12:AL:89:D2T:N	2.45	0.50
24:AX:16:H2U:H62	24:AX:16:H2U:P	2.51	0.50
26:BA:277:G:H4'	26:BA:278:A:C8	2.46	0.50
26:BA:1045:C:H41	26:BA:1111:A:H2'	1.77	0.50
26:BA:1724:G:O6	26:BA:1736:U:O4	2.29	0.50
34:BI:43:LYS:NZ	34:BI:98:GLU:HG2	2.25	0.50
51:BZ:6:LEU:HD11	51:BZ:53:VAL:HG22	1.92	0.50
59:CN:28:DA:H2''	59:CN:29:DG:C8	2.45	0.50
1:AA:590:U:H2'	1:AA:591:U:H6	1.77	0.50
1:AA:946:A:O2'	1:AA:1333:A:N3	2.31	0.50
1:AA:966:2MG:O2'	9:AI:129:LYS:O	2.22	0.50
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.47	0.50
2:AB:186:ILE:HD13	2:AB:213:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:14:GLN:HB3	6:AF:17:GLN:NE2	2.27	0.50
18:AR:20:GLU:HG3	18:AR:54:GLN:OE1	2.12	0.50
20:AT:39:ILE:HD11	20:AT:83:ILE:HD12	1.94	0.50
26:BA:2124:G:H21	26:BA:2175:C:N4	2.10	0.50
26:BA:2228:G:H2'	26:BA:2229:U:H6	1.76	0.50
44:BS:27:ILE:O	44:BS:66:HIS:NE2	2.45	0.50
61:CB:11:PRO:O	61:CB:12:ARG:HD2	2.12	0.50
63:CD:275:ARG:HH11	63:CD:298:MET:HB3	1.76	0.50
63:CD:961:SER:HB2	63:CD:981:GLU:HB2	1.94	0.50
65:CF:133:MET:HA	65:CF:147:VAL:HA	1.94	0.50
1:AA:82:G:H5'	1:AA:82:G:H8	1.77	0.49
2:AB:68:LEU:HB3	2:AB:161:LEU:HD12	1.95	0.49
22:AV:44:A:C5	62:CC:1264:GLN:NE2	2.71	0.49
22:AV:51:G:C4	22:AV:52:C:C5	3.00	0.49
26:BA:320:A:N3	30:BE:163:ASN:ND2	2.49	0.49
26:BA:396:G:OP2	50:BY:10:LYS:NZ	2.45	0.49
35:BJ:83:ALA:HB3	35:BJ:85:ILE:O	2.12	0.49
41:BP:57:ALA:O	41:BP:61:GLN:HG2	2.12	0.49
49:BX:37:ILE:HG22	49:BX:38:VAL:HG23	1.94	0.49
63:CD:67:ASP:N	63:CD:67:ASP:OD1	2.43	0.49
1:AA:1366:C:O2'	10:AJ:62:ARG:NH2	2.35	0.49
15:AO:18:ASP:O	15:AO:20:ASN:N	2.45	0.49
26:BA:284:U:O2	26:BA:356:G:C6	2.65	0.49
26:BA:1794:A:H2'	26:BA:1795:C:C6	2.47	0.49
26:BA:2314:A:H2'	26:BA:2315:G:C8	2.47	0.49
26:BA:2901:C:N3	26:BA:2902:C:N4	2.60	0.49
37:BL:108:ARG:HH12	42:BQ:34:GLU:CB	2.25	0.49
43:BR:27:ALA:HB1	43:BR:31:VAL:HB	1.94	0.49
61:CA:102:LEU:HD23	61:CA:103:ASN:N	2.27	0.49
62:CC:1058:ARG:HH21	62:CC:1240:ASP:CG	2.20	0.49
62:CC:1119:MET:HA	62:CC:1119:MET:HE3	1.95	0.49
1:AA:35:G:H2'	1:AA:36:C:C6	2.48	0.49
1:AA:346:G:OP1	42:BQ:39:ARG:NH1	2.46	0.49
1:AA:757:U:O2'	1:AA:879:C:O2	2.31	0.49
3:AC:7:PRO:HA	3:AC:10:ILE:HG22	1.94	0.49
10:AJ:25:ILE:HD11	10:AJ:92:LEU:HD11	1.95	0.49
10:AJ:42:LEU:HB2	10:AJ:71:LEU:CB	2.42	0.49
24:AX:9:A:N6	24:AX:22:G:N7	2.60	0.49
26:BA:684:G:OP1	55:B4:21:ARG:NH1	2.40	0.49
26:BA:721:A:H2'	26:BA:722:A:C8	2.46	0.49
26:BA:1796:U:H2'	26:BA:1797:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BB:89:U:OP2	27:BB:89:U:H6	1.94	0.49
33:BH:50:ARG:NH2	33:BH:51:ARG:HE	2.11	0.49
34:BI:12:VAL:O	34:BI:15:VAL:HG22	2.12	0.49
59:CN:27:DA:C6	59:CN:28:DA:C6	3.00	0.49
62:CC:680:LEU:HD23	62:CC:680:LEU:C	2.37	0.49
62:CC:811:ASN:ND2	62:CC:1097:VAL:O	2.43	0.49
63:CD:137:ARG:HG3	63:CD:142:GLU:HB2	1.94	0.49
1:AA:1090:U:HO2'	1:AA:1171:A:HO2'	1.59	0.49
6:AF:3:HIS:HB2	6:AF:92:THR:O	2.13	0.49
26:BA:140:C:H1'	26:BA:141:G:N2	2.27	0.49
26:BA:1808:A:H3'	26:BA:1809:A:C8	2.48	0.49
34:BI:26:VAL:CB	34:BI:82:ILE:HG23	2.41	0.49
1:AA:1277:C:O2'	1:AA:1278:G:P	2.70	0.49
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.94	0.49
26:BA:1176:U:O2'	26:BA:1177:G:C8	2.64	0.49
31:BF:171:ALA:O	31:BF:174:ASP:N	2.42	0.49
47:BV:94:ARG:HB2	47:BV:103:ILE:HD12	1.93	0.49
62:CC:1239:VAL:HG13	62:CC:1240:ASP:N	2.28	0.49
63:CD:291:ILE:HD13	65:CF:65:PHE:CD2	2.47	0.49
1:AA:563:A:H2'	1:AA:567:G:C8	2.48	0.49
10:AJ:6:ILE:H	10:AJ:6:ILE:HD13	1.78	0.49
26:BA:1364:G:N2	26:BA:1367:A:OP2	2.33	0.49
29:BD:110:THR:HG21	29:BD:169:ARG:HE	1.78	0.49
63:CD:53:ARG:CD	65:CF:135:ARG:HH21	2.26	0.49
3:AC:79:LYS:HD2	3:AC:80:LYS:H	1.77	0.49
26:BA:2722:G:O2'	40:BO:3:HIS:O	2.28	0.49
52:B1:9:GLN:O	52:B1:33:GLY:N	2.44	0.49
60:CT:19:DG:C4	60:CT:20:DC:C6	3.01	0.49
1:AA:874:G:C6	1:AA:875:U:C4	3.01	0.49
4:AD:163:GLU:HA	4:AD:167:LYS:HE3	1.93	0.49
10:AJ:100:ILE:HD11	65:CF:165:PHE:CE2	2.48	0.49
27:BB:42:C:C6	31:BF:66:LEU:HB2	2.48	0.49
35:BJ:109:ALA:HB2	35:BJ:128:ILE:HG13	1.94	0.49
62:CC:261:VAL:HG21	62:CC:264:GLU:HG2	1.94	0.49
63:CD:805:GLN:OE1	63:CD:1348:LYS:HB2	2.13	0.49
63:CD:1292:LEU:HD11	63:CD:1297:LYS:HB2	1.95	0.49
1:AA:195:A:C2'	1:AA:196:A:H5'	2.43	0.49
1:AA:1261:A:N6	1:AA:1274:A:HO2'	2.10	0.49
9:AI:55:VAL:HG23	9:AI:55:VAL:O	2.13	0.49
26:BA:2064:C:H2'	26:BA:2065:C:C6	2.48	0.49
38:BM:114:GLY:O	38:BM:115:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:267:ARG:HH22	62:CC:273:HIS:CE1	2.31	0.49
63:CD:425:ARG:HE	63:CD:464:ASP:CG	2.21	0.49
1:AA:664:G:H22	1:AA:741:G:H1	1.60	0.48
47:BV:83:VAL:HG13	47:BV:94:ARG:HB3	1.95	0.48
59:CN:32:DA:H5'	59:CN:32:DA:H8	1.76	0.48
60:CT:9:DC:H2'	60:CT:10:DT:C5	2.48	0.48
1:AA:1060:U:H4'	10:AJ:53:ILE:HG13	1.95	0.48
3:AC:59:ARG:HH21	3:AC:64:ILE:HD12	1.77	0.48
6:AF:43:GLY:HA2	6:AF:58:HIS:CE1	2.47	0.48
26:BA:883:G:N2	26:BA:884:U:O4	2.46	0.48
26:BA:1406:U:O2'	26:BA:1407:G:H5''	2.12	0.48
26:BA:1891:G:HO2'	26:BA:2235:G:HO2'	1.60	0.48
27:BB:52:A:N7	41:BP:64:TYR:OH	2.40	0.48
28:BC:142:HIS:HD2	28:BC:193:GLY:O	1.96	0.48
39:BN:17:ASN:O	39:BN:38:ARG:NH1	2.46	0.48
56:B5:16:LYS:HB3	56:B5:16:LYS:NZ	2.28	0.48
62:CC:377:THR:HB	65:CF:81:HIS:CE1	2.48	0.48
1:AA:147:G:O2'	1:AA:148:G:O4'	2.30	0.48
1:AA:215:C:H2'	1:AA:216:U:O4'	2.12	0.48
1:AA:843:U:H4'	1:AA:844:G:OP1	2.13	0.48
1:AA:1173:U:C2	1:AA:1174:G:C8	3.02	0.48
10:AJ:57:VAL:HG13	10:AJ:58:ASN:N	2.28	0.48
24:AX:11:C:H2'	24:AX:12:U:C6	2.48	0.48
25:AY:36:VAL:HG23	25:AY:50:ALA:HB2	1.94	0.48
26:BA:65:U:O2'	26:BA:456:C:N3	2.39	0.48
26:BA:614:A:O2'	26:BA:615:U:OP2	2.23	0.48
26:BA:929:U:H1'	52:B1:26:GLY:O	2.13	0.48
26:BA:2291:U:OP1	26:BA:2380:C:O2'	2.28	0.48
34:BI:11:ILE:O	34:BI:15:VAL:HG13	2.13	0.48
54:B3:6:ARG:HG2	54:B3:24:THR:HB	1.94	0.48
59:CN:32:DA:H1'	59:CN:33:DT:O4'	2.14	0.48
60:CT:20:DC:H2'	60:CT:21:DG:C8	2.47	0.48
1:AA:157:U:O2	1:AA:164:G:O6	2.32	0.48
1:AA:604:G:H2'	1:AA:605:U:O4'	2.13	0.48
2:AB:129:LEU:CD1	2:AB:134:ALA:HB2	2.43	0.48
4:AD:87:GLY:HA3	4:AD:197:GLU:HB3	1.95	0.48
26:BA:889:C:H2'	26:BA:890:C:H5'	1.94	0.48
26:BA:1432:G:H2'	26:BA:1433:A:C8	2.49	0.48
28:BC:132:MET:HE1	28:BC:174:LEU:HD11	1.95	0.48
34:BI:26:VAL:HG13	34:BI:115:GLY:H	1.77	0.48
47:BV:6:ARG:O	47:BV:9:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:CT:22:DC:C2	60:CT:23:DC:C5	3.01	0.48
1:AA:877:G:C2	1:AA:878:A:N7	2.82	0.48
3:AC:89:LYS:HA	63:CD:79:LYS:HE3	1.96	0.48
4:AD:50:ASP:O	4:AD:53:VAL:HG22	2.12	0.48
5:AE:99:ALA:HB2	5:AE:124:LEU:HG	1.95	0.48
15:AO:78:TYR:OH	15:AO:89:ARG:OXT	2.28	0.48
26:BA:885:C:N3	26:BA:892:A:N6	2.62	0.48
26:BA:947:A:H2'	26:BA:948:C:C6	2.48	0.48
26:BA:1007:C:OP1	36:BK:37:ARG:NH2	2.46	0.48
33:BH:16:GLY:HA3	33:BH:47:PHE:CZ	2.48	0.48
38:BM:23:ILE:HG12	44:BS:82:HIS:CD2	2.48	0.48
59:CN:28:DA:C6	59:CN:29:DG:C6	3.01	0.48
60:CT:17:DG:C6	60:CT:18:DC:C5	3.00	0.48
62:CC:493:ILE:C	62:CC:493:ILE:HD12	2.39	0.48
63:CD:813:ASP:OD1	63:CD:883:ARG:NH2	2.35	0.48
7:AG:113:ASP:O	7:AG:119:ARG:HD3	2.12	0.48
26:BA:674:G:H5''	30:BE:71:GLY:N	2.28	0.48
26:BA:863:A:O3'	27:BB:100:G:N2	2.43	0.48
26:BA:2169:A:H2'	26:BA:2170:A:H4'	1.95	0.48
34:BI:14:GLU:OE1	34:BI:57:ASN:ND2	2.46	0.48
45:BT:41:LYS:O	45:BT:44:ALA:HB3	2.12	0.48
59:CN:19:DA:H2'	65:CF:88:ARG:N	2.28	0.48
62:CC:377:THR:CG2	65:CF:81:HIS:CE1	2.97	0.48
62:CC:1238:LEU:N	62:CC:1238:LEU:HD23	2.28	0.48
63:CD:474:LEU:HD21	64:CE:27:ALA:CB	2.43	0.48
1:AA:206:C:H2'	1:AA:207:C:O4'	2.13	0.48
2:AB:205:ASP:HB2	25:AY:43:LYS:HE3	1.96	0.48
26:BA:813:U:H2'	26:BA:814:C:C6	2.49	0.48
26:BA:1251:C:OP2	43:BR:6:ARG:NH2	2.42	0.48
27:BB:55:U:HO2'	31:BF:24:SER:HG	1.41	0.48
29:BD:4:LEU:HB2	29:BD:101:PHE:HE2	1.78	0.48
1:AA:1442:G:O2'	42:BQ:114:LEU:HD22	2.13	0.48
1:AA:1516:2MG:HM21	1:AA:1519:MA6:N7	2.28	0.48
26:BA:84:A:N1	26:BA:98:G:O2'	2.46	0.48
26:BA:2885:G:O6	53:B2:40:ARG:NH1	2.46	0.48
27:BB:2:G:H2'	27:BB:3:C:C6	2.48	0.48
33:BH:122:LEU:HD11	33:BH:128:HIS:CG	2.48	0.48
42:BQ:33:VAL:O	42:BQ:33:VAL:HG12	2.14	0.48
62:CC:269:ILE:HD12	62:CC:269:ILE:N	2.29	0.48
62:CC:576:SER:OG	62:CC:577:VAL:N	2.47	0.48
62:CC:1340:GLU:CD	62:CC:1341:ASP:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:CD:158:GLN:NE2	63:CD:158:GLN:O	2.46	0.48
1:AA:1054:C:N4	24:AX:34:G:C8	2.81	0.48
8:AH:77:ARG:NE	8:AH:79:SER:O	2.47	0.48
8:AH:96:MET:HE2	8:AH:99:LEU:HB2	1.96	0.48
26:BA:287:G:H2'	26:BA:288:U:C6	2.49	0.48
26:BA:1081:U:C2	26:BA:1082:U:C5	3.02	0.48
29:BD:152:PRO:HG3	29:BD:156:PHE:CZ	2.49	0.48
33:BH:75:LEU:HD12	33:BH:77:THR:H	1.78	0.48
43:BR:70:ARG:HE	43:BR:75:SER:HA	1.79	0.48
46:BU:10:VAL:HG12	46:BU:11:LEU:HD23	1.96	0.48
62:CC:1085:MET:HE2	62:CC:1085:MET:HA	1.95	0.48
63:CD:767:LEU:HD12	63:CD:767:LEU:N	2.28	0.48
65:CF:150:GLU:HG3	65:CF:159:LYS:HB3	1.95	0.48
2:AB:194:ASP:OD1	2:AB:195:GLY:N	2.46	0.48
5:AE:106:ILE:HB	5:AE:124:LEU:HD23	1.96	0.48
26:BA:2345:G:N3	26:BA:2381:A:H2'	2.28	0.48
31:BF:57:LEU:HD13	31:BF:65:PRO:HB3	1.96	0.48
35:BJ:12:VAL:HG11	35:BJ:22:PRO:HG2	1.95	0.48
62:CC:705:GLU:OE1	62:CC:705:GLU:N	2.41	0.48
1:AA:235:C:H2'	1:AA:236:A:H8	1.79	0.47
1:AA:427:U:OP2	1:AA:428:G:O2'	2.24	0.47
4:AD:99:ASP:O	4:AD:102:VAL:HG13	2.14	0.47
6:AF:9:MET:O	6:AF:85:ILE:N	2.46	0.47
6:AF:29:ILE:HG23	6:AF:34:GLY:HA3	1.96	0.47
26:BA:1799:G:OP1	28:BC:258:ARG:HD2	2.14	0.47
30:BE:119:ILE:HB	30:BE:187:VAL:HG22	1.95	0.47
44:BS:32:THR:HG21	44:BS:60:LYS:HE3	1.96	0.47
62:CC:1133:LYS:O	62:CC:1135:GLN:NE2	2.47	0.47
63:CD:26:SER:HB3	63:CD:236:TRP:CZ2	2.49	0.47
1:AA:235:C:H2'	1:AA:236:A:C8	2.49	0.47
1:AA:736:C:H2'	1:AA:737:C:C6	2.49	0.47
1:AA:935:A:O2'	1:AA:1383:C:N3	2.37	0.47
1:AA:1223:C:P	19:AS:78:ARG:HH21	2.37	0.47
3:AC:88:ARG:HH21	63:CD:79:LYS:HB3	1.78	0.47
5:AE:37:THR:HG21	5:AE:64:MET:SD	2.54	0.47
23:AW:44:A:H2'	23:AW:45:G:O4'	2.14	0.47
26:BA:345:A:N3	26:BA:346:A:N6	2.62	0.47
62:CC:316:GLU:CD	62:CC:316:GLU:H	2.22	0.47
62:CC:529:ARG:NH2	62:CC:562:GLU:OE2	2.46	0.47
63:CD:746:LEU:HD23	63:CD:758:PRO:HB3	1.96	0.47
1:AA:1140:C:HO2'	1:AA:1141:C:C5'	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:83:ALA:HB2	2:AB:214:LEU:HB3	1.96	0.47
2:AB:164:ILE:HD13	2:AB:186:ILE:HD12	1.96	0.47
2:AB:170:HIS:CD2	2:AB:171:ILE:HG13	2.49	0.47
2:AB:187:VAL:HG21	2:AB:199:VAL:HG22	1.97	0.47
15:AO:25:THR:HG21	15:AO:70:LEU:HD13	1.95	0.47
24:AX:34:G:H2'	24:AX:35:A:C8	2.48	0.47
26:BA:2140:G:O6	26:BA:2151:U:N3	2.47	0.47
26:BA:2591:C:H2'	26:BA:2592:G:H8	1.80	0.47
26:BA:2899:A:H2'	26:BA:2900:A:C8	2.49	0.47
36:BK:17:VAL:HG23	36:BK:137:PRO:HB2	1.96	0.47
47:BV:81:ASP:OD1	47:BV:98:SER:HB3	2.14	0.47
60:CT:21:DG:H2'	60:CT:22:DC:C6	2.49	0.47
7:AG:2:PRO:HB2	7:AG:5:ARG:HH11	1.80	0.47
26:BA:851:C:H2'	26:BA:852:U:H6	1.78	0.47
26:BA:1529:G:H2'	26:BA:1530:G:C8	2.50	0.47
26:BA:1871:A:O2'	26:BA:1872:A:N7	2.48	0.47
26:BA:2315:G:HO2'	26:BA:2316:G:H8	1.62	0.47
61:CB:61:ILE:HD12	61:CB:142:MET:HB3	1.96	0.47
62:CC:1292:THR:OG1	62:CC:1293:VAL:N	2.47	0.47
63:CD:466:MET:HB2	63:CD:466:MET:HE3	1.70	0.47
63:CD:850:LYS:N	63:CD:855:ASP:O	2.33	0.47
4:AD:150:LYS:HD3	4:AD:178:MET:SD	2.54	0.47
12:AL:102:LEU:H	12:AL:102:LEU:CD1	2.26	0.47
16:AP:39:PHE:HD1	16:AP:50:THR:HG22	1.78	0.47
22:AV:32:A:H2	22:AV:33:U:H3	1.62	0.47
26:BA:1141:U:H4'	26:BA:1142:A:O4'	2.14	0.47
26:BA:2086:U:H2'	26:BA:2087:G:C8	2.49	0.47
34:BI:28:ALA:HB1	34:BI:81:LEU:HG	1.97	0.47
35:BJ:112:LYS:O	35:BJ:116:MET:N	2.39	0.47
36:BK:5:THR:HG22	36:BK:6:ALA:O	2.14	0.47
42:BQ:22:PRO:HD3	42:BQ:50:ILE:HD12	1.97	0.47
44:BS:77:PHE:CD2	44:BS:84:ARG:HB3	2.48	0.47
60:CT:19:DG:C5	60:CT:20:DC:C4	3.02	0.47
63:CD:175:GLU:CD	63:CD:175:GLU:N	2.72	0.47
63:CD:255:LEU:HG	63:CD:256:ASP:H	1.79	0.47
63:CD:849:LEU:HA	63:CD:856:ILE:HA	1.96	0.47
1:AA:1224:U:O2'	1:AA:1322:C:OP1	2.29	0.47
2:AB:146:ASN:ND2	2:AB:147:SER:N	2.63	0.47
9:AI:40:GLY:HA2	9:AI:45:ARG:NH2	2.30	0.47
13:AM:34:LEU:HD23	13:AM:41:GLU:HG3	1.95	0.47
13:AM:90:ARG:HD2	13:AM:90:ARG:HA	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:414:C:H2'	26:BA:415:A:C8	2.50	0.47
1:AA:346:G:N2	1:AA:347:G:C8	2.83	0.47
1:AA:401:C:O2'	1:AA:621:A:N3	2.42	0.47
1:AA:590:U:H2'	1:AA:591:U:C6	2.50	0.47
1:AA:1175:G:O2'	1:AA:1176:A:H8	1.98	0.47
1:AA:1384:C:H2'	1:AA:1385:G:H8	1.79	0.47
1:AA:1463:U:OP1	42:BQ:109:ARG:NE	2.41	0.47
5:AE:72:ILE:HD12	5:AE:72:ILE:O	2.13	0.47
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.95	0.47
25:AY:32:ASP:HB2	25:AY:35:VAL:HB	1.96	0.47
26:BA:673:C:OP1	30:BE:49:ARG:NH2	2.44	0.47
26:BA:989:G:OP2	52:B1:12:SER:OG	2.31	0.47
26:BA:2000:C:OP1	40:BO:5:LYS:NZ	2.48	0.47
26:BA:2114:A:C2	26:BA:2166:U:H2'	2.50	0.47
26:BA:2164:C:O2	26:BA:2164:C:H2'	2.14	0.47
26:BA:2742:G:OP2	57:B6:24:ARG:NH1	2.45	0.47
30:BE:130:LYS:HB2	30:BE:133:LEU:HD12	1.96	0.47
33:BH:11:ASN:O	33:BH:11:ASN:ND2	2.44	0.47
36:BK:117:ALA:O	36:BK:120:ARG:HB2	2.15	0.47
63:CD:87:LYS:C	65:CF:133:MET:CE	2.87	0.47
1:AA:6:G:N1	5:AE:103:THR:HG21	2.24	0.47
1:AA:73:C:O2'	1:AA:74:A:H5'	2.14	0.47
1:AA:978:A:C5	1:AA:1319:A:C2	3.03	0.47
3:AC:123:GLN:O	3:AC:128:VAL:HG23	2.15	0.47
4:AD:105:MET:HG2	4:AD:173:VAL:HB	1.95	0.47
11:AK:70:CYS:O	11:AK:74:VAL:HG23	2.14	0.47
24:AX:56:C:H5''	39:BN:59:ARG:HH22	1.80	0.47
26:BA:48:G:N2	26:BA:177:G:OP2	2.44	0.47
26:BA:833:A:H2'	26:BA:834:G:C8	2.49	0.47
26:BA:992:C:OP1	43:BR:47:TYR:OH	2.28	0.47
26:BA:1794:A:H2'	26:BA:1795:C:H6	1.80	0.47
27:BB:41:G:H8	31:BF:66:LEU:HD11	1.78	0.47
59:CN:27:DA:C2	59:CN:28:DA:C4	3.02	0.47
1:AA:72:A:C4	1:AA:73:C:C6	3.03	0.47
1:AA:429:U:H3'	4:AD:9:LEU:HD12	1.97	0.47
1:AA:1130:A:OP1	9:AI:18:ARG:NH2	2.38	0.47
3:AC:74:GLY:HA2	22:AV:35:U:H5''	1.97	0.47
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.97	0.47
12:AL:25:GLU:OE1	12:AL:59:ASN:ND2	2.35	0.47
13:AM:92:ARG:HE	26:BA:888:C:H5''	1.79	0.47
26:BA:1173:U:O2'	26:BA:1177:G:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1861:G:C2	26:BA:1862:G:C8	3.03	0.47
55:B4:41:ARG:HB2	55:B4:41:ARG:NH2	2.29	0.47
63:CD:1342:ASP:C	63:CD:1342:ASP:OD1	2.58	0.47
1:AA:553:A:H5''	12:AL:21:VAL:HG21	1.96	0.47
2:AB:44:GLU:OE2	25:AY:5:PHE:HB2	2.15	0.47
14:AN:46:LEU:O	14:AN:50:THR:HG23	2.15	0.47
18:AR:34:THR:OG1	18:AR:35:GLU:OE2	2.33	0.47
23:AW:69:C:H2'	23:AW:70:G:H8	1.80	0.47
26:BA:299:A:N3	26:BA:319:G:O2'	2.42	0.47
26:BA:532:A:N7	26:BA:2021:C:O2'	2.39	0.47
26:BA:2900:A:C6	26:BA:2901:C:N4	2.83	0.47
29:BD:149:ASN:OD1	29:BD:150:MEQ:N	2.48	0.47
43:BR:83:LEU:HD23	43:BR:83:LEU:HA	1.77	0.47
61:CA:79:LEU:HD23	61:CA:79:LEU:O	2.15	0.47
1:AA:4:U:O2'	1:AA:5:U:P	2.73	0.46
1:AA:147:G:H2'	1:AA:148:G:C8	2.49	0.46
1:AA:567:G:H2'	1:AA:568:G:O4'	2.15	0.46
7:AG:30:LEU:HD12	7:AG:105:VAL:HG13	1.97	0.46
10:AJ:56:HIS:CG	10:AJ:57:VAL:N	2.82	0.46
26:BA:2135:A:O2'	26:BA:2159:G:O2'	2.25	0.46
29:BD:8:LYS:NZ	29:BD:195:GLY:O	2.41	0.46
31:BF:41:GLY:HA2	31:BF:85:ILE:HD12	1.97	0.46
35:BJ:82:ALA:C	35:BJ:84:GLY:H	2.23	0.46
45:BT:83:LYS:HB3	45:BT:97:LEU:HD23	1.98	0.46
61:CA:179:PRO:HA	61:CA:208:ASN:ND2	2.30	0.46
1:AA:677:U:H3	1:AA:713:G:H22	1.62	0.46
1:AA:1028:C:H3'	1:AA:1029:U:C6	2.51	0.46
10:AJ:4:GLN:OE1	10:AJ:4:GLN:N	2.46	0.46
17:AQ:19:LYS:HB3	17:AQ:19:LYS:HE2	1.66	0.46
25:AY:27:VAL:O	25:AY:39:ASP:N	2.36	0.46
26:BA:784:G:H5'	26:BA:785:G:OP1	2.15	0.46
26:BA:893:C:O2'	26:BA:894:U:H6	1.98	0.46
26:BA:953:G:C2	26:BA:954:G:C8	3.03	0.46
26:BA:1064:C:N4	26:BA:1075:C:H42	2.11	0.46
26:BA:1535:A:C3'	26:BA:1536:C:H5''	2.41	0.46
26:BA:2615:U:C2	53:B2:4:GLN:HA	2.49	0.46
27:BB:37:C:N3	27:BB:48:U:O2'	2.39	0.46
31:BF:167:ARG:HD2	31:BF:179:LYS:NZ	2.30	0.46
38:BM:56:PRO:O	38:BM:59:ARG:N	2.41	0.46
45:BT:69:LEU:HD22	45:BT:107:VAL:HB	1.97	0.46
62:CC:1212:LEU:HA	62:CC:1212:LEU:HD23	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:6:G:H22	5:AE:103:THR:CG2	2.28	0.46
1:AA:958:A:C6	19:AS:55:ARG:HB2	2.49	0.46
1:AA:1382:C:C2'	1:AA:1383:C:H5'	2.46	0.46
3:AC:86:LYS:O	3:AC:89:LYS:HG2	2.15	0.46
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.97	0.46
15:AO:70:LEU:HD12	15:AO:70:LEU:HA	1.68	0.46
25:AY:50:ALA:HB1	25:AY:60:LEU:HD21	1.96	0.46
26:BA:788:A:H4'	26:BA:789:A:O5'	2.15	0.46
26:BA:1210:G:H4'	26:BA:1211:U:H5'	1.96	0.46
27:BB:116:G:H4'	41:BP:54:VAL:HG12	1.96	0.46
32:BG:156:PRO:O	32:BG:171:THR:HG22	2.16	0.46
41:BP:57:ALA:O	41:BP:60:GLU:HG2	2.14	0.46
57:B6:34:LYS:HE2	57:B6:34:LYS:HB3	1.76	0.46
62:CC:234:ASP:HB3	62:CC:238:GLN:NE2	2.29	0.46
62:CC:1204:LEU:HD23	62:CC:1204:LEU:HA	1.69	0.46
62:CC:1340:GLU:OE1	62:CC:1341:ASP:N	2.34	0.46
1:AA:70:U:H2'	1:AA:94:G:N7	2.31	0.46
1:AA:500:G:H5''	12:AL:121:ARG:NH1	2.30	0.46
1:AA:996:A:C4	1:AA:997:U:C5	3.03	0.46
3:AC:26:THR:HG22	14:AN:76:LYS:HE3	1.97	0.46
3:AC:70:THR:C	3:AC:106:VAL:HG13	2.40	0.46
3:AC:136:ARG:NH2	22:AV:30:A:N7	2.64	0.46
7:AG:109:ARG:CG	7:AG:109:ARG:HH11	2.29	0.46
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.97	0.46
9:AI:99:ARG:HH21	9:AI:104:VAL:CG2	2.27	0.46
25:AY:9:PHE:O	25:AY:12:SER:OG	2.31	0.46
26:BA:1801:A:OP2	28:BC:150:LYS:NZ	2.32	0.46
31:BF:91:LEU:C	31:BF:96:MET:HB2	2.40	0.46
39:BN:63:ILE:HD11	39:BN:105:MET:HE2	1.97	0.46
55:B4:46:LYS:HE2	55:B4:46:LYS:HB3	1.71	0.46
58:B7:8:LYS:HD3	58:B7:8:LYS:HA	1.72	0.46
61:CB:154:PRO:C	61:CB:156:SER:H	2.23	0.46
63:CD:424:ASN:ND2	63:CD:424:ASN:C	2.73	0.46
1:AA:911:U:H2'	1:AA:912:C:C6	2.50	0.46
1:AA:1492:A:OP1	12:AL:44:LYS:HD3	2.15	0.46
22:AV:52:C:H2'	22:AV:53:G:O4'	2.16	0.46
26:BA:782:A:C6	28:BC:225:MET:HE2	2.50	0.46
26:BA:1064:C:H2'	26:BA:1065:U:C6	2.50	0.46
26:BA:1857:G:N2	26:BA:1884:G:O2'	2.37	0.46
26:BA:2280:G:C2	26:BA:2281:A:C8	3.04	0.46
62:CC:28:LEU:HD23	62:CC:28:LEU:HA	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:696:ASP:CG	62:CC:697:LYS:N	2.67	0.46
62:CC:1333:LEU:O	62:CC:1335:ILE:N	2.48	0.46
62:CC:1336:ASN:HD22	62:CC:1336:ASN:C	2.23	0.46
63:CD:664:ILE:HG22	63:CD:678:ARG:HG2	1.97	0.46
63:CD:1249:ASN:OD1	63:CD:1250:ASP:N	2.48	0.46
1:AA:464:U:O2	1:AA:464:U:H2'	2.14	0.46
1:AA:714:G:N2	1:AA:777:A:N3	2.43	0.46
4:AD:72:PHE:HE1	4:AD:94:LEU:HD11	1.81	0.46
5:AE:101:GLU:N	5:AE:101:GLU:OE2	2.49	0.46
22:AV:44:A:OP1	62:CC:1259:LEU:HD21	2.15	0.46
26:BA:84:A:OP1	47:BV:6:ARG:NH1	2.48	0.46
26:BA:2322:A:N6	26:BA:2333:A:H62	2.14	0.46
35:BJ:38:CYS:SG	35:BJ:39:LYS:N	2.88	0.46
45:BT:74:ILE:HD12	45:BT:105:VAL:HG22	1.97	0.46
61:CB:34:GLY:N	61:CB:199:ASP:OD2	2.46	0.46
63:CD:393:THR:HG23	63:CD:395:LYS:H	1.80	0.46
63:CD:1143:ASP:C	63:CD:1143:ASP:OD1	2.57	0.46
2:AB:117:LEU:HD12	2:AB:120:GLN:NE2	2.31	0.46
5:AE:29:ARG:HB2	5:AE:29:ARG:NH1	2.30	0.46
7:AG:115:SER:HB3	7:AG:118:LEU:HB3	1.98	0.46
22:AV:51:G:C2	22:AV:52:C:C5	3.04	0.46
26:BA:1077:A:C2	35:BJ:134:SER:HB2	2.51	0.46
26:BA:1083:U:H5'	34:BI:53:ARG:NH1	2.25	0.46
26:BA:1473:G:C6	26:BA:1474:U:C4	3.03	0.46
26:BA:2100:G:H1	26:BA:2189:U:H3	0.71	0.46
27:BB:16:G:N2	27:BB:69:G:H1'	2.31	0.46
39:BN:42:THR:HG22	39:BN:93:VAL:HG12	1.98	0.46
40:BO:101:GLY:O	40:BO:109:PRO:HA	2.16	0.46
42:BQ:34:GLU:CD	42:BQ:39:ARG:HD3	2.40	0.46
62:CC:514:PHE:CE1	62:CC:760:ASN:HB3	2.51	0.46
63:CD:1159:ILE:HB	63:CD:1160:SER:H	1.59	0.46
1:AA:1026:G:C6	1:AA:1027:C:N4	2.83	0.46
3:AC:88:ARG:NE	63:CD:79:LYS:CD	2.71	0.46
4:AD:44:ARG:CZ	4:AD:45:LYS:H	2.27	0.46
5:AE:38:VAL:HG12	5:AE:48:PHE:CB	2.45	0.46
24:AX:19:G:H4'	24:AX:20:H2U:O5'	2.14	0.46
26:BA:2135:A:N6	26:BA:2156:G:O2'	2.49	0.46
31:BF:31:VAL:HG23	31:BF:169:LEU:HD21	1.97	0.46
43:BR:70:ARG:NE	43:BR:75:SER:HA	2.30	0.46
62:CC:1291:LEU:HD21	63:CD:1351:VAL:HG13	1.97	0.46
63:CD:265:LEU:O	63:CD:268:LEU:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:562:U:O2	12:AL:13:ALA:N	2.49	0.46
8:AH:92:LEU:HB2	8:AH:117:ARG:HD2	1.98	0.46
18:AR:41:PRO:O	18:AR:45:THR:HG22	2.16	0.46
21:AU:29:LEU:HA	21:AU:29:LEU:HD23	1.78	0.46
24:AX:5:G:H2'	24:AX:6:G:C8	2.47	0.46
26:BA:320:A:H2'	30:BE:131:THR:HG21	1.98	0.46
26:BA:1693:U:H1'	28:BC:14:ARG:HH12	1.81	0.46
26:BA:2116:G:N2	26:BA:2161:C:H5''	2.31	0.46
26:BA:2469:A:N6	26:BA:2481:G:O2'	2.49	0.46
31:BF:95:ARG:H	31:BF:95:ARG:HD2	1.81	0.46
32:BG:35:ARG:NH1	32:BG:71:LEU:HD13	2.31	0.46
35:BJ:100:ILE:HG13	35:BJ:137:LEU:HD22	1.97	0.46
59:CN:10:DG:H2''	59:CN:11:DT:H72	1.97	0.46
65:CF:116:GLN:C	65:CF:118:VAL:H	2.24	0.46
1:AA:922:G:N3	1:AA:1398:A:H2	2.14	0.46
1:AA:1175:G:N3	1:AA:1176:A:C8	2.84	0.46
2:AB:11:LYS:HA	2:AB:11:LYS:HD3	1.70	0.46
8:AH:102:ALA:HB3	8:AH:113:ASP:HB3	1.98	0.46
16:AP:48:GLU:C	16:AP:50:THR:H	2.24	0.46
26:BA:125:A:OP2	55:B4:19:ARG:HD3	2.16	0.46
26:BA:248:G:H5'	26:BA:250:G:N7	2.31	0.46
26:BA:594:U:H2'	26:BA:595:C:C6	2.51	0.46
26:BA:1255:U:C5	30:BE:68:ALA:HA	2.51	0.46
26:BA:2523:G:O2'	26:BA:2764:A:O2'	2.27	0.46
31:BF:43:ALA:HB2	31:BF:50:LEU:HB2	1.97	0.46
34:BI:80:THR:HB	34:BI:81:LEU:HD22	1.98	0.46
62:CC:38:PHE:CZ	62:CC:49:LEU:HD21	2.51	0.46
62:CC:377:THR:CB	65:CF:81:HIS:CE1	2.99	0.46
63:CD:1075:ARG:NH2	63:CD:1102:PRO:HA	2.31	0.46
4:AD:104:ARG:HB3	4:AD:171:LEU:HD11	1.97	0.45
6:AF:21:MET:N	6:AF:21:MET:HE3	2.30	0.45
22:AV:38:A:H5'	22:AV:39:C:O2	2.16	0.45
26:BA:639:U:H2'	26:BA:640:C:H6	1.77	0.45
26:BA:645:C:H2'	26:BA:647:G:C8	2.51	0.45
26:BA:1936:A:H2	26:BA:1943:U:N3	2.12	0.45
32:BG:157:TYR:CZ	32:BG:172:LYS:HE3	2.51	0.45
42:BQ:115:ASN:HD22	42:BQ:115:ASN:N	2.13	0.45
48:BW:36:ALA:O	48:BW:93:ARG:NH2	2.46	0.45
60:CT:28:DG:H5''	65:CF:18:PHE:CE1	2.51	0.45
62:CC:530:ILE:HD13	62:CC:530:ILE:HA	1.65	0.45
1:AA:91:U:H2'	1:AA:92:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1051:C:N3	1:AA:1207:2MG:N1	2.61	0.45
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.34	0.45
2:AB:3:THR:OG1	2:AB:4:VAL:N	2.49	0.45
2:AB:166:ALA:HB3	2:AB:191:SER:HB2	1.99	0.45
5:AE:81:LEU:HD21	5:AE:96:MET:HE3	1.97	0.45
7:AG:47:LEU:HA	7:AG:47:LEU:HD13	1.60	0.45
12:AL:42:PRO:HB2	12:AL:46:ASN:HB2	1.97	0.45
19:AS:3:ARG:HH11	19:AS:7:LYS:HB3	1.82	0.45
26:BA:358:U:H2'	26:BA:359:G:C8	2.52	0.45
26:BA:1614:A:C2	45:BT:93:ALA:HB2	2.52	0.45
26:BA:2265:U:OP2	26:BA:2266:A:O2'	2.26	0.45
26:BA:2324:U:H5''	26:BA:2325:G:H5''	1.97	0.45
28:BC:262:ARG:O	28:BC:265:LYS:HE2	2.16	0.45
38:BM:48:ARG:HH11	38:BM:48:ARG:HB2	1.81	0.45
62:CC:563:THR:OG1	62:CC:564:PRO:HD2	2.16	0.45
1:AA:613:C:H2'	1:AA:614:C:C6	2.52	0.45
1:AA:736:C:H2'	1:AA:737:C:H6	1.80	0.45
1:AA:1373:G:H5''	7:AG:36:LYS:HE2	1.99	0.45
3:AC:77:ILE:HG23	3:AC:81:GLY:HA2	1.99	0.45
7:AG:81:GLY:C	7:AG:83:SER:H	2.23	0.45
22:AV:49:G:H5''	62:CC:540:ARG:HH22	1.79	0.45
26:BA:1009:A:N3	26:BA:1153:C:O2'	2.40	0.45
26:BA:2125:G:H1'	26:BA:2173:A:H61	1.81	0.45
29:BD:84:LEU:HD22	29:BD:88:GLU:O	2.17	0.45
38:BM:57:LEU:HD22	56:B5:54:ASP:HB3	1.98	0.45
61:CA:102:LEU:HD23	61:CA:102:LEU:C	2.41	0.45
63:CD:952:VAL:HG13	63:CD:1014:GLY:H	1.81	0.45
63:CD:1349:GLU:H	63:CD:1349:GLU:CD	2.24	0.45
1:AA:754:C:OP1	15:AO:72:ARG:NH2	2.38	0.45
1:AA:1320:C:C2	19:AS:72:GLY:HA3	2.51	0.45
1:AA:1424:U:H2'	1:AA:1425:U:O4'	2.15	0.45
3:AC:75:ILE:HD13	22:AV:34:A:H5'	1.97	0.45
3:AC:88:ARG:HH22	63:CD:79:LYS:NZ	2.14	0.45
4:AD:192:SER:OG	4:AD:194:ASP:OD1	2.16	0.45
13:AM:3:ARG:O	13:AM:57:ARG:NE	2.48	0.45
26:BA:404:A:O2'	26:BA:405:U:P	2.74	0.45
26:BA:608:A:H2'	26:BA:609:A:C8	2.52	0.45
26:BA:686:U:H6	26:BA:788:A:N1	2.14	0.45
26:BA:1475:G:O2'	26:BA:1514:G:O6	2.34	0.45
27:BB:38:C:O4'	41:BP:100:HIS:NE2	2.50	0.45
31:BF:8:TYR:HA	31:BF:12:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BK:40:HIS:CE1	36:BK:41:LYS:HG2	2.51	0.45
40:BO:8:ARG:NH2	40:BO:43:GLU:HG2	2.32	0.45
49:BX:53:CYS:SG	49:BX:57:HIS:HA	2.56	0.45
59:CN:26:DG:C4	59:CN:27:DA:N7	2.85	0.45
63:CD:247:PRO:HA	63:CD:250:ARG:CZ	2.45	0.45
63:CD:1309:ILE:HG13	63:CD:1310:THR:N	2.31	0.45
1:AA:335:C:H2'	1:AA:336:A:H8	1.81	0.45
1:AA:562:U:H1'	12:AL:12:ARG:HB3	1.99	0.45
1:AA:1383:C:O2'	1:AA:1384:C:H5'	2.17	0.45
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.52	0.45
2:AB:133:GLU:O	2:AB:137:ARG:HB2	2.17	0.45
5:AE:83:HIS:CE1	5:AE:147:MET:HG3	2.52	0.45
26:BA:1080:A:H4'	35:BJ:126:ARG:HG2	1.98	0.45
26:BA:1355:G:C2	26:BA:1356:G:C8	3.04	0.45
26:BA:1494:A:H2'	26:BA:1495:A:H8	1.80	0.45
33:BH:56:ALA:O	33:BH:60:GLU:HG2	2.16	0.45
50:BY:33:LEU:HD23	50:BY:33:LEU:HA	1.74	0.45
62:CC:145:ILE:CG2	62:CC:456:VAL:HG22	2.46	0.45
1:AA:1240:U:OP1	7:AG:119:ARG:NH2	2.49	0.45
5:AE:153:VAL:HG11	8:AH:99:LEU:HD23	1.99	0.45
8:AH:49:PHE:HB2	8:AH:59:LEU:HD11	1.98	0.45
13:AM:59:GLU:OE2	13:AM:62:LYS:NZ	2.44	0.45
15:AO:67:LEU:HD22	15:AO:78:TYR:CE1	2.52	0.45
17:AQ:25:ILE:O	17:AQ:25:ILE:HG22	2.16	0.45
17:AQ:38:ILE:HG12	17:AQ:40:ARG:NH1	2.32	0.45
23:AW:55:PSU:O5'	23:AW:55:PSU:H6	1.99	0.45
26:BA:1084:A:H5'	34:BI:55:VAL:HB	1.98	0.45
28:BC:105:LEU:O	28:BC:107:PRO:HD3	2.17	0.45
42:BQ:103:ARG:HE	42:BQ:103:ARG:HB3	1.63	0.45
62:CC:392:GLU:CD	62:CC:392:GLU:N	2.75	0.45
62:CC:1257:GLN:NE2	63:CD:345:LYS:HD3	2.32	0.45
62:CC:1276:TRP:CE2	63:CD:801:VAL:HG21	2.52	0.45
1:AA:636:U:OP1	17:AQ:6:ARG:NH2	2.50	0.45
1:AA:1035:A:N3	1:AA:1036:A:C8	2.84	0.45
1:AA:1098:C:H2'	1:AA:1099:G:O4'	2.17	0.45
8:AH:96:MET:O	8:AH:99:LEU:HD13	2.17	0.45
24:AX:38:A:H2'	24:AX:39:PSU:O4'	2.17	0.45
25:AY:36:VAL:O	25:AY:48:ILE:HG13	2.17	0.45
26:BA:1825:U:O2'	28:BC:253:LYS:NZ	2.50	0.45
26:BA:2006:C:O2'	26:BA:2823:A:N3	2.48	0.45
37:BL:76:VAL:HG12	42:BQ:73:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BZ:6:LEU:HD22	51:BZ:56:LEU:HG	1.99	0.45
63:CD:119:SER:OG	63:CD:120:LEU:N	2.50	0.45
63:CD:317:THR:HG21	63:CD:321:LYS:HA	1.99	0.45
63:CD:1050:THR:C	63:CD:1057:SER:HB3	2.41	0.45
1:AA:530:G:N2	1:AA:1492:A:H61	2.14	0.45
1:AA:1060:U:H2'	1:AA:1061:G:H8	1.81	0.45
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.82	0.45
2:AB:79:ALA:HB1	2:AB:214:LEU:HD23	1.99	0.45
9:AI:41:ARG:HH21	9:AI:41:ARG:CG	2.29	0.45
10:AJ:37:ARG:HB3	10:AJ:37:ARG:NH1	2.32	0.45
26:BA:359:G:C5	26:BA:360:U:C5	3.05	0.45
26:BA:2038:G:H2'	26:BA:2039:U:O4'	2.17	0.45
26:BA:2287:A:N7	26:BA:2289:G:C8	2.85	0.45
26:BA:2496:C:H5'	39:BN:82:MET:HE2	1.98	0.45
31:BF:41:GLY:HA2	31:BF:85:ILE:CD1	2.47	0.45
39:BN:64:TRP:HB2	39:BN:104:GLU:HB2	1.99	0.45
40:BO:100:CYS:O	40:BO:110:MET:HB2	2.16	0.45
62:CC:222:ASP:OD1	62:CC:227:LYS:NZ	2.45	0.45
63:CD:53:ARG:HD3	65:CF:135:ARG:HH21	1.82	0.45
63:CD:120:LEU:HB3	63:CD:121:PRO:CD	2.47	0.45
63:CD:747:MET:HE2	63:CD:775:SER:HA	1.99	0.45
64:CE:45:LYS:NZ	64:CE:47:THR:OG1	2.47	0.45
1:AA:218:U:H2'	1:AA:219:U:O4'	2.17	0.45
4:AD:7:PRO:HB2	4:AD:10:LYS:HB2	1.98	0.45
12:AL:43:LYS:NZ	12:AL:89:D2T:H7	2.31	0.45
26:BA:29:U:H2'	26:BA:30:G:C8	2.52	0.45
26:BA:273:G:C6	26:BA:274:C:C4	3.05	0.45
26:BA:677:A:O2'	26:BA:2071:A:H5'	2.17	0.45
26:BA:2812:G:H2'	26:BA:2813:A:O4'	2.17	0.45
28:BC:69:ARG:HA	28:BC:69:ARG:HD2	1.77	0.45
32:BG:105:LEU:HD13	32:BG:107:LEU:HD11	1.98	0.45
51:BZ:7:ARG:NH1	51:BZ:56:LEU:HD11	2.32	0.45
51:BZ:18:LEU:HB2	51:BZ:53:VAL:HG11	1.98	0.45
62:CC:605:TYR:C	62:CC:606:LEU:HD12	2.42	0.45
63:CD:301:GLU:OE1	63:CD:312:ARG:NE	2.46	0.45
63:CD:363:LEU:HA	63:CD:363:LEU:HD12	1.73	0.45
63:CD:416:ILE:O	63:CD:416:ILE:HG23	2.15	0.45
1:AA:881:G:OP1	12:AL:9:ARG:NH2	2.50	0.45
1:AA:1169:A:OP2	1:AA:1169:A:C8	2.70	0.45
16:AP:9:HIS:O	16:AP:16:PHE:N	2.41	0.45
22:AV:41:C:O2	22:AV:41:C:C2'	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2127:G:H2'	26:BA:2128:G:C8	2.52	0.45
26:BA:2747:G:O6	26:BA:2755:C:H5''	2.16	0.45
45:BT:18:ARG:HG3	45:BT:76:VAL:HB	1.98	0.45
45:BT:22:ASP:OD1	45:BT:25:ARG:NH2	2.49	0.45
61:CB:66:HIS:CG	61:CB:68:TYR:HB3	2.52	0.45
1:AA:87:C:H2'	1:AA:88:U:C6	2.52	0.44
9:AI:55:VAL:O	9:AI:57:MET:N	2.50	0.44
26:BA:1231:U:H2'	26:BA:1232:G:H8	1.82	0.44
26:BA:2233:U:H2'	26:BA:2234:G:H8	1.81	0.44
32:BG:9:VAL:HG13	32:BG:50:LEU:HB2	1.99	0.44
33:BH:133:GLN:HG3	33:BH:139:PHE:HE1	1.81	0.44
62:CC:794:LEU:HA	62:CC:794:LEU:HD12	1.71	0.44
1:AA:928:G:H2'	1:AA:929:G:H8	1.82	0.44
4:AD:171:LEU:N	4:AD:171:LEU:HD23	2.32	0.44
25:AY:44:SER:OG	25:AY:45:GLU:N	2.50	0.44
26:BA:527:C:O2'	26:BA:2779:U:O2'	2.34	0.44
26:BA:2102:G:N1	26:BA:2188:U:C4	2.85	0.44
26:BA:2707:U:O2	40:BO:71:ARG:NH2	2.49	0.44
26:BA:2898:U:O2'	36:BK:134:ALA:O	2.32	0.44
31:BF:58:ALA:HB1	58:B7:7:PRO:HG3	1.99	0.44
32:BG:52:PHE:CZ	32:BG:72:LEU:HD22	2.52	0.44
53:B2:31:ASP:O	53:B2:35:GLY:HA2	2.16	0.44
54:B3:10:LYS:HE2	54:B3:20:PHE:CE2	2.52	0.44
60:CT:4:DT:H2''	60:CT:5:DG:H8	1.82	0.44
62:CC:528:ARG:HH11	62:CC:528:ARG:HD2	1.63	0.44
63:CD:442:ILE:HG23	63:CD:442:ILE:HD12	1.64	0.44
1:AA:684:U:O2'	11:AK:40:ASN:HB3	2.18	0.44
1:AA:1320:C:O2	19:AS:72:GLY:HA3	2.17	0.44
3:AC:70:THR:O	3:AC:106:VAL:HG13	2.18	0.44
5:AE:89:HIS:HE2	5:AE:138:ARG:NH1	2.15	0.44
7:AG:57:SER:OG	7:AG:58:GLU:N	2.48	0.44
26:BA:1095:A:H61	35:BJ:25:PRO:HD2	1.81	0.44
26:BA:2346:A:H4'	26:BA:2347:C:OP2	2.16	0.44
26:BA:2636:C:H2'	26:BA:2637:U:C6	2.52	0.44
30:BE:145:ASP:HA	30:BE:166:LYS:HB3	1.99	0.44
62:CC:1076:ILE:O	62:CC:1076:ILE:HG13	2.15	0.44
63:CD:149:GLY:HA2	63:CD:176:PHE:HB2	1.98	0.44
63:CD:340:GLN:HG3	63:CD:341:ASN:OD1	2.18	0.44
63:CD:424:ASN:ND2	63:CD:424:ASN:O	2.50	0.44
63:CD:482:ALA:O	63:CD:488:ASN:ND2	2.50	0.44
63:CD:830:ASP:OD1	63:CD:832:LYS:NZ	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1347:G:O2'	1:AA:1373:G:O6	2.30	0.44
4:AD:15:GLU:CD	4:AD:60:LYS:HB2	2.42	0.44
5:AE:10:GLU:N	5:AE:10:GLU:OE2	2.50	0.44
12:AL:7:LEU:HD23	12:AL:7:LEU:HA	1.84	0.44
18:AR:19:GLN:H	18:AR:19:GLN:HG2	1.57	0.44
26:BA:813:U:H2'	26:BA:814:C:H6	1.82	0.44
26:BA:839:U:H2'	26:BA:840:C:C6	2.53	0.44
26:BA:2081:U:H2'	26:BA:2082:A:C8	2.52	0.44
30:BE:152:GLU:HG2	30:BE:153:LEU:N	2.32	0.44
38:BM:70:LYS:O	38:BM:74:THR:HG23	2.17	0.44
59:CN:28:DA:C4	59:CN:29:DG:C5	3.06	0.44
61:CB:107:ILE:HD11	61:CB:136:GLU:HA	1.99	0.44
62:CC:616:ILE:HA	62:CC:652:TYR:O	2.17	0.44
63:CD:62:PHE:O	63:CD:101:ARG:NH2	2.46	0.44
63:CD:213:LYS:O	63:CD:213:LYS:HD3	2.17	0.44
1:AA:148:G:O2'	1:AA:149:A:C5'	2.66	0.44
1:AA:371:A:H2'	1:AA:372:C:O4'	2.17	0.44
1:AA:1178:G:C5	9:AI:99:ARG:NH1	2.85	0.44
2:AB:130:THR:HG22	2:AB:130:THR:O	2.18	0.44
3:AC:86:LYS:O	3:AC:90:VAL:HG22	2.17	0.44
14:AN:24:ARG:HG3	14:AN:48:LEU:HD11	1.99	0.44
18:AR:74:HIS:CG	18:AR:75:GLN:N	2.86	0.44
26:BA:1407:G:C2	26:BA:1408:G:C5	3.06	0.44
26:BA:2349:G:C6	26:BA:2369:A:C6	3.06	0.44
31:BF:11:GLU:HA	31:BF:14:LYS:NZ	2.33	0.44
31:BF:42:GLU:HG3	31:BF:49:LEU:HD23	1.99	0.44
48:BW:26:PHE:HZ	48:BW:47:VAL:HG11	1.83	0.44
62:CC:138:ILE:HA	62:CC:138:ILE:HD13	1.53	0.44
62:CC:261:VAL:HG21	62:CC:264:GLU:CD	2.42	0.44
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.18	0.44
10:AJ:84:VAL:HG21	65:CF:140:PRO:HB2	1.98	0.44
26:BA:69:C:O2	26:BA:73:A:O2'	2.30	0.44
26:BA:2537:U:H2'	26:BA:2538:C:C6	2.53	0.44
28:BC:108:LYS:N	28:BC:194:GLU:O	2.51	0.44
29:BD:113:SER:O	29:BD:167:ASN:HA	2.17	0.44
32:BG:24:ILE:HD11	32:BG:43:VAL:HG21	2.00	0.44
43:BR:80:ILE:HD13	43:BR:80:ILE:HA	1.85	0.44
60:CT:4:DT:C2	60:CT:5:DG:N7	2.86	0.44
62:CC:1043:ALA:O	62:CC:1046:VAL:HG22	2.17	0.44
1:AA:181:A:HO2'	1:AA:182:A:H8	1.57	0.44
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.50	0.44
5:AE:41:ASP:OD1	5:AE:45:ARG:N	2.41	0.44
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.44
20:AT:74:ARG:NH1	20:AT:74:ARG:HB2	2.33	0.44
21:AU:47:ARG:HA	21:AU:47:ARG:HD3	1.64	0.44
26:BA:2291:U:H2'	26:BA:2292:U:H6	1.83	0.44
31:BF:25:VAL:O	31:BF:28:VAL:HG12	2.17	0.44
31:BF:108:VAL:HG23	31:BF:109:PRO:CD	2.47	0.44
63:CD:265:LEU:HA	63:CD:265:LEU:HD23	1.68	0.44
63:CD:891:ASP:OD1	63:CD:1286:LYS:NZ	2.49	0.44
9:AI:115:LYS:HE2	9:AI:115:LYS:HB2	1.71	0.44
10:AJ:92:LEU:H	65:CF:167:ARG:HH12	1.66	0.44
11:AK:52:PHE:HE2	11:AK:65:VAL:HG11	1.82	0.44
14:AN:23:LYS:HE3	14:AN:23:LYS:HB2	1.82	0.44
19:AS:51:VAL:CG1	19:AS:75:ALA:HB2	2.48	0.44
24:AX:66:U:H2'	24:AX:67:C:C6	2.53	0.44
26:BA:627:A:OP1	38:BM:78:ARG:NH2	2.39	0.44
26:BA:1315:C:C2	26:BA:1338:G:N2	2.86	0.44
26:BA:2128:G:H1'	26:BA:2174:C:H5'	2.00	0.44
26:BA:2135:A:C2	26:BA:2136:G:H1'	2.52	0.44
45:BT:88:ARG:NH2	45:BT:94:ASP:OD2	2.48	0.44
63:CD:513:MET:HG3	63:CD:544:LEU:HD21	1.98	0.44
63:CD:636:GLY:O	63:CD:638:SER:N	2.49	0.44
1:AA:269:C:H2'	1:AA:270:A:H8	1.82	0.44
1:AA:429:U:H5'	4:AD:9:LEU:HD12	1.99	0.44
1:AA:1390:U:H2'	1:AA:1391:U:H6	1.82	0.44
1:AA:1497:G:H1'	1:AA:1518:MA6:H2	1.99	0.44
4:AD:161:LEU:HD23	4:AD:164:GLN:OE1	2.18	0.44
6:AF:37:HIS:HB3	6:AF:97:THR:OG1	2.18	0.44
10:AJ:88:MET:HE1	65:CF:144:PHE:CZ	2.53	0.44
12:AL:87:VAL:O	12:AL:87:VAL:HG12	2.18	0.44
26:BA:543:A:N6	26:BA:544:G:C6	2.86	0.44
26:BA:804:A:H2'	26:BA:806:C:C4	2.52	0.44
26:BA:2146:C:H4'	26:BA:2147:A:O5'	2.18	0.44
26:BA:2883:A:OP2	53:B2:50:ARG:NH1	2.50	0.44
32:BG:175:LYS:HE3	32:BG:176:LYS:HE3	1.99	0.44
35:BJ:107:GLU:O	35:BJ:110:GLN:HG2	2.18	0.44
40:BO:2:ARG:HE	40:BO:2:ARG:HB3	1.52	0.44
60:CT:10:DT:H2''	60:CT:11:DC:C6	2.53	0.44
62:CC:127:ILE:O	62:CC:127:ILE:HG13	2.18	0.44
63:CD:108:ALA:HB3	63:CD:279:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:CD:1332:LEU:HA	63:CD:1332:LEU:HD12	1.73	0.44
1:AA:143:A:H2	1:AA:220:G:H1	1.66	0.43
1:AA:1000:A:C6	1:AA:1041:G:C6	3.06	0.43
2:AB:115:LYS:HA	2:AB:118:GLU:HG2	2.00	0.43
10:AJ:89:ARG:NH2	62:CC:845:LEU:CA	2.62	0.43
26:BA:858:G:H21	26:BA:2268:A:H2'	1.82	0.43
26:BA:940:G:H5'	26:BA:941:A:OP2	2.18	0.43
26:BA:1295:C:C2	26:BA:1296:G:C8	3.06	0.43
26:BA:1509:A:O2'	26:BA:1510:G:H8	2.00	0.43
26:BA:1596:A:O2'	26:BA:1597:A:C5'	2.66	0.43
26:BA:1932:A:H2'	26:BA:1933:G:O4'	2.17	0.43
26:BA:2340:A:H5'	27:BB:41:G:H21	1.82	0.43
29:BD:4:LEU:HD23	29:BD:4:LEU:HA	1.84	0.43
36:BK:30:THR:HG22	36:BK:31:GLU:N	2.32	0.43
36:BK:122:LEU:C	36:BK:123:LYS:HG2	2.43	0.43
37:BL:53:LYS:O	37:BL:56:ASP:HB2	2.18	0.43
50:BY:3:ARG:HD2	50:BY:30:LEU:HD22	2.00	0.43
61:CA:82:LEU:HD23	61:CA:82:LEU:HA	1.65	0.43
62:CC:1278:LEU:HA	62:CC:1278:LEU:HD23	1.49	0.43
62:CC:1329:GLU:OE1	63:CD:330:MET:HE2	2.17	0.43
1:AA:399:G:H2'	1:AA:400:C:C6	2.52	0.43
1:AA:639:G:C2	1:AA:640:A:C8	3.06	0.43
9:AI:98:LEU:HD12	9:AI:98:LEU:HA	1.88	0.43
21:AU:62:ARG:O	21:AU:64:ASN:O	2.36	0.43
22:AV:37:G:H8	22:AV:37:G:H3'	1.83	0.43
26:BA:244:A:OP2	56:B5:8:ARG:NH2	2.51	0.43
26:BA:851:C:O2'	52:B1:43:ALA:O	2.33	0.43
26:BA:1174:U:H3'	26:BA:1175:A:N3	2.33	0.43
26:BA:1197:G:H2'	26:BA:1198:U:H6	1.82	0.43
26:BA:1263:U:O2'	53:B2:8:PRO:HD2	2.17	0.43
26:BA:1405:U:H2'	26:BA:1406:U:C5	2.52	0.43
26:BA:2112:G:N7	26:BA:2113:U:N3	2.67	0.43
26:BA:2135:A:C5	26:BA:2136:G:C8	3.06	0.43
26:BA:2316:G:H5'	31:BF:125:ARG:NH1	2.33	0.43
26:BA:2602:A:H4'	26:BA:2603:G:OP2	2.17	0.43
27:BB:30:C:H1'	27:BB:57:A:H61	1.83	0.43
32:BG:107:LEU:HD13	32:BG:152:ARG:HB2	2.00	0.43
60:CT:5:DG:H2'	60:CT:6:DA:C8	2.53	0.43
60:CT:6:DA:C2	60:CT:7:DA:C5	3.07	0.43
60:CT:19:DG:C6	60:CT:20:DC:N4	2.86	0.43
62:CC:1105:SER:HB2	63:CD:731:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:1238:LEU:N	62:CC:1238:LEU:CD2	2.81	0.43
63:CD:357:VAL:O	63:CD:357:VAL:HG13	2.18	0.43
1:AA:62:U:OP1	1:AA:385:C:O2'	2.35	0.43
1:AA:956:U:H2'	1:AA:957:U:O4'	2.18	0.43
1:AA:976:G:H5''	1:AA:1358:U:O2'	2.18	0.43
2:AB:60:ILE:CG2	2:AB:65:GLY:HA3	2.48	0.43
26:BA:27:G:O2'	26:BA:28:A:OP2	2.34	0.43
26:BA:271:G:C4	26:BA:272:A:C8	3.07	0.43
27:BB:24:G:C8	27:BB:56:G:C8	3.05	0.43
62:CC:571:LEU:HD23	62:CC:571:LEU:HA	1.47	0.43
62:CC:1214:ASP:C	62:CC:1214:ASP:OD1	2.61	0.43
65:CF:157:ARG:O	65:CF:158:LEU:HD12	2.18	0.43
1:AA:407:U:C2	1:AA:408:A:C8	3.07	0.43
1:AA:901:A:C5	1:AA:902:G:H1'	2.53	0.43
1:AA:996:A:C6	1:AA:997:U:O4	2.71	0.43
1:AA:1019:A:H2'	1:AA:1020:G:O4'	2.18	0.43
3:AC:55:ILE:HG23	3:AC:66:VAL:HG13	2.01	0.43
5:AE:42:GLY:O	5:AE:119:GLY:HA3	2.18	0.43
26:BA:348:A:H2'	26:BA:349:U:O4'	2.18	0.43
26:BA:396:G:N2	26:BA:2231:U:O2'	2.43	0.43
26:BA:2100:G:C6	26:BA:2190:G:C6	3.07	0.43
26:BA:2549:G:C2	26:BA:2550:G:N7	2.86	0.43
26:BA:2751:G:H2'	26:BA:2751:G:N3	2.33	0.43
29:BD:39:ASP:N	29:BD:39:ASP:OD1	2.50	0.43
34:BI:30:SER:HB2	34:BI:109:LYS:HZ1	1.82	0.43
38:BM:82:LEU:HD11	38:BM:110:VAL:HG11	2.00	0.43
43:BR:24:TYR:O	43:BR:29:SER:HB3	2.18	0.43
45:BT:97:LEU:HD12	45:BT:99:ARG:HH21	1.82	0.43
54:B3:54:ILE:HG23	54:B3:54:ILE:O	2.18	0.43
62:CC:936:ARG:HH22	62:CC:1044:PRO:HA	1.82	0.43
63:CD:500:ILE:O	63:CD:500:ILE:HG22	2.18	0.43
1:AA:477:C:H2'	1:AA:478:A:O4'	2.18	0.43
2:AB:97:LEU:HD12	2:AB:148:LEU:HD21	2.01	0.43
2:AB:217:VAL:O	2:AB:221:VAL:HG12	2.19	0.43
3:AC:175:LEU:HA	3:AC:175:LEU:HD12	1.75	0.43
26:BA:88:G:C2	26:BA:89:A:C8	3.06	0.43
26:BA:280:U:O4	26:BA:361:G:N2	2.51	0.43
26:BA:593:U:H2'	26:BA:594:U:C6	2.54	0.43
26:BA:1105:U:H2'	26:BA:1106:G:H8	1.84	0.43
26:BA:1656:C:H2'	26:BA:1657:U:H6	1.83	0.43
29:BD:55:LYS:HD3	29:BD:60:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BH:40:THR:C	33:BH:42:LYS:N	2.76	0.43
34:BI:26:VAL:HG21	34:BI:82:ILE:HD12	2.01	0.43
34:BI:81:LEU:HD22	34:BI:81:LEU:N	2.32	0.43
42:BQ:34:GLU:OE1	42:BQ:39:ARG:HD3	2.18	0.43
62:CC:129:LEU:HA	62:CC:129:LEU:HD23	1.68	0.43
62:CC:131:THR:HG22	62:CC:132:ASP:N	2.34	0.43
63:CD:499:ILE:C	63:CD:501:VAL:H	2.27	0.43
1:AA:878:A:C2	1:AA:879:C:C2	3.07	0.43
1:AA:1241:G:OP1	7:AG:35:LYS:NZ	2.51	0.43
7:AG:113:ASP:HB2	7:AG:119:ARG:CG	2.49	0.43
11:AK:92:GLY:C	11:AK:94:GLU:N	2.74	0.43
13:AM:27:LYS:NZ	13:AM:31:LYS:HE3	2.33	0.43
17:AQ:25:ILE:HD11	17:AQ:61:ILE:HD11	1.99	0.43
22:AV:37:G:C8	22:AV:37:G:H3'	2.53	0.43
25:AY:22:SER:OG	25:AY:88:LYS:NZ	2.52	0.43
26:BA:627:A:P	38:BM:78:ARG:HH21	2.39	0.43
26:BA:1837:C:O2'	26:BA:1927:A:N3	2.42	0.43
26:BA:2251:OMG:HM23	26:BA:2251:OMG:H1'	1.83	0.43
26:BA:2448:A:H3'	26:BA:2449:H2U:H61	2.00	0.43
26:BA:2477:U:O2	57:B6:4:ARG:NH2	2.52	0.43
59:CN:26:DG:C4	59:CN:27:DA:C5	3.07	0.43
61:CA:183:ILE:HG23	61:CA:183:ILE:HD12	1.69	0.43
62:CC:1281:TYR:CE2	63:CD:484:MET:HE3	2.54	0.43
65:CF:47:GLU:HG3	65:CF:64:PHE:CD1	2.44	0.43
1:AA:946:A:H2'	1:AA:947:G:C8	2.54	0.43
4:AD:147:GLU:HA	4:AD:150:LYS:HG3	1.99	0.43
4:AD:202:GLU:OE2	5:AE:112:ARG:NH1	2.51	0.43
5:AE:25:VAL:N	5:AE:28:GLY:O	2.52	0.43
14:AN:27:LEU:HA	14:AN:30:ILE:HG22	2.01	0.43
18:AR:45:THR:HG23	18:AR:47:THR:H	1.83	0.43
26:BA:580:U:O3'	43:BR:31:VAL:HG13	2.17	0.43
26:BA:1088:A:H61	35:BJ:131:THR:HA	1.84	0.43
26:BA:1775:U:O4	26:BA:1789:A:H2	2.02	0.43
26:BA:2170:A:H1'	26:BA:2171:A:C8	2.54	0.43
26:BA:2290:G:H2'	26:BA:2291:U:C6	2.54	0.43
28:BC:157:SER:O	28:BC:160:THR:OG1	2.28	0.43
34:BI:15:VAL:HB	34:BI:69:PHE:CG	2.53	0.43
35:BJ:88:GLY:O	35:BJ:97:VAL:HB	2.18	0.43
45:BT:25:ARG:HG3	45:BT:74:ILE:HG22	2.01	0.43
63:CD:576:ARG:HD3	63:CD:593:ASN:HA	2.00	0.43
1:AA:371:A:O2'	1:AA:373:A:N7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.54	0.43
9:AI:35:LEU:HD11	9:AI:48:VAL:HG11	2.00	0.43
13:AM:93:ARG:HH22	19:AS:80:TYR:HD2	1.67	0.43
17:AQ:54:GLY:N	17:AQ:57:ASP:OD2	2.49	0.43
26:BA:512:G:OP1	26:BA:1234:U:O2'	2.36	0.43
26:BA:997:G:OP1	43:BR:92:ARG:HD3	2.19	0.43
26:BA:1088:A:N1	35:BJ:134:SER:HB3	2.33	0.43
26:BA:1469:A:H2'	26:BA:1470:A:C8	2.53	0.43
26:BA:1473:G:C6	26:BA:1519:G:C6	3.07	0.43
26:BA:2124:G:H21	26:BA:2175:C:H41	1.65	0.43
33:BH:78:VAL:HG21	33:BH:103:VAL:HG22	2.00	0.43
34:BI:37:LYS:O	34:BI:41:LEU:HD23	2.19	0.43
34:BI:41:LEU:HD13	34:BI:52:MET:HG3	2.01	0.43
62:CC:69:GLN:OE1	62:CC:101:ARG:NE	2.44	0.43
62:CC:196:VAL:HG21	62:CC:209:ILE:HD11	2.00	0.43
62:CC:696:ASP:OD1	62:CC:696:ASP:N	2.45	0.43
62:CC:1327:LEU:HD23	62:CC:1327:LEU:HA	1.70	0.43
1:AA:1174:G:C2'	1:AA:1175:G:H5'	2.47	0.43
1:AA:1256:A:O2'	1:AA:1278:G:O6	2.25	0.43
6:AF:10:VAL:HA	6:AF:84:VAL:HA	1.99	0.43
11:AK:93:ARG:NH2	11:AK:112:ASP:OD2	2.52	0.43
26:BA:414:C:H2'	26:BA:415:A:H8	1.83	0.43
26:BA:710:U:N3	26:BA:711:G:N7	2.67	0.43
26:BA:1421:G:C2	26:BA:1422:G:C8	3.07	0.43
26:BA:2135:A:HO2'	26:BA:2159:G:HO2'	1.61	0.43
26:BA:2547:A:H4'	37:BL:29:HIS:CE1	2.53	0.43
38:BM:2:ARG:N	38:BM:5:THR:OG1	2.45	0.43
40:BO:42:LYS:HG2	40:BO:45:ARG:NH2	2.33	0.43
53:B2:17:ARG:C	53:B2:20:ASP:H	2.26	0.43
62:CC:569:ILE:O	62:CC:571:LEU:N	2.51	0.43
62:CC:866:ASP:C	62:CC:866:ASP:OD1	2.60	0.43
62:CC:1098:LEU:N	62:CC:1098:LEU:HD12	2.29	0.43
1:AA:999:C:N3	1:AA:1042:A:N6	2.66	0.43
1:AA:1384:C:H2'	1:AA:1385:G:C8	2.54	0.43
2:AB:71:GLY:O	2:AB:93:ASN:HA	2.19	0.43
26:BA:550:U:C2'	26:BA:551:G:H5''	2.46	0.43
26:BA:552:U:N3	26:BA:553:G:N7	2.67	0.43
26:BA:1365:A:O2'	50:BY:11:ARG:NH2	2.52	0.43
28:BC:244:PRO:HB2	28:BC:252:THR:HG22	2.01	0.43
31:BF:4:LEU:HA	31:BF:4:LEU:HD23	1.78	0.43
31:BF:59:ALA:O	58:B7:27:THR:OG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BS:59:ILE:HG23	44:BS:101:ILE:HG12	2.01	0.43
55:B4:31:LEU:HD22	55:B4:42:LEU:HD13	2.01	0.43
60:CT:17:DG:C4	60:CT:18:DC:C6	3.07	0.43
62:CC:549:ASP:OD1	62:CC:550:VAL:N	2.52	0.43
63:CD:770:LEU:HA	63:CD:770:LEU:HD13	1.70	0.43
63:CD:1233:ILE:HD13	63:CD:1233:ILE:HG21	1.76	0.43
1:AA:1061:G:H5'	10:AJ:61:ALA:HB2	2.00	0.42
2:AB:167:ASP:HB2	2:AB:191:SER:HA	2.00	0.42
3:AC:73:PRO:O	3:AC:76:VAL:N	2.52	0.42
5:AE:145:GLU:O	5:AE:147:MET:N	2.42	0.42
22:AV:27:C:H1'	22:AV:28:A:C2	2.54	0.42
22:AV:30:A:H1'	22:AV:31:U:C5	2.54	0.42
24:AX:28:G:H2'	24:AX:29:G:H8	1.83	0.42
26:BA:287:G:H2'	26:BA:288:U:H6	1.83	0.42
26:BA:534:U:N3	26:BA:535:G:N7	2.67	0.42
26:BA:2101:A:H2'	26:BA:2102:G:C8	2.54	0.42
27:BB:43:C:OP1	58:B7:2:LYS:HG2	2.19	0.42
28:BC:100:GLU:OE2	28:BC:102:ARG:NE	2.52	0.42
31:BF:179:LYS:HA	31:BF:179:LYS:HD3	1.75	0.42
44:BS:73:LYS:HE3	44:BS:86:GLN:HG2	2.01	0.42
46:BU:2:ILE:O	46:BU:2:ILE:HG22	2.19	0.42
56:B5:52:LYS:HD3	56:B5:52:LYS:HA	1.72	0.42
62:CC:100:LEU:HD23	62:CC:100:LEU:HA	1.74	0.42
63:CD:789:LYS:HE2	63:CD:789:LYS:HB3	1.62	0.42
1:AA:4:U:HO2'	1:AA:5:U:P	2.40	0.42
1:AA:575:G:O2'	1:AA:821:G:OP2	2.35	0.42
1:AA:1147:C:O2'	9:AI:7:TYR:OH	2.31	0.42
9:AI:55:VAL:HG21	9:AI:87:LEU:HD22	2.01	0.42
26:BA:144:A:H2'	26:BA:145:C:H6	1.82	0.42
26:BA:404:A:HO2'	26:BA:405:U:P	2.41	0.42
26:BA:998:C:P	43:BR:92:ARG:HH12	2.42	0.42
26:BA:1051:G:O6	26:BA:1108:U:O4	2.38	0.42
26:BA:1119:U:OP1	48:BW:83:LYS:HE2	2.19	0.42
26:BA:1333:G:C2	26:BA:1334:G:C8	3.07	0.42
26:BA:1563:U:H2'	26:BA:1564:C:C6	2.54	0.42
27:BB:55:U:C2'	27:BB:56:G:H5'	2.48	0.42
50:BY:2:SER:O	50:BY:4:VAL:N	2.52	0.42
60:CT:10:DT:H2''	60:CT:11:DC:C5	2.54	0.42
62:CC:45:GLY:O	62:CC:51:ALA:HB2	2.19	0.42
62:CC:210:LEU:HD23	62:CC:210:LEU:HA	1.60	0.42
62:CC:213:LEU:HA	62:CC:213:LEU:HD23	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:557:ARG:NH2	62:CC:611:GLU:OE1	2.44	0.42
62:CC:623:LEU:C	62:CC:623:LEU:HD12	2.44	0.42
62:CC:1096:ILE:HD13	62:CC:1096:ILE:HG21	1.65	0.42
62:CC:1336:ASN:C	62:CC:1336:ASN:ND2	2.77	0.42
63:CD:548:VAL:HG22	63:CD:549:LYS:N	2.35	0.42
63:CD:1172:LYS:HE3	63:CD:1191:PRO:HA	2.01	0.42
6:AF:52:ASN:HD21	6:AF:85:ILE:HG23	1.84	0.42
26:BA:820:A:H4'	26:BA:836:G:H22	1.85	0.42
26:BA:877:A:O2'	26:BA:900:A:N6	2.52	0.42
26:BA:1065:U:O2'	26:BA:1066:U:O5'	2.34	0.42
26:BA:2720:U:H5''	42:BQ:53:ARG:NH2	2.35	0.42
31:BF:58:ALA:HA	31:BF:63:GLN:O	2.18	0.42
49:BX:37:ILE:HD11	49:BX:82:ILE:HD11	2.02	0.42
53:B2:31:ASP:O	53:B2:35:GLY:CA	2.68	0.42
62:CC:196:VAL:HG22	62:CC:197:ARG:N	2.34	0.42
62:CC:538:LEU:HD12	62:CC:538:LEU:C	2.44	0.42
62:CC:1339:LEU:HD22	63:CD:17:PHE:CG	2.55	0.42
63:CD:264:ASP:N	63:CD:264:ASP:OD1	2.51	0.42
63:CD:488:ASN:OD1	63:CD:488:ASN:N	2.48	0.42
63:CD:700:ASN:C	63:CD:700:ASN:HD22	2.27	0.42
63:CD:903:LEU:HD13	63:CD:903:LEU:HA	1.68	0.42
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.19	0.42
11:AK:86:VAL:HG21	11:AK:93:ARG:HG3	2.02	0.42
22:AV:27:C:H1'	22:AV:28:A:H2	1.85	0.42
26:BA:236:C:H2'	26:BA:237:C:H6	1.84	0.42
26:BA:1078:U:H5''	26:BA:1079:C:OP1	2.20	0.42
26:BA:2743:U:H2'	26:BA:2744:G:O4'	2.19	0.42
35:BJ:75:ALA:CB	35:BJ:112:LYS:HE3	2.49	0.42
37:BL:79:PHE:HE1	37:BL:102:PRO:HG2	1.84	0.42
38:BM:47:ARG:HE	38:BM:47:ARG:HB2	1.57	0.42
51:BZ:14:LEU:HD23	51:BZ:14:LEU:HA	1.80	0.42
61:CA:39:LEU:O	61:CA:40:GLY:C	2.62	0.42
61:CB:34:GLY:H	61:CB:199:ASP:CG	2.25	0.42
62:CC:363:LEU:HA	62:CC:363:LEU:HD23	1.73	0.42
62:CC:447:HIS:C	62:CC:449:GLY:H	2.28	0.42
62:CC:521:LEU:HA	62:CC:521:LEU:HD12	1.74	0.42
62:CC:596:ASP:OD1	62:CC:597:GLY:N	2.38	0.42
62:CC:1014:LEU:HD12	62:CC:1017:GLN:HB3	2.00	0.42
62:CC:1257:GLN:CD	63:CD:345:LYS:HB2	2.45	0.42
63:CD:430:HIS:O	63:CD:431:ARG:C	2.61	0.42
1:AA:197:A:C6	1:AA:221:C:H4'	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1107:C:C4	1:AA:1108:G:C8	3.08	0.42
10:AJ:32:THR:HG22	10:AJ:82:LYS:HG3	2.01	0.42
22:AV:42:A:C8	22:AV:42:A:OP2	2.73	0.42
24:AX:19:G:C6	24:AX:57:G:C6	3.08	0.42
26:BA:1084:A:OP1	26:BA:1084:A:H8	2.00	0.42
28:BC:159:GLY:HA2	28:BC:195:VAL:O	2.20	0.42
29:BD:186:LEU:HD21	42:BQ:4:ILE:HD13	2.01	0.42
31:BF:43:ALA:CB	31:BF:50:LEU:HB2	2.49	0.42
45:BT:41:LYS:HE3	53:B2:22:LEU:HD11	2.00	0.42
46:BU:70:HIS:CG	46:BU:71:GLY:H	2.38	0.42
59:CN:30:DA:C6	59:CN:31:DG:C6	3.06	0.42
59:CN:36:DA:H2'	59:CN:37:DG:C8	2.54	0.42
61:CA:213:PRO:HA	61:CA:216:ALA:HB3	2.00	0.42
62:CC:139:ASN:C	62:CC:141:THR:H	2.27	0.42
62:CC:448:LEU:HA	62:CC:448:LEU:HD23	1.81	0.42
62:CC:1223:ARG:HA	62:CC:1224:PRO:HD3	1.92	0.42
63:CD:641:ILE:HA	63:CD:641:ILE:HD12	1.70	0.42
63:CD:826:ILE:HG23	63:CD:831:VAL:HG12	2.01	0.42
63:CD:978:ARG:CG	63:CD:1197:ASN:ND2	2.82	0.42
63:CD:1175:LEU:HB2	63:CD:1190:ILE:HD12	2.01	0.42
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.54	0.42
2:AB:28:LYS:HA	2:AB:31:ILE:HD12	2.00	0.42
10:AJ:19:ASP:HA	10:AJ:22:THR:HG22	2.01	0.42
14:AN:73:PHE:CZ	14:AN:78:GLY:HA2	2.55	0.42
26:BA:239:C:O2'	26:BA:622:G:O2'	2.06	0.42
26:BA:358:U:H2'	26:BA:359:G:H8	1.85	0.42
26:BA:628:G:C6	26:BA:636:G:C2	3.07	0.42
26:BA:2572:A:N6	29:BD:150:MEQ:HE1	2.35	0.42
27:BB:43:C:OP1	58:B7:1:MET:HB2	2.20	0.42
33:BH:133:GLN:HG3	33:BH:139:PHE:CE1	2.54	0.42
37:BL:123:LEU:HD23	37:BL:123:LEU:HA	1.78	0.42
60:CT:20:DC:O2	60:CT:21:DG:C8	2.73	0.42
62:CC:554:HIS:O	62:CC:555:TYR:C	2.61	0.42
62:CC:1286:THR:HG22	62:CC:1290:MET:HE2	2.02	0.42
65:CF:7:LYS:HG2	65:CF:74:VAL:HG13	2.01	0.42
2:AB:130:THR:O	2:AB:131:LYS:HB2	2.20	0.42
3:AC:64:ILE:HG22	3:AC:99:ALA:HA	2.00	0.42
4:AD:8:LYS:HB3	4:AD:21:LEU:HB3	2.01	0.42
26:BA:1113:U:OP1	32:BG:3:ARG:NH1	2.53	0.42
26:BA:1877:A:H2'	26:BA:1878:G:O4'	2.20	0.42
26:BA:2081:U:H2'	26:BA:2082:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2188:U:H3'	26:BA:2188:U:OP2	2.19	0.42
26:BA:2484:G:OP1	39:BN:44:ARG:HD3	2.20	0.42
33:BH:46:PHE:O	33:BH:51:ARG:HD2	2.19	0.42
35:BJ:58:ILE:O	35:BJ:58:ILE:HG12	2.19	0.42
37:BL:4:GLU:HG3	37:BL:22:ILE:O	2.20	0.42
37:BL:7:MET:HE1	37:BL:44:LYS:HD2	2.01	0.42
59:CN:27:DA:C5	59:CN:28:DA:N7	2.88	0.42
60:CT:4:DT:H2''	60:CT:5:DG:C8	2.55	0.42
62:CC:1304:MET:HA	62:CC:1304:MET:HE3	2.02	0.42
62:CC:1333:LEU:HA	62:CC:1333:LEU:HD23	1.85	0.42
63:CD:35:PHE:CZ	63:CD:101:ARG:HD2	2.55	0.42
63:CD:72:CYS:HB2	63:CD:87:LYS:HD3	2.02	0.42
63:CD:962:ASN:ND2	63:CD:979:ASN:O	2.51	0.42
63:CD:1350:ASN:ND2	63:CD:1358:PRO:HD3	2.34	0.42
1:AA:1004:A:N1	1:AA:1026:G:H1'	2.35	0.42
1:AA:1329:A:C5	1:AA:1330:U:C5	3.08	0.42
13:AM:41:GLU:OE1	13:AM:41:GLU:N	2.46	0.42
26:BA:918:A:N3	27:BB:80:U:O2'	2.46	0.42
26:BA:2175:C:H2'	26:BA:2176:A:N7	2.35	0.42
44:BS:48:LYS:HB2	44:BS:48:LYS:HE3	1.88	0.42
59:CN:27:DA:H1'	59:CN:28:DA:H5'	2.01	0.42
61:CA:180:VAL:HG12	61:CA:207:THR:HG22	2.02	0.42
62:CC:962:GLU:O	62:CC:966:ILE:HD13	2.20	0.42
62:CC:1176:LEU:HA	62:CC:1176:LEU:HD23	1.79	0.42
63:CD:1325:PHE:CD1	63:CD:1325:PHE:C	2.94	0.42
1:AA:829:G:O3'	2:AB:23:TRP:CH2	2.67	0.42
1:AA:1053:G:N7	1:AA:1199:U:H3'	2.35	0.42
16:AP:8:ARG:CZ	16:AP:15:PRO:HB3	2.50	0.42
22:AV:47:G:C6	22:AV:48:C:C4	3.07	0.42
22:AV:51:G:N2	60:CT:18:DC:O2	2.51	0.42
26:BA:552:U:C2	26:BA:553:G:C8	3.07	0.42
26:BA:789:A:OP2	55:B4:4:THR:HG21	2.20	0.42
26:BA:1062:G:C6	26:BA:1077:A:C6	3.08	0.42
26:BA:1113:U:H2'	26:BA:1114:C:C6	2.55	0.42
26:BA:1591:A:C6	26:BA:1592:C:C4	3.08	0.42
29:BD:170:VAL:HG12	29:BD:171:THR:H	1.85	0.42
33:BH:68:ARG:O	33:BH:72:ILE:HG12	2.20	0.42
61:CA:217:ILE:HD12	61:CA:217:ILE:HA	1.90	0.42
62:CC:204:LEU:HD21	62:CC:369:MET:SD	2.59	0.42
62:CC:217:THR:HG23	62:CC:351:LEU:HD21	2.02	0.42
62:CC:836:LEU:HA	62:CC:836:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:CD:1302:TYR:CD1	63:CD:1302:TYR:C	2.98	0.42
1:AA:15:G:O2'	5:AE:29:ARG:HD3	2.19	0.42
1:AA:1008:U:H2'	1:AA:1009:U:H6	1.76	0.42
3:AC:61:ALA:O	3:AC:62:LYS:HG2	2.20	0.42
7:AG:99:LEU:HD22	7:AG:103:TRP:CZ2	2.55	0.42
11:AK:110:ILE:O	21:AU:4:ILE:HB	2.20	0.42
19:AS:70:LYS:O	19:AS:73:GLU:N	2.53	0.42
22:AV:41:C:N4	63:CD:67:ASP:OD2	2.53	0.42
26:BA:972:A:H8	26:BA:972:A:O5'	2.02	0.42
26:BA:1624:U:N3	26:BA:1625:C:C5	2.88	0.42
26:BA:1720:U:H2'	26:BA:1721:G:O4'	2.20	0.42
26:BA:2116:G:H22	26:BA:2161:C:H5''	1.85	0.42
26:BA:2251:OMG:C8	26:BA:2450:A:H4'	2.54	0.42
26:BA:2314:A:O2'	26:BA:2315:G:H5'	2.20	0.42
26:BA:2473:U:C4	26:BA:2474:U:C5	3.07	0.42
26:BA:2590:A:H2'	26:BA:2591:C:H6	1.85	0.42
26:BA:2795:C:H2'	26:BA:2796:C:C6	2.54	0.42
35:BJ:39:LYS:H	35:BJ:39:LYS:HG2	1.51	0.42
39:BN:36:VAL:O	39:BN:98:PRO:HB3	2.19	0.42
39:BN:36:VAL:HG22	48:BW:82:TYR:HB2	2.01	0.42
43:BR:18:LEU:HD13	43:BR:18:LEU:HA	1.81	0.42
57:B6:2:LYS:HE2	57:B6:32:LYS:O	2.20	0.42
59:CN:17:DC:H6	59:CN:17:DC:H2'	1.66	0.42
59:CN:37:DG:H2''	59:CN:38:DA:OP2	2.19	0.42
61:CA:205:MET:SD	61:CA:213:PRO:HG3	2.60	0.42
62:CC:675:ASP:OD1	62:CC:675:ASP:C	2.63	0.42
62:CC:1251:TYR:CE1	62:CC:1301:ARG:NH1	2.88	0.42
63:CD:336:GLY:O	63:CD:337:ARG:C	2.62	0.42
63:CD:472:LEU:HA	63:CD:472:LEU:HD23	1.80	0.42
63:CD:554:GLU:OE1	63:CD:588:PRO:HA	2.20	0.42
63:CD:872:LEU:HD22	63:CD:877:VAL:HG21	2.02	0.42
1:AA:515:G:C6	1:AA:516:PSU:C2	3.08	0.41
1:AA:537:G:H5''	12:AL:110:ARG:NH2	2.35	0.41
1:AA:977:A:H1'	1:AA:982:U:O4	2.20	0.41
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.54	0.41
20:AT:8:LYS:O	20:AT:12:ILE:HG13	2.19	0.41
26:BA:275:C:N4	26:BA:276:U:C2	2.88	0.41
26:BA:636:G:N1	38:BM:76:GLU:OE1	2.46	0.41
26:BA:710:U:C2	26:BA:711:G:C8	3.08	0.41
26:BA:1297:C:OP1	26:BA:2710:C:H4'	2.20	0.41
26:BA:1614:A:N1	45:BT:93:ALA:HB2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2504:PSU:H6	26:BA:2504:PSU:OP1	2.03	0.41
26:BA:2636:C:H2'	26:BA:2637:U:H6	1.85	0.41
26:BA:2698:U:H2'	26:BA:2699:C:H6	1.85	0.41
46:BU:14:PRO:HD3	51:BZ:30:MET:SD	2.60	0.41
57:B6:15:LYS:O	57:B6:26:ILE:HD13	2.19	0.41
61:CA:85:LEU:HD23	61:CA:85:LEU:HA	1.84	0.41
62:CC:24:VAL:HG21	62:CC:704:MET:HE1	2.02	0.41
62:CC:473:ARG:HH11	62:CC:473:ARG:HG3	1.84	0.41
62:CC:530:ILE:HD12	62:CC:530:ILE:HG23	1.63	0.41
63:CD:174:ASP:C	63:CD:176:PHE:H	2.28	0.41
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.55	0.41
2:AB:117:LEU:HA	2:AB:120:GLN:HE21	1.85	0.41
3:AC:6:HIS:CE1	3:AC:8:ASN:HB3	2.55	0.41
6:AF:73:GLU:O	6:AF:76:THR:OG1	2.31	0.41
7:AG:76:LYS:HD2	7:AG:78:ARG:NH2	2.27	0.41
10:AJ:88:MET:HE3	10:AJ:88:MET:HB2	1.69	0.41
13:AM:25:VAL:HG13	13:AM:29:ARG:HB3	2.01	0.41
23:AW:52:G:C6	23:AW:63:G:C6	3.07	0.41
26:BA:811:U:H2'	38:BM:21:ARG:HA	2.02	0.41
26:BA:1064:C:H2'	26:BA:1065:U:C5	2.55	0.41
26:BA:2135:A:H1'	26:BA:2159:G:H1'	2.02	0.41
26:BA:2607:G:H2'	26:BA:2608:G:O4'	2.20	0.41
26:BA:2639:A:HO2'	36:BK:96:ARG:HH22	1.68	0.41
26:BA:2898:U:C2	26:BA:2899:A:C8	3.08	0.41
26:BA:2901:C:C2	26:BA:2902:C:C5	3.08	0.41
34:BI:96:PHE:HE2	34:BI:126:LEU:N	2.18	0.41
38:BM:132:ARG:HG3	38:BM:142:ILE:HD12	2.01	0.41
39:BN:18:ARG:H	39:BN:18:ARG:HG2	1.64	0.41
55:B4:25:LYS:HE3	55:B4:25:LYS:HB3	1.86	0.41
62:CC:421:SER:O	62:CC:422:LYS:C	2.62	0.41
62:CC:1336:ASN:HB2	63:CD:25:ALA:HB2	2.01	0.41
1:AA:309:A:H2'	1:AA:310:G:H8	1.85	0.41
1:AA:1368:A:OP1	9:AI:113:ARG:NH2	2.54	0.41
1:AA:1374:A:OP1	7:AG:36:LYS:NZ	2.52	0.41
2:AB:116:ASP:O	2:AB:120:GLN:HG2	2.20	0.41
5:AE:100:SER:OG	5:AE:101:GLU:OE2	2.31	0.41
6:AF:26:THR:HG23	6:AF:36:ILE:HD12	2.01	0.41
7:AG:116:MET:HA	7:AG:119:ARG:HE	1.85	0.41
25:AY:28:VAL:HG22	25:AY:38:VAL:HG22	2.02	0.41
26:BA:141:G:O2'	26:BA:142:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:543:A:C6	26:BA:544:G:C5	3.08	0.41
26:BA:1088:A:N6	35:BJ:131:THR:HA	2.35	0.41
26:BA:1261:C:OP2	45:BT:83:LYS:NZ	2.52	0.41
26:BA:2547:A:H2'	26:BA:2548:U:H6	1.84	0.41
31:BF:117:LEU:HB2	31:BF:176:PRO:O	2.20	0.41
54:B3:6:ARG:HD3	54:B3:24:THR:HB	2.02	0.41
59:CN:15:DA:H3'	65:CF:16:SER:OG	2.21	0.41
59:CN:16:DT:OP1	65:CF:16:SER:N	2.53	0.41
61:CA:188:GLU:O	61:CA:199:ASP:HA	2.21	0.41
62:CC:146:VAL:H	62:CC:146:VAL:HG22	1.59	0.41
62:CC:615:VAL:O	62:CC:615:VAL:HG13	2.20	0.41
62:CC:746:ALA:HB2	62:CC:967:LEU:HD21	2.02	0.41
62:CC:1182:ILE:HD13	62:CC:1182:ILE:HG21	1.70	0.41
63:CD:424:ASN:O	63:CD:424:ASN:CG	2.61	0.41
63:CD:755:ILE:HG22	63:CD:757:THR:H	1.85	0.41
1:AA:1229:A:OP2	13:AM:113:ARG:NH2	2.52	0.41
2:AB:43:LEU:HA	2:AB:46:THR:HB	2.03	0.41
4:AD:9:LEU:HG	4:AD:22:LYS:HE2	2.02	0.41
6:AF:11:HIS:HA	6:AF:85:ILE:HD11	2.02	0.41
10:AJ:53:ILE:HD11	10:AJ:61:ALA:HB1	2.02	0.41
26:BA:1056:G:O2'	26:BA:1086:A:O2'	2.31	0.41
26:BA:1062:G:C6	26:BA:1077:A:N1	2.89	0.41
26:BA:2705:A:H2	40:BO:64:ARG:NH1	2.18	0.41
27:BB:30:C:OP1	41:BP:3:LYS:NZ	2.45	0.41
30:BE:5:LEU:O	30:BE:9:GLN:N	2.53	0.41
30:BE:131:THR:HG22	30:BE:160:ALA:O	2.20	0.41
41:BP:51:ALA:HB3	41:BP:78:VAL:HB	2.02	0.41
60:CT:2:DT:H2''	60:CT:3:DC:H5	1.85	0.41
60:CT:20:DC:C2	60:CT:21:DG:N7	2.88	0.41
62:CC:494:ASN:C	62:CC:494:ASN:ND2	2.78	0.41
62:CC:524:ILE:HG21	62:CC:524:ILE:HD13	1.76	0.41
63:CD:327:LEU:O	63:CD:330:MET:N	2.51	0.41
63:CD:1256:ILE:HG23	63:CD:1256:ILE:HD12	1.60	0.41
1:AA:36:C:H2'	1:AA:37:U:O4'	2.21	0.41
1:AA:451:A:H2'	1:AA:481:G:O6	2.21	0.41
1:AA:523:A:N6	12:AL:89:D2T:OD1	2.34	0.41
1:AA:662:U:H2'	1:AA:663:A:C8	2.56	0.41
3:AC:75:ILE:HG12	22:AV:34:A:H8	1.85	0.41
4:AD:195:ILE:HG22	4:AD:197:GLU:OE2	2.20	0.41
6:AF:42:TRP:HZ2	6:AF:61:LEU:HD22	1.86	0.41
24:AX:28:G:H2'	24:AX:29:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:75:G:H4'	51:BZ:48:ARG:NH2	2.35	0.41
26:BA:223:A:N1	26:BA:407:G:O2'	2.50	0.41
26:BA:301:G:OP2	47:BV:82:ARG:NH1	2.53	0.41
26:BA:567:U:OP2	38:BM:29:LYS:NZ	2.53	0.41
26:BA:1042:G:O2'	26:BA:1043:C:H6	2.03	0.41
26:BA:1593:A:H2'	26:BA:1594:U:C6	2.55	0.41
26:BA:1964:G:C2	26:BA:1967:C:C5	3.08	0.41
26:BA:2056:G:C2	26:BA:2057:G:C8	3.08	0.41
26:BA:2130:U:C2	26:BA:2131:U:H5	2.38	0.41
26:BA:2178:C:H2'	26:BA:2179:C:H5	1.84	0.41
27:BB:48:U:H2'	27:BB:49:C:C6	2.55	0.41
31:BF:117:LEU:HD12	31:BF:117:LEU:HA	1.86	0.41
31:BF:140:GLU:HA	58:B7:28:VAL:HG22	2.02	0.41
33:BH:84:ALA:HA	33:BH:91:PHE:H	1.86	0.41
34:BI:51:TYR:CD2	34:BI:52:MET:N	2.88	0.41
36:BK:36:LEU:O	36:BK:51:GLY:HA3	2.20	0.41
41:BP:62:LEU:HD22	41:BP:70:ALA:HA	2.01	0.41
46:BU:54:GLU:H	46:BU:54:GLU:HG2	1.59	0.41
47:BV:26:LYS:HD3	47:BV:37:GLU:HB3	2.02	0.41
50:BY:12:PRO:HB3	50:BY:30:LEU:HD23	2.02	0.41
52:B1:59:GLU:N	52:B1:59:GLU:OE1	2.53	0.41
62:CC:606:LEU:HD12	62:CC:606:LEU:N	2.36	0.41
63:CD:201:LEU:HD23	63:CD:221:ILE:HG22	2.03	0.41
1:AA:518:C:H1'	12:AL:47:SER:CB	2.51	0.41
1:AA:674:G:N2	1:AA:717:U:O2	2.52	0.41
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.56	0.41
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	2.02	0.41
20:AT:16:LYS:HE3	20:AT:16:LYS:HB2	1.90	0.41
26:BA:1081:U:H2'	26:BA:1082:U:C6	2.54	0.41
26:BA:2056:G:H21	53:B2:2:ALA:HB3	1.85	0.41
26:BA:2113:U:C2	26:BA:2114:A:H8	2.38	0.41
28:BC:76:ALA:HB2	28:BC:96:TYR:CE1	2.56	0.41
32:BG:145:ALA:HB1	32:BG:164:TYR:HE1	1.86	0.41
42:BQ:33:VAL:HG22	42:BQ:38:LYS:CG	2.51	0.41
46:BU:25:GLU:HG3	46:BU:26:LYS:N	2.35	0.41
63:CD:579:LEU:O	63:CD:580:TRP:C	2.63	0.41
63:CD:1257:VAL:O	63:CD:1258:ARG:C	2.64	0.41
1:AA:526:C:OP2	12:AL:88:LYS:HE2	2.21	0.41
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.41
17:AQ:13:VAL:N	17:AQ:22:VAL:O	2.54	0.41
26:BA:24:G:H1'	45:BT:77:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:881:G:O6	26:BA:895:U:O4	2.39	0.41
26:BA:883:G:N3	26:BA:884:U:H5	2.18	0.41
26:BA:1108:U:C4	26:BA:1109:C:N4	2.89	0.41
26:BA:1292:G:H2'	26:BA:1293:C:C6	2.56	0.41
26:BA:1585:C:H2'	26:BA:1586:A:O4'	2.21	0.41
26:BA:1683:U:H2'	26:BA:1684:G:H8	1.85	0.41
26:BA:2001:C:H1'	26:BA:2689:U:C4	2.55	0.41
26:BA:2728:U:HO2'	26:BA:2729:G:H8	1.69	0.41
26:BA:2867:G:O2'	26:BA:2868:A:OP2	2.36	0.41
29:BD:33:ARG:NH2	29:BD:74:GLU:O	2.53	0.41
39:BN:111:GLU:OE1	39:BN:111:GLU:N	2.52	0.41
46:BU:6:ARG:HH22	46:BU:37:ASP:CG	2.29	0.41
46:BU:6:ARG:NH2	46:BU:37:ASP:OD2	2.53	0.41
59:CN:18:DG:C6	65:CF:14:ALA:HB3	2.56	0.41
61:CB:66:HIS:CE1	61:CB:68:TYR:HD1	2.39	0.41
62:CC:549:ASP:OD2	63:CD:750:PRO:HB3	2.21	0.41
62:CC:1268:GLN:OE1	63:CD:352:ARG:NH1	2.53	0.41
63:CD:416:ILE:O	63:CD:418:GLU:N	2.53	0.41
63:CD:572:THR:HG23	63:CD:573:THR:N	2.36	0.41
63:CD:871:LEU:O	63:CD:874:GLU:HB3	2.21	0.41
1:AA:88:U:C2'	1:AA:89:G:H5'	2.51	0.41
1:AA:203:G:C2	1:AA:215:C:C2	3.09	0.41
1:AA:501:C:H2'	1:AA:502:A:H8	1.86	0.41
4:AD:147:GLU:O	4:AD:150:LYS:HB2	2.20	0.41
7:AG:107:ALA:O	7:AG:111:ARG:HG3	2.20	0.41
9:AI:18:ARG:O	9:AI:65:ILE:HA	2.20	0.41
14:AN:27:LEU:HA	14:AN:27:LEU:HD23	1.87	0.41
22:AV:37:G:C8	22:AV:37:G:C4'	3.04	0.41
26:BA:1142:A:C5	26:BA:1144:A:C8	3.09	0.41
26:BA:1590:A:C6	26:BA:1591:A:C6	3.09	0.41
26:BA:2167:U:C4	26:BA:2170:A:H5''	2.56	0.41
26:BA:2834:G:H2'	26:BA:2879:A:H61	1.85	0.41
26:BA:2902:C:C2'	26:BA:2903:U:H5'	2.51	0.41
30:BE:145:ASP:OD1	30:BE:184:ASP:N	2.41	0.41
34:BI:28:ALA:CB	34:BI:81:LEU:O	2.53	0.41
34:BI:96:PHE:CZ	34:BI:125:ARG:HA	2.56	0.41
45:BT:108:SER:OG	45:BT:110:ARG:O	2.37	0.41
59:CN:28:DA:C4	59:CN:29:DG:N7	2.89	0.41
61:CA:185:TYR:CD1	61:CA:185:TYR:C	2.99	0.41
62:CC:447:HIS:C	62:CC:449:GLY:N	2.77	0.41
62:CC:783:LEU:HA	62:CC:783:LEU:HD23	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:1076:ILE:HD13	62:CC:1076:ILE:HG21	1.77	0.41
62:CC:1251:TYR:CE1	62:CC:1301:ARG:CZ	3.03	0.41
63:CD:160:LEU:HD23	63:CD:160:LEU:N	2.34	0.41
63:CD:478:LEU:HA	63:CD:478:LEU:HD23	1.63	0.41
63:CD:619:ILE:HD12	63:CD:619:ILE:HA	1.86	0.41
63:CD:1356:LEU:HA	63:CD:1356:LEU:HD23	1.85	0.41
1:AA:381:C:H2'	1:AA:382:A:O4'	2.21	0.41
1:AA:691:G:O2'	1:AA:797:C:H4'	2.20	0.41
1:AA:707:U:C2	1:AA:708:C:C5	3.09	0.41
1:AA:920:U:H2'	1:AA:921:U:C6	2.55	0.41
1:AA:1164:G:C6	1:AA:1165:U:C4	3.09	0.41
1:AA:1328:C:C4	1:AA:1329:A:N7	2.89	0.41
3:AC:3:GLN:HE21	3:AC:3:GLN:HB2	1.66	0.41
3:AC:74:GLY:CA	22:AV:35:U:H5''	2.51	0.41
3:AC:124:LEU:HD23	3:AC:124:LEU:HA	1.75	0.41
4:AD:37:ALA:HB1	4:AD:38:PRO:HD2	2.03	0.41
5:AE:72:ILE:HG21	5:AE:145:GLU:OE2	2.21	0.41
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	2.02	0.41
10:AJ:6:ILE:CD1	10:AJ:76:ILE:HB	2.49	0.41
10:AJ:35:GLN:HB2	10:AJ:77:VAL:CG2	2.51	0.41
16:AP:52:LEU:HD23	16:AP:52:LEU:HA	1.91	0.41
19:AS:79:THR:O	19:AS:79:THR:OG1	2.39	0.41
20:AT:49:LYS:HB3	20:AT:49:LYS:HE2	1.81	0.41
22:AV:25:U:O2'	22:AV:26:A:OP1	2.29	0.41
25:AY:55:ASN:ND2	25:AY:59:GLU:O	2.53	0.41
26:BA:750:A:OP1	26:BA:1615:C:N4	2.46	0.41
26:BA:879:G:H2'	26:BA:880:G:O4'	2.21	0.41
26:BA:1223:G:OP2	44:BS:90:ARG:NH1	2.45	0.41
26:BA:1405:U:H2'	26:BA:1406:U:C6	2.56	0.41
26:BA:1548:A:H2'	26:BA:1549:A:C8	2.56	0.41
26:BA:1871:A:O2'	26:BA:1872:A:C8	2.74	0.41
26:BA:2025:C:H2'	26:BA:2026:U:C6	2.56	0.41
26:BA:2571:U:O2	29:BD:148:GLN:HG2	2.21	0.41
26:BA:2583:G:H2'	26:BA:2584:U:O4'	2.21	0.41
26:BA:2602:A:H5''	26:BA:2603:G:C5'	2.51	0.41
26:BA:2898:U:C2	26:BA:2899:A:N7	2.89	0.41
27:BB:2:G:C6	27:BB:119:A:C2	3.08	0.41
29:BD:34:VAL:HG22	29:BD:50:VAL:HG12	2.03	0.41
31:BF:72:LYS:HE2	31:BF:72:LYS:HB3	1.77	0.41
35:BJ:12:VAL:HG22	35:BJ:19:PRO:HB3	2.03	0.41
47:BV:88:GLU:C	47:BV:90:GLY:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B3:21:TYR:OH	54:B3:39:PHE:O	2.27	0.41
61:CA:58:GLU:OE1	61:CA:170:ARG:HD3	2.21	0.41
61:CB:28:LEU:HD13	61:CB:28:LEU:HA	1.75	0.41
62:CC:14:ASP:OD1	62:CC:14:ASP:C	2.62	0.41
62:CC:166:SER:HB2	63:CD:1151:LYS:HE3	2.03	0.41
62:CC:660:VAL:HG13	62:CC:661:VAL:HG13	2.02	0.41
63:CD:80:HIS:O	63:CD:83:VAL:HG22	2.21	0.41
63:CD:1146:GLU:OE2	63:CD:1148:ARG:NE	2.50	0.41
65:CF:122:PRO:HB2	65:CF:123:ARG:H	1.62	0.41
1:AA:444:G:C6	1:AA:491:G:C6	3.10	0.41
1:AA:1037:C:H2'	1:AA:1038:C:C6	2.56	0.41
1:AA:1291:U:N3	1:AA:1292:G:N7	2.69	0.41
3:AC:130:PHE:CG	3:AC:131:ARG:N	2.89	0.41
9:AI:45:ARG:O	9:AI:49:ARG:HD3	2.22	0.41
20:AT:64:LYS:HD3	20:AT:64:LYS:HA	1.86	0.41
23:AW:32:OMC:HM23	23:AW:32:OMC:H1'	1.71	0.41
24:AX:49:C:C2	24:AX:50:U:C5	3.08	0.41
26:BA:2250:G:OP1	39:BN:84:LYS:NZ	2.34	0.41
26:BA:2327:A:H2'	26:BA:2328:A:C8	2.55	0.41
27:BB:45:A:C4	27:BB:46:A:C8	3.10	0.41
32:BG:141:ILE:HG13	32:BG:142:GLY:H	1.85	0.41
34:BI:12:VAL:HA	34:BI:15:VAL:HG22	2.03	0.41
60:CT:1:DC:H6	60:CT:1:DC:H2'	1.64	0.41
63:CD:1226:VAL:O	63:CD:1229:VAL:HG12	2.21	0.41
63:CD:1310:THR:O	63:CD:1310:THR:HG22	2.20	0.41
2:AB:192:ASP:OD1	2:AB:192:ASP:N	2.49	0.40
9:AI:72:ILE:HD13	9:AI:72:ILE:HA	1.91	0.40
16:AP:52:LEU:HD22	16:AP:57:ILE:HD11	2.03	0.40
22:AV:53:G:OP1	62:CC:1065:LYS:NZ	2.53	0.40
24:AX:37:MIA:O2'	26:BA:1913:A:N1	2.51	0.40
24:AX:67:C:H2'	24:AX:68:C:O4'	2.20	0.40
25:AY:9:PHE:O	25:AY:13:LEU:HG	2.20	0.40
26:BA:151:C:H2'	26:BA:152:A:C8	2.55	0.40
26:BA:359:G:C6	26:BA:360:U:C4	3.09	0.40
26:BA:1060:U:H4'	26:BA:1061:U:O5'	2.21	0.40
26:BA:2151:U:H2'	26:BA:2152:G:H8	1.86	0.40
27:BB:2:G:H2'	27:BB:3:C:H6	1.85	0.40
27:BB:7:G:OP1	41:BP:4:LYS:HE3	2.21	0.40
28:BC:160:THR:HG23	28:BC:177:ARG:HG2	2.03	0.40
30:BE:27:LEU:HG	30:BE:104:ALA:HB2	2.02	0.40
48:BW:7:GLU:O	48:BW:40:ILE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BY:5:CYS:HA	50:BY:33:LEU:HD21	2.03	0.40
51:BZ:7:ARG:HH11	51:BZ:56:LEU:HD11	1.86	0.40
60:CT:5:DG:H2'	60:CT:6:DA:O4'	2.21	0.40
62:CC:582:ASN:CG	62:CC:583:GLU:N	2.79	0.40
63:CD:1248:ILE:HD13	63:CD:1248:ILE:HG21	1.82	0.40
1:AA:89:G:H2'	1:AA:90:C:C6	2.56	0.40
1:AA:478:A:OP1	1:AA:478:A:H4'	2.20	0.40
1:AA:501:C:H2'	1:AA:502:A:C8	2.56	0.40
1:AA:1151:A:O2'	1:AA:1152:A:O4'	2.38	0.40
1:AA:1465:A:H2'	1:AA:1466:C:C6	2.57	0.40
2:AB:180:GLY:C	2:AB:181:ILE:HG13	2.46	0.40
9:AI:130:ARG:NH2	23:AW:33:U:OP2	2.45	0.40
14:AN:38:ASP:HA	14:AN:41:ARG:HD2	2.03	0.40
14:AN:83:LYS:HD3	14:AN:83:LYS:HA	1.77	0.40
20:AT:24:ARG:HA	20:AT:24:ARG:NH1	2.36	0.40
26:BA:191:A:H2'	26:BA:192:C:C6	2.57	0.40
26:BA:261:G:C2	26:BA:262:A:C8	3.10	0.40
26:BA:893:C:HO2'	26:BA:894:U:H6	1.69	0.40
26:BA:2102:G:N1	26:BA:2188:U:O4	2.54	0.40
26:BA:2557:G:H2'	26:BA:2558:C:C6	2.56	0.40
28:BC:123:ALA:O	28:BC:128:ASN:ND2	2.54	0.40
33:BH:50:ARG:CZ	33:BH:51:ARG:HE	2.34	0.40
36:BK:31:GLU:HG3	36:BK:142:ILE:HD12	2.02	0.40
43:BR:83:LEU:HD22	43:BR:88:VAL:HB	2.02	0.40
48:BW:80:HIS:ND1	48:BW:83:LYS:HB2	2.37	0.40
61:CB:66:HIS:ND1	61:CB:68:TYR:HB3	2.36	0.40
62:CC:150:HIS:ND1	62:CC:150:HIS:O	2.54	0.40
1:AA:160:A:H2'	1:AA:161:A:O4'	2.21	0.40
1:AA:255:G:C2	1:AA:272:C:C2	3.09	0.40
1:AA:256:U:H2'	1:AA:257:G:C8	2.57	0.40
1:AA:991:U:C4	1:AA:1212:U:H1'	2.56	0.40
2:AB:43:LEU:HD12	25:AY:5:PHE:CE1	2.55	0.40
3:AC:88:ARG:NH2	63:CD:80:HIS:CE1	2.90	0.40
5:AE:110:ALA:O	5:AE:114:VAL:HG12	2.21	0.40
11:AK:100:LEU:HA	11:AK:100:LEU:HD12	1.81	0.40
22:AV:37:G:C4'	22:AV:37:G:OP1	2.70	0.40
26:BA:523:C:H4'	26:BA:540:C:O2	2.22	0.40
26:BA:626:A:H2'	38:BM:78:ARG:NH2	2.35	0.40
26:BA:752:A:H3'	55:B4:1:MET:SD	2.62	0.40
26:BA:1130:U:C2	26:BA:2025:C:H5''	2.56	0.40
33:BH:78:VAL:HG23	33:BH:142:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BL:69:VAL:HG21	37:BL:106:GLU:HG2	2.03	0.40
38:BM:89:VAL:HG21	38:BM:123:ARG:HH21	1.86	0.40
42:BQ:30:VAL:HG12	42:BQ:81:VAL:HA	2.03	0.40
61:CA:27:THR:C	61:CA:28:LEU:HD12	2.46	0.40
62:CC:97:ARG:HB3	62:CC:121:GLU:HB2	2.03	0.40
62:CC:456:VAL:C	62:CC:458:GLU:H	2.29	0.40
62:CC:473:ARG:HG3	62:CC:473:ARG:NH1	2.36	0.40
62:CC:1211:ARG:NH1	62:CC:1220:GLN:OE1	2.52	0.40
62:CC:1248:THR:HG22	62:CC:1249:GLY:N	2.35	0.40
63:CD:238:ILE:HD12	63:CD:238:ILE:HG23	1.71	0.40
63:CD:374:LEU:HD23	63:CD:374:LEU:C	2.45	0.40
1:AA:868:C:H2'	1:AA:869:G:O4'	2.22	0.40
3:AC:88:ARG:NH2	63:CD:79:LYS:CG	2.62	0.40
10:AJ:6:ILE:O	10:AJ:6:ILE:HG12	2.21	0.40
26:BA:5:A:C2	26:BA:6:A:C5	3.10	0.40
26:BA:581:C:H2'	26:BA:582:A:H8	1.86	0.40
26:BA:2630:G:C5	26:BA:2894:G:C6	3.09	0.40
32:BG:121:ILE:HD12	32:BG:141:ILE:HG22	2.03	0.40
33:BH:5:LEU:CD1	33:BH:13:GLY:HA2	2.51	0.40
33:BH:41:LYS:HE2	33:BH:41:LYS:HB3	1.95	0.40
45:BT:20:VAL:O	45:BT:23:LEU:HB2	2.21	0.40
53:B2:39:LEU:HD12	53:B2:39:LEU:HA	1.88	0.40
59:CN:22:DT:C2	59:CN:22:DT:O5'	2.74	0.40
61:CA:11:PRO:HB3	61:CA:31:LEU:HD21	2.02	0.40
62:CC:130:MET:SD	62:CC:134:GLY:HA2	2.61	0.40
62:CC:145:ILE:N	62:CC:145:ILE:HD12	2.36	0.40
62:CC:675:ASP:OD1	62:CC:676:ALA:N	2.54	0.40
62:CC:678:ARG:NH1	62:CC:681:MET:SD	2.94	0.40
63:CD:157:GLN:CG	63:CD:158:GLN:H	2.34	0.40
1:AA:832:G:C2	1:AA:833:G:C8	3.10	0.40
1:AA:1251:A:H2'	1:AA:1252:A:O4'	2.21	0.40
1:AA:1312:G:O5'	19:AS:5:LEU:HD11	2.22	0.40
3:AC:101:ILE:O	22:AV:36:A:C6	2.74	0.40
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.86	0.40
21:AU:16:LEU:HD12	21:AU:16:LEU:HA	1.92	0.40
23:AW:13:C:O2'	26:BA:1924:C:H4'	2.21	0.40
25:AY:24:VAL:HB	25:AY:72:LEU:HD12	2.04	0.40
26:BA:808:G:O2'	26:BA:1254:A:H4'	2.22	0.40
26:BA:1636:U:O2'	26:BA:1760:C:O2	2.35	0.40
29:BD:170:VAL:HG12	29:BD:171:THR:N	2.37	0.40
33:BH:32:PRO:HA	50:BY:39:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:CC:647:ARG:C	62:CC:649:GLN:H	2.30	0.40
62:CC:748:ILE:O	62:CC:748:ILE:HG23	2.22	0.40
62:CC:886:LYS:HB3	62:CC:916:SER:O	2.22	0.40
63:CD:421:VAL:O	63:CD:421:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	224/241 (93%)	209 (93%)	14 (6%)	1 (0%)	30	59
3	AC	209/233 (90%)	198 (95%)	6 (3%)	5 (2%)	4	22
4	AD	203/206 (98%)	194 (96%)	8 (4%)	1 (0%)	24	54
5	AE	154/167 (92%)	140 (91%)	12 (8%)	2 (1%)	9	33
6	AF	102/131 (78%)	97 (95%)	5 (5%)	0	100	100
7	AG	151/156 (97%)	139 (92%)	11 (7%)	1 (1%)	18	47
8	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	44
9	AI	126/130 (97%)	108 (86%)	14 (11%)	4 (3%)	3	17
10	AJ	99/103 (96%)	92 (93%)	3 (3%)	4 (4%)	2	15
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	42
12	AL	119/124 (96%)	112 (94%)	5 (4%)	2 (2%)	7	28
13	AM	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	14	42
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	35
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	72 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	58/75 (77%)	55 (95%)	2 (3%)	1 (2%)	7	28
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
25	AY	87/557 (16%)	75 (86%)	12 (14%)	0	100	100
28	BC	270/273 (99%)	248 (92%)	19 (7%)	3 (1%)	11	38
29	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	54
30	BE	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
31	BF	176/179 (98%)	168 (96%)	7 (4%)	1 (1%)	21	50
32	BG	173/177 (98%)	158 (91%)	14 (8%)	1 (1%)	21	50
33	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
34	BI	128/165 (78%)	99 (77%)	24 (19%)	5 (4%)	2	15
35	BJ	139/142 (98%)	111 (80%)	24 (17%)	4 (3%)	3	19
36	BK	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
37	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
38	BM	142/144 (99%)	130 (92%)	10 (7%)	2 (1%)	9	31
39	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
40	BO	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
41	BP	115/117 (98%)	107 (93%)	7 (6%)	1 (1%)	14	42
42	BQ	112/115 (97%)	103 (92%)	8 (7%)	1 (1%)	14	42
43	BR	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
44	BS	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	40
45	BT	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
46	BU	94/100 (94%)	87 (93%)	5 (5%)	2 (2%)	5	24
47	BV	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
48	BW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
50	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
51	BZ	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
52	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
53	B2	54/57 (95%)	50 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B3	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
55	B4	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
56	B5	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
57	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
58	B7	68/70 (97%)	60 (88%)	8 (12%)	0	100	100
61	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
61	CB	215/329 (65%)	205 (95%)	9 (4%)	1 (0%)	24	54
62	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	18	47
63	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	16	44
64	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	25
65	CF	157/181 (87%)	143 (91%)	11 (7%)	3 (2%)	6	26
All	All	9264/10441 (89%)	8585 (93%)	608 (7%)	71 (1%)	18	44

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	80	LYS
5	AE	90	THR
9	AI	56	ASP
11	AK	93	ARG
12	AL	88	LYS
15	AO	19	ALA
32	BG	47	ASP
34	BI	80	THR
62	CC	165	HIS
63	CD	1159	ILE
2	AB	165	ASP
3	AC	51	SER
9	AI	13	LYS
10	AJ	57	VAL
28	BC	241	GLY
29	BD	149	ASN
31	BF	62	GLY
38	BM	36	LYS
41	BP	100	HIS
46	BU	71	GLY
61	CB	155	ALA
62	CC	47	TYR

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Mol	Chain	Res	Type
63	CD	1051	ASP
65	CF	118	VAL
65	CF	122	PRO
3	AC	60	PRO
4	AD	49	SER
7	AG	130	ASN
9	AI	5	GLN
9	AI	14	SER
12	AL	102	LEU
18	AR	72	ASP
34	BI	79	PRO
35	BJ	83	ALA
42	BQ	114	LEU
44	BS	53	PHE
62	CC	258	ASN
62	CC	1177	ARG
63	CD	119	SER
63	CD	121	PRO
63	CD	712	GLN
63	CD	854	ALA
63	CD	1200	GLU
64	CE	6	VAL
3	AC	14	ILE
13	AM	44	LYS
34	BI	81	LEU
35	BJ	64	ARG
38	BM	99	ASN
62	CC	282	VAL
62	CC	596	ASP
62	CC	1153	ALA
63	CD	586	GLY
3	AC	61	ALA
10	AJ	58	ASN
10	AJ	78	GLU
28	BC	253	LYS
46	BU	3	ARG
65	CF	123	ARG
62	CC	1223	ARG
63	CD	312	ARG
5	AE	108	GLY
34	BI	108	VAL
10	AJ	39	PRO

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Mol	Chain	Res	Type
28	BC	233	GLY
8	AH	75	ILE
34	BI	21	GLY
35	BJ	12	VAL
62	CC	1186	VAL
63	CD	500	ILE
35	BJ	22	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/199 (94%)	171 (91%)	16 (9%)	10	33
3	AC	172/190 (90%)	155 (90%)	17 (10%)	7	26
4	AD	172/173 (99%)	158 (92%)	14 (8%)	11	36
5	AE	118/126 (94%)	102 (86%)	16 (14%)	3	15
6	AF	91/112 (81%)	80 (88%)	11 (12%)	5	19
7	AG	126/129 (98%)	114 (90%)	12 (10%)	8	29
8	AH	104/105 (99%)	93 (89%)	11 (11%)	6	23
9	AI	106/107 (99%)	90 (85%)	16 (15%)	3	11
10	AJ	88/90 (98%)	76 (86%)	12 (14%)	3	15
11	AK	90/99 (91%)	84 (93%)	6 (7%)	15	41
12	AL	102/103 (99%)	93 (91%)	9 (9%)	9	31
13	AM	93/96 (97%)	83 (89%)	10 (11%)	6	22
14	AN	83/84 (99%)	74 (89%)	9 (11%)	6	22
15	AO	76/77 (99%)	72 (95%)	4 (5%)	20	47
16	AP	65/65 (100%)	60 (92%)	5 (8%)	12	37
17	AQ	74/78 (95%)	65 (88%)	9 (12%)	5	19
18	AR	52/65 (80%)	50 (96%)	2 (4%)	29	54
19	AS	72/79 (91%)	69 (96%)	3 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/66 (98%)	61 (94%)	4 (6%)	16	43
21	AU	60/61 (98%)	52 (87%)	8 (13%)	4	15
25	AY	73/461 (16%)	61 (84%)	12 (16%)	2	10
28	BC	217/218 (100%)	209 (96%)	8 (4%)	30	55
29	BD	163/163 (100%)	155 (95%)	8 (5%)	22	49
30	BE	165/165 (100%)	153 (93%)	12 (7%)	13	39
31	BF	149/150 (99%)	133 (89%)	16 (11%)	6	23
32	BG	136/138 (99%)	124 (91%)	12 (9%)	9	31
33	BH	114/114 (100%)	108 (95%)	6 (5%)	20	47
34	BI	99/123 (80%)	81 (82%)	18 (18%)	2	7
35	BJ	109/110 (99%)	91 (84%)	18 (16%)	2	10
36	BK	116/116 (100%)	107 (92%)	9 (8%)	11	37
37	BL	104/104 (100%)	97 (93%)	7 (7%)	15	41
38	BM	103/103 (100%)	92 (89%)	11 (11%)	6	23
39	BN	108/108 (100%)	100 (93%)	8 (7%)	13	38
40	BO	100/103 (97%)	96 (96%)	4 (4%)	28	53
41	BP	87/87 (100%)	79 (91%)	8 (9%)	8	29
42	BQ	99/100 (99%)	83 (84%)	16 (16%)	2	10
43	BR	89/90 (99%)	84 (94%)	5 (6%)	19	46
44	BS	84/84 (100%)	77 (92%)	7 (8%)	10	35
45	BT	93/93 (100%)	88 (95%)	5 (5%)	20	47
46	BU	83/84 (99%)	78 (94%)	5 (6%)	17	43
47	BV	84/85 (99%)	78 (93%)	6 (7%)	13	39
48	BW	78/78 (100%)	73 (94%)	5 (6%)	16	42
49	BX	58/63 (92%)	54 (93%)	4 (7%)	14	40
50	BY	67/68 (98%)	64 (96%)	3 (4%)	24	51
51	BZ	55/55 (100%)	52 (94%)	3 (6%)	19	46
52	B1	48/49 (98%)	44 (92%)	4 (8%)	10	35
53	B2	47/48 (98%)	44 (94%)	3 (6%)	16	42
54	B3	48/49 (98%)	42 (88%)	6 (12%)	4	18
55	B4	38/38 (100%)	37 (97%)	1 (3%)	40	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	B5	51/52 (98%)	48 (94%)	3 (6%)	18	44
57	B6	34/44 (77%)	32 (94%)	2 (6%)	18	44
58	B7	62/62 (100%)	60 (97%)	2 (3%)	34	58
61	CA	197/286 (69%)	193 (98%)	4 (2%)	48	65
61	CB	187/286 (65%)	177 (95%)	10 (5%)	20	47
62	CC	1139/1157 (98%)	1093 (96%)	46 (4%)	28	53
63	CD	1118/1168 (96%)	1094 (98%)	24 (2%)	47	64
64	CE	43/75 (57%)	41 (95%)	2 (5%)	23	50
65	CF	141/157 (90%)	126 (89%)	15 (11%)	6	23
All	All	7782/8638 (90%)	7250 (93%)	532 (7%)	16	40

All (532) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	14	VAL
2	AB	23	TRP
2	AB	63	ARG
2	AB	78	GLU
2	AB	105	LYS
2	AB	128	LYS
2	AB	129	LEU
2	AB	132	LYS
2	AB	135	LEU
2	AB	145	GLU
2	AB	146	ASN
2	AB	192	ASP
2	AB	199	VAL
2	AB	207	ILE
2	AB	214	LEU
2	AB	220	THR
3	AC	21	THR
3	AC	28	GLU
3	AC	35	SER
3	AC	72	ARG
3	AC	88	ARG
3	AC	97	VAL
3	AC	105	GLU
3	AC	106	VAL
3	AC	107	ARG

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Mol	Chain	Res	Type
3	AC	127	ARG
3	AC	134	MET
3	AC	153	VAL
3	AC	154	SER
3	AC	165	THR
3	AC	172	ARG
3	AC	175	LEU
3	AC	185	ASN
4	AD	17	THR
4	AD	78	GLU
4	AD	82	LEU
4	AD	83	LYS
4	AD	88	GLU
4	AD	95	GLU
4	AD	102	VAL
4	AD	116	GLN
4	AD	138	SER
4	AD	143	VAL
4	AD	147	GLU
4	AD	150	LYS
4	AD	171	LEU
4	AD	181	THR
5	AE	10	GLU
5	AE	15	LEU
5	AE	18	VAL
5	AE	39	VAL
5	AE	46	VAL
5	AE	60	ILE
5	AE	82	GLN
5	AE	94	VAL
5	AE	105	ILE
5	AE	114	VAL
5	AE	137	VAL
5	AE	138	ARG
5	AE	141	ILE
5	AE	142	ASP
5	AE	149	SER
5	AE	156	LYS
6	AF	7	VAL
6	AF	17	GLN
6	AF	21	MET
6	AF	23	GLU

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Mol	Chain	Res	Type
6	AF	29	ILE
6	AF	38	ARG
6	AF	44	ARG
6	AF	54	LEU
6	AF	71	ILE
6	AF	84	VAL
6	AF	86	ARG
7	AG	4	ARG
7	AG	7	ILE
7	AG	17	LYS
7	AG	47	LEU
7	AG	54	SER
7	AG	60	GLU
7	AG	80	VAL
7	AG	90	GLU
7	AG	109	ARG
7	AG	118	LEU
7	AG	123	GLU
7	AG	154	TYR
8	AH	22	LYS
8	AH	54	ASP
8	AH	55	THR
8	AH	73	GLU
8	AH	90	ASP
8	AH	96	MET
8	AH	99	LEU
8	AH	104	VAL
8	AH	107	SER
8	AH	117	ARG
8	AH	121	LEU
9	AI	4	ASN
9	AI	36	GLU
9	AI	41	ARG
9	AI	42	GLU
9	AI	49	ARG
9	AI	57	MET
9	AI	58	VAL
9	AI	61	LEU
9	AI	63	LEU
9	AI	84	THR
9	AI	87	LEU
9	AI	98	LEU

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Mol	Chain	Res	Type
9	AI	99	ARG
9	AI	116	VAL
9	AI	118	LEU
9	AI	123	ARG
10	AJ	3	ASN
10	AJ	6	ILE
10	AJ	7	ARG
10	AJ	14	ASP
10	AJ	17	LEU
10	AJ	18	ILE
10	AJ	27	GLU
10	AJ	36	VAL
10	AJ	37	ARG
10	AJ	57	VAL
10	AJ	97	ASP
10	AJ	102	LEU
11	AK	13	ARG
11	AK	15	GLN
11	AK	16	VAL
11	AK	33	THR
11	AK	74	VAL
11	AK	100	LEU
12	AL	5	ASN
12	AL	16	VAL
12	AL	24	LEU
12	AL	40	THR
12	AL	43	LYS
12	AL	62	GLU
12	AL	75	GLN
12	AL	102	LEU
12	AL	105	SER
13	AM	9	ILE
13	AM	34	LEU
13	AM	47	GLU
13	AM	64	VAL
13	AM	75	MET
13	AM	83	LEU
13	AM	92	ARG
13	AM	93	ARG
13	AM	104	THR
13	AM	107	ARG
14	AN	18	ASP

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Mol	Chain	Res	Type
14	AN	41	ARG
14	AN	46	LEU
14	AN	55	SER
14	AN	59	ARG
14	AN	65	ARG
14	AN	89	MET
14	AN	92	GLU
14	AN	100	SER
15	AO	22	THR
15	AO	61	SER
15	AO	64	ARG
15	AO	73	LYS
16	AP	18	GLN
16	AP	19	VAL
16	AP	42	ILE
16	AP	68	SER
16	AP	80	LYS
17	AQ	11	ARG
17	AQ	22	VAL
17	AQ	33	ILE
17	AQ	40	ARG
17	AQ	49	GLU
17	AQ	53	CYS
17	AQ	55	ILE
17	AQ	57	ASP
17	AQ	75	LEU
18	AR	29	LEU
18	AR	71	THR
19	AS	13	LEU
19	AS	51	VAL
19	AS	64	ASP
20	AT	14	SER
20	AT	24	ARG
20	AT	67	ILE
20	AT	83	ILE
21	AU	4	ILE
21	AU	13	ASP
21	AU	28	VAL
21	AU	42	THR
21	AU	47	ARG
21	AU	63	GLU
21	AU	69	ARG

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Mol	Chain	Res	Type
21	AU	70	LEU
25	AY	7	GLN
25	AY	14	LYS
25	AY	16	ILE
25	AY	17	GLU
25	AY	18	THR
25	AY	28	VAL
25	AY	33	LYS
25	AY	37	LEU
25	AY	43	LYS
25	AY	52	GLN
25	AY	68	VAL
25	AY	76	GLU
28	BC	14	ARG
28	BC	20	VAL
28	BC	54	ILE
28	BC	94	VAL
28	BC	129	THR
28	BC	130	LEU
28	BC	195	VAL
28	BC	203	ARG
29	BD	2	ILE
29	BD	13	ARG
29	BD	32	ASN
29	BD	43	ASP
29	BD	56	LYS
29	BD	77	ARG
29	BD	104	VAL
29	BD	177	VAL
30	BE	21	ARG
30	BE	40	ARG
30	BE	57	LYS
30	BE	77	ILE
30	BE	88	ARG
30	BE	111	GLU
30	BE	113	VAL
30	BE	122	GLU
30	BE	136	GLN
30	BE	152	GLU
30	BE	178	VAL
30	BE	193	VAL
31	BF	6	ASP

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Mol	Chain	Res	Type
31	BF	16	LEU
31	BF	25	VAL
31	BF	40	VAL
31	BF	49	LEU
31	BF	57	LEU
31	BF	79	ILE
31	BF	89	VAL
31	BF	95	ARG
31	BF	98	GLU
31	BF	108	VAL
31	BF	115	ARG
31	BF	117	LEU
31	BF	123	ASP
31	BF	146	VAL
31	BF	158	THR
32	BG	11	VAL
32	BG	16	ASP
32	BG	32	GLU
32	BG	87	LEU
32	BG	104	ASN
32	BG	110	SER
32	BG	117	LEU
32	BG	141	ILE
32	BG	155	GLU
32	BG	167	GLU
32	BG	168	VAL
32	BG	172	LYS
33	BH	1	MET
33	BH	11	ASN
33	BH	12	LEU
33	BH	66	ASN
33	BH	94	ILE
33	BH	122	LEU
34	BI	3	LEU
34	BI	7	ASP
34	BI	26	VAL
34	BI	27	VAL
34	BI	34	THR
34	BI	35	VAL
34	BI	41	LEU
34	BI	54	VAL
34	BI	55	VAL

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Mol	Chain	Res	Type
34	BI	74	ASP
34	BI	77	VAL
34	BI	80	THR
34	BI	81	LEU
34	BI	86	MET
34	BI	94	ARG
34	BI	107	GLU
34	BI	109	LYS
34	BI	123	ILE
35	BJ	8	VAL
35	BJ	9	LYS
35	BJ	10	LEU
35	BJ	11	GLN
35	BJ	20	SER
35	BJ	27	LEU
35	BJ	30	GLN
35	BJ	38	CYS
35	BJ	42	ASN
35	BJ	46	ASP
35	BJ	58	ILE
35	BJ	60	VAL
35	BJ	67	THR
35	BJ	72	THR
35	BJ	81	LYS
35	BJ	85	ILE
35	BJ	135	MET
35	BJ	140	GLU
36	BK	1	MET
36	BK	30	THR
36	BK	35	ARG
36	BK	43	GLU
36	BK	57	LEU
36	BK	108	MET
36	BK	123	LYS
36	BK	129	GLU
36	BK	142	ILE
37	BL	35	VAL
37	BL	41	ILE
37	BL	58	LEU
37	BL	67	LYS
37	BL	89	ASN
37	BL	99	ILE

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Mol	Chain	Res	Type
37	BL	111	LYS
38	BM	4	ASN
38	BM	30	THR
38	BM	40	SER
38	BM	47	ARG
38	BM	67	THR
38	BM	70	LYS
38	BM	84	LYS
38	BM	86	GLU
38	BM	103	ILE
38	BM	117	THR
38	BM	129	LYS
39	BN	18	ARG
39	BN	22	GLN
39	BN	59	ARG
39	BN	60	GLN
39	BN	78	LEU
39	BN	80	VAL
39	BN	100	LYS
39	BN	110	GLU
40	BO	2	ARG
40	BO	51	LEU
40	BO	65	LEU
40	BO	69	ARG
41	BP	2	ASP
41	BP	13	ARG
41	BP	54	VAL
41	BP	56	LYS
41	BP	65	THR
41	BP	98	GLN
41	BP	112	GLU
41	BP	116	GLN
42	BQ	6	LYS
42	BQ	10	GLN
42	BQ	26	VAL
42	BQ	27	GLU
42	BQ	38	LYS
42	BQ	68	GLU
42	BQ	80	VAL
42	BQ	81	VAL
42	BQ	88	ARG
42	BQ	96	LYS

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Mol	Chain	Res	Type
42	BQ	102	GLU
42	BQ	110	ILE
42	BQ	111	LYS
42	BQ	113	ARG
42	BQ	114	LEU
42	BQ	115	ASN
43	BR	11	ARG
43	BR	18	LEU
43	BR	59	GLN
43	BR	91	ASP
43	BR	117	LEU
44	BS	6	GLN
44	BS	10	LYS
44	BS	31	GLU
44	BS	39	LEU
44	BS	46	GLU
44	BS	48	LYS
44	BS	86	GLN
45	BT	19	LEU
45	BT	29	VAL
45	BT	41	LYS
45	BT	92	ARG
45	BT	96	ILE
46	BU	12	ARG
46	BU	16	VAL
46	BU	53	VAL
46	BU	73	ARG
46	BU	89	GLU
47	BV	9	ASP
47	BV	37	GLU
47	BV	43	LYS
47	BV	68	SER
47	BV	72	ILE
47	BV	88	GLU
48	BW	1	MET
48	BW	19	ARG
48	BW	45	ASP
48	BW	48	MET
48	BW	86	LEU
49	BX	32	LEU
49	BX	41	ARG
49	BX	70	GLU

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Mol	Chain	Res	Type
49	BX	83	GLU
50	BY	25	THR
50	BY	52	SER
50	BY	71	LEU
51	BZ	4	LYS
51	BZ	6	LEU
51	BZ	57	LEU
52	B1	31	ARG
52	B1	32	ILE
52	B1	35	THR
52	B1	36	VAL
53	B2	12	LYS
53	B2	29	SER
53	B2	55	ILE
54	B3	3	LYS
54	B3	5	ILE
54	B3	10	LYS
54	B3	23	THR
54	B3	29	THR
54	B3	51	GLU
55	B4	22	MET
56	B5	16	LYS
56	B5	44	LEU
56	B5	55	LEU
57	B6	26	ILE
57	B6	34	LYS
58	B7	10	GLU
58	B7	59	ARG
61	CA	7	GLU
61	CA	13	LEU
61	CA	74	VAL
61	CA	101	THR
61	CB	41	ASN
61	CB	48	LEU
61	CB	66	HIS
61	CB	76	GLU
61	CB	83	LEU
61	CB	170	ARG
61	CB	174	ASP
61	CB	187	VAL
61	CB	191	ARG
61	CB	214	GLU

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Mol	Chain	Res	Type
62	CC	20	GLN
62	CC	47	TYR
62	CC	65	ASN
62	CC	108	GLU
62	CC	116	ASP
62	CC	150	HIS
62	CC	193	ASN
62	CC	262	TYR
62	CC	292	ILE
62	CC	316	GLU
62	CC	369	MET
62	CC	494	ASN
62	CC	524	ILE
62	CC	529	ARG
62	CC	562	GLU
62	CC	568	ASN
62	CC	569	ILE
62	CC	575	LEU
62	CC	657	THR
62	CC	726	TYR
62	CC	736	VAL
62	CC	745	GLU
62	CC	772	SER
62	CC	800	MET
62	CC	815	SER
62	CC	822	VAL
62	CC	830	THR
62	CC	843	THR
62	CC	856	ASN
62	CC	888	THR
62	CC	1002	LEU
62	CC	1005	GLU
62	CC	1022	LYS
62	CC	1050	VAL
62	CC	1076	ILE
62	CC	1083	GLU
62	CC	1223	ARG
62	CC	1240	ASP
62	CC	1247	SER
62	CC	1250	SER
62	CC	1287	LEU
62	CC	1291	LEU

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Mol	Chain	Res	Type
62	CC	1298	VAL
62	CC	1304	MET
62	CC	1336	ASN
62	CC	1340	GLU
63	CD	157	GLN
63	CD	158	GLN
63	CD	244	VAL
63	CD	255	LEU
63	CD	416	ILE
63	CD	418	GLU
63	CD	488	ASN
63	CD	592	VAL
63	CD	709	ARG
63	CD	802	ASP
63	CD	826	ILE
63	CD	839	VAL
63	CD	856	ILE
63	CD	1041	ILE
63	CD	1046	ILE
63	CD	1141	VAL
63	CD	1144	LEU
63	CD	1163	VAL
63	CD	1165	PHE
63	CD	1167	LYS
63	CD	1195	GLN
63	CD	1237	VAL
63	CD	1261	LEU
63	CD	1334	GLU
64	CE	48	VAL
64	CE	53	GLU
65	CF	118	VAL
65	CF	125	LYS
65	CF	126	THR
65	CF	132	GLU
65	CF	143	ASP
65	CF	147	VAL
65	CF	151	VAL
65	CF	152	ASP
65	CF	153	TYR
65	CF	155	LYS
65	CF	158	LEU
65	CF	162	VAL

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Mol	Chain	Res	Type
65	CF	164	ILE
65	CF	169	THR
65	CF	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	120	GLN
2	AB	146	ASN
3	AC	3	GLN
4	AD	40	GLN
4	AD	59	GLN
5	AE	19	ASN
5	AE	82	GLN
6	AF	17	GLN
6	AF	55	HIS
7	AG	97	ASN
9	AI	75	GLN
11	AK	22	HIS
13	AM	8	ASN
15	AO	35	GLN
15	AO	46	HIS
16	AP	18	GLN
18	AR	54	GLN
18	AR	75	GLN
19	AS	14	HIS
20	AT	3	ASN
20	AT	20	HIS
20	AT	21	ASN
20	AT	61	GLN
20	AT	75	HIS
28	BC	197	ASN
29	BD	148	GLN
30	BE	46	GLN
30	BE	90	GLN
30	BE	165	HIS
31	BF	37	ASN
32	BG	22	GLN
33	BH	2	GLN
33	BH	20	ASN
33	BH	73	ASN

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Mol	Chain	Res	Type
34	BI	57	ASN
35	BJ	18	ASN
36	BK	130	HIS
36	BK	131	ASN
39	BN	45	GLN
40	BO	3	HIS
40	BO	18	GLN
42	BQ	56	HIS
42	BQ	115	ASN
44	BS	82	HIS
45	BT	60	HIS
47	BV	99	ASN
49	BX	76	ASN
51	BZ	36	GLN
51	BZ	58	ASN
58	B7	6	HIS
61	CA	194	GLN
62	CC	60	GLN
62	CC	238	GLN
62	CC	518	ASN
62	CC	573	ASN
62	CC	686	GLN
62	CC	955	GLN
62	CC	1008	GLN
62	CC	1111	GLN
63	CD	153	ASN
63	CD	469	HIS
63	CD	623	GLN
63	CD	861	ASN
63	CD	929	GLN
63	CD	1227	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	310 (20%)	33 (2%)
22	AV	39/53 (73%)	27 (69%)	5 (12%)
23	AW	76/77 (98%)	27 (35%)	7 (9%)
24	AX	75/76 (98%)	20 (26%)	1 (1%)
26	BA	2898/2904 (99%)	570 (19%)	71 (2%)
27	BB	119/120 (99%)	14 (11%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4739/4772 (99%)	968 (20%)	117 (2%)

All (968) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	19	A
1	AA	22	G
1	AA	29	U
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	73	C
1	AA	74	A
1	AA	75	G
1	AA	76	G
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	86	G
1	AA	89	G
1	AA	90	C
1	AA	94	G
1	AA	95	C
1	AA	96	U
1	AA	108	G
1	AA	120	A
1	AA	121	U
1	AA	122	G
1	AA	131	A
1	AA	141	G

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Mol	Chain	Res	Type
1	AA	144	G
1	AA	148	G
1	AA	149	A
1	AA	160	A
1	AA	164	G
1	AA	173	U
1	AA	181	A
1	AA	182	A
1	AA	183	C
1	AA	184	G
1	AA	196	A
1	AA	197	A
1	AA	198	G
1	AA	208	U
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	216	U
1	AA	226	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	258	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	289	G
1	AA	306	A
1	AA	316	C
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	340	U
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C

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Mol	Chain	Res	Type
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	388	G
1	AA	389	A
1	AA	392	C
1	AA	397	A
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	446	G
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	460	A
1	AA	463	U
1	AA	464	U
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	478	A
1	AA	479	U
1	AA	480	U
1	AA	481	G
1	AA	482	A
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	516	PSU
1	AA	517	G
1	AA	518	C
1	AA	521	G
1	AA	526	C
1	AA	531	U
1	AA	532	A

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Mol	Chain	Res	Type
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	587	G
1	AA	588	G
1	AA	596	A
1	AA	628	G
1	AA	633	G
1	AA	641	U
1	AA	642	A
1	AA	649	A
1	AA	650	G
1	AA	653	U
1	AA	656	G
1	AA	665	A
1	AA	687	A
1	AA	702	A
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	734	G
1	AA	747	A
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A

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Mol	Chain	Res	Type
1	AA	846	G
1	AA	849	G
1	AA	851	G
1	AA	874	G
1	AA	887	G
1	AA	902	G
1	AA	914	A
1	AA	916	U
1	AA	926	G
1	AA	927	G
1	AA	928	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	961	U
1	AA	966	2MG
1	AA	967	5MC
1	AA	969	A
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	999	C
1	AA	1004	A
1	AA	1005	A
1	AA	1008	U
1	AA	1009	U
1	AA	1017	U
1	AA	1018	G
1	AA	1020	G
1	AA	1021	A
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U

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Mol	Chain	Res	Type
1	AA	1031	C
1	AA	1032	G
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1046	A
1	AA	1065	U
1	AA	1085	U
1	AA	1086	U
1	AA	1092	A
1	AA	1094	G
1	AA	1095	U
1	AA	1099	G
1	AA	1101	A
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1151	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1167	A
1	AA	1169	A
1	AA	1171	A
1	AA	1174	G
1	AA	1175	G
1	AA	1176	A
1	AA	1184	G
1	AA	1187	G
1	AA	1196	A
1	AA	1197	A
1	AA	1211	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C

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Mol	Chain	Res	Type
1	AA	1215	G
1	AA	1227	A
1	AA	1238	A
1	AA	1239	A
1	AA	1242	G
1	AA	1257	A
1	AA	1260	G
1	AA	1276	G
1	AA	1277	C
1	AA	1278	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1311	A
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1322	C
1	AA	1323	G
1	AA	1329	A
1	AA	1332	A
1	AA	1334	G
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1378	C
1	AA	1379	G
1	AA	1381	U
1	AA	1383	C
1	AA	1396	A
1	AA	1397	C
1	AA	1404	C

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Mol	Chain	Res	Type
1	AA	1408	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1442	G
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1519	MA6
1	AA	1529	G
1	AA	1530	G
22	AV	15	C
22	AV	16	A
22	AV	23	C
22	AV	24	A
22	AV	25	U
22	AV	26	A
22	AV	28	A
22	AV	29	C
22	AV	30	A
22	AV	31	U
22	AV	32	A
22	AV	33	U
22	AV	34	A
22	AV	35	U
22	AV	36	A
22	AV	37	G
22	AV	38	A
22	AV	39	C
22	AV	40	A
22	AV	41	C
22	AV	42	A

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Mol	Chain	Res	Type
22	AV	43	A
22	AV	44	A
22	AV	45	C
22	AV	46	G
22	AV	49	G
22	AV	53	G
23	AW	6	G
23	AW	8	4SU
23	AW	14	A
23	AW	15	G
23	AW	16	C
23	AW	17	C
23	AW	17(A)	U
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	21	A
23	AW	22	G
23	AW	25	C
23	AW	31	G
23	AW	32	OMC
23	AW	47	U
23	AW	49	G
23	AW	55	PSU
23	AW	57	A
23	AW	59	A
23	AW	60	U
23	AW	61	C
23	AW	69	C
23	AW	70	G
23	AW	74	C
23	AW	75	C
23	AW	76	A
24	AX	8	4SU
24	AX	9	A
24	AX	11	C
24	AX	12	U
24	AX	16	H2U
24	AX	17	C
24	AX	18	G
24	AX	19	G
24	AX	20	H2U

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Mol	Chain	Res	Type
24	AX	22	G
24	AX	30	G
24	AX	34	G
24	AX	40	C
24	AX	41	C
24	AX	46	7MG
24	AX	47	3AU
24	AX	48	C
24	AX	57	G
24	AX	70	G
24	AX	74	C
26	BA	10	A
26	BA	14	A
26	BA	23	G
26	BA	34	U
26	BA	35	G
26	BA	45	G
26	BA	46	G
26	BA	58	G
26	BA	60	G
26	BA	62	U
26	BA	63	A
26	BA	71	A
26	BA	74	A
26	BA	75	G
26	BA	83	A
26	BA	84	A
26	BA	85	G
26	BA	99	U
26	BA	101	A
26	BA	102	U
26	BA	103	A
26	BA	110	G
26	BA	118	A
26	BA	119	A
26	BA	120	U
26	BA	122	G
26	BA	131	A
26	BA	136	G
26	BA	138	U
26	BA	139	U
26	BA	140	C

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Mol	Chain	Res	Type
26	BA	141	G
26	BA	142	A
26	BA	144	A
26	BA	149	A
26	BA	163	C
26	BA	165	A
26	BA	181	A
26	BA	196	A
26	BA	199	A
26	BA	200	U
26	BA	215	G
26	BA	216	A
26	BA	221	A
26	BA	222	A
26	BA	248	G
26	BA	249	C
26	BA	264	C
26	BA	265	A
26	BA	266	G
26	BA	270	A
26	BA	271	G
26	BA	272	A
26	BA	276	U
26	BA	278	A
26	BA	285	G
26	BA	302	C
26	BA	310	A
26	BA	311	A
26	BA	327	G
26	BA	329	G
26	BA	330	A
26	BA	361	G
26	BA	362	A
26	BA	371	A
26	BA	386	G
26	BA	396	G
26	BA	403	U
26	BA	405	U
26	BA	411	G
26	BA	412	A
26	BA	424	G
26	BA	435	C

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Mol	Chain	Res	Type
26	BA	451	U
26	BA	456	C
26	BA	477	A
26	BA	480	A
26	BA	481	G
26	BA	491	G
26	BA	501	A
26	BA	503	A
26	BA	504	A
26	BA	505	A
26	BA	508	A
26	BA	509	C
26	BA	531	C
26	BA	532	A
26	BA	533	G
26	BA	543	A
26	BA	544	G
26	BA	545	A
26	BA	550	U
26	BA	551	G
26	BA	563	A
26	BA	569	U
26	BA	573	U
26	BA	574	A
26	BA	575	A
26	BA	586	A
26	BA	603	A
26	BA	609	A
26	BA	613	A
26	BA	614	A
26	BA	615	U
26	BA	616	A
26	BA	618	G
26	BA	627	A
26	BA	637	A
26	BA	645	C
26	BA	647	G
26	BA	651	G
26	BA	654	A
26	BA	655	A
26	BA	668	A
26	BA	685	A

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Mol	Chain	Res	Type
26	BA	686	U
26	BA	696	G
26	BA	717	C
26	BA	724	U
26	BA	730	A
26	BA	738	G
26	BA	746	PSU
26	BA	747	5MU
26	BA	757	G
26	BA	764	A
26	BA	765	C
26	BA	775	G
26	BA	776	G
26	BA	777	G
26	BA	782	A
26	BA	783	A
26	BA	784	G
26	BA	785	G
26	BA	788	A
26	BA	789	A
26	BA	805	G
26	BA	812	C
26	BA	827	U
26	BA	828	U
26	BA	845	A
26	BA	846	U
26	BA	858	G
26	BA	859	G
26	BA	869	G
26	BA	878	A
26	BA	881	G
26	BA	883	G
26	BA	884	U
26	BA	885	C
26	BA	887	U
26	BA	888	C
26	BA	889	C
26	BA	890	C
26	BA	891	G
26	BA	892	A
26	BA	893	C
26	BA	895	U

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Mol	Chain	Res	Type
26	BA	896	A
26	BA	897	C
26	BA	899	A
26	BA	910	A
26	BA	914	G
26	BA	915	C
26	BA	931	U
26	BA	933	A
26	BA	940	G
26	BA	941	A
26	BA	946	C
26	BA	953	G
26	BA	961	C
26	BA	974	G
26	BA	983	A
26	BA	984	A
26	BA	985	C
26	BA	995	C
26	BA	996	A
26	BA	999	U
26	BA	1005	C
26	BA	1012	U
26	BA	1013	C
26	BA	1023	U
26	BA	1026	G
26	BA	1033	U
26	BA	1040	A
26	BA	1043	C
26	BA	1045	C
26	BA	1046	A
26	BA	1047	G
26	BA	1050	A
26	BA	1060	U
26	BA	1061	U
26	BA	1063	G
26	BA	1064	C
26	BA	1065	U
26	BA	1066	U
26	BA	1067	A
26	BA	1068	G
26	BA	1069	A
26	BA	1070	A

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Mol	Chain	Res	Type
26	BA	1074	G
26	BA	1083	U
26	BA	1084	A
26	BA	1087	G
26	BA	1088	A
26	BA	1090	A
26	BA	1107	G
26	BA	1111	A
26	BA	1112	G
26	BA	1119	U
26	BA	1122	G
26	BA	1128	G
26	BA	1129	A
26	BA	1130	U
26	BA	1132	U
26	BA	1134	A
26	BA	1135	C
26	BA	1142	A
26	BA	1169	A
26	BA	1172	C
26	BA	1173	U
26	BA	1174	U
26	BA	1175	A
26	BA	1176	U
26	BA	1177	G
26	BA	1178	C
26	BA	1179	G
26	BA	1180	U
26	BA	1186	G
26	BA	1211	U
26	BA	1212	G
26	BA	1236	G
26	BA	1238	G
26	BA	1248	G
26	BA	1253	A
26	BA	1256	G
26	BA	1265	A
26	BA	1271	G
26	BA	1272	A
26	BA	1273	U
26	BA	1301	A
26	BA	1302	A

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Mol	Chain	Res	Type
26	BA	1320	C
26	BA	1321	A
26	BA	1345	C
26	BA	1352	U
26	BA	1365	A
26	BA	1368	G
26	BA	1378	A
26	BA	1379	U
26	BA	1380	G
26	BA	1383	A
26	BA	1395	A
26	BA	1405	U
26	BA	1406	U
26	BA	1407	G
26	BA	1408	G
26	BA	1409	U
26	BA	1414	C
26	BA	1416	G
26	BA	1417	C
26	BA	1420	A
26	BA	1428	C
26	BA	1434	A
26	BA	1452	G
26	BA	1453	A
26	BA	1455	G
26	BA	1458	U
26	BA	1460	U
26	BA	1478	G
26	BA	1482	G
26	BA	1483	G
26	BA	1490	A
26	BA	1491	G
26	BA	1493	C
26	BA	1495	A
26	BA	1497	U
26	BA	1508	A
26	BA	1509	A
26	BA	1510	G
26	BA	1515	A
26	BA	1529	G
26	BA	1534	U
26	BA	1535	A

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Mol	Chain	Res	Type
26	BA	1536	C
26	BA	1537	G
26	BA	1554	U
26	BA	1558	C
26	BA	1559	U
26	BA	1566	A
26	BA	1569	A
26	BA	1578	U
26	BA	1580	A
26	BA	1583	A
26	BA	1584	U
26	BA	1589	U
26	BA	1590	A
26	BA	1592	C
26	BA	1593	A
26	BA	1594	U
26	BA	1595	C
26	BA	1596	A
26	BA	1597	A
26	BA	1608	A
26	BA	1609	A
26	BA	1610	A
26	BA	1613	G
26	BA	1618	6MZ
26	BA	1619	G
26	BA	1630	A
26	BA	1647	U
26	BA	1648	U
26	BA	1649	G
26	BA	1651	G
26	BA	1674	G
26	BA	1677	A
26	BA	1703	G
26	BA	1713	A
26	BA	1714	U
26	BA	1715	G
26	BA	1718	G
26	BA	1729	U
26	BA	1730	C
26	BA	1732	C
26	BA	1738	G
26	BA	1742	U

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Mol	Chain	Res	Type
26	BA	1750	G
26	BA	1755	A
26	BA	1758	U
26	BA	1761	C
26	BA	1764	C
26	BA	1773	A
26	BA	1791	A
26	BA	1800	C
26	BA	1801	A
26	BA	1808	A
26	BA	1811	G
26	BA	1816	C
26	BA	1829	A
26	BA	1833	C
26	BA	1848	A
26	BA	1858	A
26	BA	1859	U
26	BA	1862	G
26	BA	1864	U
26	BA	1869	G
26	BA	1870	C
26	BA	1872	A
26	BA	1873	G
26	BA	1905	C
26	BA	1906	G
26	BA	1907	G
26	BA	1912	A
26	BA	1913	A
26	BA	1914	C
26	BA	1917	PSU
26	BA	1918	A
26	BA	1919	A
26	BA	1929	G
26	BA	1930	G
26	BA	1931	U
26	BA	1936	A
26	BA	1938	A
26	BA	1939	5MU
26	BA	1955	U
26	BA	1960	A
26	BA	1965	C
26	BA	1966	A

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Mol	Chain	Res	Type
26	BA	1967	C
26	BA	1970	A
26	BA	1971	U
26	BA	1972	G
26	BA	1987	A
26	BA	1991	U
26	BA	1992	G
26	BA	1993	U
26	BA	1997	C
26	BA	2002	G
26	BA	2022	U
26	BA	2023	C
26	BA	2026	U
26	BA	2031	A
26	BA	2033	A
26	BA	2043	C
26	BA	2051	A
26	BA	2052	A
26	BA	2055	C
26	BA	2056	G
26	BA	2060	A
26	BA	2061	G
26	BA	2062	A
26	BA	2063	C
26	BA	2069	G7M
26	BA	2093	G
26	BA	2097	A
26	BA	2099	U
26	BA	2100	G
26	BA	2101	A
26	BA	2102	G
26	BA	2107	G
26	BA	2108	A
26	BA	2110	G
26	BA	2111	U
26	BA	2113	U
26	BA	2115	G
26	BA	2116	G
26	BA	2117	A
26	BA	2118	U
26	BA	2121	G
26	BA	2122	U

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Mol	Chain	Res	Type
26	BA	2124	G
26	BA	2125	G
26	BA	2126	A
26	BA	2128	G
26	BA	2129	C
26	BA	2132	U
26	BA	2133	G
26	BA	2134	A
26	BA	2138	G
26	BA	2139	U
26	BA	2141	G
26	BA	2142	A
26	BA	2146	C
26	BA	2147	A
26	BA	2154	A
26	BA	2157	G
26	BA	2158	A
26	BA	2159	G
26	BA	2161	C
26	BA	2162	G
26	BA	2163	A
26	BA	2164	C
26	BA	2165	C
26	BA	2167	U
26	BA	2169	A
26	BA	2170	A
26	BA	2171	A
26	BA	2172	U
26	BA	2173	A
26	BA	2178	C
26	BA	2181	U
26	BA	2182	U
26	BA	2183	A
26	BA	2185	U
26	BA	2187	U
26	BA	2188	U
26	BA	2190	G
26	BA	2197	U
26	BA	2198	A
26	BA	2199	A
26	BA	2203	U
26	BA	2204	G

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Mol	Chain	Res	Type
26	BA	2210	U
26	BA	2211	G
26	BA	2212	A
26	BA	2213	U
26	BA	2225	A
26	BA	2226	C
26	BA	2229	U
26	BA	2238	G
26	BA	2239	G
26	BA	2245	U
26	BA	2246	G
26	BA	2250	G
26	BA	2251	OMG
26	BA	2252	G
26	BA	2268	A
26	BA	2278	A
26	BA	2283	C
26	BA	2287	A
26	BA	2294	G
26	BA	2297	A
26	BA	2305	U
26	BA	2308	G
26	BA	2309	A
26	BA	2315	G
26	BA	2322	A
26	BA	2325	G
26	BA	2333	A
26	BA	2335	A
26	BA	2336	A
26	BA	2347	C
26	BA	2350	C
26	BA	2361	G
26	BA	2372	U
26	BA	2376	A
26	BA	2383	G
26	BA	2385	C
26	BA	2402	U
26	BA	2403	C
26	BA	2406	A
26	BA	2410	G
26	BA	2423	U
26	BA	2424	C

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Mol	Chain	Res	Type
26	BA	2425	A
26	BA	2426	A
26	BA	2429	G
26	BA	2430	A
26	BA	2431	U
26	BA	2435	A
26	BA	2441	U
26	BA	2445	2MG
26	BA	2448	A
26	BA	2449	H2U
26	BA	2470	G
26	BA	2474	U
26	BA	2476	A
26	BA	2478	A
26	BA	2491	U
26	BA	2498	OMC
26	BA	2502	G
26	BA	2503	2MA
26	BA	2505	G
26	BA	2512	C
26	BA	2513	A
26	BA	2518	A
26	BA	2520	C
26	BA	2525	G
26	BA	2529	G
26	BA	2535	G
26	BA	2547	A
26	BA	2552	OMU
26	BA	2554	U
26	BA	2566	A
26	BA	2567	G
26	BA	2573	C
26	BA	2574	G
26	BA	2585	U
26	BA	2586	U
26	BA	2603	G
26	BA	2609	U
26	BA	2610	C
26	BA	2611	C
26	BA	2613	U
26	BA	2629	U
26	BA	2630	G

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Mol	Chain	Res	Type
26	BA	2663	G
26	BA	2671	G
26	BA	2682	A
26	BA	2689	U
26	BA	2690	U
26	BA	2714	G
26	BA	2726	A
26	BA	2744	G
26	BA	2748	A
26	BA	2757	A
26	BA	2762	C
26	BA	2777	G
26	BA	2778	A
26	BA	2791	G
26	BA	2797	U
26	BA	2798	U
26	BA	2799	G
26	BA	2800	A
26	BA	2801	G
26	BA	2818	U
26	BA	2820	A
26	BA	2825	G
26	BA	2849	U
26	BA	2859	G
26	BA	2861	U
26	BA	2867	G
26	BA	2872	A
26	BA	2879	A
26	BA	2880	C
26	BA	2883	A
26	BA	2884	U
26	BA	2885	G
26	BA	2891	U
26	BA	2902	C
26	BA	2903	U
27	BB	13	G
27	BB	16	G
27	BB	35	C
27	BB	36	C
27	BB	41	G
27	BB	45	A
27	BB	56	G

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Mol	Chain	Res	Type
27	BB	64	G
27	BB	66	A
27	BB	88	C
27	BB	89	U
27	BB	90	C
27	BB	99	A
27	BB	109	A

All (117) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	70	U
1	AA	148	G
1	AA	181	A
1	AA	183	C
1	AA	197	A
1	AA	209	U
1	AA	421	U
1	AA	428	G
1	AA	481	G
1	AA	587	G
1	AA	641	U
1	AA	701	U
1	AA	793	U
1	AA	843	U
1	AA	873	A
1	AA	961	U
1	AA	991	U
1	AA	992	U
1	AA	1024	G
1	AA	1129	C
1	AA	1166	G
1	AA	1196	A
1	AA	1211	U
1	AA	1213	A
1	AA	1214	C
1	AA	1277	C
1	AA	1299	A
1	AA	1319	A
1	AA	1363	A

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Mol	Chain	Res	Type
1	AA	1396	A
1	AA	1447	A
22	AV	25	U
22	AV	36	A
22	AV	37	G
22	AV	40	A
22	AV	41	C
23	AW	15	G
23	AW	16	C
23	AW	17(A)	U
23	AW	18	G
23	AW	19	G
23	AW	20	H2U
23	AW	60	U
24	AX	19	G
26	BA	33	C
26	BA	62	U
26	BA	70	G
26	BA	71	A
26	BA	101	A
26	BA	138	U
26	BA	140	C
26	BA	142	A
26	BA	196	A
26	BA	199	A
26	BA	271	G
26	BA	310	A
26	BA	404	A
26	BA	503	A
26	BA	685	A
26	BA	764	A
26	BA	776	G
26	BA	784	G
26	BA	788	A
26	BA	883	G
26	BA	884	U
26	BA	887	U
26	BA	888	C
26	BA	892	A
26	BA	894	U
26	BA	984	A
26	BA	1045	C

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Mol	Chain	Res	Type
26	BA	1060	U
26	BA	1064	C
26	BA	1067	A
26	BA	1069	A
26	BA	1070	A
26	BA	1109	C
26	BA	1111	A
26	BA	1128	G
26	BA	1173	U
26	BA	1174	U
26	BA	1300	G
26	BA	1320	C
26	BA	1344	U
26	BA	1395	A
26	BA	1405	U
26	BA	1407	G
26	BA	1490	A
26	BA	1494	A
26	BA	1509	A
26	BA	1583	A
26	BA	1584	U
26	BA	1596	A
26	BA	1608	A
26	BA	1912	A
26	BA	1913	A
26	BA	1918	A
26	BA	2062	A
26	BA	2197	U
26	BA	2198	A
26	BA	2210	U
26	BA	2212	A
26	BA	2225	A
26	BA	2250	G
26	BA	2296	U
26	BA	2308	G
26	BA	2425	A
26	BA	2573	C
26	BA	2585	U
26	BA	2602	A
26	BA	2610	C
26	BA	2756	U
26	BA	2797	U

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Mol	Chain	Res	Type
26	BA	2798	U
26	BA	2873	A

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

53 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	PSU	AX	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.89	5 (22%)
24	7MG	AX	46	24	20,25,27	3.27	10 (50%)	27,37,42	2.22	8 (29%)
26	1MG	BA	745	26	22,26,27	2.72	5 (22%)	33,39,42	1.82	7 (21%)
1	UR3	AA	1498	1,66	19,22,23	2.59	7 (36%)	26,32,35	1.31	1 (3%)
1	MA6	AA	1518	1	23,26,27	1.54	6 (26%)	34,38,41	3.87	11 (32%)
26	PSU	BA	1911	26	18,21,22	1.07	1 (5%)	22,30,33	1.77	3 (13%)
26	3TD	BA	1915	26	18,22,23	4.47	10 (55%)	22,32,35	1.91	4 (18%)
26	5MU	BA	1939	26	19,22,23	1.42	4 (21%)	28,32,35	2.29	6 (21%)
26	PSU	BA	2604	26	18,21,22	1.01	1 (5%)	22,30,33	1.67	3 (13%)
26	5MC	BA	1962	26	18,22,23	3.97	7 (38%)	26,32,35	1.14	1 (3%)
26	2MG	BA	2445	26	23,26,27	2.77	9 (39%)	32,38,41	2.85	13 (40%)
26	PSU	BA	2605	26	18,21,22	1.04	1 (5%)	22,30,33	1.96	6 (27%)
26	G7M	BA	2069	26	23,26,27	2.60	9 (39%)	35,39,42	2.58	12 (34%)
1	PSU	AA	516	1	18,21,22	1.05	2 (11%)	22,30,33	2.04	7 (31%)
24	MIA	AX	37	24	21,24,32	1.76	4 (19%)	31,35,47	2.03	9 (29%)
26	H2U	BA	2449	26	18,21,22	2.82	5 (27%)	21,30,33	2.13	5 (23%)
26	PSU	BA	2457	26	18,21,22	1.05	1 (5%)	22,30,33	2.00	6 (27%)
24	5MU	AX	54	24	19,22,23	1.34	5 (26%)	28,32,35	2.09	6 (21%)
26	PSU	BA	746	66,26	18,21,22	1.03	1 (5%)	22,30,33	2.12	8 (36%)
1	2MG	AA	1207	1,66	23,26,27	2.82	9 (39%)	32,38,41	2.83	13 (40%)
12	D2T	AL	89	12	7,9,10	1.11	0	6,11,13	2.48	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	AA	1402	1	20,23,24	3.40	9 (45%)	26,32,35	1.01	2 (7%)
23	OMC	AW	32	23	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	1.99	5 (23%)
23	PSU	AW	55	23	18,21,22	1.04	1 (5%)	22,30,33	1.98	7 (31%)
26	5MU	BA	747	26	19,22,23	1.41	4 (21%)	28,32,35	2.16	6 (21%)
26	6MZ	BA	1618	26	22,25,26	2.73	4 (18%)	30,36,39	2.30	10 (33%)
24	3AU	AX	47	24	18,21,29	3.40	8 (44%)	26,30,43	1.64	4 (15%)
29	MEQ	BD	150	29	8,9,10	0.86	0	5,10,12	0.92	0
24	PSU	AX	39	24	18,21,22	1.14	1 (5%)	22,30,33	1.78	5 (22%)
1	MA6	AA	1519	1	23,26,27	1.58	6 (26%)	34,38,41	3.88	11 (32%)
24	PSU	AX	32	24,66	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
26	OMU	BA	2552	26	19,22,23	3.01	7 (36%)	26,31,34	1.71	5 (19%)
26	2MA	BA	2503	66,26	22,25,26	4.00	10 (45%)	33,37,40	2.59	10 (30%)
26	PSU	BA	2504	26	18,21,22	1.06	3 (16%)	22,30,33	2.05	6 (27%)
26	2MG	BA	1835	26	23,26,27	2.77	9 (39%)	32,38,41	2.90	13 (40%)
1	5MC	AA	1407	1	18,22,23	3.89	7 (38%)	26,32,35	0.97	1 (3%)
39	4D4	BN	81	39	9,11,12	2.41	2 (22%)	8,13,15	0.86	0
26	PSU	BA	955	66,26	18,21,22	1.07	2 (11%)	22,30,33	1.74	4 (18%)
1	G7M	AA	527	1	23,26,27	2.53	9 (39%)	35,39,42	2.61	12 (34%)
24	H2U	AX	16	24	18,21,22	3.05	5 (27%)	21,30,33	2.01	5 (23%)
1	2MG	AA	1516	1	23,26,27	2.73	9 (39%)	32,38,41	2.78	13 (40%)
26	OMG	BA	2251	23,26	23,26,27	2.53	8 (34%)	33,38,41	2.10	11 (33%)
24	4SU	AX	8	24	18,21,22	4.12	8 (44%)	26,30,33	2.26	5 (19%)
1	2MG	AA	966	1	23,26,27	2.82	9 (39%)	32,38,41	2.71	15 (46%)
24	H2U	AX	20	24	18,21,22	3.15	5 (27%)	21,30,33	1.95	4 (19%)
26	6MZ	BA	2030	26	22,25,26	2.63	5 (22%)	30,36,39	2.53	10 (33%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.11	6 (21%)
26	OMC	BA	2498	26	19,22,23	2.91	8 (42%)	26,31,34	0.87	1 (3%)
26	PSU	BA	2580	26	18,21,22	1.05	2 (11%)	22,30,33	2.07	6 (27%)
1	5MC	AA	967	1	18,22,23	3.99	7 (38%)	26,32,35	1.03	1 (3%)
26	PSU	BA	1917	26	18,21,22	0.99	1 (5%)	22,30,33	1.80	5 (22%)
23	4SU	AW	8	23	18,21,22	4.16	8 (44%)	26,30,33	2.28	5 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	AX	55	24	-	4/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	2/7/34/38	0/3/3/3
26	1MG	BA	745	26	-	0/7/25/26	0/3/3/3
1	UR3	AA	1498	1,66	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	1/11/29/30	0/3/3/3
26	PSU	BA	1911	26	-	1/7/25/26	0/2/2/2
26	3TD	BA	1915	26	-	3/7/25/26	0/2/2/2
26	5MU	BA	1939	26	-	2/7/25/26	0/2/2/2
26	PSU	BA	2604	26	-	0/7/25/26	0/2/2/2
26	5MC	BA	1962	26	-	0/7/25/26	0/2/2/2
26	2MG	BA	2445	26	-	2/9/27/28	0/3/3/3
26	PSU	BA	2605	26	-	0/7/25/26	0/2/2/2
26	G7M	BA	2069	26	-	2/7/25/26	0/3/3/3
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/7/25/34	0/3/3/3
26	H2U	BA	2449	26	-	2/7/38/39	0/2/2/2
26	PSU	BA	2457	26	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
26	PSU	BA	746	66,26	-	2/7/25/26	0/2/2/2
1	2MG	AA	1207	1,66	-	2/9/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
23	OMC	AW	32	23	-	3/9/27/28	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2
26	5MU	BA	747	26	-	0/7/25/26	0/2/2/2
26	6MZ	BA	1618	26	-	4/9/27/28	0/3/3/3
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
29	MEQ	BD	150	29	-	4/8/9/11	-
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/11/29/30	0/3/3/3
24	PSU	AX	32	24,66	-	2/7/25/26	0/2/2/2
26	OMU	BA	2552	26	-	2/9/27/28	0/2/2/2
26	2MA	BA	2503	66,26	-	2/7/25/26	0/3/3/3
26	PSU	BA	2504	26	-	0/7/25/26	0/2/2/2
26	2MG	BA	1835	26	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	4D4	BN	81	39	-	4/11/12/14	-
26	PSU	BA	955	66,26	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/7/25/26	0/3/3/3
24	H2U	AX	16	24	-	4/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
26	OMG	BA	2251	23,26	-	0/9/27/28	0/3/3/3
24	4SU	AX	8	24	-	1/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
26	6MZ	BA	2030	26	-	3/9/27/28	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
26	OMC	BA	2498	26	-	2/9/27/28	0/2/2/2
26	PSU	BA	2580	26	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
26	PSU	BA	1917	26	-	2/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	2/7/25/26	0/2/2/2

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2503	2MA	C4-N3	12.32	1.49	1.34
26	BA	1915	3TD	C6-C5	11.99	1.49	1.35
26	BA	1618	6MZ	C6-N6	11.41	1.46	1.34
26	BA	2030	6MZ	C6-N6	10.61	1.45	1.34
1	AA	967	5MC	C6-C5	10.01	1.51	1.34
1	AA	1407	5MC	C6-C5	9.87	1.50	1.34
24	AX	20	H2U	C2-N1	9.80	1.49	1.35
26	BA	1915	3TD	C2-N1	9.77	1.49	1.37
26	BA	1962	5MC	C6-C5	9.68	1.50	1.34
23	AW	8	4SU	C4-N3	9.40	1.47	1.37
23	AW	20	H2U	C2-N1	9.32	1.48	1.35
24	AX	16	H2U	C2-N1	9.26	1.48	1.35
24	AX	8	4SU	C4-N3	9.09	1.47	1.37
26	BA	2449	H2U	C2-N1	8.17	1.47	1.35
1	AA	1207	2MG	C2-N3	8.02	1.47	1.31
26	BA	2445	2MG	C2-N3	8.02	1.47	1.31
26	BA	1835	2MG	C2-N3	7.99	1.47	1.31
24	AX	8	4SU	C2-N1	7.96	1.51	1.38
1	AA	966	2MG	C2-N3	7.87	1.47	1.31
26	BA	745	1MG	C2-N3	7.83	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	8	4SU	C2-N1	7.69	1.50	1.38
1	AA	1516	2MG	C2-N3	7.68	1.46	1.31
26	BA	1962	5MC	C4-N3	7.57	1.46	1.34
24	AX	47	3AU	C2-N1	7.52	1.50	1.38
1	AA	967	5MC	C4-N3	7.31	1.46	1.34
26	BA	2503	2MA	C6-N1	7.20	1.45	1.35
26	BA	2503	2MA	C2-N3	7.07	1.46	1.34
1	AA	1407	5MC	C4-N3	7.04	1.46	1.34
24	AX	47	3AU	C6-C5	6.99	1.51	1.35
26	BA	2552	OMU	C2-N3	6.96	1.50	1.38
1	AA	1402	4OC	C4-N3	6.94	1.44	1.32
1	AA	967	5MC	C2-N3	6.87	1.50	1.36
26	BA	1962	5MC	C2-N3	6.78	1.50	1.36
23	AW	8	4SU	C2-N3	6.67	1.49	1.38
26	BA	2251	OMG	C4-N3	6.61	1.50	1.34
24	AX	20	H2U	C2-N3	6.57	1.49	1.38
1	AA	1407	5MC	C2-N3	6.55	1.49	1.36
23	AW	20	H2U	C2-N3	6.54	1.49	1.38
24	AX	16	H2U	C2-N3	6.51	1.49	1.38
1	AA	1402	4OC	C6-C5	6.48	1.50	1.35
23	AW	32	OMC	C2-N3	6.47	1.49	1.36
24	AX	8	4SU	C2-N3	6.46	1.49	1.38
24	AX	47	3AU	C2-N3	6.45	1.49	1.38
1	AA	1498	UR3	C2-N1	6.26	1.47	1.38
26	BA	2498	OMC	C2-N3	6.16	1.48	1.36
26	BA	1915	3TD	C6-N1	6.15	1.46	1.36
39	BN	81	4D4	CZ-NE	6.11	1.45	1.33
26	BA	2552	OMU	C6-C5	6.11	1.49	1.35
1	AA	1498	UR3	C6-C5	6.09	1.49	1.35
26	BA	2449	H2U	C2-N3	6.05	1.48	1.38
23	AW	8	4SU	C6-C5	6.04	1.49	1.35
24	AX	8	4SU	C6-C5	6.03	1.49	1.35
23	AW	32	OMC	C6-C5	5.98	1.49	1.35
24	AX	46	7MG	C4-N9	5.96	1.44	1.37
24	AX	46	7MG	C4-N3	5.95	1.48	1.34
1	AA	1402	4OC	C2-N3	5.92	1.48	1.36
24	AX	46	7MG	C2-N3	5.92	1.47	1.33
26	BA	2069	G7M	C4-N3	5.90	1.48	1.34
24	AX	37	MIA	C6-N6	5.89	1.48	1.34
26	BA	745	1MG	C4-N3	5.88	1.48	1.34
1	AA	527	G7M	C4-N3	5.87	1.48	1.34
26	BA	2552	OMU	C2-N1	5.85	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2498	OMC	C6-C5	5.79	1.48	1.35
26	BA	2503	2MA	C2-N1	5.69	1.44	1.34
23	AW	8	4SU	C5-C4	5.63	1.49	1.42
26	BA	2069	G7M	C5-N7	-5.61	1.32	1.39
23	AW	8	4SU	C4-S4	-5.49	1.58	1.68
24	AX	8	4SU	C5-C4	5.49	1.49	1.42
24	AX	8	4SU	C4-S4	-5.45	1.58	1.68
26	BA	2251	OMG	C2-N2	5.42	1.47	1.34
26	BA	2251	OMG	C2-N3	5.40	1.46	1.33
1	AA	967	5MC	C4-N4	5.38	1.48	1.34
26	BA	745	1MG	C2-N2	5.37	1.43	1.34
26	BA	2445	2MG	C4-N3	5.37	1.47	1.34
26	BA	1962	5MC	C4-N4	5.36	1.48	1.34
26	BA	1835	2MG	C4-N3	5.30	1.46	1.34
1	AA	967	5MC	C6-N1	5.26	1.47	1.38
1	AA	1207	2MG	C4-N3	5.25	1.46	1.34
23	AW	32	OMC	C4-N3	5.23	1.45	1.34
1	AA	1407	5MC	C4-N4	5.23	1.47	1.34
26	BA	1962	5MC	C6-N1	5.23	1.47	1.38
1	AA	1407	5MC	C6-N1	5.17	1.46	1.38
1	AA	966	2MG	C4-N3	5.16	1.46	1.34
24	AX	47	3AU	C4-N3	5.14	1.47	1.38
1	AA	527	G7M	C5-N7	-5.13	1.33	1.39
1	AA	1516	2MG	C4-N3	5.11	1.46	1.34
26	BA	2069	G7M	C2-N3	5.08	1.45	1.33
23	AW	20	H2U	C4-N3	5.07	1.46	1.37
26	BA	2498	OMC	C4-N3	5.04	1.44	1.34
24	AX	16	H2U	C4-N3	4.97	1.46	1.37
26	BA	1915	3TD	C1'-C5	-4.94	1.38	1.50
24	AX	20	H2U	C4-N3	4.92	1.46	1.37
23	AW	32	OMC	C4-N4	4.86	1.45	1.33
1	AA	527	G7M	C2-N3	4.82	1.44	1.33
24	AX	46	7MG	C2-N2	4.81	1.45	1.34
1	AA	1402	4OC	C4-N4	4.78	1.45	1.35
26	BA	2498	OMC	C4-N4	4.78	1.45	1.33
1	AA	1402	4OC	O2-C2	-4.70	1.15	1.23
1	AA	966	2MG	C2-N2	4.70	1.43	1.33
26	BA	1962	5MC	C2-N1	4.67	1.50	1.40
1	AA	1498	UR3	C2-N3	4.67	1.48	1.39
26	BA	2069	G7M	C2-N2	4.63	1.45	1.34
1	AA	1207	2MG	C2-N2	4.59	1.43	1.33
26	BA	2503	2MA	C5-C6	4.55	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C2-N2	4.55	1.45	1.34
26	BA	2449	H2U	C4-N3	4.54	1.45	1.37
26	BA	1835	2MG	C2-N2	4.53	1.43	1.33
26	BA	2445	2MG	C2-N2	4.51	1.43	1.33
23	AW	32	OMC	C2-N1	4.41	1.49	1.40
1	AA	1516	2MG	C2-N2	4.39	1.43	1.33
1	AA	967	5MC	C2-N1	4.39	1.49	1.40
1	AA	1402	4OC	C5-C4	4.37	1.50	1.40
1	AA	1407	5MC	C2-N1	4.35	1.49	1.40
24	AX	46	7MG	C5-C4	4.31	1.43	1.37
1	AA	966	2MG	C2-N1	4.25	1.43	1.36
1	AA	1402	4OC	C2-N1	4.22	1.49	1.40
26	BA	1915	3TD	C2-N3	4.22	1.47	1.38
26	BA	2552	OMU	C4-N3	4.07	1.45	1.38
1	AA	1207	2MG	C2-N1	4.07	1.43	1.36
24	AX	46	7MG	C2-N1	4.05	1.47	1.37
24	AX	46	7MG	C5-C6	4.05	1.52	1.42
1	AA	1516	2MG	C2-N1	3.95	1.43	1.36
26	BA	2498	OMC	C2-N1	3.94	1.48	1.40
26	BA	2445	2MG	C2-N1	3.92	1.43	1.36
26	BA	2552	OMU	O4-C4	-3.84	1.17	1.24
26	BA	1835	2MG	O6-C6	-3.82	1.16	1.23
1	AA	1516	2MG	O6-C6	-3.73	1.16	1.23
26	BA	1835	2MG	C2-N1	3.71	1.42	1.36
26	BA	2445	2MG	O6-C6	-3.70	1.16	1.23
1	AA	1518	MA6	C6-N6	3.64	1.47	1.36
26	BA	2503	2MA	C8-N7	3.62	1.38	1.31
1	AA	1519	MA6	C6-N6	3.61	1.47	1.36
1	AA	966	2MG	O6-C6	-3.59	1.16	1.23
1	AA	1516	2MG	C5-N7	-3.56	1.32	1.39
1	AA	1207	2MG	O6-C6	-3.54	1.16	1.23
24	AX	39	PSU	C6-C5	3.52	1.39	1.35
1	AA	1207	2MG	C5-N7	-3.50	1.32	1.39
24	AX	46	7MG	O6-C6	-3.50	1.16	1.23
26	BA	745	1MG	C5-N7	-3.49	1.32	1.39
24	AX	55	PSU	C6-C5	3.45	1.39	1.35
26	BA	745	1MG	C5-C6	3.43	1.54	1.45
1	AA	1402	4OC	CM4-N4	3.41	1.51	1.45
24	AX	32	PSU	C6-C5	3.39	1.39	1.35
24	AX	46	7MG	C6-N1	3.37	1.45	1.38
26	BA	1835	2MG	C5-N7	-3.37	1.32	1.39
26	BA	2445	2MG	C5-N7	-3.34	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	47	3AU	C6-N1	3.28	1.45	1.38
1	AA	966	2MG	C5-N7	-3.26	1.32	1.39
26	BA	2069	G7M	C5-C6	3.25	1.52	1.43
26	BA	2498	OMC	C6-N1	3.19	1.45	1.38
1	AA	527	G7M	C5-C6	3.16	1.52	1.43
26	BA	2552	OMU	O2-C2	-3.15	1.17	1.23
26	BA	2030	6MZ	C5-C4	-3.14	1.33	1.39
1	AA	1519	MA6	C5-C4	-3.12	1.33	1.39
1	AA	1402	4OC	C6-N1	3.11	1.45	1.38
26	BA	1939	5MU	C4-N3	-3.11	1.33	1.38
24	AX	8	4SU	C6-N1	3.11	1.45	1.38
24	AX	8	4SU	O2-C2	-3.10	1.17	1.23
23	AW	8	4SU	C6-N1	3.10	1.45	1.38
23	AW	8	4SU	O2-C2	-3.08	1.17	1.23
23	AW	55	PSU	C6-C5	3.07	1.38	1.35
23	AW	32	OMC	C6-N1	3.03	1.45	1.38
26	BA	1911	PSU	C6-C5	3.03	1.38	1.35
26	BA	746	PSU	C6-C5	3.02	1.38	1.35
24	AX	46	7MG	C5-N7	3.00	1.44	1.35
26	BA	1915	3TD	O2-C2	-2.98	1.17	1.23
26	BA	2251	OMG	C5-N7	-2.98	1.33	1.39
26	BA	1915	3TD	O4-C4	-2.97	1.16	1.23
26	BA	1915	3TD	C4-N3	2.97	1.46	1.40
26	BA	747	5MU	C4-N3	-2.95	1.33	1.38
1	AA	966	2MG	C6-N1	2.93	1.44	1.38
26	BA	2604	PSU	C6-C5	2.92	1.38	1.35
24	AX	47	3AU	O4-C4	-2.91	1.18	1.24
1	AA	966	2MG	C4-N9	-2.90	1.30	1.38
26	BA	2580	PSU	C6-C5	2.90	1.38	1.35
26	BA	2503	2MA	C6-N6	-2.90	1.26	1.34
1	AA	1207	2MG	C6-N1	2.90	1.44	1.38
26	BA	955	PSU	C6-C5	2.89	1.38	1.35
26	BA	2457	PSU	C6-C5	2.89	1.38	1.35
23	AW	32	OMC	O2-C2	-2.88	1.18	1.23
1	AA	1518	MA6	C10-N6	2.88	1.52	1.45
1	AA	527	G7M	O6-C6	-2.87	1.18	1.23
26	BA	2498	OMC	O2-C2	-2.87	1.18	1.23
1	AA	516	PSU	C6-C5	2.87	1.38	1.35
1	AA	1518	MA6	C5-C4	-2.85	1.33	1.39
26	BA	2605	PSU	C6-C5	2.84	1.38	1.35
1	AA	1519	MA6	C10-N6	2.83	1.52	1.45
24	AX	37	MIA	C4-N9	-2.80	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1618	6MZ	C5-N7	-2.80	1.33	1.39
1	AA	1519	MA6	C8-N9	-2.79	1.32	1.37
24	AX	47	3AU	C5-C4	2.77	1.49	1.43
24	AX	54	5MU	C4-N3	-2.75	1.33	1.38
26	BA	1917	PSU	C6-C5	2.70	1.38	1.35
26	BA	747	5MU	C6-N1	-2.70	1.33	1.38
1	AA	1498	UR3	C6-N1	2.70	1.44	1.38
26	BA	2503	2MA	C5-N7	-2.69	1.33	1.39
23	AW	54	5MU	C4-N3	-2.68	1.33	1.38
1	AA	1516	2MG	C6-N1	2.67	1.43	1.38
26	BA	2069	G7M	O6-C6	-2.66	1.18	1.23
26	BA	1939	5MU	C6-N1	-2.66	1.33	1.38
24	AX	37	MIA	C5-N7	-2.66	1.34	1.39
26	BA	2030	6MZ	C5-N7	-2.63	1.34	1.39
26	BA	2251	OMG	C2-N1	2.63	1.44	1.37
26	BA	1618	6MZ	C5-C4	-2.63	1.34	1.39
26	BA	1835	2MG	C6-N1	2.61	1.43	1.38
26	BA	2069	G7M	C2-N1	2.61	1.44	1.37
1	AA	527	G7M	C4-N9	-2.59	1.31	1.38
26	BA	2445	2MG	C6-N1	2.58	1.43	1.38
1	AA	1516	2MG	C4-N9	-2.58	1.31	1.38
26	BA	1962	5MC	O2-C2	-2.58	1.18	1.23
23	AW	54	5MU	C6-C5	2.57	1.38	1.34
26	BA	1939	5MU	C2-N3	-2.57	1.33	1.38
26	BA	747	5MU	C6-C5	2.57	1.38	1.34
26	BA	1939	5MU	C6-C5	2.57	1.38	1.34
1	AA	1407	5MC	O2-C2	-2.57	1.19	1.23
1	AA	1518	MA6	C8-N9	-2.56	1.32	1.37
26	BA	1915	3TD	C10-N3	2.55	1.51	1.47
39	BN	81	4D4	CZ-NH1	2.55	1.45	1.34
26	BA	1915	3TD	O4'-C1'	-2.53	1.40	1.43
24	AX	47	3AU	O2-C2	-2.52	1.18	1.23
26	BA	2030	6MZ	C8-N9	-2.52	1.33	1.37
1	AA	1207	2MG	C4-N9	-2.51	1.31	1.38
26	BA	2251	OMG	C6-N1	2.51	1.43	1.38
26	BA	2449	H2U	O2-C2	-2.51	1.18	1.23
26	BA	2504	PSU	C6-C5	2.50	1.38	1.35
26	BA	2251	OMG	O6-C6	-2.47	1.18	1.23
1	AA	967	5MC	O2-C2	-2.46	1.19	1.23
1	AA	1498	UR3	O4-C4	-2.46	1.18	1.23
26	BA	2069	G7M	C4-N9	-2.44	1.31	1.38
24	AX	20	H2U	O4-C4	-2.43	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C2-N1	2.42	1.43	1.37
23	AW	54	5MU	C6-N1	-2.42	1.33	1.38
26	BA	2251	OMG	C5-C6	2.41	1.53	1.44
26	BA	2552	OMU	C6-N1	2.41	1.43	1.38
26	BA	747	5MU	C2-N3	-2.40	1.33	1.38
24	AX	37	MIA	C5-C4	-2.40	1.34	1.39
26	BA	1835	2MG	C4-N9	-2.40	1.31	1.38
1	AA	966	2MG	C5-C6	2.40	1.53	1.44
24	AX	54	5MU	C6-N1	-2.39	1.34	1.38
26	BA	2503	2MA	CM2-C2	2.37	1.56	1.49
23	AW	20	H2U	O2-C2	-2.37	1.18	1.23
1	AA	1498	UR3	O2-C2	-2.37	1.18	1.22
26	BA	2503	2MA	C8-N9	-2.36	1.33	1.37
26	BA	2445	2MG	C5-C6	2.36	1.53	1.44
26	BA	2449	H2U	O4-C4	-2.35	1.18	1.23
1	AA	1207	2MG	C5-C6	2.34	1.53	1.44
24	AX	54	5MU	C2-N3	-2.33	1.33	1.38
26	BA	1835	2MG	C5-C6	2.33	1.53	1.44
24	AX	16	H2U	O2-C2	-2.33	1.18	1.23
24	AX	54	5MU	C6-C5	2.32	1.38	1.34
23	AW	32	OMC	C5-C4	2.31	1.48	1.42
26	BA	2069	G7M	C6-N1	2.31	1.43	1.38
23	AW	54	5MU	C4-C5	2.27	1.48	1.44
1	AA	1518	MA6	C8-N7	2.26	1.35	1.31
26	BA	2445	2MG	C4-N9	-2.26	1.32	1.38
1	AA	527	G7M	C6-N1	2.25	1.43	1.38
24	AX	16	H2U	O4-C4	-2.25	1.18	1.23
1	AA	1519	MA6	C5-N7	-2.22	1.34	1.39
24	AX	20	H2U	O2-C2	-2.22	1.19	1.23
1	AA	1516	2MG	C5-C6	2.21	1.52	1.44
26	BA	1618	6MZ	C8-N9	-2.21	1.33	1.37
23	AW	20	H2U	O4-C4	-2.16	1.18	1.23
23	AW	54	5MU	C2-N3	-2.14	1.34	1.38
1	AA	1519	MA6	C8-N7	2.13	1.35	1.31
26	BA	2498	OMC	C5-C4	2.12	1.47	1.42
1	AA	1518	MA6	C5-N7	-2.12	1.35	1.39
26	BA	2504	PSU	O4'-C1'	-2.09	1.40	1.43
1	AA	516	PSU	C4-C5	-2.09	1.38	1.44
26	BA	955	PSU	C4-C5	-2.09	1.38	1.44
26	BA	2580	PSU	C4-C5	-2.04	1.38	1.44
26	BA	2504	PSU	C4-C5	-2.04	1.38	1.44
1	AA	1498	UR3	C5-C4	2.03	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	54	5MU	C4-C5	2.02	1.48	1.44
26	BA	2030	6MZ	C6-N1	-2.02	1.31	1.35
24	AX	32	PSU	C4-C5	-2.01	1.38	1.44

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-16.51	99.03	117.08
1	AA	1519	MA6	N1-C6-N6	-16.20	99.37	117.08
1	AA	1518	MA6	C5-C6-N6	9.15	141.24	125.30
1	AA	1519	MA6	C5-C6-N6	8.73	140.50	125.30
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34
1	AA	1207	2MG	C1'-N9-C8	-8.03	103.83	126.70
26	BA	1835	2MG	C1'-N9-C8	-8.01	103.89	126.70
26	BA	2445	2MG	C1'-N9-C8	-7.95	104.07	126.70
24	AX	8	4SU	C4-N3-C2	-7.83	119.73	127.34
24	AX	46	7MG	C5-C4-N3	-7.48	120.08	127.80
1	AA	1516	2MG	C1'-N9-C8	-7.44	105.52	126.70
26	BA	2503	2MA	C1'-N9-C8	-7.44	110.34	127.14
1	AA	1207	2MG	C1'-N9-C4	7.26	148.07	126.50
26	BA	2449	H2U	C4-N3-C2	-7.25	119.78	125.79
26	BA	2445	2MG	C1'-N9-C4	7.21	147.91	126.50
26	BA	1835	2MG	C1'-N9-C4	7.17	147.81	126.50
24	AX	16	H2U	C4-N3-C2	-6.94	120.03	125.79
1	AA	1516	2MG	C1'-N9-C4	6.88	146.94	126.50
1	AA	966	2MG	C1'-N9-C8	-6.83	107.25	126.70
24	AX	20	H2U	C4-N3-C2	-6.81	120.14	125.79
23	AW	20	H2U	C4-N3-C2	-6.78	120.17	125.79
26	BA	2069	G7M	C1'-N9-C8	-6.68	104.20	126.74
26	BA	2069	G7M	C1'-N9-C4	6.64	146.22	126.50
26	BA	2030	6MZ	C9-N6-C6	-6.59	117.20	122.87
1	AA	527	G7M	C1'-N9-C8	-6.47	104.88	126.74
26	BA	1835	2MG	C2-N3-C4	6.41	119.99	112.04
1	AA	1207	2MG	C2-N3-C4	6.35	119.91	112.04
26	BA	2445	2MG	C2-N3-C4	6.29	119.84	112.04
1	AA	966	2MG	C2-N3-C4	6.12	119.63	112.04
1	AA	1516	2MG	C2-N3-C4	6.11	119.62	112.04
1	AA	527	G7M	C1'-N9-C4	6.03	144.41	126.50
1	AA	527	G7M	CN7-N7-C5	5.87	134.06	126.77
26	BA	1915	3TD	N1-C2-N3	5.84	120.75	116.14
26	BA	1939	5MU	C4-N3-C2	-5.84	119.79	127.35
1	AA	966	2MG	C1'-N9-C4	5.77	143.64	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2030	6MZ	N1-C2-N3	-5.63	119.79	128.60
26	BA	1939	5MU	N3-C2-N1	5.62	122.35	114.89
26	BA	2503	2MA	N9-C8-N7	-5.61	106.23	113.91
1	AA	1519	MA6	C5-C4-N3	-5.61	119.43	126.75
23	AW	8	4SU	C5-C4-N3	5.55	119.83	114.69
1	AA	1519	MA6	N1-C2-N3	-5.53	119.96	128.60
26	BA	1618	6MZ	C5-C4-N3	-5.50	119.57	126.75
26	BA	2069	G7M	CN7-N7-C5	5.50	133.60	126.77
26	BA	2503	2MA	C4-N9-C1'	5.47	139.63	126.59
26	BA	745	1MG	C5-C4-N3	-5.45	119.62	128.46
24	AX	8	4SU	C5-C4-N3	5.40	119.70	114.69
26	BA	747	5MU	C4-N3-C2	-5.39	120.37	127.35
26	BA	1618	6MZ	N1-C2-N3	-5.34	120.25	128.60
26	BA	747	5MU	N3-C2-N1	5.29	121.92	114.89
24	AX	37	MIA	N3-C2-N1	-5.22	120.44	128.60
1	AA	1518	MA6	N1-C2-N3	-5.21	120.44	128.60
26	BA	2030	6MZ	N9-C8-N7	-5.20	106.80	113.91
23	AW	54	5MU	C4-N3-C2	-5.20	120.62	127.35
24	AX	54	5MU	C4-N3-C2	-5.19	120.64	127.35
26	BA	2552	OMU	C4-N3-C2	-5.19	119.74	126.58
26	BA	2503	2MA	C5-C4-N3	-5.17	121.38	127.19
1	AA	1518	MA6	C5-C4-N3	-5.15	120.04	126.75
24	AX	37	MIA	C5-C4-N3	-5.01	120.21	126.75
1	AA	1498	UR3	C4-N3-C2	-4.96	119.89	124.56
23	AW	54	5MU	N3-C2-N1	4.95	121.46	114.89
26	BA	2504	PSU	N1-C2-N3	4.91	120.69	115.13
1	AA	527	G7M	CN7-N7-C8	-4.91	117.27	124.84
24	AX	47	3AU	C4-N3-C2	-4.90	120.12	126.58
26	BA	2605	PSU	C4-N3-C2	-4.88	119.31	126.34
26	BA	2457	PSU	C4-N3-C2	-4.88	119.31	126.34
26	BA	2504	PSU	C4-N3-C2	-4.84	119.37	126.34
24	AX	54	5MU	N3-C2-N1	4.77	121.22	114.89
24	AX	55	PSU	C4-N3-C2	-4.76	119.48	126.34
26	BA	746	PSU	C4-N3-C2	-4.76	119.49	126.34
26	BA	2251	OMG	C5-C4-N3	-4.75	120.75	128.46
26	BA	1835	2MG	C2-N1-C6	-4.74	119.03	124.48
24	AX	55	PSU	N1-C2-N3	4.71	120.46	115.13
26	BA	1939	5MU	C5-C4-N3	4.70	119.32	115.31
26	BA	2605	PSU	N1-C2-N3	4.69	120.44	115.13
26	BA	1911	PSU	C4-N3-C2	-4.69	119.59	126.34
26	BA	2251	OMG	C1'-N9-C8	-4.69	113.36	126.70
1	AA	1519	MA6	N9-C8-N7	-4.67	107.53	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	1939	5MU	C5-C6-N1	-4.66	118.54	123.34
24	AX	54	5MU	C5-C4-N3	4.65	119.28	115.31
26	BA	1917	PSU	C4-N3-C2	-4.64	119.66	126.34
26	BA	2445	2MG	C5-C4-N3	-4.61	120.97	128.46
26	BA	2457	PSU	N1-C2-N3	4.60	120.34	115.13
26	BA	2580	PSU	C4-N3-C2	-4.60	119.72	126.34
26	BA	955	PSU	C4-N3-C2	-4.57	119.75	126.34
24	AX	39	PSU	C4-N3-C2	-4.56	119.76	126.34
1	AA	1516	2MG	C2-N1-C6	-4.56	119.24	124.48
1	AA	1518	MA6	N9-C8-N7	-4.54	107.70	113.91
1	AA	1207	2MG	C5-C4-N3	-4.54	121.10	128.46
26	BA	1835	2MG	C5-C4-N3	-4.54	121.10	128.46
26	BA	2604	PSU	C4-N3-C2	-4.52	119.83	126.34
26	BA	2030	6MZ	C5-C4-N3	-4.52	120.85	126.75
1	AA	516	PSU	C4-N3-C2	-4.52	119.83	126.34
24	AX	32	PSU	C4-N3-C2	-4.51	119.85	126.34
1	AA	1207	2MG	C2-N1-C6	-4.48	119.32	124.48
26	BA	2069	G7M	CN7-N7-C8	-4.48	117.93	124.84
26	BA	2580	PSU	N1-C2-N3	4.48	120.20	115.13
24	AX	46	7MG	C2-N3-C4	4.48	120.28	112.30
26	BA	747	5MU	C5-C4-N3	4.45	119.11	115.31
24	AX	32	PSU	N1-C2-N3	4.42	120.14	115.13
26	BA	746	PSU	N1-C2-N3	4.41	120.13	115.13
26	BA	1917	PSU	N1-C2-N3	4.41	120.13	115.13
26	BA	1618	6MZ	C4-C5-C6	4.40	120.22	116.81
23	AW	55	PSU	C4-N3-C2	-4.40	120.00	126.34
26	BA	1911	PSU	N1-C2-N3	4.39	120.11	115.13
26	BA	747	5MU	O4-C4-C5	-4.39	119.82	124.90
26	BA	2445	2MG	C2-N1-C6	-4.38	119.44	124.48
24	AX	39	PSU	N1-C2-N3	4.36	120.07	115.13
24	AX	37	MIA	N9-C8-N7	-4.33	107.99	113.91
23	AW	55	PSU	N1-C2-N3	4.31	120.02	115.13
23	AW	54	5MU	C5-C4-N3	4.31	118.99	115.31
1	AA	1516	2MG	C5-C4-N3	-4.30	121.48	128.46
26	BA	1915	3TD	C4-N3-C2	-4.22	120.03	124.61
1	AA	966	2MG	C2-N1-C6	-4.21	119.64	124.48
1	AA	516	PSU	N1-C2-N3	4.20	119.89	115.13
26	BA	1618	6MZ	N9-C8-N7	-4.16	108.22	113.91
26	BA	2604	PSU	N1-C2-N3	4.15	119.83	115.13
24	AX	54	5MU	O4-C4-C5	-4.14	120.10	124.90
1	AA	527	G7M	C5-C6-N1	4.11	120.36	111.79
1	AA	527	G7M	C2-N3-C4	4.10	119.60	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	955	PSU	N1-C2-N3	4.09	119.76	115.13
1	AA	1519	MA6	C4-C5-C6	4.07	120.44	115.88
26	BA	2251	OMG	C2-N3-C4	4.07	119.55	112.30
1	AA	1518	MA6	C4-C5-C6	4.03	120.39	115.88
12	AL	89	D2T	CB1-SB-CB	4.02	109.71	102.44
26	BA	2503	2MA	C4-N9-C8	3.96	110.02	105.73
26	BA	2069	G7M	C2-N3-C4	3.95	119.34	112.30
24	AX	47	3AU	N3-C2-N1	3.95	120.13	114.89
24	AX	8	4SU	N3-C2-N1	3.94	120.12	114.89
1	AA	527	G7M	O6-C6-C5	-3.91	119.24	128.06
26	BA	2251	OMG	N9-C8-N7	-3.84	106.15	113.39
26	BA	1939	5MU	O4-C4-C5	-3.84	120.45	124.90
23	AW	54	5MU	C5-C6-N1	-3.84	119.39	123.34
23	AW	8	4SU	N3-C2-N1	3.83	119.98	114.89
26	BA	2069	G7M	C5-C6-N1	3.81	119.75	111.79
23	AW	54	5MU	O4-C4-C5	-3.80	120.50	124.90
26	BA	2069	G7M	O6-C6-C5	-3.79	119.52	128.06
26	BA	2552	OMU	N3-C2-N1	3.74	119.86	114.89
24	AX	54	5MU	C5-C6-N1	-3.74	119.49	123.34
1	AA	966	2MG	C5-C4-N3	-3.74	122.39	128.46
1	AA	966	2MG	N9-C8-N7	-3.71	106.41	113.39
26	BA	747	5MU	C5-C6-N1	-3.70	119.53	123.34
1	AA	1519	MA6	N3-C4-N9	3.68	133.14	127.08
26	BA	745	1MG	N9-C4-N3	3.66	133.29	125.94
1	AA	1519	MA6	C2-N3-C4	3.61	120.29	111.75
26	BA	745	1MG	C2-N3-C4	3.61	120.10	111.98
26	BA	2069	G7M	C5-C4-N3	-3.59	121.26	128.15
26	BA	1962	5MC	C5-C6-N1	-3.58	119.65	123.34
26	BA	1618	6MZ	C2-N3-C4	3.53	120.09	111.75
26	BA	2503	2MA	C5-N7-C8	3.51	108.50	103.51
23	AW	8	4SU	C5-C4-S4	-3.51	119.95	124.47
26	BA	1939	5MU	O2-C2-N1	-3.50	118.13	122.79
1	AA	1516	2MG	CM2-N2-C2	-3.48	116.16	123.86
1	AA	1518	MA6	C2-N1-C6	3.46	119.92	111.75
1	AA	1407	5MC	C5-C6-N1	-3.45	119.79	123.34
26	BA	2030	6MZ	C4-N9-C8	3.41	109.42	105.73
26	BA	1618	6MZ	N3-C4-N9	3.41	132.69	127.08
24	AX	8	4SU	C5-C4-S4	-3.40	120.09	124.47
26	BA	2030	6MZ	C5-N7-C8	3.40	108.33	103.51
1	AA	1519	MA6	C2-N1-C6	3.39	119.76	111.75
24	AX	37	MIA	C2-N3-C4	3.38	119.73	111.75
24	AX	46	7MG	O6-C6-C5	-3.37	119.52	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2251	OMG	N9-C4-N3	3.33	132.62	125.94
26	BA	2030	6MZ	C2-N3-C4	3.33	119.61	111.75
26	BA	2552	OMU	C5-C4-N3	3.31	119.80	114.84
26	BA	2030	6MZ	C4-C5-C6	3.29	119.36	116.81
1	AA	527	G7M	C5-C4-N3	-3.29	121.84	128.15
26	BA	1835	2MG	N9-C8-N7	-3.29	107.19	113.39
1	AA	1518	MA6	N3-C4-N9	3.29	132.50	127.08
24	AX	20	H2U	C5-C4-N3	3.28	120.34	116.65
26	BA	2251	OMG	C1'-N9-C4	3.28	136.24	126.50
1	AA	1518	MA6	C2-N3-C4	3.28	119.49	111.75
24	AX	47	3AU	C5-C4-N3	3.27	119.74	114.84
26	BA	746	PSU	O2'-C2'-C3'	3.27	122.40	111.82
1	AA	1519	MA6	C5-N7-C8	3.21	108.07	103.51
26	BA	745	1MG	N9-C8-N7	-3.21	107.35	113.39
26	BA	2449	H2U	C5-C4-N3	3.17	120.21	116.65
26	BA	2503	2MA	N3-C2-N1	-3.17	119.90	125.72
26	BA	2445	2MG	N9-C8-N7	-3.14	107.48	113.39
24	AX	16	H2U	N3-C2-N1	3.12	119.95	116.65
26	BA	1618	6MZ	C5-N7-C8	3.11	107.93	103.51
1	AA	516	PSU	O4'-C1'-C2'	3.09	109.50	105.14
26	BA	2251	OMG	C2-N1-C6	-3.07	119.50	125.10
24	AX	37	MIA	C5-N7-C8	3.07	107.87	103.51
23	AW	20	H2U	N3-C2-N1	3.06	119.89	116.65
1	AA	1207	2MG	N9-C8-N7	-3.05	107.64	113.39
23	AW	55	PSU	O2-C2-N1	-3.05	119.43	122.79
1	AA	1518	MA6	C5-N7-C8	3.04	107.83	103.51
1	AA	1516	2MG	N9-C8-N7	-3.03	107.69	113.39
24	AX	46	7MG	C2-N1-C6	-3.01	119.61	125.10
26	BA	2069	G7M	C2-N1-C6	-3.01	119.62	125.10
24	AX	46	7MG	N9-C4-N3	3.00	129.96	125.47
24	AX	55	PSU	O2-C2-N1	-3.00	119.49	122.79
1	AA	527	G7M	C2-N1-C6	-2.98	119.66	125.10
26	BA	2552	OMU	O4-C4-C5	-2.98	119.92	125.16
26	BA	2503	2MA	N3-C4-N9	2.98	131.12	126.99
26	BA	2449	H2U	N3-C2-N1	2.97	119.79	116.65
26	BA	1835	2MG	CM2-N2-C2	-2.93	117.38	123.86
12	AL	89	D2T	O-C-CA	-2.93	117.10	124.78
26	BA	1835	2MG	C5-C6-N1	2.90	120.56	113.19
26	BA	2580	PSU	O4'-C1'-C2'	2.88	109.20	105.14
24	AX	54	5MU	O2-C2-N1	-2.87	118.98	122.79
26	BA	746	PSU	C3'-C2'-C1'	2.86	104.97	101.64
26	BA	2449	H2U	O2-C2-N1	-2.85	119.53	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	2504	PSU	O2-C2-N1	-2.84	119.66	122.79
26	BA	2030	6MZ	N3-C4-N9	2.83	131.74	127.08
26	BA	2605	PSU	O2-C2-N1	-2.81	119.69	122.79
24	AX	47	3AU	O4-C4-C5	-2.81	120.22	125.16
24	AX	37	MIA	N3-C4-N9	2.79	131.68	127.08
1	AA	966	2MG	N1-C2-N3	-2.77	119.66	123.95
24	AX	20	H2U	C5-C6-N1	2.77	120.75	111.61
1	AA	516	PSU	C3'-C2'-C1'	2.77	104.86	101.64
26	BA	2069	G7M	N9-C4-N3	2.76	131.48	125.94
1	AA	1519	MA6	C4-N9-C8	2.76	108.72	105.73
26	BA	2251	OMG	C5-C6-N1	2.75	120.16	113.19
26	BA	2449	H2U	C5-C6-N1	2.74	120.66	111.61
23	AW	20	H2U	C5-C6-N1	2.74	120.64	111.61
26	BA	2580	PSU	O2-C2-N1	-2.73	119.78	122.79
26	BA	2580	PSU	C3'-C2'-C1'	2.73	104.82	101.64
1	AA	967	5MC	C5-C6-N1	-2.73	120.53	123.34
1	AA	527	G7M	N9-C4-N3	2.72	131.40	125.94
26	BA	1917	PSU	O2-C2-N1	-2.71	119.80	122.79
23	AW	20	H2U	C5-C4-N3	2.71	119.70	116.65
1	AA	1518	MA6	C4-N9-C8	2.71	108.67	105.73
24	AX	16	H2U	C5-C4-N3	2.71	119.69	116.65
24	AX	16	H2U	C5-C6-N1	2.70	120.50	111.61
1	AA	966	2MG	O3'-C3'-C4'	2.68	118.81	111.05
1	AA	966	2MG	C5-C6-N1	2.68	119.99	113.19
1	AA	1516	2MG	C5-C6-N1	2.67	119.97	113.19
26	BA	745	1MG	C1'-N9-C4	-2.67	118.58	126.50
26	BA	2445	2MG	C5-C6-N1	2.66	119.95	113.19
1	AA	527	G7M	N9-C8-N7	-2.65	105.66	112.21
26	BA	2445	2MG	CM2-N2-C2	-2.64	118.02	123.86
1	AA	1207	2MG	C5-C6-N1	2.62	119.84	113.19
26	BA	2504	PSU	C6-N1-C2	-2.62	120.01	122.68
24	AX	46	7MG	C5-C6-N1	2.61	120.10	112.31
26	BA	745	1MG	C5-C6-N1	2.61	119.96	114.91
1	AA	1402	4OC	CM4-N4-C4	-2.61	117.36	122.45
23	AW	55	PSU	C3'-C2'-C1'	2.60	104.66	101.64
24	AX	16	H2U	O2-C2-N1	-2.59	119.85	123.11
1	AA	1207	2MG	O6-C6-C5	-2.59	119.73	126.60
1	AA	1516	2MG	O6-C6-C5	-2.58	119.74	126.60
23	AW	54	5MU	O2-C2-N1	-2.57	119.36	122.79
23	AW	20	H2U	O2-C2-N1	-2.56	119.89	123.11
26	BA	2457	PSU	O2-C2-N1	-2.56	119.97	122.79
26	BA	1835	2MG	O6-C6-C5	-2.55	119.84	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	747	5MU	O2-C2-N1	-2.55	119.40	122.79
1	AA	966	2MG	O6-C6-C5	-2.53	119.89	126.60
26	BA	746	PSU	O2-C2-N1	-2.50	120.04	122.79
23	AW	55	PSU	C6-N1-C2	-2.50	120.13	122.68
1	AA	516	PSU	O2-C2-N1	-2.48	120.06	122.79
1	AA	1207	2MG	N1-C2-N3	-2.47	120.14	123.95
26	BA	2445	2MG	N1-C2-N3	-2.46	120.14	123.95
26	BA	2503	2MA	CM2-C2-N1	2.46	120.99	117.15
26	BA	1835	2MG	N1-C2-N3	-2.45	120.17	123.95
24	AX	55	PSU	C6-C5-C4	2.44	119.91	118.20
26	BA	2445	2MG	O6-C6-C5	-2.44	120.13	126.60
26	BA	2251	OMG	O6-C6-C5	-2.43	120.16	126.60
26	BA	2251	OMG	C8-N7-C5	2.43	108.63	104.24
24	AX	20	H2U	N3-C2-N1	2.42	119.22	116.65
1	AA	516	PSU	C6-N1-C2	-2.41	120.22	122.68
26	BA	1917	PSU	C6-N1-C2	-2.39	120.24	122.68
1	AA	966	2MG	C4-C5-N7	-2.37	106.97	110.72
26	BA	2503	2MA	C4-C5-N7	-2.36	107.74	110.62
1	AA	1516	2MG	N1-C2-N3	-2.36	120.30	123.95
24	AX	46	7MG	C5-C4-N9	2.36	109.97	106.68
26	BA	746	PSU	C6-C5-C4	2.34	119.83	118.20
1	AA	966	2MG	C8-N7-C5	2.33	108.46	104.24
23	AW	55	PSU	O2'-C2'-C3'	2.33	119.35	111.82
26	BA	2457	PSU	O4'-C1'-C2'	2.32	108.42	105.14
24	AX	32	PSU	C6-N1-C2	-2.31	120.32	122.68
1	AA	966	2MG	CM2-N2-C2	-2.31	118.76	123.86
26	BA	2504	PSU	C6-C5-C4	2.30	119.81	118.20
26	BA	2069	G7M	N9-C8-N7	-2.30	106.52	112.21
1	AA	1402	4OC	C6-C5-C4	2.30	119.78	116.96
12	AL	89	D2T	OD2-CG-CB	2.30	118.11	113.15
26	BA	2580	PSU	C6-N1-C2	-2.30	120.34	122.68
26	BA	2605	PSU	C6-N1-C2	-2.28	120.35	122.68
26	BA	2498	OMC	O3'-C3'-C2'	2.28	117.65	111.17
26	BA	2251	OMG	C8-N9-C4	2.28	110.38	106.05
26	BA	1618	6MZ	C9-N6-C6	-2.27	120.92	122.87
26	BA	1835	2MG	C8-N7-C5	2.27	108.34	104.24
1	AA	527	G7M	N2-C2-N1	2.26	121.52	116.71
24	AX	55	PSU	C6-N1-C2	-2.23	120.40	122.68
26	BA	2504	PSU	O2'-C2'-C3'	2.23	119.04	111.82
26	BA	2445	2MG	C8-N7-C5	2.23	108.27	104.24
23	AW	32	OMC	O2-C2-N3	-2.22	118.71	122.33
23	AW	8	4SU	O2-C2-N1	-2.22	119.83	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	1911	PSU	O2-C2-N1	-2.21	120.36	122.79
24	AX	39	PSU	O4'-C1'-C2'	2.21	108.25	105.14
24	AX	46	7MG	C4-C5-N7	2.21	110.43	106.13
24	AX	37	MIA	C4-C5-N7	-2.20	107.93	110.62
1	AA	966	2MG	C6-C5-N7	2.20	134.34	130.25
24	AX	32	PSU	O2-C2-N1	-2.19	120.38	122.79
26	BA	1917	PSU	O4'-C1'-C2'	2.19	108.23	105.14
24	AX	39	PSU	O2-C2-N1	-2.18	120.39	122.79
24	AX	8	4SU	C1'-N1-C2	2.18	121.52	117.57
24	AX	37	MIA	C4-N9-C8	2.18	108.09	105.73
26	BA	2604	PSU	O2-C2-N1	-2.17	120.40	122.79
1	AA	1207	2MG	CM2-N2-C2	-2.17	119.06	123.86
26	BA	955	PSU	C6-N1-C2	-2.17	120.46	122.68
26	BA	745	1MG	C8-N7-C5	2.17	108.16	104.24
26	BA	2445	2MG	N9-C4-N3	2.16	130.28	125.94
26	BA	955	PSU	O2-C2-N1	-2.15	120.42	122.79
26	BA	1835	2MG	C4-C5-N7	-2.15	107.31	110.72
1	AA	1516	2MG	C4-C5-N7	-2.14	107.34	110.72
26	BA	2030	6MZ	C4-C5-N7	-2.12	108.03	110.62
24	AX	39	PSU	C6-N1-C2	-2.12	120.52	122.68
1	AA	1516	2MG	C5-C4-N9	2.11	109.45	105.63
23	AW	55	PSU	O4'-C1'-C2'	2.10	108.11	105.14
26	BA	2605	PSU	C6-C5-C4	2.10	119.67	118.20
1	AA	1516	2MG	C8-N7-C5	2.10	108.03	104.24
26	BA	1915	3TD	C6-C5-C4	2.09	119.66	118.22
26	BA	746	PSU	O2'-C2'-C1'	2.08	116.20	111.23
12	AL	89	D2T	CB-CA-N	2.08	113.53	109.10
1	AA	1207	2MG	N9-C4-N3	2.07	130.09	125.94
1	AA	1207	2MG	C8-N7-C5	2.07	107.98	104.24
26	BA	2605	PSU	O4'-C1'-C2'	2.05	108.03	105.14
26	BA	2069	G7M	N2-C2-N1	2.04	121.06	116.71
26	BA	2445	2MG	C4-C5-N7	-2.04	107.50	110.72
26	BA	1835	2MG	N9-C4-N3	2.04	130.03	125.94
26	BA	746	PSU	C6-N1-C2	-2.03	120.61	122.68
1	AA	1207	2MG	C4-C5-N7	-2.03	107.50	110.72
26	BA	2457	PSU	C6-C5-C4	2.02	119.61	118.20
26	BA	2552	OMU	C1'-N1-C2	2.02	121.23	117.57
1	AA	516	PSU	O2'-C2'-C3'	2.02	118.36	111.82
26	BA	1618	6MZ	C4-N9-C8	2.02	107.91	105.73
26	BA	1618	6MZ	C1'-N9-C8	-2.02	122.58	127.14
26	BA	1915	3TD	O4'-C1'-C2'	2.01	107.98	105.14
1	AA	966	2MG	O4'-C4'-C3'	-2.01	101.13	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	37	MIA	C5-C4-N9	2.00	108.11	105.78
26	BA	2457	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	32	PSU	C2'-C1'-C5-C4
24	AX	46	7MG	O4'-C4'-C5'-O5'
39	BN	81	4D4	O-C-CA-CB
39	BN	81	4D4	CA-CB-CG-CD
23	AW	20	H2U	O4'-C1'-N1-C6
23	AW	20	H2U	C2'-C1'-N1-C2
23	AW	20	H2U	C2'-C1'-N1-C6
23	AW	32	OMC	C1'-C2'-O2'-CM2
26	BA	746	PSU	C2'-C1'-C5-C6
26	BA	746	PSU	O4'-C1'-C5-C6
26	BA	1618	6MZ	N1-C6-N6-C9
26	BA	1618	6MZ	O4'-C4'-C5'-O5'
26	BA	1618	6MZ	C3'-C4'-C5'-O5'
26	BA	1915	3TD	O4'-C1'-C5-C4
26	BA	1915	3TD	C2'-C1'-C5-C6
26	BA	1915	3TD	O4'-C1'-C5-C6
26	BA	2552	OMU	O4'-C4'-C5'-O5'
1	AA	967	5MC	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
24	AX	46	7MG	C3'-C4'-C5'-O5'
24	AX	55	PSU	O4'-C4'-C5'-O5'
23	AW	8	4SU	C3'-C4'-C5'-O5'
23	AW	55	PSU	C3'-C4'-C5'-O5'
26	BA	1917	PSU	C3'-C4'-C5'-O5'
26	BA	1917	PSU	O4'-C4'-C5'-O5'
26	BA	2030	6MZ	O4'-C4'-C5'-O5'
26	BA	2503	2MA	O4'-C4'-C5'-O5'
26	BA	2552	OMU	C3'-C4'-C5'-O5'
29	BD	150	MEQ	CA-CB-CG-CD
1	AA	516	PSU	C3'-C4'-C5'-O5'
1	AA	967	5MC	C3'-C4'-C5'-O5'
24	AX	55	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
23	AW	8	4SU	O4'-C4'-C5'-O5'
23	AW	20	H2U	C3'-C4'-C5'-O5'
23	AW	55	PSU	O4'-C4'-C5'-O5'
26	BA	2449	H2U	O4'-C4'-C5'-O5'
26	BA	2449	H2U	C3'-C4'-C5'-O5'
26	BA	2498	OMC	C3'-C4'-C5'-O5'
29	BD	150	MEQ	NE2-CD-CG-CB
29	BD	150	MEQ	OE1-CD-CG-CB
1	AA	1207	2MG	O4'-C4'-C5'-O5'
26	BA	2498	OMC	O4'-C4'-C5'-O5'
39	BN	81	4D4	OB-CB-CG-CD
23	AW	20	H2U	O4'-C4'-C5'-O5'
26	BA	2445	2MG	C3'-C4'-C5'-O5'
26	BA	2030	6MZ	C3'-C4'-C5'-O5'
26	BA	2030	6MZ	N1-C6-N6-C9
29	BD	150	MEQ	C-CA-CB-CG
24	AX	16	H2U	C2'-C1'-N1-C6
26	BA	2503	2MA	C3'-C4'-C5'-O5'
1	AA	1518	MA6	C5-C6-N6-C10
24	AX	20	H2U	C2'-C1'-N1-C2
23	AW	20	H2U	C4'-C5'-O5'-P
24	AX	20	H2U	C2'-C1'-N1-C6
26	BA	1618	6MZ	C5-C6-N6-C9
26	BA	2445	2MG	O4'-C4'-C5'-O5'
24	AX	47	3AU	C4'-C5'-O5'-P
26	BA	1911	PSU	O4'-C4'-C5'-O5'
26	BA	1939	5MU	O4'-C4'-C5'-O5'
1	AA	527	G7M	C4'-C5'-O5'-P
23	AW	20	H2U	O4'-C1'-N1-C2
26	BA	2069	G7M	C4'-C5'-O5'-P
24	AX	47	3AU	O4'-C4'-C5'-O5'
24	AX	16	H2U	O4'-C1'-N1-C2
24	AX	16	H2U	C2'-C1'-N1-C2
24	AX	55	PSU	O4'-C1'-C5-C6
39	BN	81	4D4	N-CA-CB-CG
1	AA	1519	MA6	C4'-C5'-O5'-P
1	AA	1207	2MG	C3'-C4'-C5'-O5'
23	AW	55	PSU	C4'-C5'-O5'-P
12	AL	89	D2T	CG-CB-SB-CB1
24	AX	32	PSU	O4'-C1'-C5-C6
24	AX	55	PSU	O4'-C1'-C5-C6
23	AW	32	OMC	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
26	BA	1939	5MU	C3'-C4'-C5'-O5'
24	AX	8	4SU	C2'-C1'-N1-C2
1	AA	516	PSU	O4'-C4'-C5'-O5'
26	BA	2069	G7M	O4'-C4'-C5'-O5'
1	AA	967	5MC	C4'-C5'-O5'-P
24	AX	16	H2U	C4'-C5'-O5'-P
24	AX	20	H2U	C4'-C5'-O5'-P
23	AW	32	OMC	C2'-C1'-N1-C6

There are no ring outliers.

24 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
26	BA	1915	3TD	3	0
26	BA	2605	PSU	1	0
1	AA	516	PSU	1	0
24	AX	37	MIA	1	0
26	BA	2449	H2U	1	0
24	AX	54	5MU	1	0
1	AA	1207	2MG	3	0
12	AL	89	D2T	3	0
23	AW	32	OMC	1	0
23	AW	55	PSU	1	0
29	BD	150	MEQ	2	0
24	AX	39	PSU	1	0
1	AA	1519	MA6	1	0
26	BA	2504	PSU	1	0
1	AA	527	G7M	1	0
24	AX	16	H2U	1	0
1	AA	1516	2MG	1	0
26	BA	2251	OMG	2	0
1	AA	966	2MG	2	0
24	AX	20	H2U	3	0
26	BA	2030	6MZ	1	0
1	AA	967	5MC	1	0
26	BA	1917	PSU	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 484 ligands modelled in this entry, 483 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
67	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	PHE	AX	101	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	AX	101	PHE	CA-CB-CG-CD1
67	AX	101	PHE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

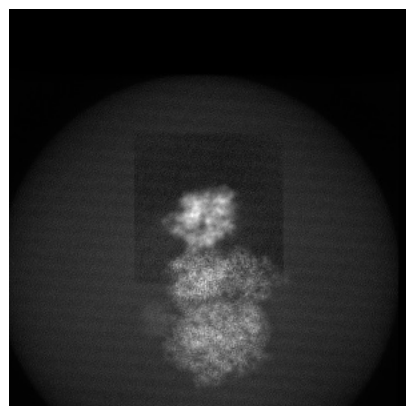
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11418. These allow visual inspection of the internal detail of the map and identification of artifacts.

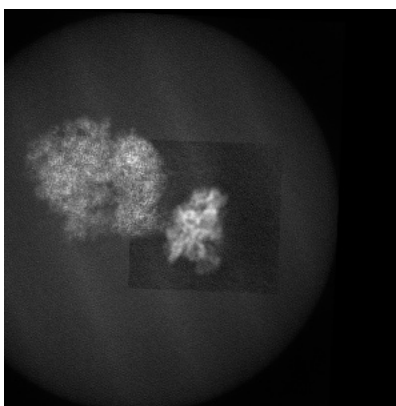
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

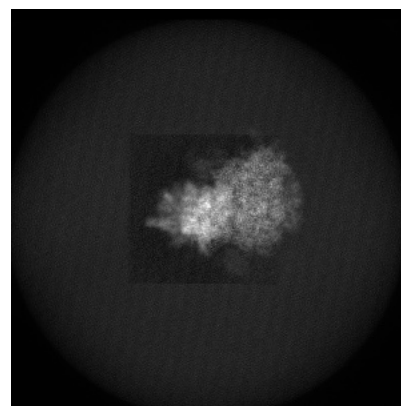
6.1.1 Primary map



X

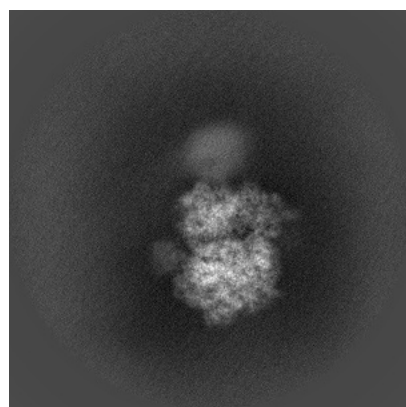


Y

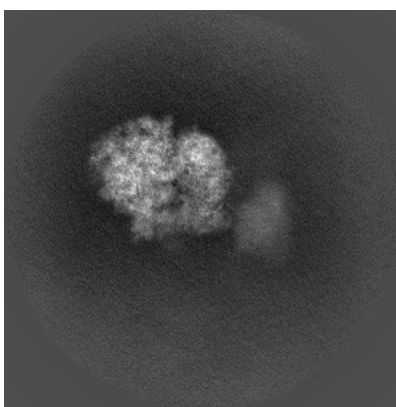


Z

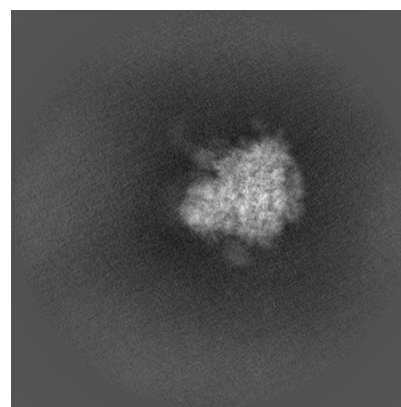
6.1.2 Raw map



X



Y

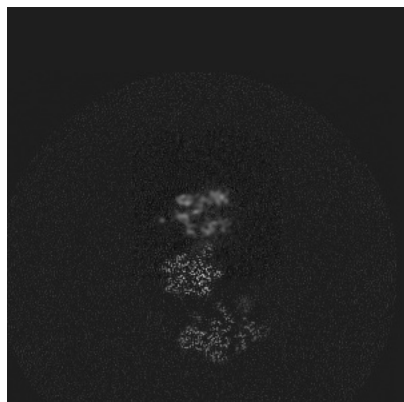


Z

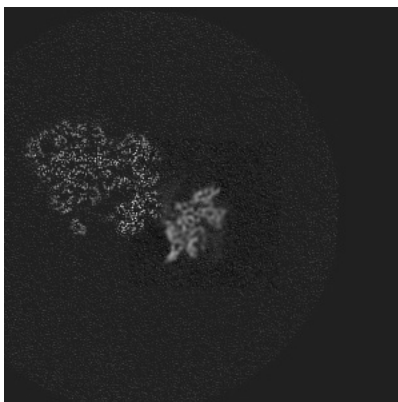
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

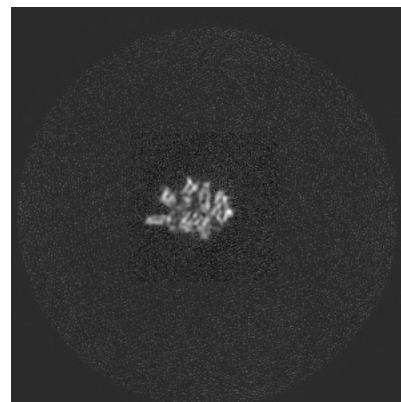
6.2.1 Primary map



X Index: 320

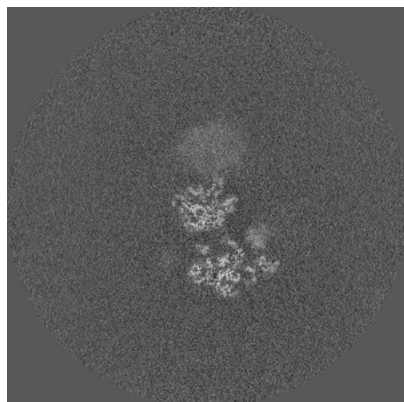


Y Index: 320

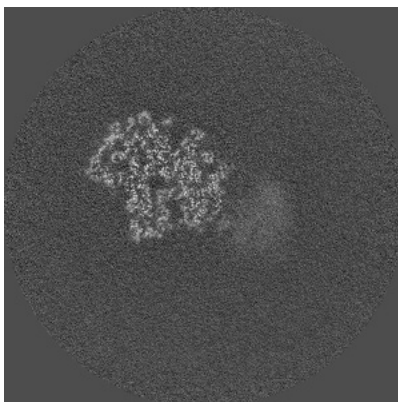


Z Index: 320

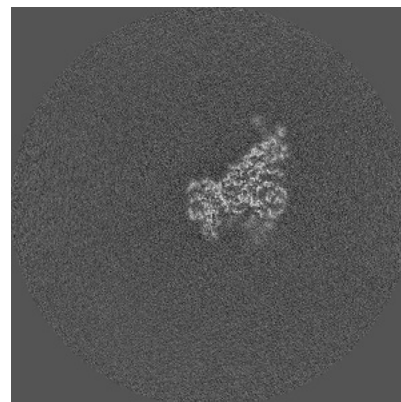
6.2.2 Raw map



X Index: 320



Y Index: 320

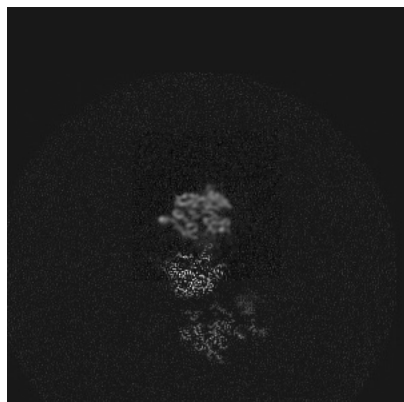


Z Index: 320

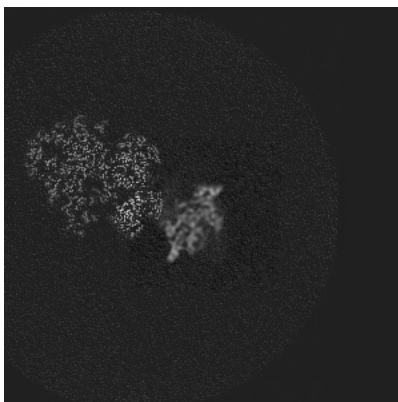
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

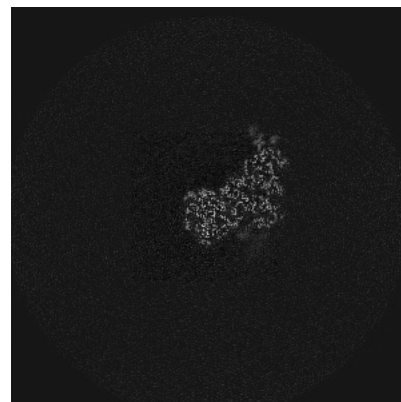
6.3.1 Primary map



X Index: 315

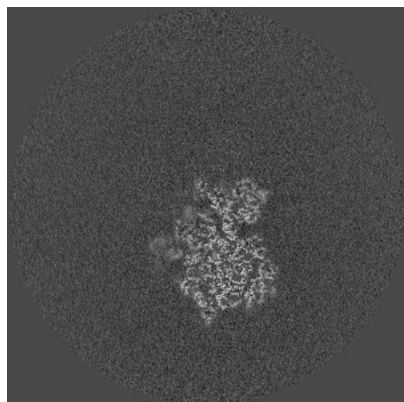


Y Index: 315

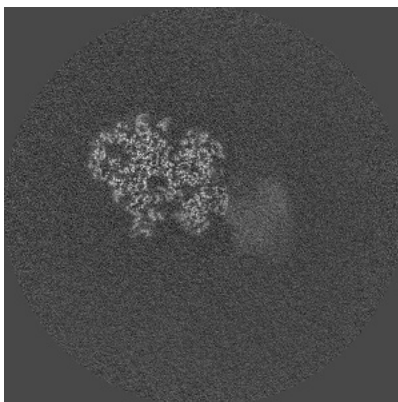


Z Index: 212

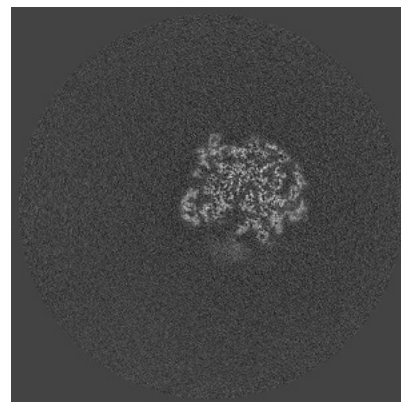
6.3.2 Raw map



X Index: 377



Y Index: 331

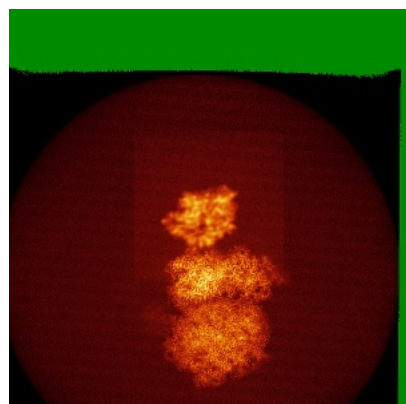


Z Index: 229

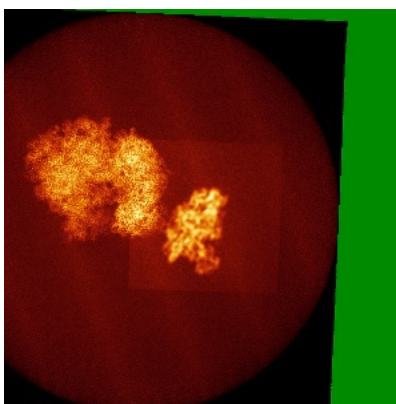
The images above show the largest variance slices of the map in three orthogonal directions.

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

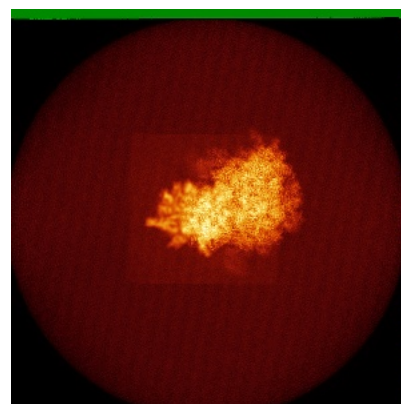
6.4.1 Primary map



X

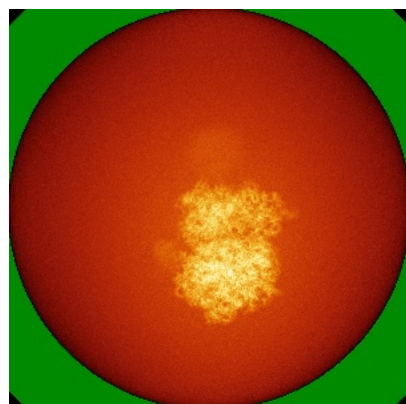


Y

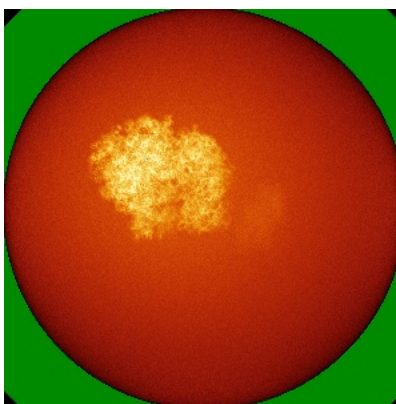


Z

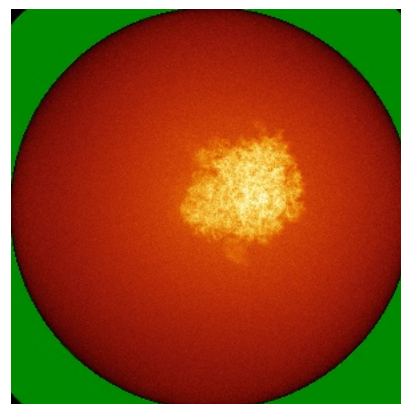
6.4.2 Raw map



X



Y

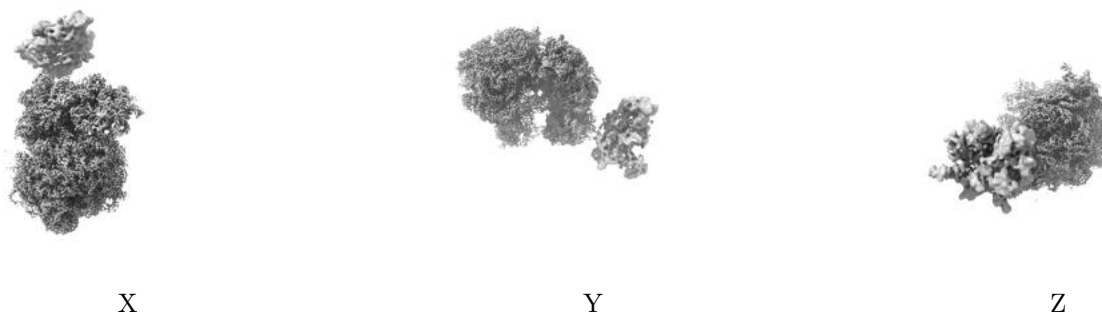


Z

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.

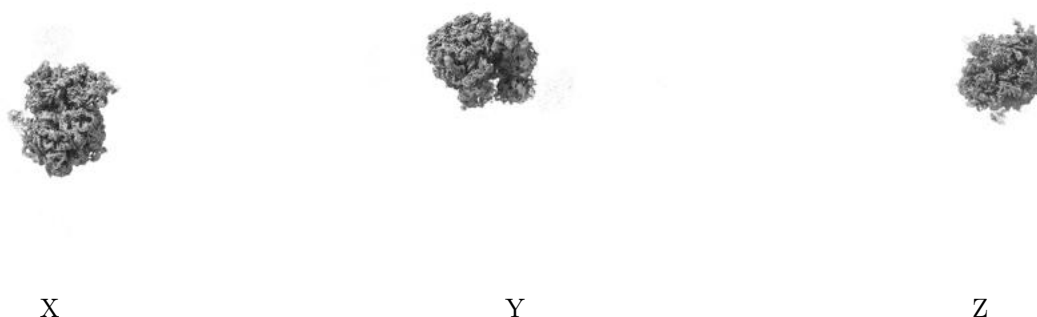
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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.

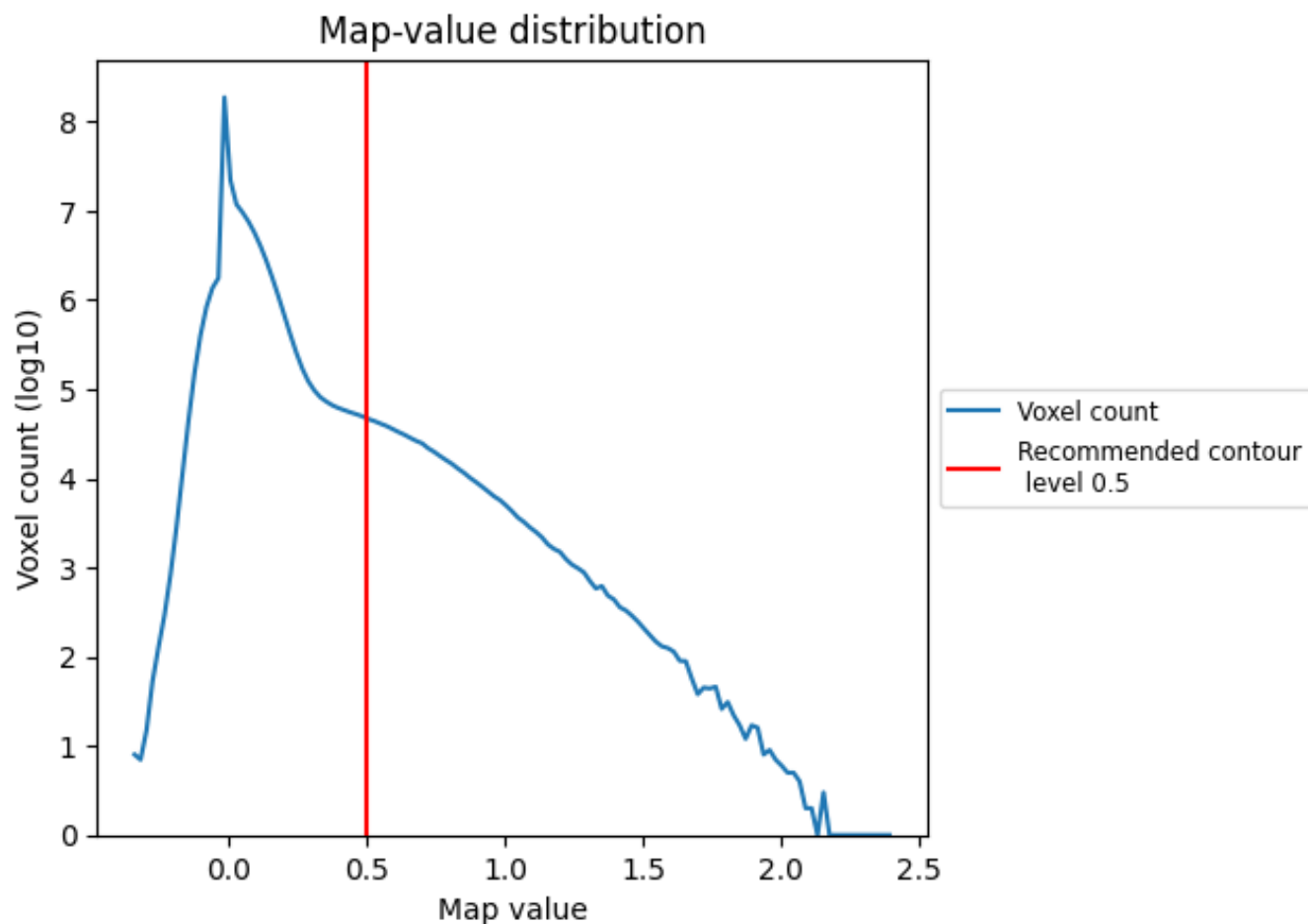
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

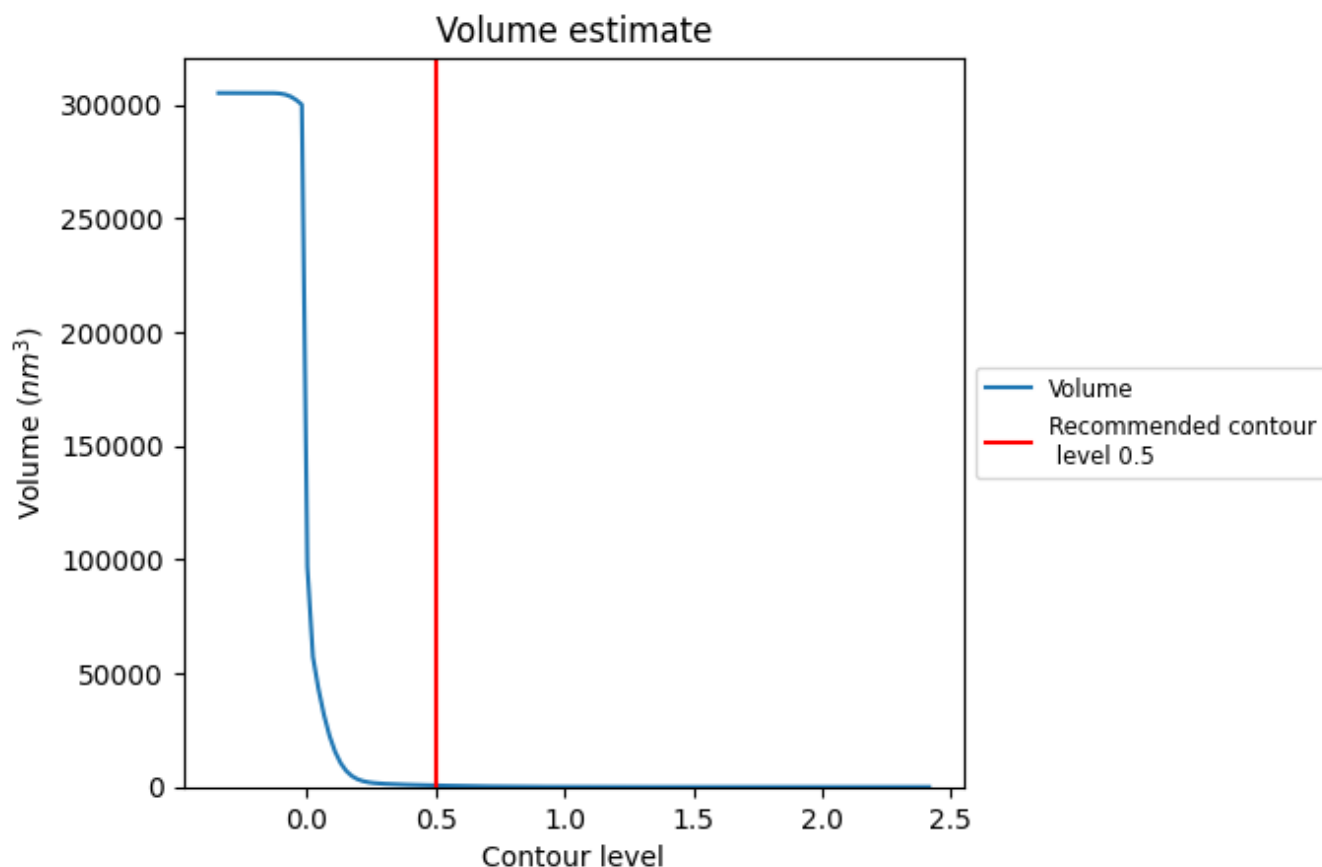
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

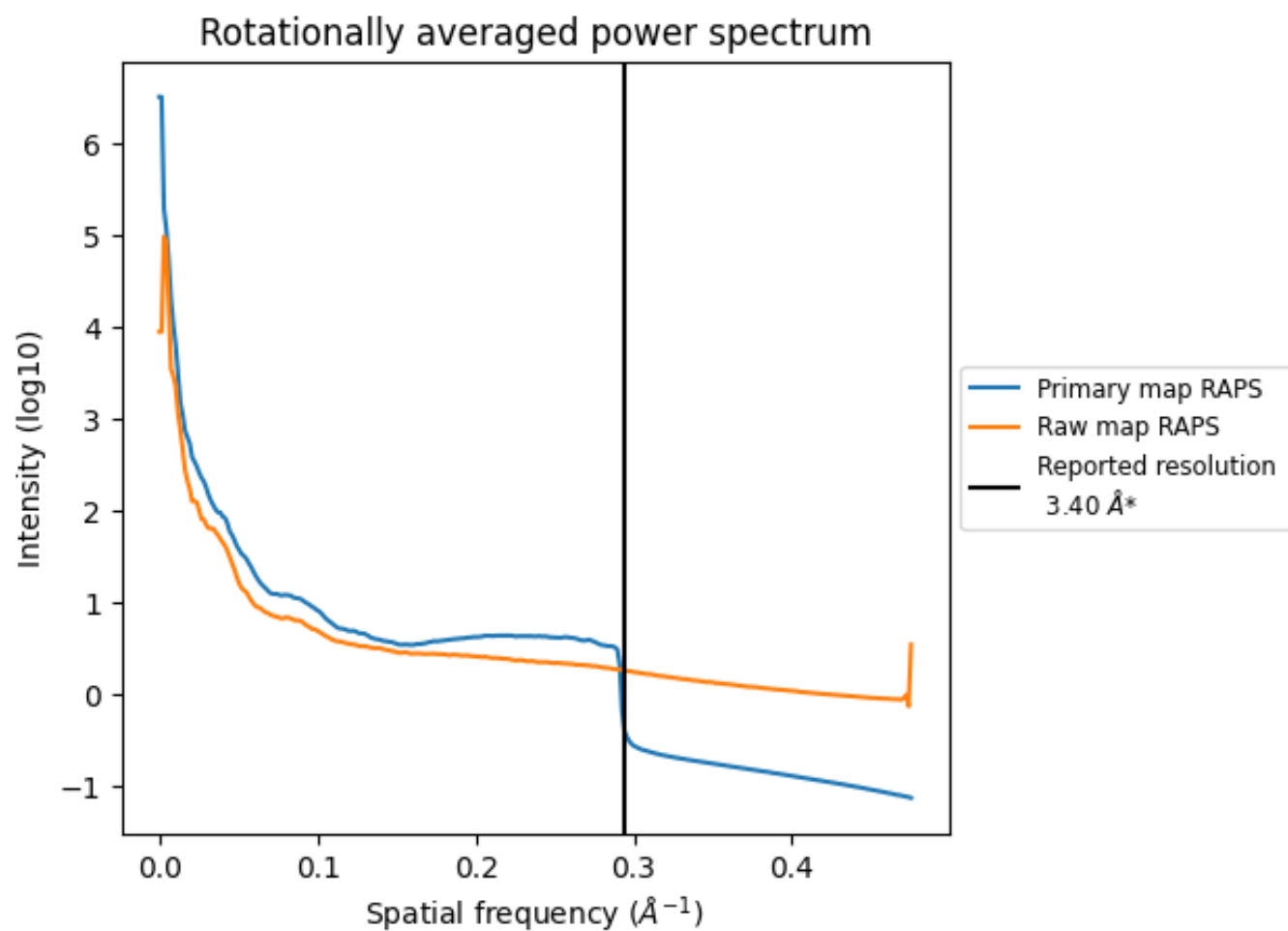
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm^3 ; this corresponds to an approximate mass of 591 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

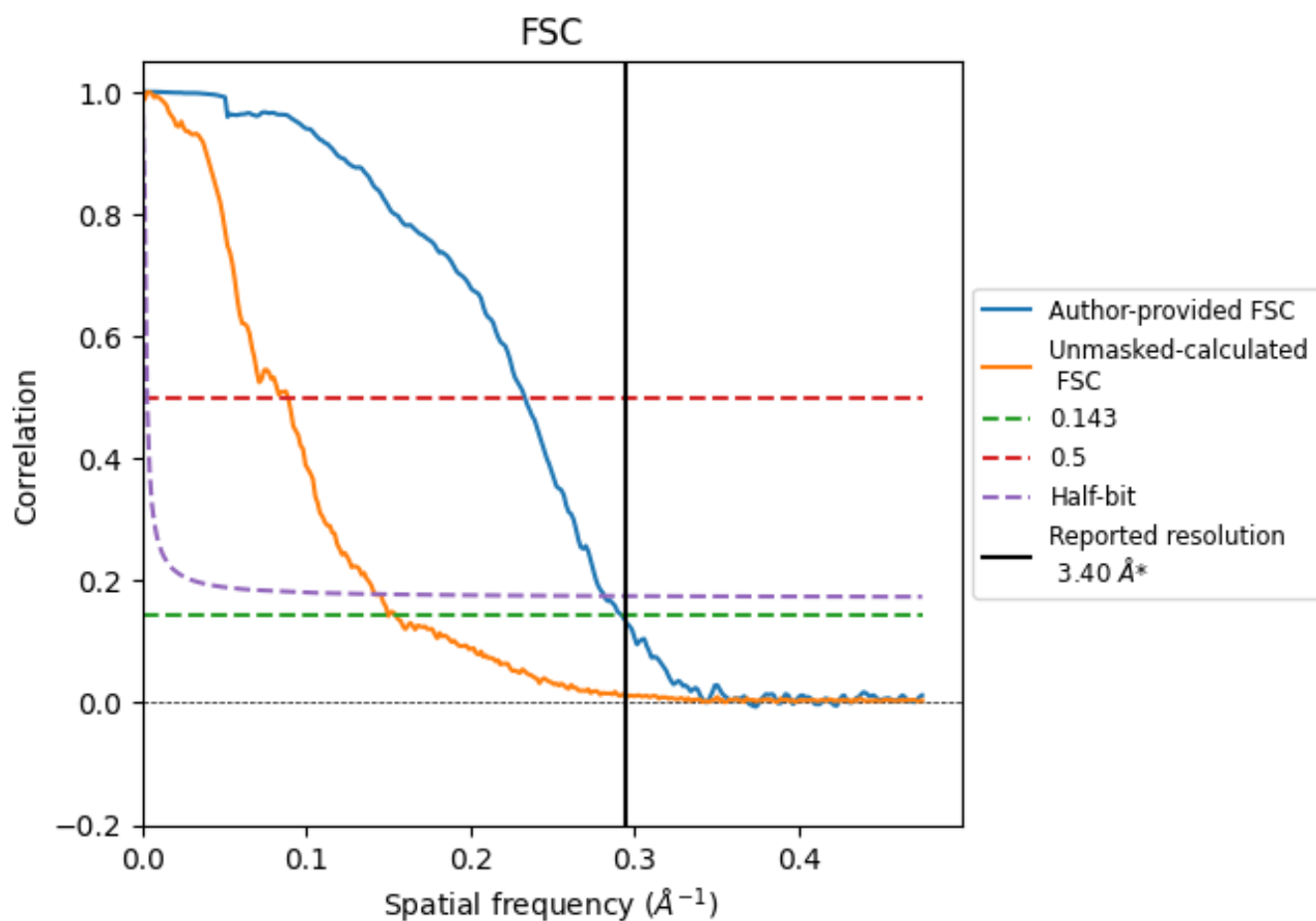


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

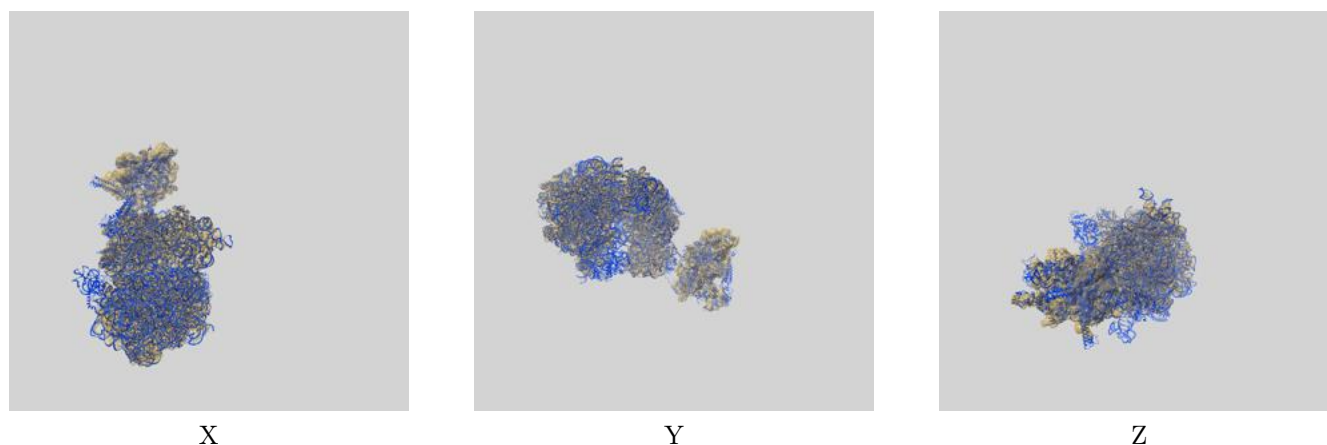
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.29	3.55
Unmasked-calculated*	6.67	11.26	7.04

*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 6.67 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

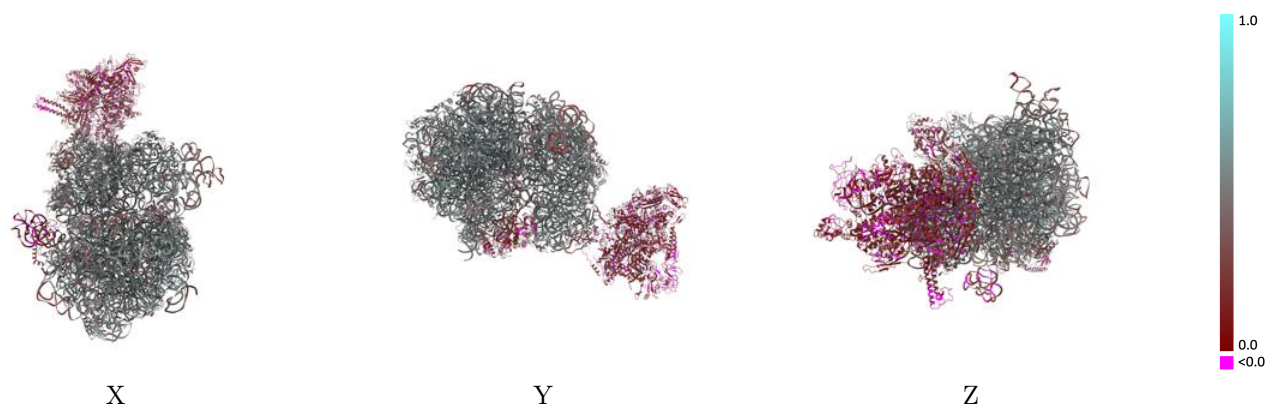
This section contains information regarding the fit between EMDB map EMD-11418 and PDB model 6ZTJ. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



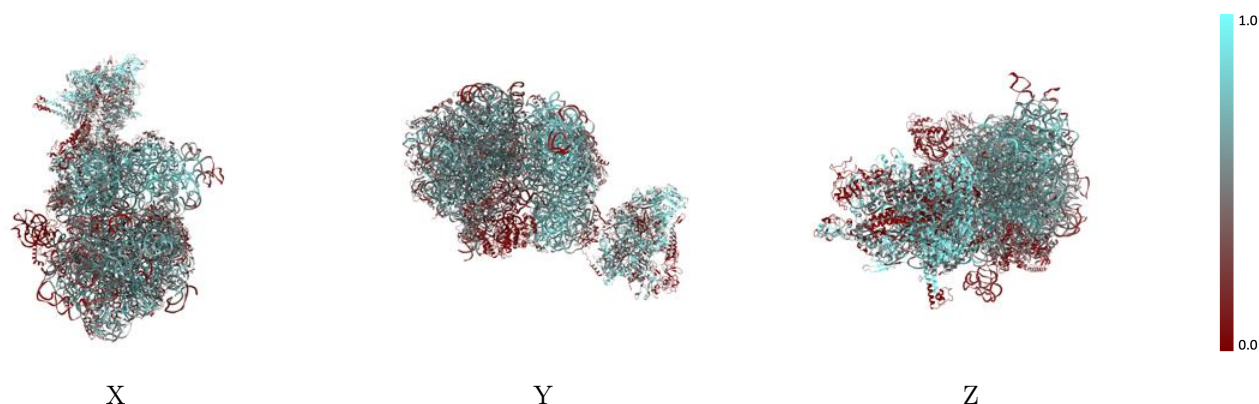
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



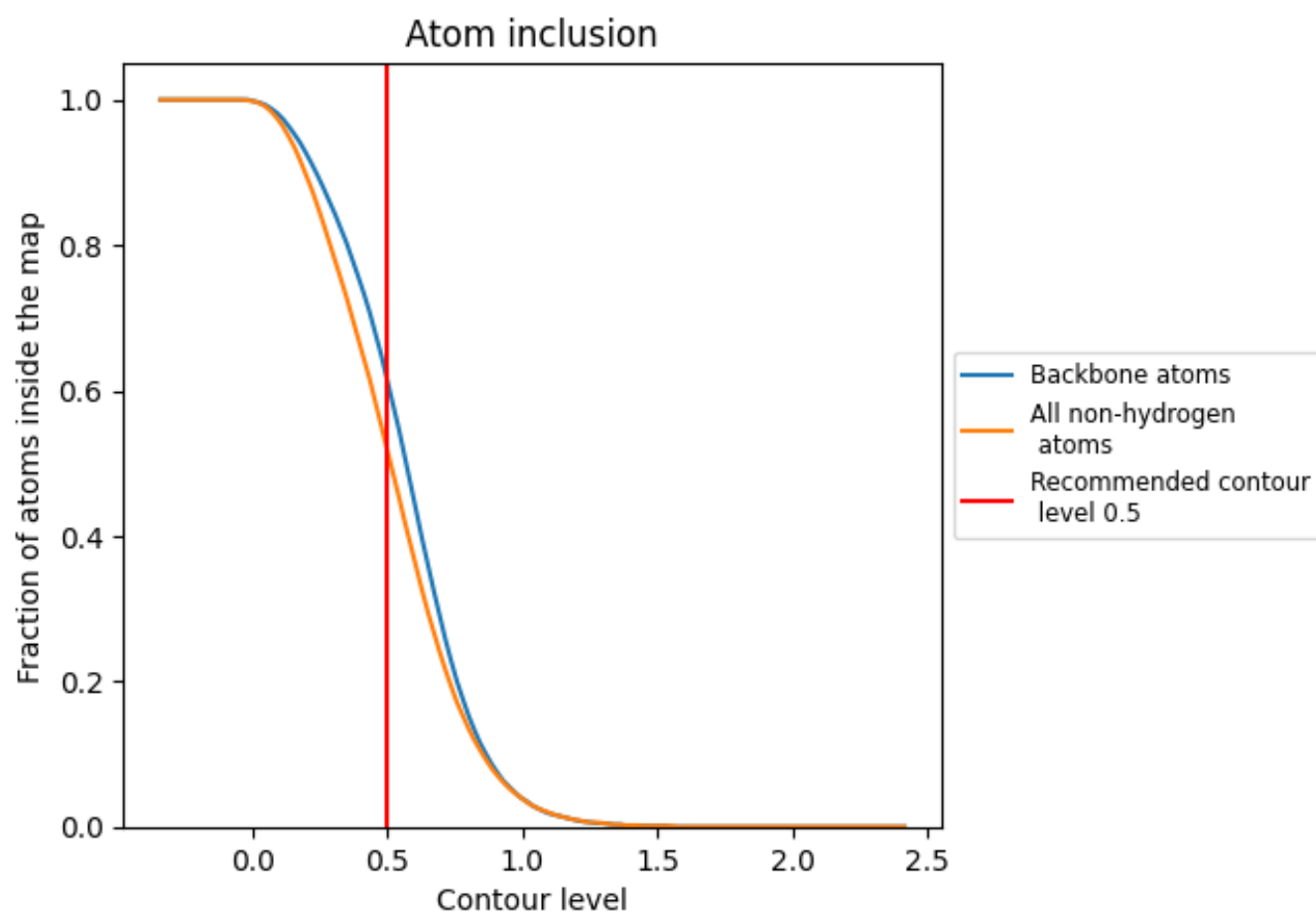
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5180	 0.4150
AA	 0.7250	 0.4790
AB	 0.2420	 0.4180
AC	 0.5560	 0.4950
AD	 0.4380	 0.4710
AE	 0.4830	 0.4930
AF	 0.3760	 0.4510
AG	 0.4690	 0.4420
AH	 0.5060	 0.4900
AI	 0.6160	 0.4900
AJ	 0.5020	 0.4680
AK	 0.4000	 0.4740
AL	 0.5550	 0.5060
AM	 0.5480	 0.4710
AN	 0.6560	 0.5010
AO	 0.4880	 0.4850
AP	 0.5740	 0.4990
AQ	 0.4870	 0.4810
AR	 0.4250	 0.4720
AS	 0.6600	 0.4980
AT	 0.5270	 0.4910
AU	 0.2450	 0.3910
AV	 0.2890	 0.3010
AW	 0.3570	 0.4410
AX	 0.2030	 0.4340
AY	 0.0020	 0.3590
B1	 0.4440	 0.4930
B2	 0.3480	 0.4970
B3	 0.0210	 0.4460
B4	 0.5150	 0.5320
B5	 0.4520	 0.5190
B6	 0.3900	 0.5070
B7	 0.0130	 0.3290
BA	 0.5490	 0.4720
BB	 0.4510	 0.4660



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Chain	Atom inclusion	Q-score
BC	 0.4470	 0.5170
BD	 0.4280	 0.5090
BE	 0.3860	 0.4830
BF	 0.1270	 0.4160
BG	 0.1860	 0.4270
BH	 0.0360	 0.2540
BI	 0.0000	 0.1480
BJ	 0.0000	 0.1760
BK	 0.4600	 0.5090
BL	 0.3980	 0.4990
BM	 0.4070	 0.5000
BN	 0.3830	 0.5110
BO	 0.4630	 0.5160
BP	 0.2660	 0.4710
BQ	 0.3510	 0.4880
BR	 0.5450	 0.5190
BS	 0.4320	 0.5130
BT	 0.4660	 0.5030
BU	 0.3240	 0.4730
BV	 0.3770	 0.4770
BW	 0.3100	 0.4850
BX	 0.4360	 0.5110
BY	 0.3910	 0.4940
BZ	 0.2660	 0.4410
CA	 0.6040	 0.1270
CB	 0.6620	 0.1250
CC	 0.4760	 0.1230
CD	 0.4330	 0.1080
CE	 0.3200	 0.1200
CF	 0.2340	 0.1990
CN	 0.4140	 0.1560
CT	 0.5740	 0.1830