Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 09:45 am BST

PDB ID	:	6ZTM
EMDB ID	:	EMD-11420
Title	:	E. coli 70S-RNAP expressome complex in collided state without NusG
Authors	:	Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on	:	2020-07-20
Resolution	:	3.30 Å(reported)
Based on initial models	:	6ALH, 4YBB

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 (i) 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 (i)) were used in the production of this report:

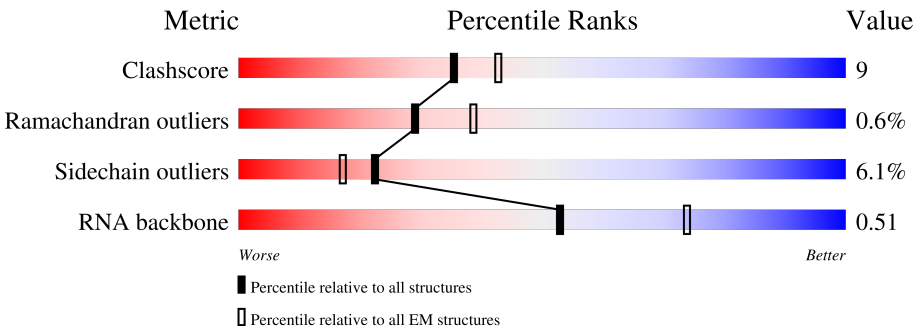
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	AA	1542	58% 33% 7% ••
2	AB	241	71% 20% • 6%
3	AC	233	58% 27% 5% 10%
4	AD	206	66% 30% •
5	AE	167	65% 25% •• 7%
6	AF	131	49% 24% 6% 21%
7	AG	156	65% 29% • •

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Mol	Chain	Length	Quality of chain
8	AH	130	70% 25% 5%
9	AI	130	55% 38% 5%
10	AJ	103	48% 41% 9%
11	AK	129	66% 23% 10%
12	AL	124	69% 26%
13	AM	118	61% 33%
14	AN	101	71% 26%
15	AO	89	70% 26%
16	AP	82	89% 11%
17	AQ	84	68% 20% 6% 6%
18	AR	75	47% 21% 28%
19	AS	92	61% 27% 10%
20	AT	87	76% 20%
21	AU	71	69% 25%
22	AV	57	16% 14% 16% 7% 47%
23	AW	77	48% 30% 21%
24	AX	76	33% 51% 12%
25	BA	2904	63% 28% 7%
26	BB	120	67% 30%
27	BC	273	77% 21%
28	BD	209	78% 19%
29	BE	201	75% 23%
30	BF	179	54% 41% 5%
31	BG	177	70% 26%
32	BH	149	64% 31% 5%

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Mol	Chain	Length	Quality of chain
33	BK	142	80% 18% •
34	BL	123	71% 28% •
35	BM	144	72% 25% •
36	BN	136	71% 29%
37	BO	127	77% 14% • 6%
38	BP	117	64% 33% •
39	BQ	115	72% 24% • •
40	BR	118	80% 19% • •
41	BS	103	71% 28% •
42	BT	110	76% 22% •
43	BU	100	68% 21% 6% 5%
44	BV	104	74% 24% • •
45	BW	94	71% 27% • •
46	BX	85	74% 13% • 11%
47	BY	78	72% 27% •
48	BZ	63	81% 14% • •
49	B1	59	69% 24% 5% •
50	B2	57	60% 33% 5% •
51	B3	55	64% 31% • •
52	B4	46	76% 24%
53	B5	65	68% 29% • •
54	B6	50	58% 18% 24%
55	CN	39	26% 41% 10% 23%
56	CT	39	15% 36% 26% 23%
57	CA	329	60% 8% • 30%

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Mol	Chain	Length	Quality of chain
57	CB	329	56% 9% • 33%
58	CC	1342	76% 18% • •
59	CD	1407	77% 17% • 5%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 171689 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
			Total	C	N	O	P		
1	AA	1533	32907	14682	6037	10655	1533	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	209	1640	1038	308	291	3	0	0

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

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

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

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

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
			Total	C	N	O	S		
6	AF	104	848	536	153	152	7	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	100	800	500	153	146	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AK	116	866	534	170	159	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	122	949	587	195	163	4	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	79	641	406	120	112	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	54	443	281	81	81	0	0

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	AV	30	636	285	115	206	30	0	0

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

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

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

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

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	BA	2901	62290	27795	11458	20136	2901	0	0

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BU	95	757	479	141	135	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BZ	62	501	308	98	94	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a DNA chain called Non-template DNA strand.

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

- Molecule 56 is a DNA chain called Template DNA strand.

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

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

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

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta.

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

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta'.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	AA	119	119	119	0
60	AW	2	2	2	0

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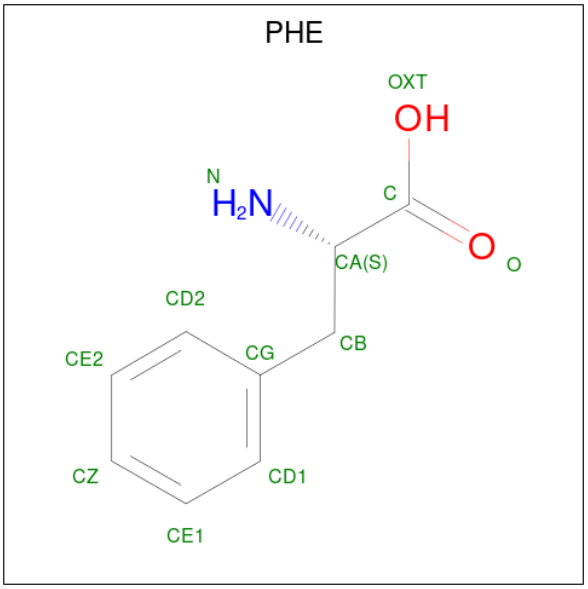
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	BA	294	294	294	0
			Total	Mg	
60	BB	2	2	2	0
			Total	Mg	
60	BC	1	1	1	0
			Total	Mg	
60	BO	1	1	1	0
			Total	Mg	
60	B2	1	1	1	0
			Total	Mg	
60	CD	1	1	1	0

- Molecule 61 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

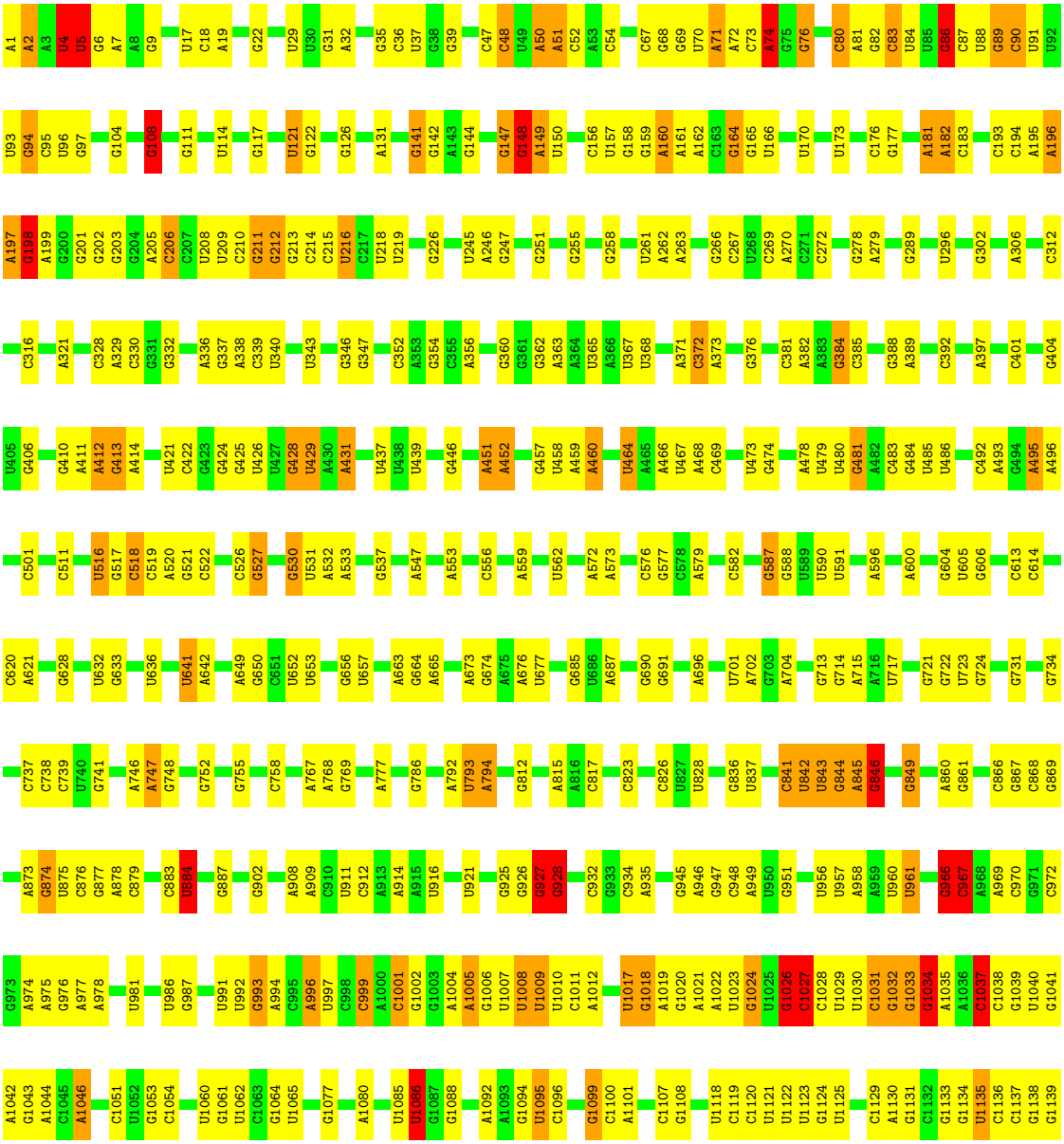
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	B6	1	1	1	0
			Total	Zn	
62	CD	2	2	2	0

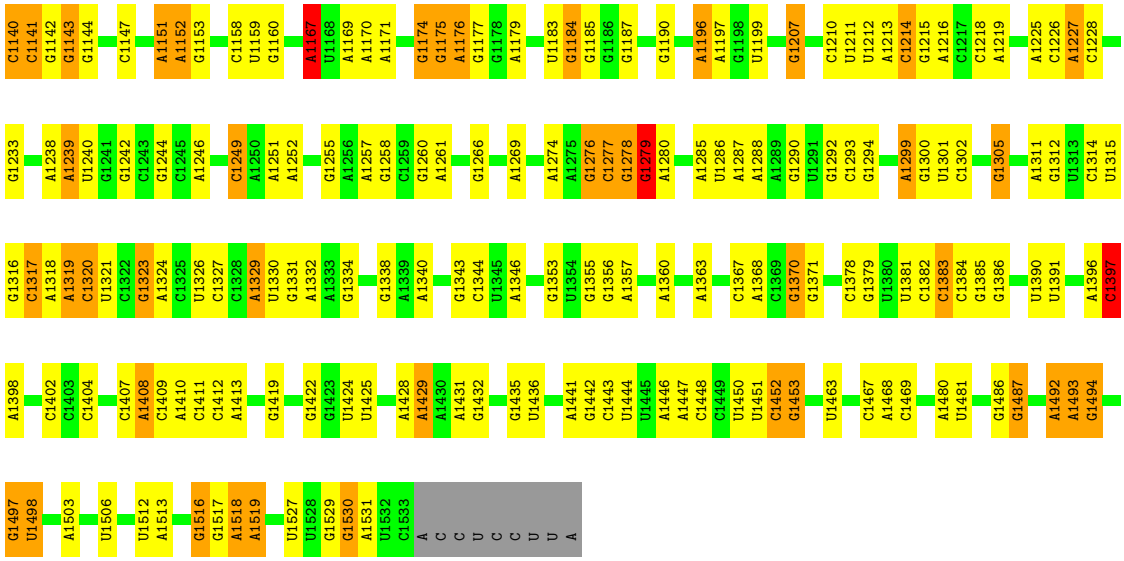
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

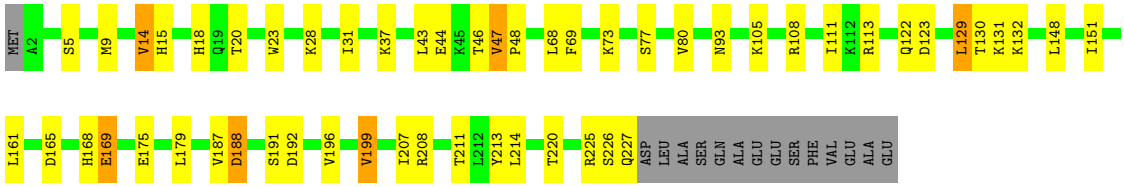
Chain AA: 58% 33% 7% ••





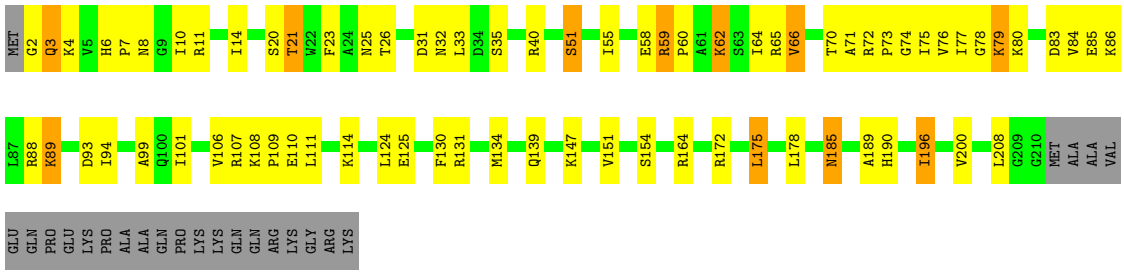
- Molecule 2: 30S ribosomal protein S2

Chain AB:



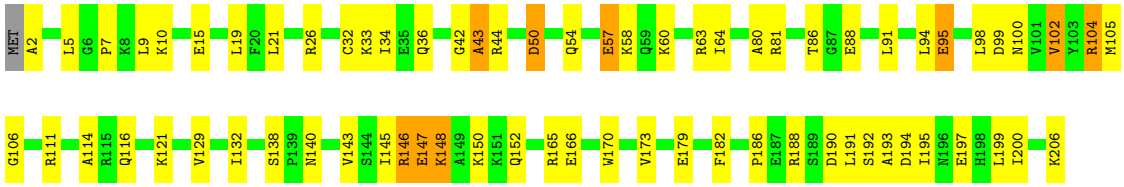
- Molecule 3: 30S ribosomal protein S3

Chain AC:



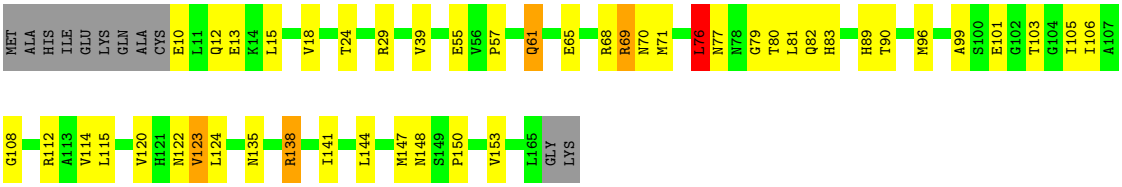
- Molecule 4: 30S ribosomal protein S4

Chain AD:



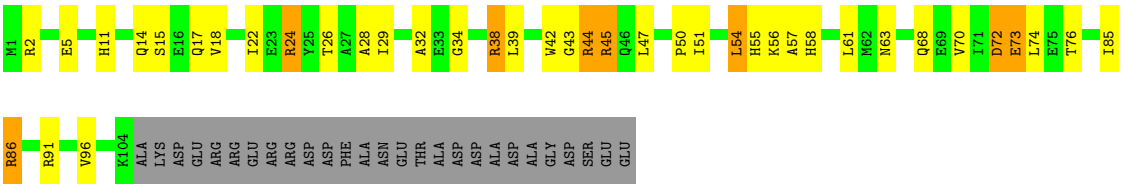
- Molecule 5: 30S ribosomal protein S5

Chain AE:



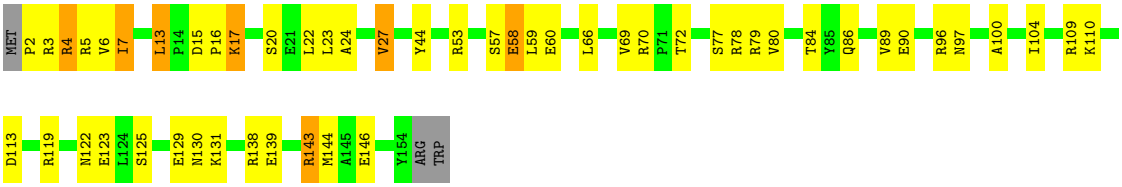
- Molecule 6: 30S ribosomal protein S6

Chain AF:



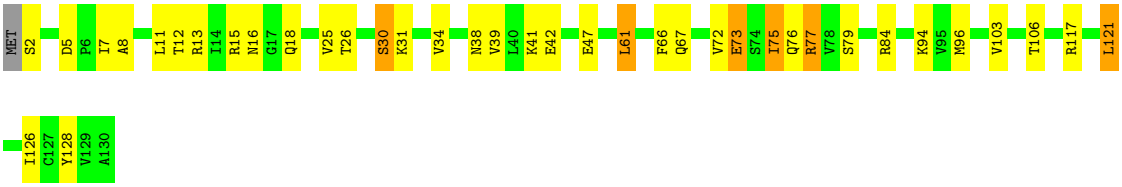
- Molecule 7: 30S ribosomal protein S7

Chain AG:



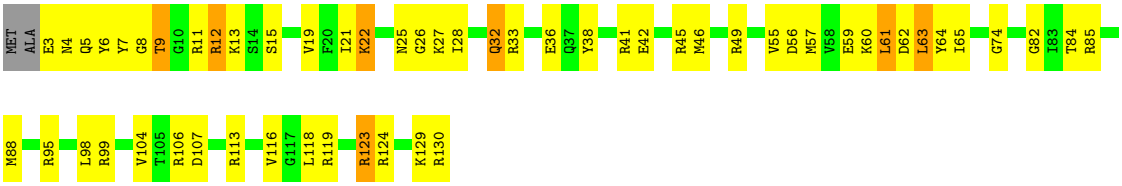
- Molecule 8: 30S ribosomal protein S8

Chain AH:



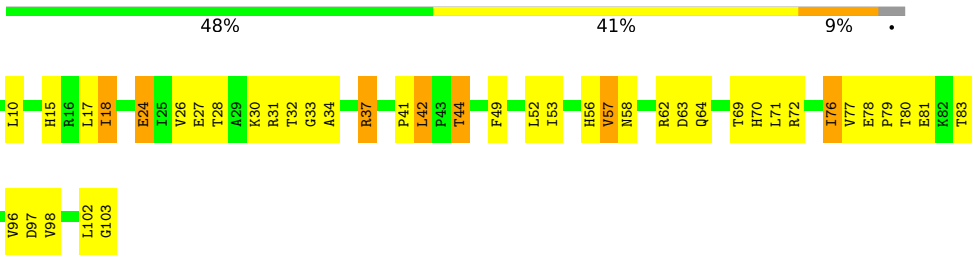
- Molecule 9: 30S ribosomal protein S9

Chain AI:



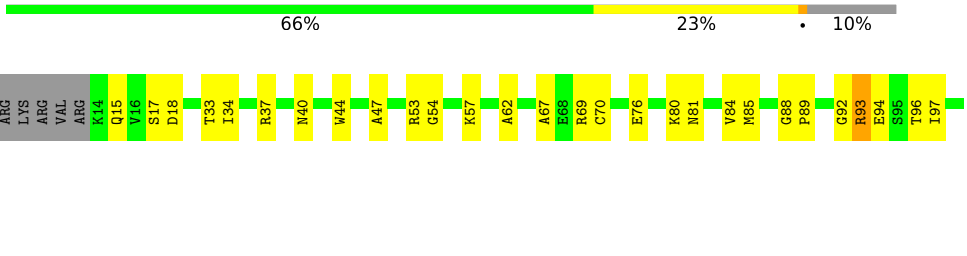
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



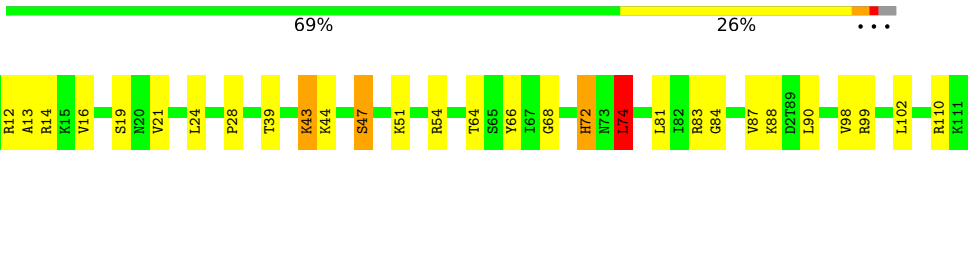
- Molecule 11: 30S ribosomal protein S11

Chain AK:



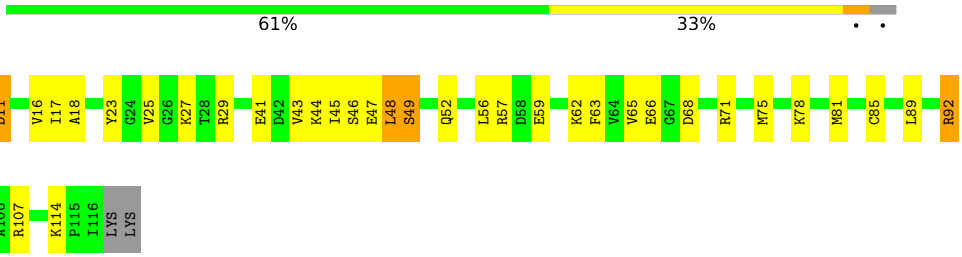
- Molecule 12: 30S ribosomal protein S12

Chain AL:



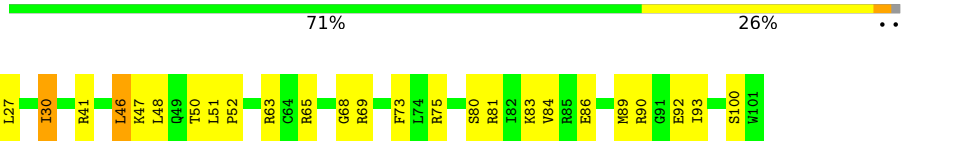
- Molecule 13: 30S ribosomal protein S13

Chain AM:



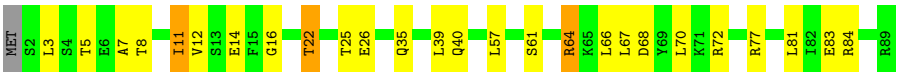
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 15: 30S ribosomal protein S15

Chain AO: 70% 26%



• Molecule 16: 30S ribosomal protein S16

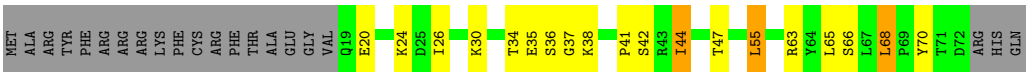
Chain AP: 89% 11%

• Molecule 17: 30S ribosomal protein S17

Chain AQ: 68% 20% 6% 6%

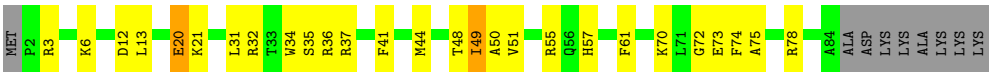
• Molecule 18: 30S ribosomal protein S18

Chain AR: 47% 21% 28%



• Molecule 19: 30S ribosomal protein S19

Chain AS: 61% 27% 10%

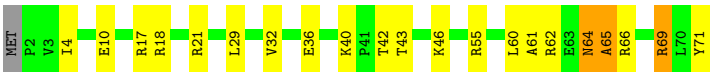


• Molecule 20: 30S ribosomal protein S20

Chain AT: 76% 20%

• Molecule 21: 30S ribosomal protein S21

Chain AU: 69% 25%



• Molecule 22: mRNA

Chain AV: 16% 14% 16% 7% 47%

A C A A A G G A G G U A U U14 C15 A16 U19 C23 A24 U25 A26 C27 A C A U A U A U A G A C A C A34 C37 A38 A39 A40 C41 G42 G43 C44 G45 C46 G47 C48 G49

• Molecule 23: tRNA(fmet) P-site

Chain AW: 48% 30% 21%

C1 G2 G6 G7 U8 A14 G15 C16 C17 U17A G18 G19 U20 A21 G22 C25 G31 C32 U33 A44 G45 A46 U47 C48 G49 U50 G53 U54 U55 C56 A57 A58 A59 U60 C61 G64 C69 G70 C74 C75 A76

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

Chain AX: 33% 51% 12%

G1 G5 G6 A7 U8 A9 G10 C11 U12 C13 A14 G15 U16 C17 G18 G19 U20 A21 G22 A23 G24 C25 A26 G27 G28 U32 U33 G34 A35 A36 A37 A38 U39 C40 C41 C42 C43 G44 U45 G46 3AU47 C48 C49 U50 U51 G52 G53 U54 U55 C56 G57 A58 U59 G63 A64 G65 U66

G71 C74 C75 A76

• Molecule 25: 23S ribosomal RNA

Chain BA: 63% 28% 7%

G1 A10 C11 U12 A13 A14 U18 G23 G27 A28 C33 U34 G35 G39 U40 A44 G45 G46 A52 A53 G58 U59 G60 C61 U62 A63 A64 U65 C66 U67 G68 A71 U72 A73 A74 G75 U78 G81 U82 A83 A84 G85 U92 G93 G98 U99

U100 A101 U102 G110 A111 U112 A118 A119 U120 G121 G122 A125 A131 C132 U133 G134 U135 G136 U137 U138 U139 C140 G141 A142 C143 A144 C145 A149 C163 C164 A165 U166 A167 G168 A172 A173 A181 A191 C192 A196 A197 C198 A199 U200 C201 A207 C208 C209 C210

G215 A216 A219 G220 A221 A222 U234 C239 C240 A241 A244 G245 G248 C249 G250 G263 C264 A265 G266 A270 G271 A272 G273 C274 C275 U276 G277 A278 A279 U280 U284 G285 G289 U290 G301 C302 A310 A311 G327 U328 G329 A330 C335 C353 A354

U355 G356 C357 U358 G359 U360 G361 A362 U365 C366 G370 A371 G386 G389 G396 G400 U403 A404 U405 G411 A412 C413 C414 A415 G424 U427 C435 A443 C444 U451 C456 G463 U464 G465 A466 G467 G468 C475 G476 A477 A478 A479 A480 G481

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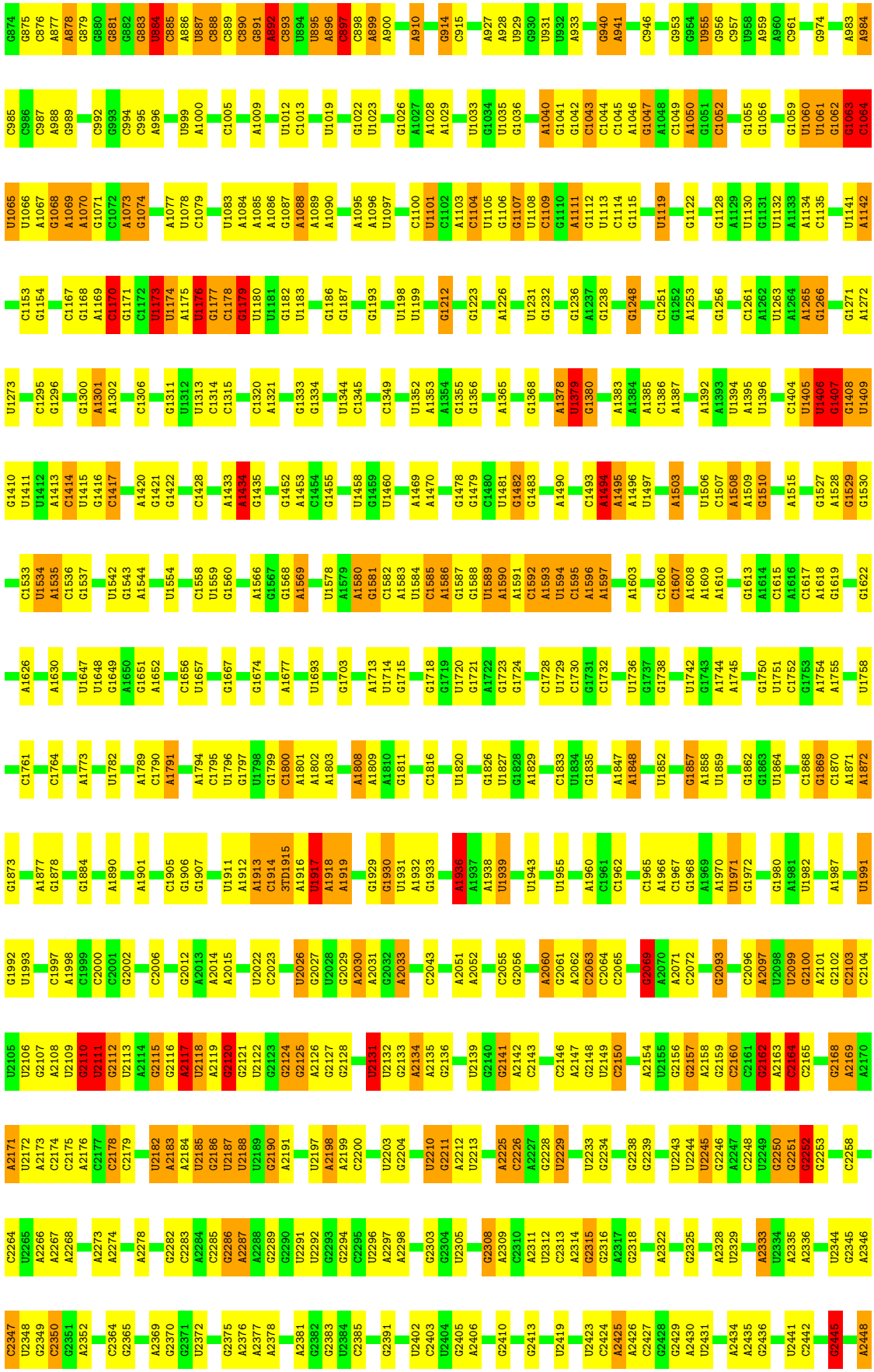
A614 U615 A616 G617 G618 G622 A626 A627 A637 G638 U639 C640 C645 U646 G647 G651 U652 U653 A654 A655 A668 A677 A685 U686 A693 G696 G711 C717 A721 A722 C723 U724 G728 G729 A730 G738 A742 A743 U744 G745 U746 U747 A752

G757 A764 C765 G768 G775 G776 A782 A783 G784 G785 A788 A789 U790 C791 A792 A804 G805 C806 U811 C812 U827 U828 A829 A833 G834 U839 C840 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 A866 C867 U868 G869 U870 U871 U872 C873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C985 C986 C987 A988 G989 C992 G993 C994 C995 A996 U999 A1000 C1005 A1009 U1012 C1013 U1019 G1022 U1023 G1026 A1027 A1028 A1029 U1033 G1034 U1035 G1036 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 G1055 G1056 G1059 U1060 U1061 G1062 G1063 C1064
U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 A1077 U1078 C1079 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 A1095 A1096 U1097 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 U1119 G1122 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 U1141 A1142
C1153 G1154 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 G1186 G1187 G1193 U1198 U1199 G1212 G1223 A1226 U1231 G1232 G1236 A1237 G1238 G1248 C1251 G1252 A1253 G1256 C1261 A1262 U1263 A1264 A1265 G1266 G1271 A1272
U1273 C1295 G1296 G1300 A1301 A1302 C1306 G1311 U1312 U1313 C1314 C1315 C1320 A1321 G1333 G1334 U1344 C1345 C1349 U1352 A1353 A1354 G1355 G1356 A1365 G1368 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394 A1395 U1396 C1404 U1405 U1406 G1407 G1408 U1409
G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 A1420 G1421 G1422 C1428 A1433 A1434 G1435 G1452 A1453 C1454 G1455 U1458 G1459 U1460 A1469 A1470 G1478 G1479 C1480 U1481 G1482 G1483 A1490 C1493 A1494 A1495 A1496 U1497 A1503 U1506 C1507 A1508 A1509 G1510 A1515 G1527 A1528 G1529 G1530
C1533 U1534 A1535 C1536 G1537 U1542 G1543 A1544 U1554 C1558 U1559 G1560 A1566 G1567 G1568 A1569 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1603 C1606 C1607 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1622
A1626 A1630 U1647 U1648 G1649 A1650 G1651 A1652 C1656 U1657 G1667 G1674 A1677 U1693 G1703 A1713 U1714 G1715 G1718 G1719 U1720 G1721 A1722 G1723 G1724 C1728 U1729 C1730 G1731 C1732 U1736 G1737 G1738 U1742 G1743 A1744 A1745 G1750 U1751 C1752 G1753 A1754 A1755 U1758
C1761 C1764 A1773 U1782 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 A1808 A1809 A1810 G1811 C1816 U1820 G1826 U1827 G1828 A1829 C1833 U1834 G1835 A1847 A1848 U1852 G1857 A1858 U1859 G1862 G1863 U1864 C1868 G1869 C1870 A1871 A1872
G1873 A1877 G1878 G1884 A1890 A1901 C1905 G1906 G1907 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 U1943 U1955 A1960 C1961 C1962 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 G1980 A1981 U1982 A1987 U1991
G1992 U1993 C1997 A1998 C1999 C2000 C2001 G2002 C2006 G2012 A2013 A2014 A2015 U2022 C2023 U2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 C2043 A2051 A2052 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 G2069 A2070 A2071 C2072 G2093 C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104
U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 U2131 U2132 G2133 A2134 A2135 G2136 U2139 G2140 G2141 A2142 C2143 C2146 A2147 G2148 U2149 C2150 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 G2168 A2169 A2170
A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2197 A2198 A2199 C2200 U2203 G2204 U2210 G2211 A2212 U2213 A2225 C2226 A2227 U2228 U2229 U2233 G2234 G2238 G2239 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253 C2258
C2264 U2265 A2266 A2267 A2268 A2273 A2274 A2278 G2282 C2283 A2284 C2285 G2286 A2287 A2288 G2289 G2290 U2291 U2292 G2293 G2294 C2295 U2296 A2297 A2298 G2303 G2304 U2305 G2308 A2309 C2310 A2311 U2312 C2313 A2314 G2315 G2316 A2317 G2318 A2322 G2325 A2328 U2329 A2333 U2334 A2335 A2336 U2344 U2345 A2346
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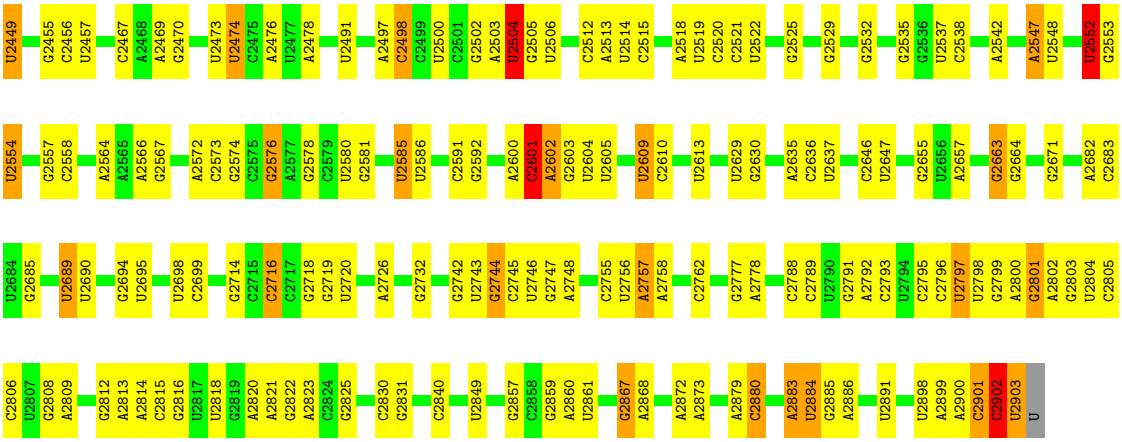
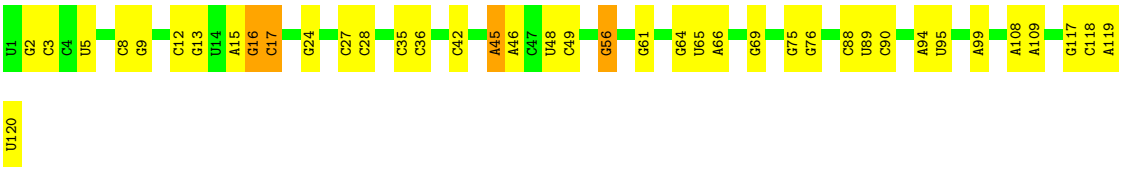


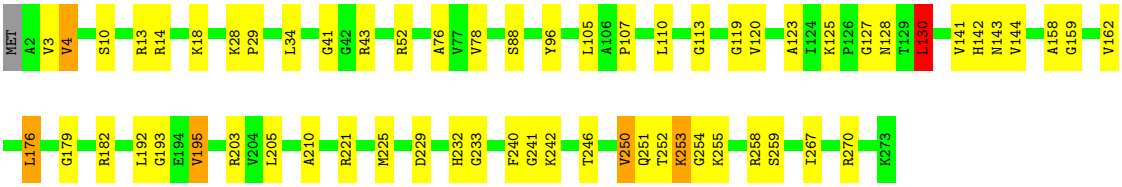
- Molecule 26: 5S ribosomal RNA

Chain BB:



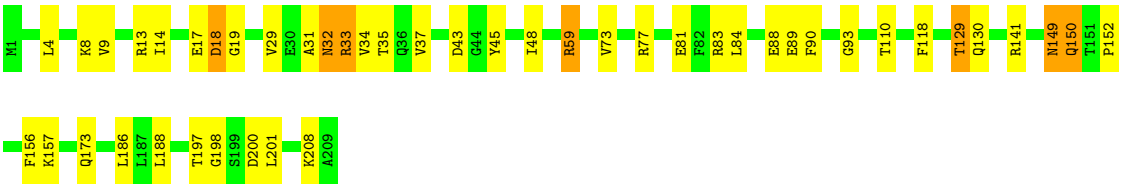
- Molecule 27: 50S ribosomal protein L2

Chain BC:



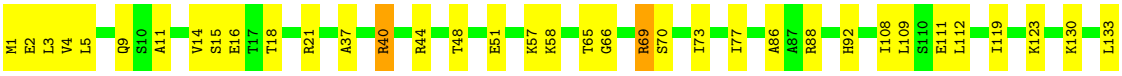
- Molecule 28: 50S ribosomal protein L3

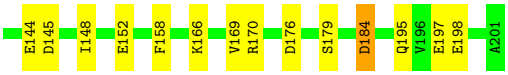
Chain BD:



- Molecule 29: 50S ribosomal protein L4

Chain BE:



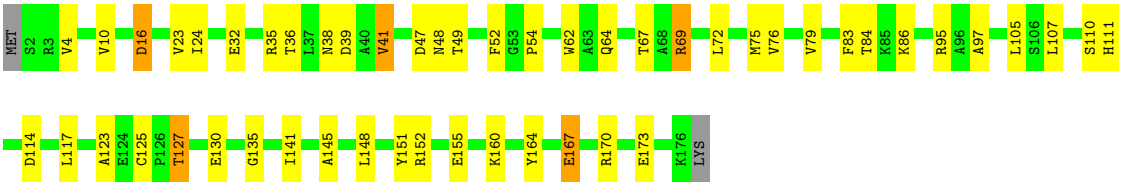


• Molecule 30: 50S ribosomal protein L5

Chain BF:

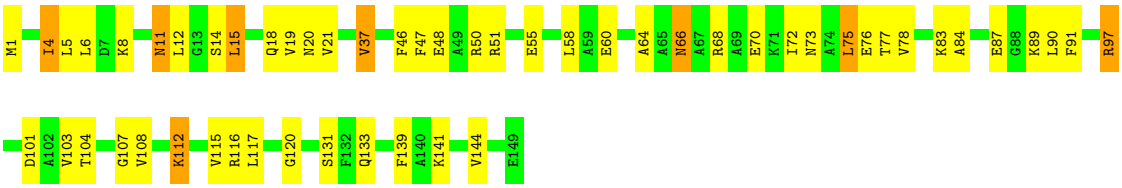
• Molecule 31: 50S ribosomal protein L6

Chain BG:



• Molecule 32: 50S ribosomal protein L9

Chain BH:

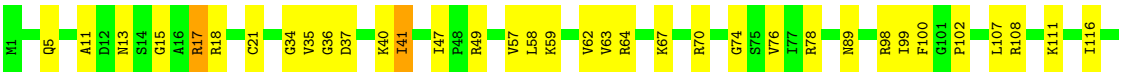


• Molecule 33: 50S ribosomal protein L13

Chain BK:

• Molecule 34: 50S ribosomal protein L14

Chain BL:



L123

- Molecule 35: 50S ribosomal protein L15

Chain BM: 72% 25% •

M1 R2 T5 A9 S12 K13 K14 K17 R21 L27 G28 K29 T30 R33 K36 G37 S40 L57 L61 P62 K63 T67 K70 E76 V77 R78 L79 S80 D81 K84 V85 V89 A98 N99 F107 I111 L112 A113 G114 E115 V116

V120 R123 R126 K129 R132 I142 E143 E144

- Molecule 36: 50S ribosomal protein L16

Chain BN: 71% 29%

M1 L2 Q3 K8 H13 K14 G15 R16 N17 R18 G19 L20 D25 F31 G32 L33 K34 A35 V36 G37 R38 R55 R59 W64 I65 R66 V67 K71 P77 L78 A79 V80 4D481 W92 I96 Q97 P98 L102 Y103 E104 M105 D106 G107 E110 E115 A116

F117 K123 K127 F130 V131 T132 K133 T134 V135 M136

- Molecule 37: 50S ribosomal protein L17

Chain BO: 77% 14% • 6%

M1 R2 K5 R8 N13 M20 F21 M24 L38 P39 L44 E49 T53 L54 L65 R69 E82 R86 R90 C100 G101 P109 M110 E120 LYS ALA GLU ALA ALA ALA GLU

- Molecule 38: 50S ribosomal protein L18

Chain BP: 64% 33% •

M1 D2 S5 A6 R7 R13 A14 R15 R25 L26 V27 R30 T31 H34 I35 Y36 A37 Q38 Y39 I40 V47 L48 V49 A50 A51 S52 E55 K56 A57 E60 Q61 N67 K68 D69 V74 V78 R81 D89 F92 S95 G96 F97 Q98 Y99 H100

G101 R102 V103 L106 A107 R111 Q116 F117

- Molecule 39: 50S ribosomal protein L19

Chain BQ: 72% 24% • •

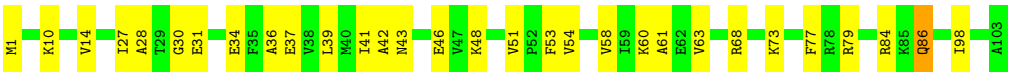
MET S2 N3 I4 L8 E11 Q12 M13 K14 S19 V26 V32 V33 E34 R39 L40 R51 N52 R53 V73 S78 P79 V80 R88 R89 G90 A91 Y98 Y99 L100 R101 E102 R103 T104 R109 I110 K111 E112 R113 L114 N115

- Molecule 40: 50S ribosomal protein L20

Chain BR: 80% 19% ••

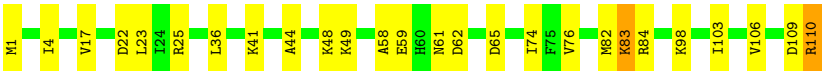
• Molecule 41: 50S ribosomal protein L21

Chain BS: 71% 28% •



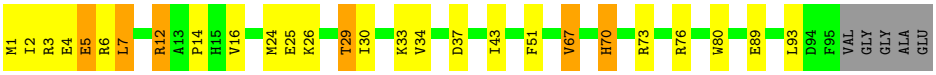
• Molecule 42: 50S ribosomal protein L22

Chain BT: 76% 22% •



• Molecule 43: 50S ribosomal protein L23

Chain BU: 68% 21% 6% 5%



• Molecule 44: 50S ribosomal protein L24

Chain BV: 74% 24% ••

• Molecule 45: 50S ribosomal protein L25

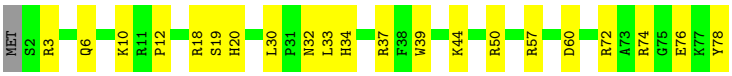
Chain BW: 71% 27% ••

• Molecule 46: 50S ribosomal protein L27

Chain BX: 74% 13% • 11%

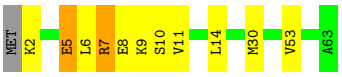
• Molecule 47: 50S ribosomal protein L28

Chain BY: 72% 27%



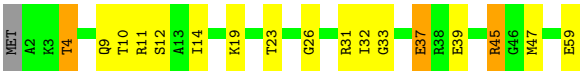
• Molecule 48: 50S ribosomal protein L29

Chain BZ: 81% 14%



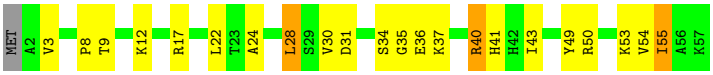
• Molecule 49: 50S ribosomal protein L30

Chain B1: 69% 24% 5%



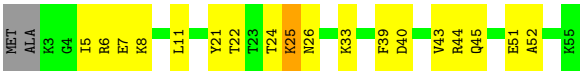
• Molecule 50: 50S ribosomal protein L32

Chain B2: 60% 33% 5%



• Molecule 51: 50S ribosomal protein L33

Chain B3: 64% 31%

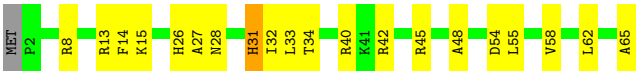


• Molecule 52: 50S ribosomal protein L34

Chain B4: 76% 24%

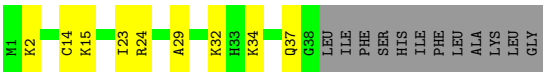
• Molecule 53: 50S ribosomal protein L35

Chain B5: 68% 29%



• Molecule 54: 50S ribosomal protein L36

Chain B6: 58% 18% 24%

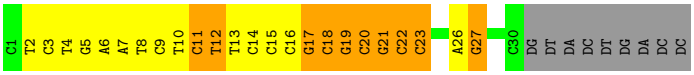


• Molecule 55: Non-template DNA strand

Chain CN: 26% 41% 10% 23%

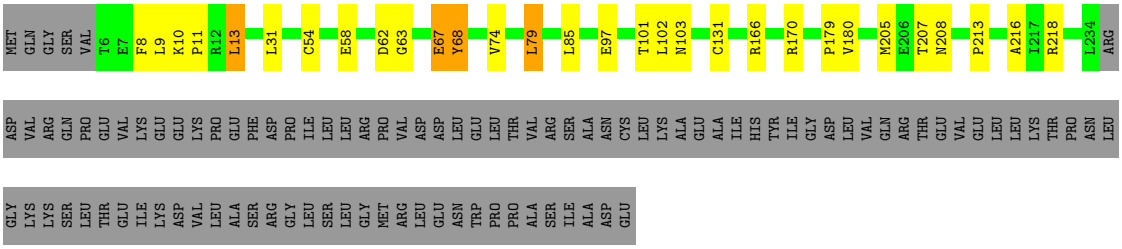
• Molecule 56: Template DNA strand

Chain CT: 15% 36% 26% 23%



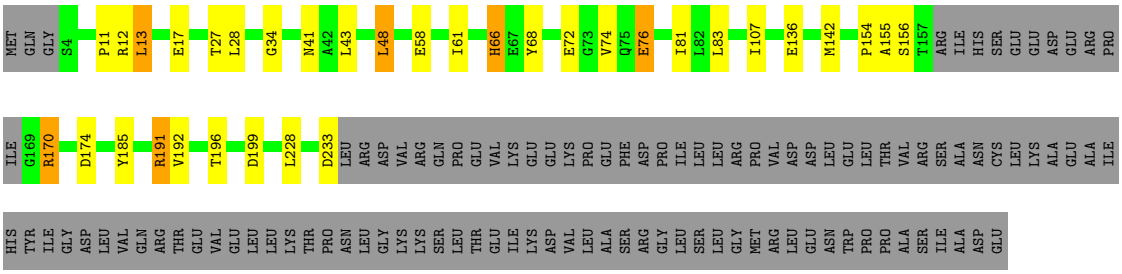
• Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain CA: 60% 8% • 30%



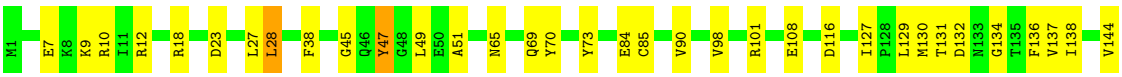
• Molecule 57: DNA-directed RNA polymerase subunit alpha

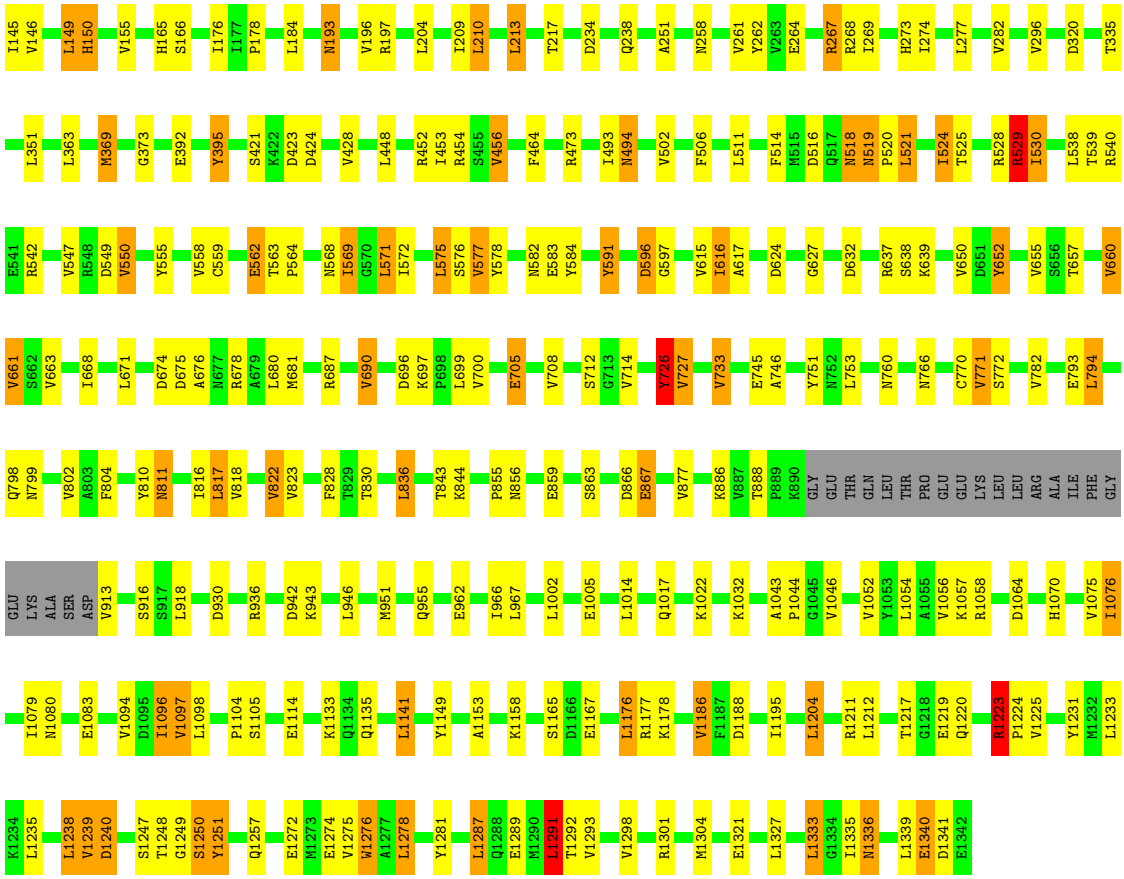
Chain CB: 56% 9% • 33%



• Molecule 58: DNA-directed RNA polymerase subunit beta

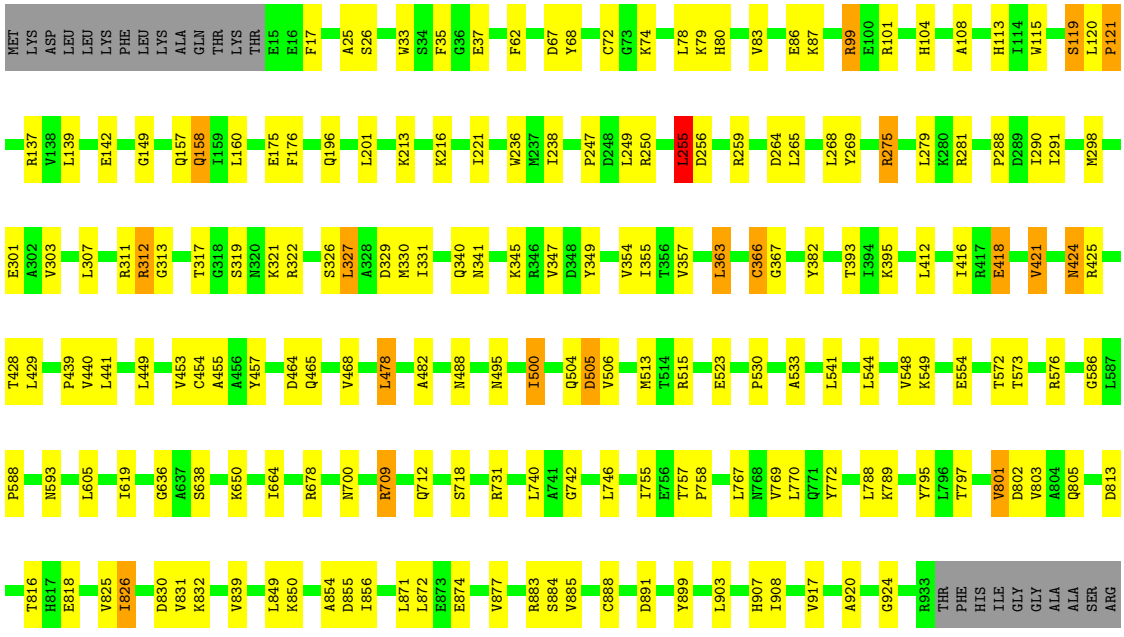
Chain CC: 76% 18% • •

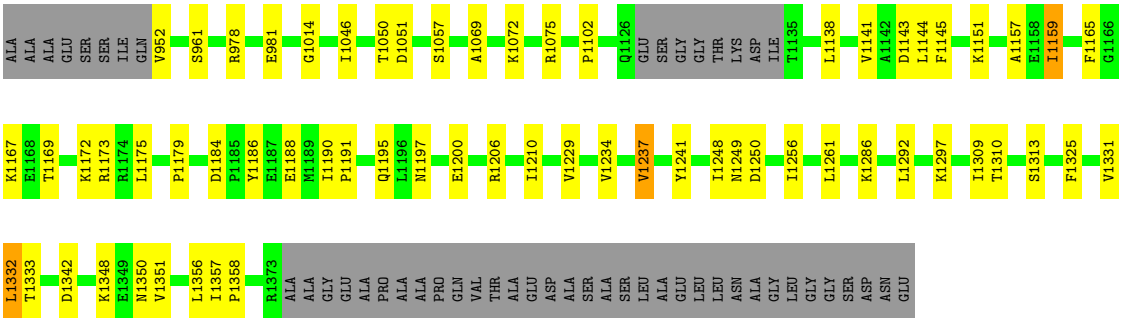




- Molecule 59: DNA-directed RNA polymerase subunit beta'

Chain CD: 77% 17% • 5%




ALA
ALA
ALA
GLU
SER
SER
ILE
GLN
V952
S961
R978
E981
G1014
I1046
T1050
D1051
S1057
A1069
K1072
R1075
P1102
Q1126
GLU
SER
GLY
GLY
THR
LYS
ASP
ILE
T1135
L1138
V1141
A1142
D1143
L1144
F1145
K1151
A1157
E1158
I1159
F1165
G1166
K1167
E1168
T1169
K1172
R1173
R1174
L1175
P1179
D1184
P1185
Y1186
E1187
E1188
M1189
I1190
P1191
Q1195
L1196
N1197
E1200
R1206
I1210
V1229
V1234
V1237
Y1241
I1248
N1249
D1250
I1256
L1261
K1286
L1292
K1297
I1309
T1310
S1313
F1325
V1331
L1332
T1333
D1342
K1348
E1349
N1350
V1351
L1356
I1357
P1358
R1373
ALA
ALA
GLY
GLU
ALA
PRO
ALA
ALA
PRO
GLN
VAL
THR
ALA
GLU
ASP
ALA
SER
ALA
SER
LEU
ALA
GLU
LEU
LEU
ASN
ALA
GLY
LEU
GLY
GLY
SER
ASP
ASN
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.13	1/36569 (0.0%)	1.04	68/57044 (0.1%)
2	AB	0.35	0/1796	0.56	0/2420
3	AC	0.42	0/1667	0.58	0/2246
4	AD	0.51	0/1665	0.62	0/2227
5	AE	0.50	0/1161	0.68	1/1563 (0.1%)
6	AF	0.44	0/867	0.58	0/1171
7	AG	0.34	0/1219	0.61	1/1635 (0.1%)
8	AH	0.54	0/989	0.60	1/1326 (0.1%)
9	AI	0.43	0/1043	0.62	0/1387
10	AJ	0.41	0/810	0.70	1/1094 (0.1%)
11	AK	0.40	0/882	0.57	0/1191
12	AL	0.59	0/954	0.72	1/1279 (0.1%)
13	AM	0.36	0/900	0.55	0/1204
14	AN	0.40	0/817	0.52	0/1088
15	AO	0.45	0/722	0.56	0/964
16	AP	0.63	0/659	0.62	0/884
17	AQ	0.53	0/650	0.71	1/871 (0.1%)
18	AR	0.43	0/449	0.47	0/604
19	AS	0.42	0/680	0.58	0/915
20	AT	0.47	0/676	0.53	0/895
21	AU	0.37	0/598	0.57	1/792 (0.1%)
22	AV	1.89	28/709 (3.9%)	1.72	32/1099 (2.9%)
23	AW	0.73	1/1725 (0.1%)	1.04	2/2687 (0.1%)
24	AX	0.60	1/1584 (0.1%)	0.85	0/2463
25	BA	1.01	2/69187 (0.0%)	1.01	148/107927 (0.1%)
26	BB	0.72	0/2872	0.90	1/4478 (0.0%)
27	BC	0.50	0/2131	0.64	1/2863 (0.0%)
28	BD	0.47	0/1576	0.60	0/2119
29	BE	0.44	0/1571	0.65	2/2113 (0.1%)
30	BF	0.33	0/1444	0.59	0/1937
31	BG	0.38	0/1333	0.59	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BH	0.30	0/1122	0.65	2/1515 (0.1%)
33	BK	0.47	0/1152	0.54	0/1551
34	BL	0.46	0/956	0.62	0/1279
35	BM	0.44	0/1061	0.64	0/1412
36	BN	0.43	0/1081	0.57	0/1443
37	BO	0.46	0/973	0.62	0/1301
38	BP	0.36	0/910	0.59	0/1219
39	BQ	0.43	0/929	0.58	0/1242
40	BR	0.59	0/960	0.56	0/1278
41	BS	0.48	0/829	0.67	0/1107
42	BT	0.43	0/864	0.58	0/1156
43	BU	0.41	0/764	0.57	0/1021
44	BV	0.41	0/797	0.58	0/1062
45	BW	0.42	0/766	0.61	1/1025 (0.1%)
46	BX	0.45	0/589	0.56	0/779
47	BY	0.46	0/635	0.52	0/848
48	BZ	0.34	0/502	0.51	0/667
49	B1	0.40	0/453	0.61	0/605
50	B2	0.47	0/450	0.73	0/599
51	B3	0.36	0/443	0.65	0/587
52	B4	0.48	0/380	0.61	0/498
53	B5	0.40	0/513	0.65	0/676
54	B6	0.47	0/302	0.65	0/397
55	CN	1.77	13/693 (1.9%)	1.24	3/1068 (0.3%)
56	CT	2.53	39/676 (5.8%)	1.33	9/1039 (0.9%)
57	CA	1.13	7/1797 (0.4%)	0.91	2/2436 (0.1%)
57	CB	0.80	1/1703 (0.1%)	0.86	3/2308 (0.1%)
58	CC	1.41	120/10581 (1.1%)	0.97	31/14275 (0.2%)
59	CD	1.12	58/10532 (0.6%)	0.91	15/14219 (0.1%)
All	All	0.98	271/183318 (0.1%)	0.94	327/270903 (0.1%)

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
10	AJ	0	1
12	AL	0	1
13	AM	0	2
22	AV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BA	0	2
27	BC	0	1
37	BO	0	1
46	BX	0	1
53	B5	0	1
All	All	0	14

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.65	1.48	1.61
24	AX	1	G	OP3-P	-10.51	1.48	1.61
56	CT	18	DC	C3'-O3'	-10.28	1.30	1.44
59	CD	1357	ILE	C-N	-9.69	1.15	1.34
56	CT	14	DC	C3'-O3'	-9.60	1.31	1.44
56	CT	12	DT	N1-C2	-9.40	1.30	1.38
22	AV	47	G	N3-C4	-9.20	1.29	1.35
58	CC	146	VAL	CB-CG1	-8.96	1.34	1.52
58	CC	144	VAL	CB-CG1	-8.85	1.34	1.52
56	CT	15	DC	C3'-O3'	-8.75	1.32	1.44
56	CT	16	DC	N1-C6	-8.74	1.31	1.37
22	AV	46	C	N1-C6	-8.69	1.31	1.37
58	CC	146	VAL	CB-CG2	-8.53	1.34	1.52
59	CD	457	TYR	CD2-CE2	-8.38	1.26	1.39
58	CC	802	VAL	CB-CG1	-8.37	1.35	1.52
56	CT	16	DC	C3'-O3'	-8.37	1.33	1.44
58	CC	712	SER	CA-C	-8.30	1.31	1.52
59	CD	457	TYR	CE2-CZ	-8.29	1.27	1.38
56	CT	13	DT	N1-C2	-8.27	1.31	1.38
56	CT	22	DC	N1-C6	-8.19	1.32	1.37
22	AV	47	G	C6-N1	-8.16	1.33	1.39
59	CD	421	VAL	CB-CG2	-7.84	1.36	1.52
58	CC	655	VAL	CB-CG1	-7.83	1.36	1.52
58	CC	663	VAL	CB-CG2	-7.82	1.36	1.52
55	CN	28	DA	C3'-O3'	-7.82	1.33	1.44
56	CT	18	DC	N1-C6	-7.76	1.32	1.37
55	CN	28	DA	N3-C4	-7.75	1.30	1.34
22	AV	49	G	N7-C5	-7.66	1.34	1.39
58	CC	591	TYR	CG-CD1	-7.65	1.29	1.39
59	CD	457	TYR	CD1-CE1	-7.64	1.27	1.39
58	CC	136	PHE	CB-CG	-7.63	1.38	1.51
58	CC	591	TYR	CD2-CE2	-7.58	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CD	1145	PHE	CB-CG	-7.58	1.38	1.51
58	CC	818	VAL	CB-CG2	-7.52	1.37	1.52
55	CN	26	DG	C3'-O3'	-7.41	1.34	1.44
58	CC	1239	VAL	CB-CG2	-7.38	1.37	1.52
59	CD	1141	VAL	CB-CG1	-7.27	1.37	1.52
56	CT	19	DG	N7-C5	-7.21	1.34	1.39
58	CC	708	VAL	CB-CG1	-7.21	1.37	1.52
59	CD	453	VAL	CB-CG1	-7.12	1.37	1.52
58	CC	708	VAL	CB-CG2	-7.09	1.38	1.52
58	CC	137	VAL	CB-CG2	-7.07	1.38	1.52
58	CC	591	TYR	CD1-CE1	-7.07	1.28	1.39
22	AV	47	G	N1-C2	-7.06	1.32	1.37
58	CC	578	TYR	CE2-CZ	-7.05	1.29	1.38
58	CC	802	VAL	CB-CG2	-7.03	1.38	1.52
22	AV	43	G	N7-C5	-7.01	1.35	1.39
22	AV	48	C	N1-C6	-7.00	1.32	1.37
56	CT	16	DC	N1-C2	-6.99	1.33	1.40
58	CC	591	TYR	CE1-CZ	-6.96	1.29	1.38
22	AV	46	C	N3-C4	-6.95	1.29	1.33
22	AV	46	C	N1-C2	-6.93	1.33	1.40
58	CC	663	VAL	CB-CG1	-6.92	1.38	1.52
22	AV	47	G	C5-C4	-6.90	1.33	1.38
59	CD	457	TYR	CE1-CZ	-6.89	1.29	1.38
56	CT	14	DC	N1-C6	-6.85	1.33	1.37
58	CC	1289	GLU	CB-CG	-6.83	1.39	1.52
58	CC	652	TYR	CD1-CE1	-6.82	1.29	1.39
58	CC	822	VAL	CB-CG1	-6.79	1.38	1.52
58	CC	577	VAL	CB-CG1	-6.76	1.38	1.52
58	CC	448	LEU	CA-C	-6.75	1.35	1.52
59	CD	801	VAL	CB-CG2	-6.75	1.38	1.52
58	CC	1094	VAL	CB-CG1	-6.70	1.38	1.52
58	CC	464	PHE	CB-CG	-6.66	1.40	1.51
56	CT	13	DT	C4-C5	-6.63	1.39	1.45
58	CC	530	ILE	CB-CG2	-6.63	1.32	1.52
58	CC	144	VAL	CB-CG2	-6.62	1.39	1.52
22	AV	43	G	C6-N1	-6.59	1.34	1.39
58	CC	1251	TYR	CE1-CZ	-6.57	1.30	1.38
58	CC	558	VAL	CB-CG1	-6.56	1.39	1.52
58	CC	705	GLU	CG-CD	-6.54	1.42	1.51
58	CC	578	TYR	CD2-CE2	-6.50	1.29	1.39
59	CD	772	TYR	CD2-CE2	-6.49	1.29	1.39
59	CD	424	ASN	CB-CG	-6.46	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	47	G	N7-C5	-6.45	1.35	1.39
58	CC	591	TYR	CE2-CZ	-6.45	1.30	1.38
58	CC	652	TYR	CE1-CZ	-6.41	1.30	1.38
58	CC	1097	VAL	CB-CG1	-6.41	1.39	1.52
59	CD	801	VAL	CB-CG1	-6.40	1.39	1.52
58	CC	727	VAL	CB-CG2	-6.39	1.39	1.52
58	CC	799	ASN	CB-CG	-6.39	1.36	1.51
58	CC	591	TYR	CB-CG	-6.36	1.42	1.51
59	CD	421	VAL	CB-CG1	-6.34	1.39	1.52
59	CD	33	TRP	CB-CG	-6.34	1.38	1.50
58	CC	519	ASN	CB-CG	-6.31	1.36	1.51
58	CC	1225	VAL	CB-CG2	-6.30	1.39	1.52
59	CD	803	VAL	CB-CG1	-6.29	1.39	1.52
56	CT	17	DG	N3-C4	-6.29	1.31	1.35
58	CC	1281	TYR	CD2-CE2	-6.28	1.29	1.39
22	AV	47	G	C2-N3	-6.27	1.27	1.32
59	CD	917	VAL	CB-CG1	-6.24	1.39	1.52
58	CC	1186	VAL	CB-CG2	-6.22	1.39	1.52
22	AV	47	G	C5-C6	-6.19	1.36	1.42
59	CD	1237	VAL	CB-CG2	-6.19	1.39	1.52
58	CC	578	TYR	CD1-CE1	-6.18	1.30	1.39
58	CC	1094	VAL	CB-CG2	-6.15	1.40	1.52
58	CC	823	VAL	CB-CG2	-6.11	1.40	1.52
58	CC	1149	TYR	CD2-CE2	-6.09	1.30	1.39
58	CC	1231	TYR	CE2-CZ	-6.09	1.30	1.38
59	CD	468	VAL	CB-CG2	-6.08	1.40	1.52
22	AV	45	G	N3-C4	-6.08	1.31	1.35
58	CC	1239	VAL	CB-CG1	-6.06	1.40	1.52
58	CC	1075	VAL	CB-CG2	-6.04	1.40	1.52
56	CT	20	DC	N1-C6	-6.04	1.33	1.37
59	CD	303	VAL	CB-CG2	-6.04	1.40	1.52
59	CD	1145	PHE	CD2-CE2	-6.04	1.27	1.39
57	CA	68	TYR	CD1-CE1	-6.03	1.30	1.39
22	AV	48	C	N1-C2	-6.03	1.34	1.40
56	CT	12	DT	C4-C5	-6.03	1.39	1.45
58	CC	518	ASN	CB-CG	-6.02	1.37	1.51
58	CC	726	TYR	CD1-CE1	-6.00	1.30	1.39
58	CC	1231	TYR	CD2-CE2	-5.99	1.30	1.39
58	CC	818	VAL	CB-CG1	-5.96	1.40	1.52
22	AV	49	G	C5-C6	-5.94	1.36	1.42
22	AV	46	C	C4-C5	-5.92	1.38	1.43
59	CD	1145	PHE	CD1-CE1	-5.91	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	47	G	N9-C4	-5.90	1.33	1.38
58	CC	660	VAL	CB-CG1	-5.88	1.40	1.52
59	CD	888	CYS	CB-SG	-5.87	1.72	1.81
58	CC	661	VAL	CB-CG2	-5.87	1.40	1.52
56	CT	21	DG	C3'-O3'	-5.87	1.36	1.44
59	CD	1241	TYR	CE1-CZ	-5.87	1.30	1.38
55	CN	13	DC	C3'-O3'	-5.87	1.36	1.44
58	CC	751	TYR	CE1-CZ	-5.86	1.30	1.38
55	CN	30	DA	N9-C8	-5.85	1.33	1.37
59	CD	795	TYR	CE1-CZ	-5.85	1.30	1.38
59	CD	899	TYR	CE2-CZ	-5.85	1.30	1.38
57	CA	97	GLU	CB-CG	-5.84	1.41	1.52
22	AV	45	G	C6-N1	-5.82	1.35	1.39
59	CD	772	TYR	CD1-CE1	-5.82	1.30	1.39
57	CA	68	TYR	CE1-CZ	-5.82	1.30	1.38
55	CN	28	DA	C6-N1	-5.80	1.31	1.35
58	CC	1052	VAL	CB-CG1	-5.79	1.40	1.52
58	CC	453	ILE	CB-CG2	-5.77	1.34	1.52
56	CT	19	DG	C3'-O3'	-5.77	1.36	1.44
58	CC	1281	TYR	CE2-CZ	-5.77	1.31	1.38
22	AV	49	G	C6-N1	-5.76	1.35	1.39
59	CD	354	VAL	CB-CG1	-5.76	1.40	1.52
57	CA	54	CYS	CB-SG	-5.75	1.72	1.81
59	CD	347	VAL	CB-CG2	-5.74	1.40	1.52
56	CT	22	DC	N3-C4	-5.74	1.29	1.33
58	CC	816	ILE	CB-CG2	-5.74	1.35	1.52
56	CT	27	DG	C3'-O3'	-5.73	1.36	1.44
58	CC	506	PHE	CG-CD1	-5.73	1.30	1.38
58	CC	700	VAL	CB-CG2	-5.73	1.40	1.52
58	CC	877	VAL	CB-CG2	-5.72	1.40	1.52
56	CT	11	DC	C3'-O3'	-5.71	1.36	1.44
56	CT	17	DG	N7-C5	-5.68	1.35	1.39
58	CC	1251	TYR	CD1-CE1	-5.68	1.30	1.39
55	CN	29	DG	N7-C5	-5.64	1.35	1.39
58	CC	660	VAL	CB-CG2	-5.64	1.41	1.52
58	CC	578	TYR	CG-CD1	-5.62	1.31	1.39
56	CT	15	DC	C4'-C3'	-5.62	1.47	1.52
59	CD	795	TYR	CD2-CE2	-5.62	1.30	1.39
58	CC	73	TYR	CE1-CZ	-5.61	1.31	1.38
58	CC	577	VAL	CB-CG2	-5.61	1.41	1.52
56	CT	13	DT	C3'-O3'	-5.60	1.36	1.44
58	CC	1096	ILE	CB-CG2	-5.60	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CD	269	TYR	CE1-CZ	-5.60	1.31	1.38
59	CD	772	TYR	CE2-CZ	-5.60	1.31	1.38
56	CT	16	DC	N3-C4	-5.60	1.30	1.33
59	CD	1331	VAL	CB-CG2	-5.59	1.41	1.52
58	CC	559	CYS	CB-SG	-5.58	1.72	1.81
59	CD	899	TYR	CE1-CZ	-5.58	1.31	1.38
58	CC	690	VAL	CB-CG2	-5.57	1.41	1.52
55	CN	28	DA	C5-C6	-5.57	1.36	1.41
59	CD	349	TYR	CE2-CZ	-5.57	1.31	1.38
59	CD	366	CYS	CB-SG	-5.57	1.72	1.81
59	CD	899	TYR	CD2-CE2	-5.57	1.30	1.39
57	CA	9	LEU	C-N	-5.57	1.21	1.34
22	AV	49	G	N3-C4	-5.55	1.31	1.35
58	CC	828	PHE	CE2-CZ	-5.55	1.26	1.37
58	CC	1056	VAL	CB-CG2	-5.54	1.41	1.52
58	CC	798	GLN	CA-CB	-5.54	1.41	1.53
58	CC	782	VAL	CB-CG1	-5.53	1.41	1.52
58	CC	1275	VAL	CB-CG1	-5.52	1.41	1.52
58	CC	674	ASP	CB-CG	-5.51	1.40	1.51
56	CT	17	DG	N9-C4	-5.49	1.33	1.38
58	CC	1276	TRP	CB-CG	-5.48	1.40	1.50
56	CT	12	DT	C1'-N1	-5.47	1.39	1.47
58	CC	811	ASN	CB-CG	-5.47	1.38	1.51
58	CC	652	TYR	CD2-CE2	-5.46	1.31	1.39
1	AA	312	C	N1-C6	-5.44	1.33	1.37
58	CC	810	TYR	CE2-CZ	-5.43	1.31	1.38
58	CC	456	VAL	CB-CG1	-5.42	1.41	1.52
22	AV	43	G	N3-C4	-5.41	1.31	1.35
57	CA	131	CYS	CB-SG	-5.41	1.73	1.81
58	CC	823	VAL	CB-CG1	-5.41	1.41	1.52
58	CC	73	TYR	CE2-CZ	-5.40	1.31	1.38
59	CD	468	VAL	CB-CG1	-5.39	1.41	1.52
25	BA	545	A	C1'-N9	-5.38	1.39	1.46
59	CD	465	GLN	CB-CG	-5.38	1.38	1.52
56	CT	20	DC	C4-C5	-5.37	1.38	1.43
58	CC	137	VAL	CB-CG1	-5.37	1.41	1.52
58	CC	690	VAL	CB-CG1	-5.37	1.41	1.52
58	CC	584	TYR	CD2-CE2	-5.37	1.31	1.39
58	CC	804	PHE	CD1-CE1	-5.36	1.28	1.39
58	CC	98	VAL	CB-CG2	-5.36	1.41	1.52
59	CD	355	ILE	CB-CG2	-5.36	1.36	1.52
58	CC	456	VAL	CB-CG2	-5.35	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CT	19	DG	C5-C4	-5.34	1.34	1.38
22	AV	41	C	N1-C2	-5.34	1.34	1.40
58	CC	591	TYR	CG-CD2	-5.34	1.32	1.39
59	CD	269	TYR	CD1-CE1	-5.33	1.31	1.39
59	CD	453	VAL	CB-CG2	-5.33	1.41	1.52
59	CD	1237	VAL	CB-CG1	-5.33	1.41	1.52
56	CT	12	DT	C2-N3	-5.33	1.33	1.37
55	CN	29	DG	N9-C8	-5.32	1.34	1.37
56	CT	11	DC	N3-C4	-5.32	1.30	1.33
59	CD	1333	THR	CB-CG2	-5.31	1.34	1.52
58	CC	136	PHE	CG-CD1	-5.30	1.30	1.38
56	CT	17	DG	C3'-O3'	-5.29	1.37	1.44
56	CT	23	DC	N1-C6	-5.29	1.33	1.37
59	CD	803	VAL	CB-CG2	-5.28	1.41	1.52
58	CC	733	VAL	CB-CG1	-5.28	1.41	1.52
57	CB	185	TYR	CB-CG	-5.28	1.43	1.51
58	CC	770	CYS	CB-SG	-5.26	1.73	1.81
58	CC	428	VAL	CB-CG2	-5.26	1.41	1.52
58	CC	930	ASP	CB-CG	-5.25	1.40	1.51
58	CC	1231	TYR	CE1-CZ	-5.25	1.31	1.38
58	CC	520	PRO	CB-CG	-5.25	1.23	1.50
58	CC	1149	TYR	CD1-CE1	-5.25	1.31	1.39
59	CD	428	THR	CA-CB	-5.25	1.39	1.53
56	CT	16	DC	C2-O2	-5.24	1.19	1.24
58	CC	155	VAL	CB-CG2	-5.24	1.41	1.52
58	CC	616	ILE	CB-CG2	-5.23	1.36	1.52
59	CD	769	VAL	CB-CG1	-5.22	1.41	1.52
58	CC	1149	TYR	CE1-CZ	-5.22	1.31	1.38
58	CC	578	TYR	CG-CD2	-5.21	1.32	1.39
58	CC	395	TYR	CD2-CE2	-5.21	1.31	1.39
58	CC	555	TYR	CD1-CE1	-5.21	1.31	1.39
58	CC	804	PHE	CD2-CE2	-5.21	1.28	1.39
55	CN	29	DG	N3-C4	-5.20	1.31	1.35
22	AV	48	C	C4-C5	-5.20	1.38	1.43
56	CT	17	DG	C5-C6	-5.20	1.37	1.42
59	CD	457	TYR	CG-CD1	-5.20	1.32	1.39
58	CC	70	TYR	CD2-CE2	-5.19	1.31	1.39
59	CD	1145	PHE	CG-CD1	-5.18	1.30	1.38
58	CC	502	VAL	CB-CG2	-5.17	1.42	1.52
58	CC	714	VAL	CB-CG1	-5.17	1.42	1.52
59	CD	347	VAL	CB-CG1	-5.17	1.42	1.52
22	AV	46	C	C2-N3	-5.16	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CC	584	TYR	CD1-CE1	-5.16	1.31	1.39
59	CD	115	TRP	CG-CD1	-5.15	1.29	1.36
58	CC	1149	TYR	CE2-CZ	-5.15	1.31	1.38
58	CC	550	VAL	CB-CG2	-5.12	1.42	1.52
55	CN	30	DA	N9-C4	-5.12	1.34	1.37
56	CT	17	DG	C6-N1	-5.11	1.35	1.39
58	CC	771	VAL	CB-CG2	-5.11	1.42	1.52
55	CN	28	DA	C5-C4	-5.11	1.35	1.38
58	CC	751	TYR	CE2-CZ	-5.10	1.31	1.38
59	CD	382	TYR	CD2-CE2	-5.10	1.31	1.39
59	CD	1234	VAL	CB-CG1	-5.09	1.42	1.52
59	CD	795	TYR	CD1-CE1	-5.09	1.31	1.39
59	CD	1229	VAL	CB-CG1	-5.08	1.42	1.52
59	CD	506	VAL	CB-CG2	-5.08	1.42	1.52
58	CC	547	VAL	CB-CG2	-5.07	1.42	1.52
58	CC	572	ILE	CB-CG2	-5.07	1.37	1.52
58	CC	373	GLY	C-N	-5.07	1.22	1.34
25	BA	548	U	C1'-N1	5.06	1.56	1.48
22	AV	43	G	C5-C6	-5.06	1.37	1.42
55	CN	30	DA	C3'-O3'	-5.06	1.37	1.44
59	CD	115	TRP	CB-CG	-5.03	1.41	1.50
56	CT	12	DT	C2-O2	-5.01	1.18	1.22
58	CC	1289	GLU	CG-CD	-5.01	1.44	1.51
22	AV	45	G	C5-C4	-5.00	1.34	1.38
56	CT	16	DC	C4-C5	-5.00	1.39	1.43
58	CC	1272	GLU	CB-CG	-5.00	1.42	1.52
59	CD	269	TYR	CD2-CE2	-5.00	1.31	1.39
56	CT	19	DG	C5-C6	-5.00	1.37	1.42
57	CA	67	GLU	CG-CD	5.00	1.59	1.51

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1027	C	C6-N1-C2	-25.80	109.98	120.30
1	AA	1027	C	C2-N1-C1'	18.88	139.57	118.80
1	AA	1027	C	C5-C6-N1	18.21	130.11	121.00
1	AA	1027	C	C6-N1-C1'	-15.29	102.45	120.80
25	BA	2131	U	O4'-C1'-N1	-14.14	96.89	108.20
25	BA	1104	C	C6-N1-C2	-11.64	115.64	120.30
25	BA	1047	G	O4'-C1'-N9	11.03	117.02	108.20
25	BA	1077	A	O4'-C1'-N9	10.57	116.65	108.20
56	CT	19	DG	O4'-C1'-N9	10.21	115.14	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1173	U	C5'-C4'-O4'	-9.90	97.22	109.10
22	AV	48	C	C6-N1-C2	-9.74	116.40	120.30
29	BE	69	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	AA	1034	G	C8-N9-C1'	-9.48	114.67	127.00
1	AA	1034	G	C8-N9-C4	-9.47	102.61	106.40
1	AA	452	A	O4'-C1'-N9	9.35	115.68	108.20
25	BA	2902	C	N1-C2-O2	9.27	124.46	118.90
1	AA	812	G	O4'-C1'-N9	9.13	115.50	108.20
1	AA	641	U	P-O3'-C3'	9.02	130.53	119.70
25	BA	1728	C	C2-N1-C1'	-8.90	109.01	118.80
25	BA	1857	G	O4'-C1'-N9	8.89	115.31	108.20
25	BA	884	U	N1-C1'-C2'	-8.86	102.26	112.00
1	AA	108	G	O4'-C1'-N9	-8.73	101.22	108.20
1	AA	206	C	C2-N1-C1'	8.46	128.11	118.80
25	BA	1936	A	O4'-C1'-N9	-8.45	101.44	108.20
22	AV	41	C	O5'-P-OP2	-8.37	98.17	105.70
25	BA	2164	C	N1-C2-O2	8.32	123.89	118.90
25	BA	1104	C	C2-N1-C1'	8.27	127.90	118.80
22	AV	48	C	N1-C2-O2	-8.23	113.96	118.90
25	BA	2164	C	O4'-C1'-N1	-8.19	101.64	108.20
25	BA	1176	U	O4'-C1'-N1	8.18	114.75	108.20
1	AA	1001	C	O4'-C1'-N1	7.96	114.57	108.20
22	AV	45	G	O5'-P-OP1	-7.94	98.55	105.70
25	BA	1064	C	C6-N1-C2	-7.94	117.12	120.30
25	BA	136	G	C8-N9-C1'	-7.92	116.70	127.00
22	AV	40	A	C8-N9-C4	7.92	108.97	105.80
1	AA	1167	A	O4'-C1'-N9	7.87	114.50	108.20
45	BW	20	LEU	CA-CB-CG	7.87	133.40	115.30
25	BA	2506	U	N1-C1'-C2'	-7.87	103.35	112.00
1	AA	4	U	P-O3'-C3'	7.84	129.11	119.70
1	AA	884	U	C6-N1-C2	-7.78	116.33	121.00
58	CC	210	LEU	CA-CB-CG	-7.65	97.70	115.30
58	CC	571	LEU	CB-CG-CD2	-7.61	98.06	111.00
25	BA	136	G	C4-N9-C1'	7.56	136.33	126.50
25	BA	653	U	N1-C2-O2	7.54	128.08	122.80
25	BA	2601	C	O4'-C1'-N1	7.53	114.23	108.20
1	AA	1432	G	O4'-C1'-N9	7.53	114.23	108.20
25	BA	2902	C	N3-C2-O2	-7.53	116.63	121.90
25	BA	783	A	C2-N3-C4	7.47	114.34	110.60
25	BA	1170	C	C2-N1-C1'	7.44	126.99	118.80
1	AA	206	C	O4'-C1'-N1	-7.43	102.26	108.20
25	BA	2131	U	C2-N1-C1'	7.39	126.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1728	C	C6-N1-C1'	7.39	129.66	120.80
25	BA	652	U	N3-C2-O2	-7.36	117.05	122.20
25	BA	1104	C	C6-N1-C1'	-7.36	111.97	120.80
25	BA	2286	G	O4'-C1'-N9	7.35	114.08	108.20
22	AV	47	G	C2-N3-C4	-7.34	108.23	111.90
29	BE	69	ARG	NE-CZ-NH2	-7.33	116.63	120.30
22	AV	49	G	C6-C5-N7	-7.30	126.02	130.40
22	AV	47	G	N1-C2-N3	7.26	128.26	123.90
56	CT	18	DC	O5'-P-OP1	-7.25	99.17	105.70
58	CC	794	LEU	CB-CG-CD1	-7.22	98.73	111.00
1	AA	928	G	N9-C1'-C2'	-7.18	104.10	112.00
25	BA	653	U	C2-N1-C1'	7.16	126.29	117.70
58	CC	149	LEU	CB-CG-CD1	-7.12	98.89	111.00
22	AV	49	G	C4-C5-N7	7.12	113.65	110.80
58	CC	1238	LEU	CB-CG-CD1	-7.09	98.94	111.00
1	AA	206	C	C5-C6-N1	7.08	124.54	121.00
27	BC	130	LEU	CA-CB-CG	7.07	131.56	115.30
25	BA	2186	G	C4-C5-N7	-7.06	107.98	110.80
25	BA	652	U	C2-N1-C1'	7.05	126.16	117.70
1	AA	464	U	N1-C2-O2	-7.04	117.88	122.80
25	BA	1052	C	C6-N1-C2	-6.99	117.50	120.30
25	BA	2576	G	O4'-C1'-N9	-6.99	102.61	108.20
25	BA	2901	C	N1-C2-O2	6.99	123.09	118.90
25	BA	2164	C	N3-C2-O2	-6.99	117.01	121.90
1	AA	1026	G	P-O3'-C3'	6.94	128.02	119.70
25	BA	884	U	O4'-C1'-N1	-6.93	102.66	108.20
25	BA	2131	U	N3-C2-O2	-6.90	117.37	122.20
22	AV	46	C	N1-C2-O2	-6.89	114.76	118.90
25	BA	653	U	N3-C2-O2	-6.87	117.39	122.20
25	BA	2110	G	O4'-C1'-N9	-6.81	102.75	108.20
22	AV	49	G	C5-N7-C8	-6.80	100.90	104.30
25	BA	2174	C	C2-N1-C1'	6.80	126.28	118.80
25	BA	2186	G	C6-N1-C2	-6.80	121.02	125.10
1	AA	927	G	N9-C1'-C2'	-6.74	104.59	112.00
57	CB	48	LEU	CA-CB-CG	6.74	130.79	115.30
58	CC	575	LEU	CB-CG-CD2	-6.73	99.56	111.00
25	BA	2131	U	N1-C2-O2	6.72	127.50	122.80
22	AV	49	G	C8-N9-C4	-6.71	103.71	106.40
25	BA	897	C	C5-C6-N1	6.70	124.35	121.00
25	BA	2150	C	C2-N1-C1'	6.70	126.17	118.80
59	CD	307	LEU	CA-CB-CG	-6.69	99.92	115.30
1	AA	1034	G	C4-N9-C1'	6.69	135.19	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1064	C	O4'-C1'-N1	6.68	113.55	108.20
25	BA	1179	G	C4-C5-N7	6.68	113.47	110.80
25	BA	2186	G	N9-C4-C5	6.62	108.05	105.40
1	AA	1027	C	N3-C4-C5	-6.62	119.25	121.90
25	BA	1434	A	O4'-C1'-N9	6.60	113.48	108.20
22	AV	45	G	O3'-P-O5'	-6.60	91.46	104.00
5	AE	76	LEU	CA-CB-CG	6.55	130.37	115.30
59	CD	478	LEU	CA-CB-CG	-6.55	100.23	115.30
25	BA	2120	G	C4-N9-C1'	6.53	134.99	126.50
25	BA	652	U	N1-C2-O2	6.52	127.37	122.80
1	AA	108	G	C4-N9-C1'	6.50	134.95	126.50
25	BA	1728	C	O4'-C1'-N1	6.48	113.38	108.20
25	BA	62	U	C2-N1-C1'	6.46	125.45	117.70
58	CC	213	LEU	CA-CB-CG	-6.42	100.54	115.30
59	CD	449	LEU	CB-CG-CD1	-6.41	100.11	111.00
59	CD	1332	LEU	CB-CG-CD2	-6.39	100.14	111.00
32	BH	107	GLY	N-CA-C	6.37	129.03	113.10
25	BA	2110	G	N9-C4-C5	-6.36	102.86	105.40
58	CC	521	LEU	CB-CG-CD1	-6.32	100.25	111.00
56	CT	17	DG	O4'-C1'-N9	6.32	112.42	108.00
1	AA	431	A	N1-C6-N6	-6.32	114.81	118.60
25	BA	1064	C	C6-N1-C1'	6.31	128.38	120.80
1	AA	206	C	C6-N1-C2	-6.31	117.78	120.30
58	CC	1287	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	AA	431	A	O4'-C1'-N9	6.29	113.23	108.20
25	BA	1266	G	O4'-C1'-N9	6.29	113.23	108.20
25	BA	2120	G	C8-N9-C1'	-6.28	118.83	127.00
25	BA	1179	G	C6-C5-N7	-6.28	126.63	130.40
56	CT	16	DC	O4'-C1'-N1	6.28	112.39	108.00
58	CC	511	LEU	CB-CG-CD1	-6.28	100.33	111.00
1	AA	1027	C	N3-C4-N4	6.25	122.38	118.00
25	BA	2391	G	O4'-C1'-N9	6.21	113.17	108.20
58	CC	1076	ILE	CG1-CB-CG2	-6.21	97.74	111.40
25	BA	136	G	C6-C5-N7	-6.20	126.68	130.40
22	AV	49	G	N7-C8-N9	6.20	116.20	113.10
25	BA	1104	C	C5-C6-N1	6.18	124.09	121.00
22	AV	42	G	C5-C6-N1	6.18	114.59	111.50
55	CN	26	DG	O4'-C4'-C3'	-6.18	102.03	104.50
58	CC	817	LEU	CB-CG-CD1	-6.18	100.50	111.00
25	BA	1494	A	P-O3'-C3'	6.17	127.11	119.70
1	AA	1037	C	O4'-C1'-N1	6.15	113.12	108.20
25	BA	893	C	N1-C2-O2	-6.14	115.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	121	U	C5'-C4'-O4'	-6.12	101.75	109.10
1	AA	530	G	C4-N9-C1'	-6.10	118.57	126.50
25	BA	2286	G	C4-N9-C1'	6.09	134.41	126.50
1	AA	1008	U	C6-N1-C2	-6.08	117.35	121.00
25	BA	1170	C	C6-N1-C1'	-6.07	113.52	120.80
22	AV	41	C	O4'-C1'-N1	6.07	113.05	108.20
25	BA	2131	U	C6-N1-C1'	-6.05	112.73	121.20
25	BA	1064	C	C2-N1-C1'	-6.04	112.16	118.80
25	BA	2252	G	N9-C1'-C2'	-6.04	105.36	112.00
58	CC	529	ARG	CA-CB-CG	6.04	126.68	113.40
59	CD	1144	LEU	CB-CG-CD1	-6.02	100.77	111.00
25	BA	897	C	C6-N1-C2	-6.01	117.89	120.30
25	BA	885	C	N3-C2-O2	-5.98	117.71	121.90
1	AA	1027	C	C4-C5-C6	-5.97	114.41	117.40
59	CD	255	LEU	CA-CB-CG	5.97	129.04	115.30
25	BA	301	G	O4'-C1'-N9	5.97	112.98	108.20
22	AV	48	C	N1-C2-N3	5.97	123.38	119.20
59	CD	363	LEU	CB-CG-CD1	-5.95	100.89	111.00
25	BA	1379	U	C5'-C4'-O4'	5.94	116.23	109.10
25	BA	1179	G	N9-C4-C5	-5.94	103.03	105.40
22	AV	43	G	C6-C5-N7	-5.94	126.84	130.40
25	BA	62	U	N1-C2-O2	5.93	126.95	122.80
25	BA	1313	U	C2-N1-C1'	5.92	124.81	117.70
55	CN	25	DG	C1'-O4'-C4'	-5.92	104.18	110.10
59	CD	307	LEU	CB-CG-CD2	-5.92	100.94	111.00
25	BA	2160	C	C6-N1-C2	-5.91	117.94	120.30
25	BA	2174	C	C5-C6-N1	5.91	123.95	121.00
25	BA	1936	A	N1-C2-N3	5.89	132.25	129.30
56	CT	18	DC	O4'-C1'-N1	5.89	112.12	108.00
59	CD	605	LEU	CB-CG-CD2	-5.89	100.99	111.00
57	CA	13	LEU	CA-CB-CG	5.88	128.83	115.30
25	BA	2186	G	N1-C2-N3	5.88	127.43	123.90
58	CC	1278	LEU	CB-CG-CD2	-5.87	101.02	111.00
25	BA	1406	U	C5-C6-N1	5.86	125.63	122.70
25	BA	222	A	O4'-C1'-N9	-5.86	103.51	108.20
58	CC	1204	LEU	CA-CB-CG	-5.86	101.82	115.30
59	CD	327	LEU	CB-CG-CD2	-5.85	101.06	111.00
21	AU	64	ASN	N-CA-C	-5.84	95.23	111.00
25	BA	2103	C	C2-N3-C4	-5.84	116.98	119.90
56	CT	20	DC	O5'-P-OP2	-5.83	100.45	105.70
58	CC	1291	LEU	CB-CG-CD2	-5.82	101.10	111.00
25	BA	2808	G	O4'-C1'-N9	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	44	C	C6-N1-C2	-5.81	117.97	120.30
7	AG	13	LEU	CA-CB-CG	5.80	128.63	115.30
1	AA	846	G	C4-N9-C1'	5.79	134.03	126.50
25	BA	2103	C	N1-C2-N3	5.76	123.24	119.20
58	CC	1141	LEU	CB-CG-CD1	-5.76	101.20	111.00
25	BA	884	U	C6-N1-C1'	-5.76	113.13	121.20
25	BA	1179	G	N1-C6-O6	5.76	123.36	119.90
1	AA	206	C	C6-N1-C1'	-5.75	113.90	120.80
58	CC	452	ARG	NE-CZ-NH1	-5.73	117.44	120.30
57	CB	228	LEU	CA-CB-CG	-5.72	102.13	115.30
1	AA	883	C	C6-N1-C2	-5.72	118.01	120.30
25	BA	199	A	O4'-C1'-N9	5.72	112.78	108.20
1	AA	1034	G	N3-C4-N9	-5.71	122.58	126.00
22	AV	42	G	N1-C6-O6	-5.71	116.48	119.90
25	BA	2581	G	O4'-C1'-N9	5.70	112.76	108.20
25	BA	2120	G	C6-C5-N7	-5.68	126.99	130.40
22	AV	40	A	O4'-C1'-N9	5.68	112.75	108.20
25	BA	60	G	O4'-C1'-N9	-5.68	103.66	108.20
25	BA	2160	C	C2-N1-C1'	5.68	125.05	118.80
59	CD	1332	LEU	CB-CG-CD1	-5.65	101.39	111.00
25	BA	1170	C	C5-C6-N1	5.64	123.82	121.00
58	CC	802	VAL	CG1-CB-CG2	-5.63	101.88	110.90
1	AA	846	G	C8-N9-C1'	-5.63	119.68	127.00
25	BA	370	G	O4'-C1'-N9	-5.63	103.70	108.20
25	BA	613	A	P-O3'-C3'	-5.63	112.95	119.70
25	BA	2150	C	C6-N1-C1'	-5.62	114.06	120.80
1	AA	1034	G	C5-N7-C8	-5.61	101.50	104.30
25	BA	2111	U	N1-C2-O2	5.59	126.71	122.80
57	CB	13	LEU	CA-CB-CG	5.58	128.13	115.30
22	AV	37	C	C2-N1-C1'	5.57	124.93	118.80
25	BA	353	C	N1-C2-O2	5.57	122.24	118.90
22	AV	49	G	C4-N9-C1'	5.56	133.73	126.50
1	AA	452	A	C4-N9-C1'	5.56	136.30	126.30
22	AV	47	G	C8-N9-C4	-5.55	104.18	106.40
17	AQ	75	LEU	CA-CB-CG	5.54	128.05	115.30
25	BA	897	C	C2-N1-C1'	5.54	124.90	118.80
25	BA	1936	A	C2-N3-C4	-5.54	107.83	110.60
1	AA	1009	U	N1-C2-O2	5.53	126.67	122.80
59	CD	412	LEU	CB-CG-CD1	-5.53	101.60	111.00
25	BA	2286	G	C8-N9-C1'	-5.52	119.83	127.00
25	BA	1349	C	C6-N1-C2	-5.51	118.09	120.30
25	BA	2110	G	C8-N9-C1'	-5.51	119.83	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	892	A	O4'-C1'-N9	5.51	112.61	108.20
25	BA	2186	G	N3-C2-N2	-5.51	116.04	119.90
58	CC	836	LEU	CB-CG-CD2	-5.50	101.64	111.00
59	CD	449	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	AA	86	G	O5'-P-OP1	5.49	117.29	110.70
1	AA	1009	U	N3-C2-O2	-5.49	118.35	122.20
58	CC	28	LEU	CA-CB-CG	-5.49	102.66	115.30
1	AA	1008	U	N3-C2-O2	-5.49	118.36	122.20
22	AV	47	G	C5-N7-C8	-5.49	101.56	104.30
25	BA	2187	U	O4'-C1'-N1	5.46	112.57	108.20
1	AA	108	G	C8-N9-C1'	-5.45	119.91	127.00
58	CC	184	LEU	CB-CG-CD1	-5.45	101.74	111.00
25	BA	2150	C	N1-C2-O2	5.44	122.17	118.90
1	AA	999	C	C6-N1-C2	-5.43	118.13	120.30
1	AA	1027	C	C2-N3-C4	5.43	122.61	119.90
25	BA	783	A	N3-C4-C5	-5.42	123.01	126.80
59	CD	1138	LEU	CB-CG-CD2	-5.41	101.81	111.00
25	BA	27	G	O4'-C1'-N9	5.41	112.53	108.20
22	AV	43	G	C4-N9-C1'	5.40	133.51	126.50
25	BA	2111	U	C2-N1-C1'	5.40	124.17	117.70
10	AJ	87	LEU	CA-CB-CG	5.39	127.70	115.30
1	AA	1167	A	C5'-C4'-O4'	5.39	115.57	109.10
25	BA	136	G	N3-C4-N9	5.37	129.22	126.00
1	AA	148	G	O4'-C1'-N9	5.37	112.50	108.20
58	CC	671	LEU	CB-CG-CD2	-5.37	101.88	111.00
22	AV	40	A	N7-C8-N9	-5.36	111.12	113.80
22	AV	41	C	C6-N1-C1'	-5.36	114.37	120.80
1	AA	1249	C	C6-N1-C2	-5.35	118.16	120.30
25	BA	1607	C	C6-N1-C2	-5.35	118.16	120.30
1	AA	1086	U	C2-N1-C1'	5.35	124.12	117.70
1	AA	439	U	N3-C2-O2	-5.34	118.46	122.20
25	BA	2150	C	C5-C6-N1	5.34	123.67	121.00
58	CC	1064	ASP	CB-CG-OD2	5.33	123.10	118.30
8	AH	61	LEU	CA-CB-CG	5.32	127.54	115.30
25	BA	2103	C	C6-N1-C2	-5.32	118.17	120.30
22	AV	49	G	N9-C1'-C2'	5.31	120.91	114.00
25	BA	2506	U	C5'-C4'-O4'	-5.31	102.73	109.10
25	BA	136	G	N9-C4-C5	-5.31	103.28	105.40
25	BA	2150	C	C6-N1-C2	-5.31	118.18	120.30
25	BA	1313	U	N1-C2-O2	5.30	126.51	122.80
25	BA	2164	C	C2-N1-C1'	5.30	124.63	118.80
25	BA	1415	U	O4'-C1'-N1	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	CC	1054	LEU	CB-CG-CD2	-5.30	102.00	111.00
23	AW	22	G	C8-N9-C1'	-5.29	120.12	127.00
58	CC	210	LEU	CB-CG-CD2	-5.28	102.02	111.00
25	BA	1052	C	N1-C2-O2	-5.28	115.73	118.90
56	CT	8	DT	N3-C4-O4	5.28	123.07	119.90
25	BA	1176	U	P-O3'-C3'	5.28	126.03	119.70
56	CT	12	DT	N3-C4-O4	5.28	123.06	119.90
25	BA	892	A	C4-N9-C1'	-5.26	116.83	126.30
1	AA	1086	U	O4'-C1'-N1	5.26	112.41	108.20
1	AA	961	U	C5'-C4'-O4'	5.26	115.41	109.10
25	BA	2110	G	C4-C5-N7	5.25	112.90	110.80
25	BA	783	A	C8-N9-C4	-5.24	103.70	105.80
1	AA	117	G	C6-C5-N7	-5.24	127.26	130.40
1	AA	2	A	O4'-C1'-N9	-5.23	104.01	108.20
1	AA	121	U	O4'-C1'-N1	-5.23	104.02	108.20
25	BA	137	U	P-O3'-C3'	5.23	125.97	119.70
58	CC	1176	LEU	CB-CG-CD2	-5.22	102.13	111.00
25	BA	2111	U	N3-C2-O2	-5.21	118.55	122.20
25	BA	1077	A	N9-C1'-C2'	5.21	120.77	114.00
58	CC	1333	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	AA	1279	G	C4-N9-C1'	5.19	133.24	126.50
25	BA	1179	G	C5-C6-O6	-5.18	125.49	128.60
56	CT	13	DT	N3-C4-O4	5.18	123.01	119.90
25	BA	1407	G	C4-C5-N7	5.18	112.87	110.80
25	BA	1311	G	O4'-C1'-N9	5.17	112.34	108.20
25	BA	2186	G	C6-C5-N7	5.17	133.50	130.40
25	BA	12	U	N3-C2-O2	-5.16	118.59	122.20
25	BA	2162	G	P-O3'-C3'	5.15	125.89	119.70
25	BA	2174	C	C6-N1-C2	-5.15	118.24	120.30
1	AA	793	U	O4'-C1'-N1	-5.15	104.08	108.20
22	AV	34	A	P-O3'-C3'	5.15	125.88	119.70
22	AV	47	G	N3-C4-N9	-5.15	122.91	126.00
58	CC	616	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	AA	1249	C	C2-N1-C1'	5.14	124.45	118.80
26	BB	17	C	O4'-C1'-N1	5.14	112.31	108.20
32	BH	15	LEU	CA-CB-CG	5.13	127.11	115.30
1	AA	74	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	1397	C	P-O3'-C3'	5.12	125.84	119.70
12	AL	74	LEU	CA-CB-CG	5.12	127.07	115.30
25	BA	1728	C	C5-C6-N1	-5.11	118.44	121.00
1	AA	198	G	N9-C1'-C2'	-5.10	106.39	112.00
25	BA	1407	G	C6-C5-N7	-5.10	127.34	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1063	G	N1-C6-O6	-5.10	116.84	119.90
25	BA	1313	U	N3-C2-O2	-5.09	118.64	122.20
25	BA	404	A	O4'-C1'-N9	5.09	112.27	108.20
25	BA	1212	G	O4'-C1'-N9	5.08	112.26	108.20
1	AA	999	C	C6-N1-C1'	-5.07	114.71	120.80
59	CD	788	LEU	CB-CG-CD1	-5.07	102.38	111.00
25	BA	1607	C	C2-N1-C1'	5.07	124.38	118.80
25	BA	884	U	C5-C4-O4	-5.07	122.86	125.90
25	BA	404	A	P-O3'-C3'	5.06	125.77	119.70
25	BA	1062	G	N3-C4-N9	5.06	129.04	126.00
23	AW	74	C	N1-C2-O2	5.06	121.94	118.90
25	BA	136	G	C4-C5-N7	5.06	112.82	110.80
58	CC	1233	LEU	CA-CB-CG	5.06	126.93	115.30
25	BA	2117	A	O4'-C1'-N9	5.04	112.23	108.20
1	AA	5	U	C2-N1-C1'	5.04	123.75	117.70
22	AV	42	G	C6-N1-C2	-5.03	122.08	125.10
1	AA	1008	U	O4'-C1'-N1	5.02	112.22	108.20
57	CA	79	LEU	CB-CG-CD1	-5.02	102.47	111.00
25	BA	1063	G	O3'-P-O5'	5.01	113.53	104.00
25	BA	1406	U	C3'-C2'-C1'	5.01	105.51	101.50
55	CN	21	DC	O4'-C1'-N1	5.01	111.51	108.00
58	CC	918	LEU	CA-CB-CG	-5.00	103.79	115.30
1	AA	1227	A	O4'-C1'-N9	-5.00	104.20	108.20
25	BA	1314	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	884	U	Sidechain
10	AJ	42	LEU	Mainchain
12	AL	43	LYS	Peptide
13	AM	48	LEU	Peptide
13	AM	49	SER	Peptide
22	AV	41	C	Sidechain
53	B5	31	HIS	Peptide
25	BA	1052	C	Sidechain
25	BA	1104	C	Sidechain
27	BC	176	LEU	Mainchain
37	BO	100	CYS	Mainchain

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Mol	Chain	Res	Type	Group
46	BX	54	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32907	0	16571	400	0
2	AB	1765	0	1792	35	0
3	AC	1640	0	1713	99	0
4	AD	1643	0	1706	58	0
5	AE	1148	0	1195	40	0
6	AF	848	0	846	31	0
7	AG	1203	0	1254	34	0
8	AH	979	0	1031	26	0
9	AI	1031	0	1076	50	0
10	AJ	800	0	839	39	0
11	AK	866	0	874	17	0
12	AL	949	0	1008	24	0
13	AM	891	0	952	37	0
14	AN	805	0	844	21	0
15	AO	714	0	734	13	0
16	AP	649	0	666	4	0
17	AQ	641	0	682	13	0
18	AR	443	0	466	14	0
19	AS	663	0	688	21	0
20	AT	670	0	719	14	0
21	AU	590	0	629	19	0
22	AV	636	0	327	19	0
23	AW	1645	0	842	26	0
24	AX	1624	0	823	35	0
25	BA	62290	0	31344	614	0
26	BB	2569	0	1301	24	0
27	BC	2092	0	2167	40	0
28	BD	1566	0	1618	31	0
29	BE	1552	0	1618	28	0
30	BF	1420	0	1457	63	0
31	BG	1313	0	1358	34	0
32	BH	1111	0	1148	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BK	1129	0	1162	17	0
34	BL	947	0	1023	25	0
35	BM	1052	0	1127	26	0
36	BN	1075	0	1153	23	0
37	BO	960	0	999	15	0
38	BP	900	0	935	26	0
39	BQ	917	0	962	23	0
40	BR	947	0	1019	20	0
41	BS	816	0	839	15	0
42	BT	857	0	922	17	0
43	BU	757	0	820	20	0
44	BV	789	0	844	18	0
45	BW	753	0	780	17	0
46	BX	582	0	599	8	0
47	BY	625	0	652	13	0
48	BZ	501	0	531	7	0
49	B1	449	0	488	9	0
50	B2	444	0	458	17	0
51	B3	436	0	477	13	0
52	B4	377	0	418	10	0
53	B5	504	0	572	14	0
54	B6	301	0	341	7	0
55	CN	618	0	339	27	0
56	CT	606	0	338	36	0
57	CA	1775	0	1800	15	0
57	CB	1684	0	1713	19	0
58	CC	10415	0	10432	214	0
59	CD	10375	0	10597	176	0
60	AA	119	0	0	0	0
60	AW	2	0	0	0	0
60	B2	1	0	0	0	0
60	BA	294	0	0	0	0
60	BB	2	0	0	0	0
60	BC	1	0	0	0	0
60	BO	1	0	0	0	0
60	CD	1	0	0	0	0
61	AX	11	0	8	1	0
62	B6	1	0	0	0	0
62	CD	2	0	0	0	0
All	All	171689	0	122636	2452	0

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

All (2452) 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:109:PRO:HD2	58:CC:859:GLU:CG	1.58	1.34
4:AD:193:ALA:CA	59:CD:86:GLU:OE2	1.73	1.32
5:AE:10:GLU:HG3	59:CD:78:LEU:CD1	1.77	1.15
3:AC:109:PRO:HD2	58:CC:859:GLU:HG3	1.21	1.15
4:AD:191:LEU:O	59:CD:86:GLU:OE1	1.60	1.15
5:AE:10:GLU:HG3	59:CD:78:LEU:HD13	1.27	1.11
3:AC:78:GLY:O	58:CC:943:LYS:HD2	1.51	1.11
3:AC:80:LYS:NZ	58:CC:946:LEU:HD22	1.70	1.05
3:AC:77:ILE:CG2	58:CC:943:LYS:HE2	1.86	1.04
3:AC:108:LYS:HA	58:CC:859:GLU:HG3	1.40	1.03
1:AA:1175:G:HO2'	1:AA:1176:A:H8	1.10	0.99
4:AD:194:ASP:HB3	59:CD:74:LYS:NZ	1.79	0.97
30:BF:55:ALA:O	30:BF:59:ALA:N	1.97	0.97
1:AA:181:A:HO2'	1:AA:182:A:H8	1.12	0.97
3:AC:107:ARG:HH21	58:CC:863:SER:HB3	1.30	0.97
3:AC:109:PRO:CD	58:CC:859:GLU:HG3	1.93	0.97
24:AX:26:A:N6	24:AX:44:G:H1	1.62	0.96
3:AC:77:ILE:HG21	58:CC:943:LYS:HE2	1.47	0.96
25:BA:284:U:H3	25:BA:356:G:H1	1.05	0.96
3:AC:107:ARG:O	58:CC:859:GLU:CG	2.15	0.95
24:AX:26:A:H61	24:AX:44:G:H1	0.98	0.95
4:AD:194:ASP:HB3	59:CD:74:LYS:HZ3	1.28	0.94
25:BA:2141:G:H2'	25:BA:2142:A:H8	1.32	0.94
41:BS:73:LYS:HE3	41:BS:86:GLN:HG2	1.49	0.94
25:BA:2312:U:H5'	30:BF:85:ILE:HD11	1.50	0.93
21:AU:61:ALA:O	21:AU:65:ALA:HB3	1.68	0.93
46:BX:65:GLY:HA2	46:BX:85:GLU:HG2	1.49	0.93
25:BA:1040:A:N6	25:BA:1115:G:H1	1.65	0.93
32:BH:47:PHE:HA	32:BH:51:ARG:HB2	1.49	0.92
25:BA:2135:A:N6	25:BA:2156:G:O2'	2.02	0.91
25:BA:2118:U:OP1	25:BA:2148:G:O2'	1.86	0.91
25:BA:2308:G:O6	25:BA:2311:A:N7	2.03	0.91
30:BF:54:ALA:O	30:BF:58:ALA:N	2.02	0.91
3:AC:79:LYS:HE2	58:CC:942:ASP:HA	1.51	0.90
4:AD:193:ALA:HA	59:CD:86:GLU:OE2	0.98	0.90
13:AM:44:LYS:HB2	13:AM:47:GLU:HG2	1.53	0.90
1:AA:481:G:O2'	1:AA:483:C:N4	2.05	0.90
25:BA:1827:U:OP2	27:BC:221:ARG:NH1	2.05	0.89
13:AM:92:ARG:HD2	25:BA:888:C:H3'	1.55	0.89
25:BA:1040:A:H61	25:BA:1115:G:H1	1.10	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:109:PRO:CD	58:CC:859:GLU:CG	2.48	0.88
21:AU:61:ALA:O	21:AU:64:ASN:O	1.90	0.88
25:BA:1936:A:H2	25:BA:1943:U:H3	1.17	0.88
3:AC:107:ARG:HE	58:CC:863:SER:HB3	1.39	0.87
5:AE:10:GLU:CG	59:CD:78:LEU:CD1	2.51	0.87
25:BA:1724:G:H1	25:BA:1736:U:H3	1.19	0.87
44:BV:96:PHE:O	44:BV:100:SER:HA	1.73	0.87
25:BA:2141:G:H2'	25:BA:2142:A:C8	2.10	0.87
3:AC:107:ARG:O	58:CC:859:GLU:CD	2.13	0.86
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.08	0.86
25:BA:1198:U:H4'	40:BR:9:ILE:HD11	1.56	0.86
25:BA:1998:A:OP2	28:BD:141:ARG:NH2	2.08	0.86
50:B2:30:VAL:HG22	50:B2:37:LYS:HG2	1.58	0.86
2:AB:187:VAL:HG11	2:AB:199:VAL:HG12	1.57	0.86
1:AA:1452:C:H4'	1:AA:1453:G:H5"	1.57	0.86
45:BW:20:LEU:HD21	45:BW:27:PRO:HD3	1.57	0.85
25:BA:2880:C:O2'	37:BO:90:ARG:NH1	2.09	0.85
3:AC:107:ARG:NH2	58:CC:863:SER:HB3	1.91	0.85
3:AC:80:LYS:HZ1	58:CC:946:LEU:HD22	1.36	0.85
3:AC:77:ILE:HG22	58:CC:943:LYS:HE2	1.57	0.84
22:AV:46:C:H2'	22:AV:47:G:H8	1.43	0.84
5:AE:10:GLU:CG	59:CD:78:LEU:HD13	2.06	0.83
1:AA:1261:A:N6	1:AA:1274:A:O2'	2.12	0.83
3:AC:107:ARG:O	58:CC:859:GLU:HB3	1.78	0.83
3:AC:109:PRO:HD2	58:CC:859:GLU:CD	1.99	0.83
31:BG:170:ARG:NH2	54:B6:29:ALA:O	2.11	0.83
25:BA:1178:C:H2'	25:BA:1179:G:C8	2.15	0.82
25:BA:1534:U:H2'	25:BA:1535:A:H5"	1.60	0.82
25:BA:1481:U:H3	25:BA:1510:G:H1	1.25	0.82
25:BA:890:C:H3'	25:BA:891:G:H4'	1.62	0.82
25:BA:1590:A:H2'	25:BA:1591:A:C8	2.15	0.81
1:AA:73:C:N4	1:AA:94:G:O6	2.13	0.81
4:AD:147:GLU:HA	4:AD:150:LYS:HB2	1.62	0.81
29:BE:5:LEU:O	29:BE:9:GLN:HA	1.80	0.81
34:BL:36:GLY:N	34:BL:62:VAL:O	2.13	0.81
25:BA:276:U:O2'	25:BA:278:A:N7	2.12	0.81
1:AA:1051:C:O2	1:AA:1207:2MG:N2	2.13	0.81
1:AA:1006:G:H2'	1:AA:1007:U:H6	1.45	0.80
23:AW:15:G:H22	23:AW:48:C:H42	1.28	0.80
25:BA:2285:C:OP2	51:B3:6:ARG:NH1	2.13	0.80
29:BE:15:SER:HB3	29:BE:18:THR:HG22	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:47:G:H2'	22:AV:48:C:H6	1.44	0.80
25:BA:883:G:N2	25:BA:884:U:O4	2.14	0.80
12:AL:83:ARG:NH1	12:AL:84:GLY:O	2.14	0.80
59:CD:429:LEU:H	59:CD:429:LEU:HD22	1.46	0.80
25:BA:1918:A:O2'	25:BA:1919:A:N7	2.15	0.80
25:BA:2110:G:OP1	25:BA:2143:C:O2'	1.99	0.80
4:AD:194:ASP:HA	59:CD:74:LYS:CE	2.11	0.80
57:CB:191:ARG:HB3	57:CB:196:THR:HG23	1.64	0.80
25:BA:881:G:H1	25:BA:895:U:H3	1.30	0.80
3:AC:107:ARG:CZ	58:CC:863:SER:O	2.29	0.79
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.15	0.79
30:BF:114:PHE:HE2	30:BF:176:PRO:HB2	1.46	0.79
3:AC:80:LYS:HZ2	58:CC:946:LEU:HD22	1.47	0.79
1:AA:522:C:O2	1:AA:527:G7M:N2	2.13	0.79
3:AC:107:ARG:O	58:CC:859:GLU:OE1	2.00	0.79
24:AX:16:H2U:N3	24:AX:59:U:O2	2.14	0.79
11:AK:88:GLY:O	11:AK:93:ARG:NH1	2.16	0.79
3:AC:109:PRO:CD	58:CC:859:GLU:OE2	2.30	0.78
3:AC:107:ARG:HE	58:CC:863:SER:CB	1.94	0.78
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.82	0.78
25:BA:1529:G:H1	25:BA:1542:U:H3	1.32	0.78
21:AU:10:GLU:OE2	21:AU:18:ARG:NH2	2.17	0.78
25:BA:550:U:H2'	25:BA:551:G:H8	1.47	0.78
1:AA:582:C:OP2	1:AA:758:C:N4	2.17	0.77
3:AC:107:ARG:O	58:CC:859:GLU:CB	2.33	0.77
25:BA:483:A:H5"	44:BV:47:LYS:HD2	1.67	0.77
25:BA:2107:G:H1	25:BA:2182:U:H3	0.81	0.77
25:BA:2162:G:OP2	25:BA:2164:C:N4	2.14	0.77
25:BA:2467:C:O2	36:BN:123:LYS:NZ	2.16	0.77
25:BA:2792:A:H2'	25:BA:2793:C:C6	2.20	0.77
20:AT:44:LYS:NZ	20:AT:83:ILE:O	2.18	0.77
12:AL:110:ARG:NH1	12:AL:112:GLN:O	2.18	0.77
59:CD:1186:TYR:OH	59:CD:1188:GLU:OE1	2.01	0.77
25:BA:475:C:O2	25:BA:479:A:N6	2.16	0.77
25:BA:2901:C:H2'	25:BA:2902:C:C6	2.20	0.77
56:CT:18:DC:H2'	56:CT:19:DG:C8	2.19	0.77
14:AN:46:LEU:HD12	19:AS:13:LEU:HD13	1.67	0.77
25:BA:284:U:O2	25:BA:356:G:N2	2.17	0.77
25:BA:1100:C:H2'	25:BA:1101:U:H6	1.49	0.76
19:AS:31:LEU:HB2	19:AS:49:ILE:HG22	1.66	0.76
1:AA:664:G:H22	1:AA:741:G:H1	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:78:VAL:HG21	32:BH:103:VAL:HG22	1.67	0.76
25:BA:1040:A:N1	25:BA:1115:G:N2	2.33	0.76
31:BG:164:TYR:HB2	31:BG:167:GLU:HB3	1.66	0.76
1:AA:160:A:N6	1:AA:346:G:O6	2.18	0.76
1:AA:1382:C:O2'	7:AG:79:ARG:NH2	2.18	0.76
4:AD:194:ASP:CB	59:CD:74:LYS:NZ	2.48	0.76
57:CA:62:ASP:OD1	57:CA:63:GLY:N	2.19	0.76
1:AA:1160:G:OP2	2:AB:131:LYS:NZ	2.19	0.76
4:AD:192:SER:O	59:CD:86:GLU:OE2	2.04	0.76
3:AC:189:ALA:HB3	3:AC:196:ILE:HG23	1.67	0.76
9:AI:84:THR:HG23	9:AI:98:LEU:HD13	1.67	0.76
39:BQ:113:ARG:O	39:BQ:115:ASN:ND2	2.19	0.76
25:BA:1071:G:O6	25:BA:1100:C:N4	2.19	0.75
25:BA:2718:G:O4'	25:BA:2718:G:O2'	1.93	0.75
25:BA:444:C:OP1	29:BE:40:ARG:NH2	2.19	0.75
57:CB:74:VAL:HG21	57:CB:81:ILE:HD11	1.66	0.75
3:AC:107:ARG:NE	58:CC:863:SER:HB3	2.00	0.75
30:BF:56:ASP:O	30:BF:60:ILE:HB	1.87	0.75
5:AE:101:GLU:OE2	5:AE:122:ASN:ND2	2.20	0.75
25:BA:783:A:H2'	25:BA:783:A:N3	2.00	0.75
25:BA:877:A:O2'	25:BA:900:A:N6	2.19	0.74
25:BA:878:A:N6	25:BA:899:A:O2'	2.21	0.74
25:BA:2831:G:OP2	28:BD:59:ARG:NH2	2.21	0.74
54:B6:23:ILE:HB	54:B6:37:GLN:HB3	1.68	0.74
59:CD:816:THR:OG1	59:CD:818:GLU:OE1	2.04	0.74
25:BA:1916:A:H2'	25:BA:1917:PSU:C6	2.23	0.74
17:AQ:79:VAL:HG22	17:AQ:80:GLU:HG3	1.70	0.74
22:AV:46:C:H2'	22:AV:47:G:C8	2.21	0.74
25:BA:1494:A:O2'	25:BA:1495:A:OP1	2.05	0.74
25:BA:1782:U:O2'	25:BA:2609:U:H5"	1.87	0.74
50:B2:54:VAL:HG23	50:B2:55:ILE:HD12	1.69	0.74
1:AA:1463:U:H5"	39:BQ:109:ARG:HH11	1.53	0.73
5:AE:10:GLU:CB	59:CD:78:LEU:HD12	2.18	0.73
25:BA:443:A:C5	29:BE:40:ARG:HD2	2.23	0.73
1:AA:198:G:H2'	1:AA:199:A:H8	1.53	0.73
1:AA:263:A:OP2	20:AT:74:ARG:NH1	2.21	0.73
3:AC:108:LYS:CA	58:CC:859:GLU:HG3	2.17	0.73
38:BP:56:LYS:O	38:BP:60:GLU:HB2	1.89	0.73
44:BV:28:VAL:HG22	44:BV:34:VAL:HG12	1.69	0.73
1:AA:1006:G:O6	1:AA:1024:G:N2	2.20	0.73
44:BV:17:LYS:NZ	44:BV:40:ASN:OD1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BO:82:GLU:OE2	37:BO:86:ARG:NH2	2.20	0.73
1:AA:951:G:OP2	13:AM:101:ARG:NH2	2.21	0.73
8:AH:41:LYS:NZ	8:AH:47:GLU:O	2.21	0.73
59:CD:1179:PRO:HD2	59:CD:1184:ASP:HA	1.69	0.73
25:BA:1100:C:H2'	25:BA:1101:U:C6	2.23	0.73
1:AA:1086:U:O4	1:AA:1099:G:N1	2.18	0.72
13:AM:92:ARG:HB2	25:BA:888:C:H5'	1.71	0.72
35:BM:37:GLY:N	35:BM:40:SER:OG	2.22	0.72
58:CC:10:ARG:NH2	58:CC:793:GLU:OE1	2.21	0.72
3:AC:109:PRO:CD	58:CC:859:GLU:CD	2.57	0.72
25:BA:2069:G7M:N2	25:BA:2442:C:O2	2.16	0.72
25:BA:2099:U:H3	25:BA:2190:G:H1	1.34	0.72
36:BN:14:LYS:O	36:BN:71:LYS:NZ	2.22	0.72
2:AB:44:GLU:N	2:AB:44:GLU:OE2	2.21	0.72
3:AC:108:LYS:HA	58:CC:859:GLU:CG	2.18	0.72
30:BF:110:ARG:NH1	30:BF:136:ILE:O	2.20	0.72
5:AE:10:GLU:CG	59:CD:78:LEU:HD12	2.20	0.72
30:BF:56:ASP:O	30:BF:60:ILE:N	2.21	0.72
44:BV:99:ASN:OD1	44:BV:101:GLU:HG2	1.89	0.72
25:BA:1592:C:H2'	25:BA:1593:A:H8	1.55	0.72
24:AX:26:A:N1	24:AX:44:G:N2	2.38	0.71
3:AC:79:LYS:CE	58:CC:942:ASP:HA	2.20	0.71
25:BA:729:G:OP1	27:BC:10:SER:OG	2.08	0.71
4:AD:192:SER:C	59:CD:86:GLU:OE2	2.18	0.71
58:CC:27:LEU:O	58:CC:528:ARG:NH1	2.24	0.71
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.06	0.71
14:AN:63:ARG:NH1	14:AN:68:GLY:O	2.24	0.71
25:BA:1406:U:C2'	25:BA:1407:G:H5"	2.20	0.71
25:BA:1592:C:H2'	25:BA:1593:A:C8	2.24	0.71
5:AE:10:GLU:CB	59:CD:78:LEU:CD1	2.69	0.71
17:AQ:76:VAL:HG23	17:AQ:77:ARG:HD2	1.73	0.71
25:BA:1693:U:O2	27:BC:14:ARG:NH1	2.24	0.71
24:AX:51:U:H2'	24:AX:52:G:H8	1.54	0.71
1:AA:974:A:OP1	14:AN:69:ARG:NH2	2.24	0.71
25:BA:881:G:O6	25:BA:895:U:O4	2.09	0.71
25:BA:1065:U:O2'	25:BA:1066:U:O4'	2.08	0.71
59:CD:454:CYS:SG	59:CD:455:ALA:N	2.64	0.71
25:BA:1529:G:O6	25:BA:1542:U:O4	2.08	0.70
25:BA:1481:U:O2	25:BA:1510:G:N2	2.24	0.70
1:AA:412:A:H62	1:AA:431:A:H61	1.39	0.70
1:AA:841:C:O2'	1:AA:843:U:OP2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.24	0.70
25:BA:137:U:O2'	25:BA:138:U:OP1	2.08	0.70
1:AA:1277:C:O2'	1:AA:1278:G:H5"	1.91	0.70
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.25	0.70
27:BC:29:PRO:HG2	27:BC:34:LEU:HD11	1.74	0.70
59:CD:1157:ALA:HB2	59:CD:1210:ILE:HD11	1.74	0.70
1:AA:35:G:N3	12:AL:115:SER:OG	2.25	0.70
22:AV:47:G:H2'	22:AV:48:C:C6	2.25	0.70
1:AA:181:A:O2'	1:AA:194:C:N4	2.24	0.70
23:AW:50:U:H3	23:AW:64:G:H1	1.38	0.70
44:BV:48:PRO:HG3	44:BV:56:GLY:HA3	1.74	0.70
1:AA:356:A:N3	1:AA:368:U:O2'	2.25	0.70
25:BA:2168:G:O2'	25:BA:2169:A:OP1	2.09	0.70
16:AP:55:ASP:OD1	16:AP:56:ARG:N	2.25	0.70
1:AA:83:C:O2	1:AA:86:G:N1	2.16	0.69
29:BE:1:MET:HB3	29:BE:14:VAL:HG23	1.72	0.69
47:BY:72:ARG:NH1	47:BY:78:TYR:OH	2.25	0.69
1:AA:437:U:H5"	4:AD:152:GLN:HE22	1.56	0.69
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.27	0.69
4:AD:104:ARG:HA	4:AD:104:ARG:HH11	1.58	0.69
1:AA:1017:U:O2'	1:AA:1018:G:O4'	2.10	0.69
13:AM:81:MET:O	13:AM:92:ARG:NH1	2.25	0.69
1:AA:927:G:O2'	1:AA:928:G:H5'	1.93	0.69
25:BA:1223:G:OP1	41:BS:68:ARG:NH2	2.25	0.69
25:BA:2795:C:H2'	25:BA:2796:C:C6	2.28	0.69
58:CC:624:ASP:OD1	58:CC:627:GLY:N	2.25	0.69
8:AH:106:THR:HB	8:AH:121:LEU:HD12	1.72	0.69
38:BP:89:ASP:OD1	38:BP:89:ASP:N	2.26	0.69
1:AA:1329:A:H5'	13:AM:29:ARG:HD2	1.74	0.69
25:BA:627:A:OP1	35:BM:78:ARG:NH2	2.19	0.69
25:BA:2106:U:H2'	25:BA:2107:G:H8	1.55	0.69
1:AA:86:G:H4'	1:AA:86:G:OP1	1.92	0.69
3:AC:107:ARG:HH21	58:CC:863:SER:CB	2.06	0.69
17:AQ:9:GLN:NE2	17:AQ:60:GLU:OE2	2.25	0.69
25:BA:1040:A:N6	25:BA:1115:G:N1	2.26	0.69
28:BD:35:THR:HG22	28:BD:73:VAL:HG21	1.73	0.69
36:BN:35:ALA:HB2	36:BN:102:LEU:HD11	1.75	0.69
7:AG:57:SER:OG	7:AG:58:GLU:OE2	2.08	0.69
59:CD:504:GLN:NE2	59:CD:505:ASP:OD1	2.18	0.69
8:AH:77:ARG:NH1	8:AH:79:SER:O	2.26	0.68
25:BA:550:U:H2'	25:BA:551:G:C8	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1901:A:OP2	27:BC:253:LYS:NZ	2.26	0.68
10:AJ:10:LEU:HB3	10:AJ:18:ILE:HD11	1.74	0.68
1:AA:195:A:O2'	1:AA:196:A:H5'	1.93	0.68
25:BA:1177:G:O2'	25:BA:1178:C:O5'	2.08	0.68
1:AA:518:C:HO2'	1:AA:530:G:N2	1.91	0.68
1:AA:1005:A:N6	1:AA:1024:G:O2'	2.27	0.68
25:BA:1607:C:N4	25:BA:1622:G:OP2	2.26	0.68
42:BT:82:MET:SD	42:BT:84:ARG:NH1	2.67	0.68
28:BD:8:LYS:O	28:BD:198:GLY:N	2.21	0.68
1:AA:823:C:HO2'	8:AH:2:SER:N	1.92	0.68
25:BA:1585:C:H2'	25:BA:1586:A:H8	1.59	0.68
27:BC:107:PRO:HD2	27:BC:110:LEU:HD22	1.75	0.68
25:BA:1044:C:O2'	25:BA:1111:A:N1	2.26	0.68
25:BA:2720:U:OP1	39:BQ:53:ARG:NH2	2.27	0.68
35:BM:107:PHE:HB3	35:BM:126:ARG:HH12	1.57	0.68
42:BT:22:ASP:OD1	42:BT:25:ARG:NH2	2.27	0.68
4:AD:194:ASP:HA	59:CD:74:LYS:HE3	1.74	0.67
31:BG:145:ALA:HB1	31:BG:164:TYR:HE1	1.59	0.67
56:CT:19:DG:H2'	56:CT:20:DC:C6	2.29	0.67
1:AA:198:G:H2'	1:AA:199:A:C8	2.30	0.67
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.27	0.67
13:AM:59:GLU:OE2	13:AM:62:LYS:NZ	2.27	0.67
1:AA:4:U:O2'	1:AA:5:U:O5'	2.10	0.67
25:BA:2683:C:OP1	39:BQ:51:ARG:NH1	2.27	0.67
25:BA:125:A:OP2	52:B4:19:ARG:NH2	2.24	0.67
1:AA:1290:G:O2'	9:AI:41:ARG:NH2	2.27	0.67
3:AC:107:ARG:CZ	58:CC:863:SER:HB3	2.25	0.67
3:AC:80:LYS:NZ	58:CC:946:LEU:CD2	2.55	0.67
4:AD:43:ALA:O	4:AD:44:ARG:NH1	2.27	0.67
1:AA:1397:C:H5'	22:AV:23:C:H41	1.58	0.67
9:AI:25:ASN:HB3	9:AI:27:LYS:HE2	1.74	0.67
25:BA:1068:G:N2	25:BA:1095:A:O3'	2.27	0.67
9:AI:42:GLU:OE2	9:AI:49:ARG:NH2	2.27	0.67
25:BA:1869:G:N2	25:BA:1871:A:O2'	2.27	0.67
25:BA:2857:G:N2	25:BA:2860:A:OP2	2.23	0.67
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.29	0.66
1:AA:1249:C:H5	1:AA:1288:A:H62	1.43	0.66
23:AW:69:C:H2'	23:AW:70:G:H8	1.60	0.66
1:AA:4:U:HO2'	1:AA:5:U:C5'	2.07	0.66
1:AA:1422:G:O2'	34:BL:49:ARG:NH2	2.28	0.66
2:AB:43:LEU:O	2:AB:47:VAL:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:93:ASP:OD1	3:AC:94:ILE:N	2.28	0.66
25:BA:2683:C:O2	34:BL:70:ARG:NH2	2.28	0.66
36:BN:106:ASP:OD1	36:BN:107:GLY:N	2.29	0.66
35:BM:78:ARG:HG2	35:BM:113:ALA:HB3	1.77	0.66
9:AI:116:VAL:HG13	10:AJ:62:ARG:HH21	1.61	0.66
17:AQ:40:ARG:HA	17:AQ:40:ARG:HE	1.59	0.66
25:BA:1494:A:HO2'	25:BA:1495:A:P	2.18	0.66
25:BA:2175:C:H2'	25:BA:2176:A:C8	2.30	0.66
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.31	0.66
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.75	0.66
9:AI:21:ILE:HD13	9:AI:63:LEU:HB3	1.77	0.66
23:AW:21:A:N6	23:AW:46:A:O2'	2.29	0.66
25:BA:1857:G:O2'	25:BA:1884:G:N2	2.27	0.66
25:BA:1914:C:H2'	25:BA:1915:3TD:H6	1.77	0.66
25:BA:2364:C:OP1	46:BX:55:ARG:NH1	2.28	0.66
3:AC:58:GLU:OE1	3:AC:65:ARG:NH1	2.29	0.66
3:AC:79:LYS:HE2	58:CC:942:ASP:CA	2.23	0.66
25:BA:639:U:H2'	25:BA:640:C:C6	2.30	0.66
36:BN:20:LEU:HD13	45:BW:81:PRO:HG2	1.78	0.66
12:AL:54:ARG:HB2	12:AL:54:ARG:HH11	1.59	0.66
31:BG:47:ASP:OD1	31:BG:48:ASN:N	2.24	0.66
32:BH:4:ILE:HG13	32:BH:18:GLN:HG3	1.78	0.66
4:AD:146:ARG:HH21	4:AD:148:LYS:HD3	1.61	0.65
14:AN:86:GLU:OE2	14:AN:90:ARG:NH2	2.29	0.65
25:BA:2328:A:H2'	25:BA:2329:U:C6	2.31	0.65
25:BA:491:G:O6	42:BT:49:LYS:NZ	2.27	0.65
25:BA:889:C:H2'	25:BA:890:C:H5'	1.79	0.65
45:BW:36:ALA:O	45:BW:93:ARG:NH2	2.25	0.65
4:AD:194:ASP:N	59:CD:74:LYS:HE2	2.11	0.65
27:BC:78:VAL:O	27:BC:113:GLY:N	2.29	0.65
1:AA:1239:A:H62	1:AA:1299:A:H62	1.44	0.65
23:AW:15:G:H22	23:AW:48:C:N4	1.94	0.65
25:BA:1154:G:OP2	40:BR:58:ARG:NH2	2.28	0.65
25:BA:2291:U:H2'	25:BA:2292:U:C6	2.32	0.65
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.29	0.65
45:BW:55:GLU:OE1	45:BW:55:GLU:N	2.29	0.65
55:CN:32:DA:H5'	55:CN:32:DA:C8	2.32	0.65
1:AA:411:A:OP1	4:AD:26:ARG:NH1	2.29	0.65
1:AA:1276:G:O2'	1:AA:1277:C:H5'	1.97	0.65
6:AF:43:GLY:HA2	6:AF:58:HIS:CE1	2.31	0.65
1:AA:1100:C:OP1	21:AU:69:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1317:C:O2	19:AS:37:ARG:NH2	2.29	0.65
24:AX:37:MIA:O2'	25:BA:1913:A:N1	2.28	0.65
25:BA:1064:C:O2'	25:BA:1065:U:O4'	2.15	0.65
47:BY:12:PRO:HB3	47:BY:30:LEU:HD23	1.78	0.65
22:AV:45:G:H5"	58:CC:540:ARG:NH2	2.11	0.65
28:BD:4:LEU:HD23	28:BD:29:VAL:HG11	1.79	0.65
56:CT:17:DG:C5	56:CT:18:DC:C5	2.84	0.65
8:AH:94:LYS:HD3	8:AH:117:ARG:HH12	1.62	0.65
57:CA:8:PHE:O	57:CA:10:LYS:NZ	2.26	0.64
6:AF:14:GLN:OE1	6:AF:14:GLN:N	2.31	0.64
24:AX:51:U:H2'	24:AX:52:G:C8	2.32	0.64
25:BA:1594:U:H2'	25:BA:1595:C:C6	2.31	0.64
1:AA:1051:C:N3	1:AA:1207:2MG:N1	2.35	0.64
46:BX:59:LEU:HD12	46:BX:80:ILE:HD12	1.78	0.64
1:AA:1006:G:H2'	1:AA:1007:U:C6	2.29	0.64
6:AF:29:ILE:HG23	6:AF:34:GLY:HA3	1.79	0.64
31:BG:52:PHE:CD1	31:BG:69:ARG:HB2	2.32	0.64
51:B3:6:ARG:HG2	51:B3:24:THR:HB	1.79	0.64
25:BA:613:A:N6	25:BA:616:A:N1	2.46	0.64
1:AA:1383:C:H2'	1:AA:1384:C:C6	2.33	0.64
25:BA:2102:G:N2	25:BA:2187:U:O2	2.31	0.64
56:CT:19:DG:C6	56:CT:20:DC:C4	2.86	0.64
58:CC:18:ARG:NH1	58:CC:1188:ASP:OD1	2.31	0.64
1:AA:1174:G:H2'	1:AA:1175:G:H5'	1.80	0.64
25:BA:994:C:OP2	40:BR:54:LYS:NZ	2.31	0.64
25:BA:2243:U:H2'	25:BA:2244:U:C6	2.32	0.64
16:AP:48:GLU:OE1	16:AP:51:ARG:NH2	2.30	0.64
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.31	0.64
25:BA:2795:C:H2'	25:BA:2796:C:H6	1.63	0.64
53:B5:42:ARG:HG3	53:B5:45:ARG:HH12	1.63	0.64
31:BG:35:ARG:NH1	31:BG:75:MET:SD	2.71	0.64
1:AA:1451:U:OP2	1:AA:1452:C:N4	2.31	0.63
3:AC:108:LYS:HD3	58:CC:859:GLU:HB2	1.80	0.63
4:AD:194:ASP:CA	59:CD:74:LYS:CE	2.76	0.63
56:CT:19:DG:C5	56:CT:20:DC:C5	2.86	0.63
24:AX:27:G:H2'	24:AX:28:G:H8	1.63	0.63
25:BA:1036:G:H1	25:BA:1119:U:H3	1.43	0.63
58:CC:251:ALA:HB2	58:CC:269:ILE:HD11	1.80	0.63
1:AA:246:A:N1	1:AA:278:G:O2'	2.29	0.63
21:AU:64:ASN:O	21:AU:66:ARG:N	2.30	0.63
25:BA:62:U:O2'	25:BA:63:A:N7	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1009:A:OP2	33:BK:39:LYS:NZ	2.31	0.63
37:BO:24:MET:HG2	37:BO:44:LEU:HD22	1.79	0.63
59:CD:429:LEU:HD22	59:CD:429:LEU:N	2.12	0.63
35:BM:80:SER:O	35:BM:84:LYS:HD3	1.98	0.63
23:AW:15:G:N2	23:AW:48:C:H42	1.96	0.63
25:BA:1261:C:OP2	42:BT:83:LYS:NZ	2.32	0.63
25:BA:2135:A:N6	25:BA:2156:G:HO2'	1.96	0.63
1:AA:1452:C:H4'	1:AA:1453:G:C5'	2.29	0.63
3:AC:25:ASN:OD1	3:AC:26:THR:N	2.32	0.63
12:AL:72:HIS:HB2	12:AL:74:LEU:HD23	1.79	0.63
25:BA:2282:G:O2'	25:BA:2425:A:N6	2.32	0.63
56:CT:9:DC:H2'	56:CT:10:DT:C6	2.34	0.63
58:CC:582:ASN:OD1	58:CC:583:GLU:N	2.31	0.63
25:BA:1534:U:C2'	25:BA:1535:A:H5"	2.28	0.63
56:CT:19:DG:H2'	56:CT:20:DC:H6	1.63	0.63
7:AG:79:ARG:HG3	7:AG:84:THR:HG22	1.80	0.62
25:BA:1108:U:H2'	25:BA:1109:C:C6	2.34	0.62
25:BA:1226:A:OP1	40:BR:16:LYS:NZ	2.28	0.62
30:BF:58:ALA:HB2	30:BF:65:PRO:HD3	1.81	0.62
1:AA:160:A:N6	1:AA:343:U:O2'	2.32	0.62
2:AB:47:VAL:HG13	2:AB:48:PRO:HD3	1.81	0.62
8:AH:76:GLN:HE21	8:AH:128:TYR:HD2	1.47	0.62
23:AW:15:G:O6	23:AW:48:C:O2	2.16	0.62
25:BA:1108:U:H2'	25:BA:1109:C:H6	1.63	0.62
1:AA:1233:G:OP1	9:AI:119:ARG:NH2	2.32	0.62
25:BA:1404:C:H2'	25:BA:1405:U:H5'	1.82	0.62
41:BS:1:MET:HG3	41:BS:43:ASN:HA	1.80	0.62
25:BA:2102:G:H2'	25:BA:2103:C:C6	2.34	0.62
30:BF:98:GLU:OE1	30:BF:102:ARG:NH1	2.26	0.62
13:AM:52:GLN:OE1	13:AM:52:GLN:N	2.33	0.62
1:AA:201:G:H2'	1:AA:202:G:C8	2.34	0.62
25:BA:1019:U:OP1	25:BA:1035:U:O2'	2.13	0.62
25:BA:1406:U:H2'	25:BA:1407:G:H5"	1.80	0.62
25:BA:2333:A:OP2	46:BX:77:ARG:NH2	2.28	0.62
32:BH:97:ARG:HA	32:BH:112:LYS:HB3	1.81	0.62
34:BL:34:GLY:N	34:BL:37:ASP:OD2	2.31	0.62
59:CD:576:ARG:NH1	59:CD:593:ASN:O	2.32	0.62
1:AA:932:C:H3'	7:AG:3:ARG:HD2	1.82	0.62
1:AA:1343:G:H1'	9:AI:123:ARG:HH12	1.65	0.62
3:AC:62:LYS:N	3:AC:62:LYS:HE3	2.13	0.62
1:AA:986:U:H2'	1:AA:987:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:225:ARG:O	2:AB:227:GLN:NE2	2.33	0.62
13:AM:68:ASP:OD1	13:AM:71:ARG:NH2	2.33	0.62
25:BA:1527:G:N1	25:BA:1544:A:OP2	2.30	0.62
25:BA:2187:U:H2'	25:BA:2188:U:C6	2.34	0.62
25:BA:2245:U:O2'	25:BA:2436:G:OP2	2.16	0.62
32:BH:75:LEU:HD23	32:BH:75:LEU:H	1.64	0.62
4:AD:194:ASP:CB	59:CD:74:LYS:HZ1	2.11	0.62
9:AI:88:MET:HG3	9:AI:95:ARG:HG2	1.81	0.62
11:AK:89:PRO:HB3	21:AU:32:VAL:HG21	1.80	0.62
25:BA:1585:C:O2'	25:BA:1586:A:O4'	2.12	0.62
7:AG:23:LEU:O	7:AG:27:VAL:HG13	2.00	0.61
23:AW:17:C:OP1	23:AW:60:U:O2'	2.18	0.61
25:BA:265:A:N1	25:BA:427:U:O2'	2.29	0.61
49:B1:4:THR:OG1	49:B1:37:GLU:OE2	2.17	0.61
24:AX:6:G:H2'	24:AX:7:A:C8	2.35	0.61
25:BA:2071:A:H2'	25:BA:2072:C:C6	2.35	0.61
28:BD:48:ILE:HG23	28:BD:84:LEU:HD11	1.82	0.61
55:CN:38:DA:H2"	55:CN:39:DG:N7	2.14	0.61
4:AD:166:GLU:OE2	4:AD:166:GLU:N	2.22	0.61
25:BA:2107:G:O6	25:BA:2182:U:O4	2.18	0.61
32:BH:116:ARG:HB2	32:BH:131:SER:HB2	1.82	0.61
58:CC:638:SER:OG	58:CC:639:LYS:N	2.32	0.61
1:AA:1135:U:O2'	1:AA:1138:G:N1	2.33	0.61
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.36	0.61
3:AC:79:LYS:HE3	58:CC:943:LYS:N	2.16	0.61
13:AM:23:TYR:HB3	13:AM:66:GLU:HB3	1.82	0.61
57:CB:27:THR:C	57:CB:28:LEU:HD22	2.19	0.61
1:AA:1383:C:H2'	1:AA:1384:C:H6	1.64	0.61
1:AA:302:G:OP1	12:AL:14:ARG:NH2	2.33	0.61
1:AA:1018:G:H2'	1:AA:1019:A:H8	1.66	0.61
2:AB:148:LEU:HD22	2:AB:151:ILE:HD11	1.82	0.61
10:AJ:92:LEU:HD23	10:AJ:98:VAL:HG11	1.83	0.61
25:BA:1404:C:C2'	25:BA:1405:U:H5'	2.31	0.61
45:BW:20:LEU:HD23	45:BW:21:ARG:N	2.16	0.61
5:AE:10:GLU:HB3	59:CD:78:LEU:HD12	1.81	0.61
7:AG:70:ARG:NH2	7:AG:97:ASN:OD1	2.33	0.61
59:CD:504:GLN:HG3	59:CD:505:ASP:H	1.65	0.61
27:BC:123:ALA:O	27:BC:128:ASN:ND2	2.34	0.61
29:BE:148:ILE:HB	29:BE:169:VAL:HG12	1.81	0.61
39:BQ:115:ASN:HD22	39:BQ:115:ASN:N	1.98	0.61
47:BY:3:ARG:HD2	47:BY:30:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1492:A:O2'	1:AA:1493:A:H5'	2.01	0.60
3:AC:109:PRO:HD2	58:CC:859:GLU:HG2	1.69	0.60
20:AT:42:GLY:HA2	20:AT:86:LEU:HD11	1.83	0.60
29:BE:48:THR:HG23	29:BE:86:ALA:HB3	1.82	0.60
5:AE:150:PRO:HA	5:AE:153:VAL:HG22	1.83	0.60
10:AJ:44:THR:HA	10:AJ:69:THR:O	2.01	0.60
1:AA:673:A:H2'	1:AA:674:G:C8	2.37	0.60
25:BA:1871:A:O2'	25:BA:1872:A:N7	2.35	0.60
25:BA:2252:G:H2'	25:BA:2253:G:H8	1.66	0.60
1:AA:518:C:O2'	1:AA:530:G:N2	2.33	0.60
1:AA:1179:A:OP2	9:AI:95:ARG:NH2	2.22	0.60
25:BA:2830:C:H3'	28:BD:59:ARG:HH22	1.65	0.60
3:AC:124:LEU:HD13	3:AC:196:ILE:HD13	1.84	0.60
3:AC:164:ARG:NH2	22:AV:25:U:O2'	2.35	0.60
25:BA:792:A:N3	25:BA:2072:C:O2'	2.31	0.60
1:AA:202:G:H21	1:AA:466:A:H61	1.48	0.60
24:AX:8:4SU:O2'	24:AX:21:A:N1	2.34	0.60
25:BA:645:C:H2'	25:BA:647:G:C8	2.36	0.60
25:BA:1469:A:H2'	25:BA:1470:A:C8	2.37	0.60
1:AA:1498:UR3:OP2	22:AV:16:A:O2'	2.20	0.60
17:AQ:25:ILE:HB	17:AQ:42:THR:HG23	1.81	0.60
25:BA:138:U:H6	25:BA:141:G:H1	1.49	0.60
36:BN:31:PHE:HD1	36:BN:132:THR:HG22	1.66	0.60
57:CA:67:GLU:OE1	58:CC:1057:LYS:NZ	2.33	0.60
28:BD:45:TYR:HB2	28:BD:83:ARG:HH11	1.66	0.60
59:CD:441:LEU:HD22	59:CD:441:LEU:N	2.16	0.60
1:AA:844:G:H2'	1:AA:845:A:C2	2.35	0.59
10:AJ:53:ILE:HD11	10:AJ:63:ASP:HB2	1.84	0.59
25:BA:2883:A:OP2	50:B2:50:ARG:NH1	2.35	0.59
39:BQ:91:ALA:HB2	39:BQ:113:ARG:HB2	1.84	0.59
58:CC:525:THR:HG21	58:CC:687:ARG:HH11	1.67	0.59
59:CD:797:THR:HG22	59:CD:924:GLY:HA3	1.83	0.59
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.65	0.59
25:BA:871:U:H2'	25:BA:872:U:C6	2.37	0.59
25:BA:1064:C:O2'	25:BA:1065:U:H5'	2.03	0.59
25:BA:2103:C:O2	25:BA:2186:G:N2	2.34	0.59
59:CD:1169:THR:OG1	59:CD:1173:ARG:HB3	2.02	0.59
25:BA:64:A:H2'	25:BA:65:U:C6	2.37	0.59
25:BA:210:C:OP1	52:B4:29:GLN:NE2	2.34	0.59
25:BA:1595:C:O2'	25:BA:1596:A:H5'	2.01	0.59
28:BD:34:VAL:O	28:BD:93:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BG:86:LYS:HZ2	31:BG:86:LYS:HB3	1.68	0.59
55:CN:27:DA:C4	55:CN:28:DA:C8	2.90	0.59
25:BA:335:C:OP2	44:BV:82:ARG:NH2	2.35	0.59
58:CC:705:GLU:HB3	58:CC:794:LEU:H	1.67	0.59
1:AA:1344:C:P	9:AI:124:ARG:HH11	2.25	0.59
1:AA:339:C:OP1	34:BL:13:ASN:ND2	2.35	0.59
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.35	0.59
25:BA:443:A:C6	29:BE:40:ARG:HD2	2.38	0.59
25:BA:896:A:O2'	25:BA:897:C:H6	1.85	0.59
25:BA:1169:A:H2'	25:BA:1170:C:H6	1.67	0.59
34:BL:59:LYS:NZ	34:BL:89:ASN:O	2.35	0.59
44:BV:96:PHE:O	44:BV:100:SER:CA	2.50	0.59
1:AA:90:C:H2'	1:AA:91:U:H6	1.67	0.59
25:BA:2134:A:N7	25:BA:2157:G:O2'	2.36	0.59
30:BF:136:ILE:HG12	30:BF:143:TYR:HD1	1.68	0.59
32:BH:73:ASN:ND2	32:BH:76:GLU:HA	2.17	0.59
56:CT:20:DC:H2'	56:CT:21:DG:H8	1.68	0.59
59:CD:256:ASP:O	59:CD:259:ARG:NH2	2.22	0.59
1:AA:636:U:H5'	17:AQ:6:ARG:HE	1.66	0.59
1:AA:1390:U:H2'	1:AA:1391:U:C6	2.37	0.59
32:BH:8:LYS:NZ	32:BH:14:SER:OG	2.30	0.59
58:CC:23:ASP:OD1	58:CC:23:ASP:N	2.34	0.59
25:BA:1529:G:H2'	25:BA:1530:G:H8	1.68	0.59
38:BP:1:MET:O	38:BP:5:SER:CB	2.51	0.59
59:CD:429:LEU:H	59:CD:429:LEU:CD2	2.13	0.59
1:AA:464:U:O2'	1:AA:466:A:N7	2.23	0.59
4:AD:7:PRO:HB2	4:AD:10:LYS:HB2	1.84	0.59
4:AD:50:ASP:OD1	4:AD:50:ASP:N	2.34	0.59
25:BA:140:C:H1'	25:BA:141:G:N2	2.17	0.59
29:BE:16:GLU:N	29:BE:16:GLU:OE2	2.32	0.59
32:BH:104:THR:HA	32:BH:108:VAL:O	2.03	0.59
55:CN:26:DG:OP2	58:CC:542:ARG:NH1	2.35	0.59
1:AA:925:G:C6	1:AA:927:G:N7	2.71	0.58
3:AC:74:GLY:H	58:CC:867:GLU:CB	1.66	0.58
6:AF:26:THR:HG21	6:AF:39:LEU:HD22	1.85	0.58
22:AV:40:A:O2'	22:AV:41:C:OP2	2.21	0.58
25:BA:1069:A:H4'	25:BA:1070:A:C8	2.38	0.58
59:CD:1069:ALA:HA	59:CD:1072:LYS:HB2	1.85	0.58
1:AA:82:G:O3'	1:AA:83:C:H4'	2.03	0.58
25:BA:987:C:O2'	25:BA:1000:A:N3	2.34	0.58
30:BF:56:ASP:N	30:BF:56:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BP:38:GLN:HE21	38:BP:47:VAL:HG11	1.68	0.58
41:BS:14:VAL:HG21	41:BS:98:ILE:HG13	1.83	0.58
25:BA:1494:A:H2'	25:BA:1495:A:C8	2.38	0.58
30:BF:118:SER:C	30:BF:120:LYS:H	2.07	0.58
31:BG:83:PHE:HB2	31:BG:141:ILE:HD12	1.85	0.58
13:AM:16:VAL:HG13	13:AM:17:ILE:HD12	1.86	0.58
27:BC:41:GLY:O	27:BC:43:ARG:NH1	2.34	0.58
31:BG:41:VAL:HG12	31:BG:64:GLN:HB3	1.85	0.58
31:BG:127:THR:HG23	31:BG:130:GLU:H	1.67	0.58
1:AA:746:A:H2'	1:AA:747:A:C8	2.38	0.58
34:BL:17:ARG:HA	34:BL:17:ARG:HE	1.68	0.58
37:BO:101:GLY:O	37:BO:110:MET:N	2.36	0.58
56:CT:17:DG:C6	56:CT:18:DC:C4	2.91	0.58
56:CT:18:DC:H2'	56:CT:19:DG:H8	1.65	0.58
3:AC:110:GLU:OE1	3:AC:110:GLU:N	2.36	0.58
7:AG:17:LYS:HG3	7:AG:44:TYR:CZ	2.38	0.58
38:BP:51:ALA:HB3	38:BP:78:VAL:HB	1.83	0.58
2:AB:68:LEU:HB3	2:AB:161:LEU:HD12	1.84	0.58
25:BA:535:G:N2	40:BR:56:GLN:OE1	2.35	0.58
31:BG:95:ARG:HH22	31:BG:97:ALA:HB2	1.69	0.58
35:BM:85:VAL:HG23	35:BM:98:ALA:HB2	1.84	0.58
59:CD:650:LYS:HE3	59:CD:742:GLY:O	2.02	0.58
1:AA:205:A:H2'	1:AA:206:C:C6	2.39	0.58
13:AM:92:ARG:NH1	25:BA:889:C:OP1	2.37	0.58
25:BA:172:A:H2'	25:BA:173:A:C8	2.39	0.58
25:BA:219:A:N3	25:BA:234:U:O2'	2.36	0.58
56:CT:26:DA:H2"	56:CT:27:DG:C8	2.39	0.58
58:CC:696:ASP:CG	58:CC:697:LYS:H	2.06	0.58
9:AI:46:MET:N	9:AI:49:ARG:HH21	2.02	0.58
25:BA:141:G:H2'	25:BA:142:A:O4'	2.04	0.58
25:BA:895:U:O2'	25:BA:896:A:H2'	2.04	0.58
25:BA:927:A:H2'	25:BA:928:A:C8	2.39	0.58
25:BA:2448:A:O2'	25:BA:2449:H2U:H52	2.04	0.58
26:BB:8:C:O3'	38:BP:25:ARG:NH1	2.36	0.58
58:CC:525:THR:HG21	58:CC:687:ARG:NH1	2.18	0.58
59:CD:515:ARG:NH2	59:CD:718:SER:O	2.37	0.58
9:AI:12:ARG:HD2	9:AI:74:GLY:HA2	1.85	0.58
15:AO:14:GLU:OE1	15:AO:84:ARG:NH2	2.37	0.58
25:BA:614:A:O2'	25:BA:615:U:OP2	2.21	0.58
1:AA:1053:G:HO2'	1:AA:1199:U:H5	1.52	0.57
25:BA:135:U:H2'	25:BA:136:G:O4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2370:G:O2'	51:B3:44:ARG:NH1	2.37	0.57
1:AA:67:C:H2'	1:AA:68:G:C8	2.38	0.57
1:AA:80:C:N3	1:AA:81:A:N6	2.53	0.57
1:AA:713:G:H2'	1:AA:714:G:C8	2.40	0.57
38:BP:1:MET:O	38:BP:5:SER:HB3	2.04	0.57
58:CC:421:SER:H	58:CC:424:ASP:HB2	1.69	0.57
58:CC:591:TYR:OH	58:CC:637:ARG:NH2	2.36	0.57
1:AA:362:G:N2	1:AA:365:U:OP2	2.37	0.57
4:AD:194:ASP:HB3	59:CD:74:LYS:HZ1	1.66	0.57
6:AF:63:ASN:ND2	6:AF:96:VAL:HG21	2.19	0.57
9:AI:62:ASP:OD1	9:AI:63:LEU:N	2.38	0.57
25:BA:1433:A:H2'	25:BA:1434:A:C8	2.39	0.57
11:AK:17:SER:O	11:AK:80:LYS:N	2.27	0.57
25:BA:728:G:H4'	27:BC:13:ARG:HD3	1.85	0.57
37:BO:2:ARG:NE	37:BO:2:ARG:O	2.37	0.57
5:AE:12:GLN:OE1	59:CD:79:LYS:HD2	2.05	0.57
6:AF:17:GLN:HG2	32:BH:87:GLU:HG3	1.86	0.57
22:AV:44:C:H2'	22:AV:45:G:O4'	2.04	0.57
1:AA:51:A:N7	1:AA:114:U:O2'	2.36	0.57
25:BA:1105:U:H2'	25:BA:1106:G:H8	1.69	0.57
25:BA:1248:G:OP1	29:BE:44:ARG:NH1	2.38	0.57
56:CT:19:DG:C4	56:CT:20:DC:C5	2.93	0.57
10:AJ:81:GLU:N	10:AJ:81:GLU:OE2	2.38	0.57
13:AM:68:ASP:HA	13:AM:71:ARG:HH21	1.70	0.57
25:BA:1915:3TD:H2'	25:BA:1916:A:C8	2.40	0.57
58:CC:12:ARG:HH21	58:CC:793:GLU:CD	2.07	0.57
58:CC:726:TYR:HB3	58:CC:733:VAL:CG1	2.34	0.57
4:AD:140:ASN:N	4:AD:182:PHE:O	2.38	0.57
7:AG:77:SER:OG	7:AG:86:GLN:OE1	2.17	0.57
45:BW:20:LEU:HD21	45:BW:26:PHE:HA	1.87	0.57
57:CB:76:GLU:H	57:CB:76:GLU:CD	2.08	0.57
1:AA:966:2MG:H5"	1:AA:967:5MC:OP2	2.05	0.57
25:BA:1068:G:N2	25:BA:1095:A:O2'	2.31	0.57
34:BL:5:GLN:N	34:BL:21:CYS:O	2.37	0.57
1:AA:104:G:OP1	20:AT:16:LYS:NZ	2.31	0.56
1:AA:413:G:O2'	1:AA:428:G:N2	2.39	0.56
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.40	0.56
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.70	0.56
25:BA:277:G:H2'	25:BA:361:G:C6	2.40	0.56
25:BA:1056:G:H4'	25:BA:1086:A:H8	1.70	0.56
25:BA:1315:C:O2'	25:BA:1392:A:N3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2333:A:P	46:BX:77:ARG:HH22	2.27	0.56
26:BB:28:C:H5"	38:BP:31:THR:HG21	1.87	0.56
1:AA:76:G:O6	1:AA:93:U:O4	2.22	0.56
1:AA:148:G:O2'	1:AA:149:A:O5'	2.23	0.56
1:AA:413:G:N2	1:AA:428:G:H1'	2.20	0.56
25:BA:2244:U:O2'	25:BA:2245:U:H5'	2.05	0.56
29:BE:145:ASP:HB3	29:BE:184:ASP:HB2	1.87	0.56
44:BV:74:ASN:HB3	44:BV:96:PHE:CE1	2.41	0.56
3:AC:107:ARG:O	58:CC:859:GLU:HG3	2.03	0.56
7:AG:113:ASP:O	7:AG:119:ARG:NE	2.37	0.56
13:AM:46:SER:OG	13:AM:47:GLU:OE2	2.20	0.56
23:AW:15:G:N1	23:AW:48:C:N3	2.49	0.56
24:AX:20:H2U:O2'	24:AX:21:A:H5"	2.06	0.56
25:BA:100:U:O2'	44:BV:91:LYS:NZ	2.39	0.56
29:BE:48:THR:OG1	29:BE:51:GLU:OE1	2.22	0.56
32:BH:84:ALA:HB2	32:BH:90:LEU:HD12	1.87	0.56
44:BV:62:GLU:OE1	44:BV:62:GLU:N	2.39	0.56
4:AD:95:GLU:HG2	4:AD:191:LEU:HD21	1.87	0.56
7:AG:138:ARG:HH21	7:AG:139:GLU:HG2	1.70	0.56
25:BA:653:U:O2	25:BA:653:U:H2'	2.06	0.56
25:BA:2519:U:O4'	25:BA:2542:A:N6	2.37	0.56
59:CD:160:LEU:HD23	59:CD:160:LEU:H	1.71	0.56
1:AA:1033:G:H2'	1:AA:1034:G:H8	1.70	0.56
2:AB:208:ARG:O	2:AB:211:THR:OG1	2.22	0.56
29:BE:130:LYS:HB2	29:BE:133:LEU:HD12	1.87	0.56
58:CC:267:ARG:NE	58:CC:268:ARG:O	2.37	0.56
7:AG:7:ILE:HD13	7:AG:7:ILE:H	1.71	0.56
24:AX:34:G:H2'	24:AX:35:A:C8	2.41	0.56
25:BA:888:C:H1'	25:BA:889:C:H1'	1.86	0.56
25:BA:1914:C:H2'	25:BA:1915:3TD:C6	2.35	0.56
32:BH:50:ARG:NH1	32:BH:51:ARG:HE	2.04	0.56
1:AA:111:G:O6	1:AA:330:C:N4	2.27	0.56
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.29	0.56
25:BA:172:A:H2'	25:BA:173:A:H8	1.71	0.56
30:BF:98:GLU:HG3	30:BF:99:PHE:N	2.21	0.56
55:CN:28:DA:H2"	55:CN:29:DG:H8	1.70	0.56
1:AA:1135:U:HO2'	1:AA:1138:G:H1	1.53	0.56
23:AW:69:C:H2'	23:AW:70:G:C8	2.40	0.56
43:BU:6:ARG:NH2	43:BU:37:ASP:OD2	2.36	0.56
58:CC:320:ASP:N	58:CC:320:ASP:OD1	2.37	0.56
5:AE:69:ARG:HG3	5:AE:70:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1591:A:H2'	25:BA:1592:C:H6	1.70	0.56
25:BA:2135:A:O2'	25:BA:2160:C:H5'	2.06	0.56
31:BG:148:LEU:HA	31:BG:151:TYR:HD2	1.70	0.56
46:BX:37:ILE:HG22	46:BX:38:VAL:HG23	1.88	0.56
59:CD:523:GLU:CD	59:CD:709:ARG:HH22	2.07	0.56
1:AA:160:A:N6	1:AA:343:U:HO2'	2.05	0.55
1:AA:946:A:H2'	1:AA:947:G:C8	2.41	0.55
11:AK:92:GLY:O	11:AK:94:GLU:N	2.38	0.55
25:BA:1306:C:H41	25:BA:1606:C:H2'	1.72	0.55
30:BF:5:HIS:HB2	30:BF:97:TRP:CG	2.42	0.55
36:BN:77:PRO:HG2	36:BN:80:VAL:HG11	1.87	0.55
26:BB:119:A:H2'	26:BB:120:U:C6	2.40	0.55
29:BE:5:LEU:O	29:BE:9:GLN:CA	2.51	0.55
46:BX:53:CYS:SG	46:BX:57:HIS:HA	2.46	0.55
3:AC:80:LYS:HZ1	58:CC:946:LEU:CD2	2.14	0.55
4:AD:42:GLY:O	4:AD:44:ARG:N	2.38	0.55
25:BA:2119:A:H8	25:BA:2119:A:O5'	1.88	0.55
25:BA:2352:A:N6	25:BA:2365:G:O2'	2.39	0.55
25:BA:2840:C:H5"	37:BO:53:THR:HG21	1.88	0.55
1:AA:90:C:H2'	1:AA:91:U:C6	2.40	0.55
25:BA:856:G:H2'	25:BA:857:G:C8	2.41	0.55
32:BH:84:ALA:HA	32:BH:91:PHE:H	1.72	0.55
41:BS:30:GLY:N	41:BS:63:VAL:O	2.38	0.55
43:BU:34:VAL:HG21	43:BU:43:ILE:HD11	1.87	0.55
58:CC:696:ASP:OD1	58:CC:697:LYS:N	2.39	0.55
58:CC:1176:LEU:O	58:CC:1178:LYS:N	2.40	0.55
59:CD:495:ASN:OD1	59:CD:495:ASN:N	2.37	0.55
5:AE:10:GLU:HB2	59:CD:78:LEU:HB2	1.89	0.55
25:BA:136:G:H4'	25:BA:136:G:OP1	2.05	0.55
25:BA:2111:U:O4'	25:BA:2118:U:O2'	2.24	0.55
29:BE:158:PHE:HA	29:BE:169:VAL:HG21	1.89	0.55
19:AS:32:ARG:HG3	19:AS:57:HIS:CD2	2.41	0.55
25:BA:84:A:N1	25:BA:98:G:O2'	2.34	0.55
25:BA:1594:U:H2'	25:BA:1595:C:H6	1.70	0.55
25:BA:2104:C:H5	25:BA:2186:G:N2	2.05	0.55
35:BM:2:ARG:N	35:BM:5:THR:OG1	2.27	0.55
57:CB:13:LEU:HA	57:CB:28:LEU:HD13	1.89	0.55
1:AA:126:G:OP1	1:AA:605:U:O2'	2.20	0.55
1:AA:339:C:OP2	34:BL:98:ARG:NH2	2.40	0.55
1:AA:1032:G:H21	1:AA:1033:G:H4'	1.72	0.55
15:AO:25:THR:HG23	15:AO:66:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1251:C:OP2	40:BR:6:ARG:NH2	2.39	0.55
4:AD:88:GLU:OE1	4:AD:88:GLU:N	2.39	0.55
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	1.88	0.55
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.87	0.55
25:BA:567:U:OP2	35:BM:29:LYS:NZ	2.39	0.55
25:BA:2115:G:H2'	25:BA:2117:A:OP2	2.07	0.55
25:BA:2788:C:O2'	25:BA:2809:A:N3	2.38	0.55
50:B2:31:ASP:O	50:B2:35:GLY:HA2	2.06	0.55
1:AA:945:G:C2	1:AA:946:A:C8	2.95	0.55
1:AA:1119:C:OP1	9:AI:85:ARG:NH1	2.40	0.55
3:AC:109:PRO:HD2	58:CC:859:GLU:OE2	2.02	0.55
25:BA:1417:C:H1'	25:BA:1586:A:N1	2.22	0.55
30:BF:126:GLY:HA2	30:BF:163:ASP:HA	1.88	0.55
1:AA:993:G:O2'	1:AA:994:A:N7	2.39	0.55
9:AI:33:ARG:HH11	9:AI:38:TYR:HA	1.71	0.55
12:AL:54:ARG:HB2	12:AL:54:ARG:NH1	2.21	0.55
33:BK:60:ASP:OD2	33:BK:61:LYS:NZ	2.38	0.55
51:B3:22:THR:HG23	53:B5:34:THR:HG23	1.89	0.55
1:AA:147:G:O2'	1:AA:148:G:O4'	2.25	0.54
1:AA:205:A:H2'	1:AA:206:C:H6	1.71	0.54
1:AA:215:C:H2'	1:AA:216:U:O4'	2.06	0.54
6:AF:24:ARG:HH12	6:AF:28:ALA:HB2	1.71	0.54
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.89	0.54
25:BA:1056:G:HO2'	25:BA:1086:A:HO2'	1.50	0.54
25:BA:2698:U:H2'	25:BA:2699:C:C6	2.42	0.54
55:CN:34:DT:H6	55:CN:34:DT:H5'	1.70	0.54
58:CC:1165:SER:O	58:CC:1167:GLU:N	2.37	0.54
1:AA:1124:G:N2	1:AA:1125:U:O4	2.26	0.54
3:AC:107:ARG:NE	58:CC:863:SER:O	2.40	0.54
5:AE:148:ASN:ND2	8:AH:73:GLU:OE1	2.40	0.54
8:AH:31:LYS:O	8:AH:34:VAL:HG22	2.07	0.54
15:AO:3:LEU:HB2	15:AO:35:GLN:OE1	2.06	0.54
24:AX:43:C:H2'	24:AX:44:G:C8	2.41	0.54
25:BA:1193:G:OP1	35:BM:14:LYS:NZ	2.29	0.54
44:BV:18:ASP:HA	44:BV:21:LYS:HZ3	1.70	0.54
1:AA:1018:G:H2'	1:AA:1019:A:C8	2.42	0.54
1:AA:1318:A:H5"	19:AS:3:ARG:HH22	1.72	0.54
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.89	0.54
23:AW:1:C:H2'	23:AW:2:G:C8	2.43	0.54
25:BA:244:A:OP2	53:B5:8:ARG:NH2	2.40	0.54
34:BL:17:ARG:HA	34:BL:17:ARG:NE	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CC:423:ASP:N	58:CC:423:ASP:OD1	2.33	0.54
58:CC:1070:HIS:NE2	58:CC:1114:GLU:OE1	2.41	0.54
58:CC:1321:GLU:OE2	59:CD:99:ARG:NH1	2.41	0.54
59:CD:37:GLU:HB2	59:CD:104:HIS:CE1	2.41	0.54
1:AA:714:G:H2'	1:AA:715:A:C8	2.42	0.54
3:AC:79:LYS:CE	58:CC:943:LYS:N	2.70	0.54
7:AG:143:ARG:HG3	7:AG:144:MET:N	2.22	0.54
9:AI:116:VAL:HG13	10:AJ:62:ARG:NH2	2.21	0.54
1:AA:1007:U:H2'	1:AA:1008:U:C6	2.42	0.54
25:BA:1808:A:H3'	25:BA:1809:A:C8	2.43	0.54
25:BA:2190:G:H2'	25:BA:2191:A:O4'	2.07	0.54
26:BB:24:G:N7	26:BB:56:G:H2'	2.22	0.54
31:BG:95:ARG:HH12	31:BG:97:ALA:HB2	1.71	0.54
58:CC:7:GLU:O	58:CC:9:LYS:N	2.35	0.54
1:AA:837:U:O2	1:AA:849:G:O6	2.25	0.54
13:AM:4:ILE:HG23	13:AM:57:ARG:HG2	1.88	0.54
19:AS:20:GLU:OE1	19:AS:21:LYS:N	2.40	0.54
25:BA:2314:A:H2'	25:BA:2315:G:C8	2.42	0.54
32:BH:73:ASN:HD22	32:BH:76:GLU:HA	1.72	0.54
24:AX:37:MIA:H2'	24:AX:38:A:O4'	2.07	0.54
41:BS:27:ILE:HG21	41:BS:63:VAL:HG21	1.89	0.54
1:AA:1240:U:O4	7:AG:109:ARG:NH1	2.41	0.54
3:AC:125:GLU:OE2	3:AC:190:HIS:N	2.38	0.54
5:AE:76:LEU:HD13	5:AE:79:GLY:H	1.73	0.54
8:AH:8:ALA:O	8:AH:12:THR:HG23	2.07	0.54
15:AO:25:THR:HG21	15:AO:70:LEU:HD13	1.89	0.54
25:BA:1724:G:N2	25:BA:1736:U:O2	2.37	0.54
25:BA:2178:C:H2'	25:BA:2179:C:C5	2.43	0.54
25:BA:2258:C:O2'	25:BA:2427:C:OP2	2.19	0.54
33:BK:56:VAL:HB	33:BK:124:VAL:HG13	1.89	0.54
51:B3:33:LYS:HG2	51:B3:52:ALA:HB2	1.90	0.54
4:AD:98:LEU:O	4:AD:102:VAL:HG12	2.08	0.54
25:BA:956:G:N7	36:BN:14:LYS:NZ	2.47	0.54
25:BA:1405:U:O2'	25:BA:1406:U:O4'	2.26	0.54
25:BA:2547:A:H2'	25:BA:2548:U:C6	2.43	0.54
55:CN:31:DG:H2"	55:CN:32:DA:C8	2.42	0.54
58:CC:524:ILE:HG22	58:CC:525:THR:N	2.22	0.54
1:AA:31:G:O2'	1:AA:48:C:N4	2.41	0.54
1:AA:1318:A:H5"	19:AS:3:ARG:NH2	2.23	0.54
8:AH:5:ASP:OD1	8:AH:77:ARG:NH2	2.39	0.54
25:BA:1826:G:O2'	25:BA:1971:U:OP2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BU:33:LYS:HG2	43:BU:80:TRP:CZ3	2.43	0.54
55:CN:26:DG:C6	55:CN:27:DA:N6	2.76	0.54
58:CC:1079:ILE:HG23	58:CC:1079:ILE:O	2.08	0.54
1:AA:1184:G:C2	1:AA:1185:G:C8	2.96	0.53
6:AF:44:ARG:HB2	6:AF:44:ARG:HH11	1.71	0.53
25:BA:1301:A:H2	25:BA:1626:A:H2	1.55	0.53
25:BA:1506:U:H2'	25:BA:1507:C:C6	2.43	0.53
25:BA:1595:C:H2'	25:BA:1596:A:C8	2.43	0.53
30:BF:60:ILE:HD13	30:BF:140:GLU:HB2	1.90	0.53
31:BG:24:ILE:HG21	31:BG:72:LEU:HD21	1.90	0.53
6:AF:32:ALA:CB	6:AF:70:VAL:HG11	2.39	0.53
10:AJ:56:HIS:ND1	10:AJ:57:VAL:HG22	2.23	0.53
14:AN:81:ARG:O	14:AN:84:VAL:HG22	2.08	0.53
25:BA:285:G:O6	25:BA:355:U:O2	2.26	0.53
25:BA:1042:G:HO2'	25:BA:1043:C:H6	1.56	0.53
36:BN:66:ARG:NH1	36:BN:104:GLU:OE1	2.33	0.53
38:BP:57:ALA:O	38:BP:61:GLN:HG2	2.08	0.53
59:CD:367:GLY:HA2	59:CD:440:VAL:O	2.08	0.53
1:AA:337:G:H2'	1:AA:338:A:C8	2.42	0.53
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.90	0.53
25:BA:1095:A:H2'	25:BA:1096:A:C8	2.43	0.53
25:BA:1421:G:C2	25:BA:1422:G:C8	2.96	0.53
25:BA:1869:G:N2	25:BA:1872:A:OP2	2.40	0.53
58:CC:12:ARG:NE	58:CC:793:GLU:OE2	2.36	0.53
58:CC:178:PRO:HB3	58:CC:395:TYR:CZ	2.44	0.53
1:AA:73:C:C2'	1:AA:74:A:H5'	2.38	0.53
1:AA:1210:C:O4'	1:AA:1214:C:N4	2.41	0.53
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.44	0.53
2:AB:15:HIS:HB3	2:AB:43:LEU:HD21	1.89	0.53
2:AB:168:HIS:ND1	2:AB:169:GLU:OE1	2.42	0.53
25:BA:995:C:OP2	40:BR:54:LYS:HE3	2.08	0.53
25:BA:1529:G:O6	25:BA:1542:U:C4	2.61	0.53
25:BA:1789:A:OP1	27:BC:221:ARG:HG3	2.08	0.53
50:B2:28:LEU:HD12	50:B2:37:LYS:HB3	1.90	0.53
57:CB:191:ARG:NH2	57:CB:192:VAL:O	2.42	0.53
1:AA:197:A:H4'	1:AA:198:G:O5'	2.06	0.53
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.42	0.53
5:AE:89:HIS:NE2	5:AE:138:ARG:HG3	2.24	0.53
10:AJ:6:ILE:HB	10:AJ:76:ILE:HG23	1.90	0.53
25:BA:645:C:H2'	25:BA:647:G:N7	2.23	0.53
25:BA:898:C:C4	25:BA:899:A:C8	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2405:G:OP1	35:BM:70:LYS:NZ	2.40	0.53
25:BA:2636:C:H2'	25:BA:2637:U:C6	2.43	0.53
56:CT:21:DG:C6	56:CT:22:DC:N4	2.77	0.53
58:CC:538:LEU:HD12	58:CC:539:THR:N	2.23	0.53
1:AA:492:C:H2'	1:AA:493:A:C8	2.44	0.53
1:AA:496:A:H2'	1:AA:496:A:N3	2.24	0.53
24:AX:21:A:O2'	24:AX:46:7MG:O6	2.18	0.53
24:AX:27:G:H2'	24:AX:28:G:C8	2.42	0.53
32:BH:115:VAL:O	32:BH:116:ARG:NH1	2.41	0.53
1:AA:108:G:C6	20:AT:10:ARG:HG3	2.43	0.53
7:AG:53:ARG:HH12	7:AG:122:ASN:HA	1.74	0.53
11:AK:92:GLY:C	11:AK:94:GLU:H	2.11	0.53
30:BF:25:VAL:O	30:BF:28:VAL:HG12	2.08	0.53
38:BP:7:ARG:NH1	38:BP:95:SER:O	2.41	0.53
1:AA:412:A:H62	1:AA:431:A:N6	2.05	0.53
2:AB:77:SER:HB2	2:AB:93:ASN:HB2	1.90	0.53
2:AB:188:ASP:OD1	2:AB:188:ASP:N	2.31	0.53
10:AJ:87:LEU:HD12	10:AJ:88:MET:N	2.23	0.53
25:BA:273:G:H2'	25:BA:274:C:O4'	2.09	0.53
25:BA:1084:A:H2'	25:BA:1085:A:C8	2.44	0.53
58:CC:150:HIS:CE1	58:CC:454:ARG:HG3	2.43	0.53
59:CD:825:VAL:HG13	59:CD:825:VAL:O	2.08	0.53
1:AA:1382:C:C2'	1:AA:1383:C:H5'	2.39	0.53
1:AA:1397:C:OP2	5:AE:29:ARG:NH2	2.29	0.53
57:CA:218:ARG:NH1	57:CB:233:ASP:OD1	2.42	0.53
59:CD:312:ARG:HG2	59:CD:313:GLY:N	2.24	0.53
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.74	0.53
6:AF:44:ARG:HB2	6:AF:44:ARG:NH1	2.24	0.53
6:AF:47:LEU:HD21	6:AF:57:ALA:HB3	1.90	0.53
14:AN:26:GLU:O	14:AN:30:ILE:HG22	2.08	0.53
25:BA:144:A:H2'	25:BA:145:C:C6	2.44	0.53
25:BA:886:A:N6	25:BA:892:A:H1'	2.24	0.53
25:BA:1980:G:O2'	25:BA:1982:U:OP2	2.26	0.53
30:BF:34:ILE:HG12	30:BF:156:ILE:HG12	1.91	0.53
32:BH:46:PHE:O	32:BH:51:ARG:HD2	2.09	0.53
59:CD:441:LEU:HD22	59:CD:441:LEU:H	1.73	0.53
1:AA:522:C:N3	1:AA:527:G7M:N1	2.41	0.52
1:AA:932:C:O3'	7:AG:4:ARG:NH2	2.42	0.52
4:AD:15:GLU:HG3	4:AD:60:LYS:HA	1.91	0.52
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.42	0.52
25:BA:2636:C:H2'	25:BA:2637:U:H6	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:108:ARG:O	2:AB:111:ILE:HG12	2.09	0.52
4:AD:80:ALA:HA	4:AD:86:THR:HG22	1.91	0.52
6:AF:47:LEU:HD13	6:AF:51:ILE:HG13	1.92	0.52
25:BA:1042:G:O2'	25:BA:1043:C:H6	1.92	0.52
25:BA:2900:A:C6	25:BA:2901:C:N4	2.77	0.52
27:BC:259:SER:O	27:BC:259:SER:OG	2.26	0.52
38:BP:99:TYR:OH	38:BP:111:ARG:NH1	2.41	0.52
59:CD:35:PHE:CD1	59:CD:101:ARG:HB3	2.44	0.52
1:AA:921:U:O2	5:AE:24:THR:OG1	2.28	0.52
13:AM:29:ARG:HH12	13:AM:63:PHE:HB3	1.75	0.52
25:BA:2285:C:P	51:B3:6:ARG:HH12	2.32	0.52
30:BF:94:GLU:HG3	30:BF:95:ARG:N	2.25	0.52
32:BH:83:LYS:O	32:BH:91:PHE:HB3	2.09	0.52
39:BQ:32:VAL:HG12	39:BQ:34:GLU:HG2	1.92	0.52
39:BQ:88:ARG:HH21	39:BQ:112:GLU:HG3	1.73	0.52
2:AB:129:LEU:HD12	2:AB:130:THR:H	1.73	0.52
9:AI:22:LYS:HG2	9:AI:62:ASP:HB3	1.90	0.52
10:AJ:76:ILE:HG12	10:AJ:79:PRO:HG3	1.91	0.52
13:AM:11:ASP:HA	13:AM:45:ILE:HB	1.91	0.52
14:AN:48:LEU:HD12	14:AN:51:LEU:HD12	1.90	0.52
25:BA:1028:A:H2'	25:BA:1029:A:C8	2.45	0.52
25:BA:1169:A:H2'	25:BA:1170:C:C6	2.43	0.52
25:BA:1568:G:N7	27:BC:28:LYS:NZ	2.57	0.52
25:BA:1596:A:O2'	25:BA:1597:A:H5'	2.09	0.52
25:BA:1615:C:OP2	25:BA:1617:C:N4	2.24	0.52
28:BD:37:VAL:HG21	28:BD:90:PHE:O	2.09	0.52
31:BG:145:ALA:HB1	31:BG:164:TYR:CE1	2.41	0.52
58:CC:1340:GLU:OE1	58:CC:1341:ASP:N	2.34	0.52
9:AI:26:GLY:HA2	9:AI:61:LEU:O	2.10	0.52
59:CD:978:ARG:HD3	59:CD:1197:ASN:O	2.09	0.52
1:AA:866:C:C4	1:AA:867:G:H1'	2.44	0.52
1:AA:1497:G:H1'	1:AA:1518:MA6:H2	1.91	0.52
9:AI:36:GLU:OE1	9:AI:36:GLU:N	2.38	0.52
25:BA:240:C:OP2	25:BA:241:A:O2'	2.23	0.52
31:BG:10:VAL:HA	31:BG:49:THR:HG22	1.90	0.52
31:BG:86:LYS:HB3	31:BG:86:LYS:NZ	2.24	0.52
1:AA:613:C:OP1	4:AD:81:ARG:NH1	2.37	0.52
25:BA:639:U:H2'	25:BA:640:C:H6	1.72	0.52
25:BA:1479:G:HO2'	25:BA:1560:G:HO2'	1.52	0.52
30:BF:31:VAL:HG23	30:BF:169:LEU:HD21	1.92	0.52
34:BL:63:VAL:HA	34:BL:107:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:437:U:H5"	4:AD:152:GLN:NE2	2.23	0.52
2:AB:187:VAL:HG23	2:AB:191:SER:HB2	1.91	0.52
25:BA:887:U:O2'	25:BA:888:C:H5"	2.10	0.52
30:BF:11:GLU:HB3	30:BF:15:LYS:HE3	1.92	0.52
31:BG:107:LEU:HD13	31:BG:152:ARG:HB2	1.91	0.52
31:BG:148:LEU:HA	31:BG:151:TYR:CD2	2.45	0.52
34:BL:102:PRO:HB2	34:BL:123:LEU:HD23	1.92	0.52
59:CD:1313:SER:HG	59:CD:1325:PHE:HE2	1.57	0.52
13:AM:65:VAL:HG22	13:AM:66:GLU:HG2	1.92	0.52
23:AW:76:A:HO3'	25:BA:2063:C:HO2'	1.57	0.52
24:AX:6:G:H2'	24:AX:7:A:H8	1.75	0.52
25:BA:1113:U:H2'	25:BA:1114:C:C6	2.45	0.52
25:BA:1168:G:H2'	25:BA:1169:A:C8	2.45	0.52
25:BA:1266:G:OP2	50:B2:17:ARG:NE	2.41	0.52
25:BA:2252:G:H2'	25:BA:2253:G:C8	2.45	0.52
30:BF:11:GLU:O	30:BF:15:LYS:HG3	2.10	0.52
41:BS:61:ALA:HB2	41:BS:98:ILE:HD13	1.92	0.52
58:CC:193:ASN:HD22	58:CC:193:ASN:N	2.08	0.52
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.45	0.52
3:AC:58:GLU:HG3	3:AC:65:ARG:HB3	1.92	0.52
5:AE:10:GLU:HB2	59:CD:78:LEU:CB	2.40	0.52
8:AH:66:PHE:CD2	8:AH:67:GLN:HG3	2.45	0.52
10:AJ:34:ALA:HB2	10:AJ:83:THR:HG21	1.92	0.52
30:BF:100:PHE:O	30:BF:104:ILE:HG22	2.09	0.52
35:BM:61:LEU:O	53:B5:13:ARG:NE	2.37	0.52
58:CC:726:TYR:CD1	58:CC:727:VAL:N	2.78	0.52
1:AA:159:G:N2	1:AA:162:A:OP2	2.43	0.51
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.45	0.51
9:AI:57:MET:HG2	9:AI:60:LYS:HD2	1.92	0.51
25:BA:357:C:H2'	25:BA:358:U:H6	1.74	0.51
25:BA:1173:U:C2	25:BA:1176:U:O2	2.63	0.51
25:BA:1667:G:O2'	25:BA:1991:U:O4	2.24	0.51
28:BD:77:ARG:NH1	28:BD:200:ASP:OD1	2.44	0.51
29:BE:170:ARG:NH2	29:BE:176:ASP:OD1	2.42	0.51
58:CC:85:CYS:SG	58:CC:90:VAL:HG23	2.50	0.51
58:CC:296:VAL:O	58:CC:335:THR:HB	2.10	0.51
59:CD:801:VAL:HG12	59:CD:920:ALA:HB3	1.91	0.51
1:AA:89:G:H2'	1:AA:90:C:C6	2.44	0.51
1:AA:363:A:C6	12:AL:28:PRO:HD2	2.45	0.51
3:AC:80:LYS:HZ2	58:CC:946:LEU:CD2	2.19	0.51
21:AU:62:ARG:O	21:AU:66:ARG:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2102:G:N1	25:BA:2187:U:C2	2.79	0.51
42:BT:1:MET:N	42:BT:110:ARG:HH11	2.07	0.51
43:BU:4:GLU:HA	43:BU:7:LEU:HD22	1.92	0.51
1:AA:925:G:C2	1:AA:927:G:C8	2.99	0.51
8:AH:7:ILE:HB	8:AH:77:ARG:NH2	2.25	0.51
24:AX:41:C:H2'	24:AX:42:C:C6	2.46	0.51
25:BA:134:G:H2'	25:BA:135:U:C6	2.46	0.51
25:BA:1174:U:H2'	25:BA:1175:A:C8	2.45	0.51
58:CC:519:ASN:C	58:CC:519:ASN:OD1	2.46	0.51
1:AA:218:U:H2'	1:AA:219:U:O4'	2.11	0.51
3:AC:77:ILE:HG22	58:CC:943:LYS:CE	2.34	0.51
5:AE:80:THR:HA	5:AE:120:VAL:HG13	1.93	0.51
13:AM:52:GLN:O	13:AM:56:LEU:HG	2.10	0.51
25:BA:1754:A:N1	25:BA:2716:C:O2'	2.40	0.51
30:BF:55:ALA:O	30:BF:59:ALA:HB3	2.11	0.51
42:BT:4:ILE:HG12	42:BT:106:VAL:HG22	1.92	0.51
59:CD:301:GLU:OE1	59:CD:312:ARG:NH1	2.37	0.51
11:AK:47:ALA:HB1	11:AK:62:ALA:HB1	1.90	0.51
25:BA:2124:G:N1	25:BA:2175:C:N3	2.59	0.51
49:B1:9:GLN:O	49:B1:33:GLY:N	2.44	0.51
59:CD:288:PRO:HD2	59:CD:291:ILE:HD12	1.93	0.51
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.45	0.51
10:AJ:5:ARG:HB2	10:AJ:77:VAL:HA	1.92	0.51
14:AN:83:LYS:HA	14:AN:86:GLU:HG3	1.92	0.51
25:BA:1820:U:O2'	27:BC:158:ALA:HB3	2.11	0.51
30:BF:83:TYR:O	30:BF:85:ILE:HG23	2.11	0.51
59:CD:275:ARG:HH11	59:CD:298:MET:HB3	1.76	0.51
1:AA:1:A:H2'	1:AA:2:A:C8	2.45	0.51
1:AA:1062:U:O4	3:AC:3:GLN:NE2	2.43	0.51
9:AI:119:ARG:NH1	9:AI:123:ARG:HE	2.08	0.51
25:BA:1059:G:N7	25:BA:1060:U:H2'	2.25	0.51
25:BA:2315:G:HO2'	25:BA:2316:G:H8	1.58	0.51
25:BA:2886:A:C5	50:B2:40:ARG:NH2	2.79	0.51
31:BG:135:GLY:N	31:BG:141:ILE:HD11	2.26	0.51
58:CC:705:GLU:CD	58:CC:705:GLU:H	2.14	0.51
1:AA:1039:G:H2'	1:AA:1040:U:C6	2.46	0.51
3:AC:86:LYS:O	3:AC:89:LYS:HG3	2.11	0.51
25:BA:1585:C:H2'	25:BA:1586:A:C8	2.42	0.51
25:BA:2120:G:O2'	25:BA:2121:G:H5'	2.10	0.51
27:BC:252:THR:HG23	27:BC:253:LYS:HG3	1.93	0.51
29:BE:195:GLN:O	29:BE:198:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CC:811:ASN:ND2	58:CC:1097:VAL:O	2.43	0.51
59:CD:1075:ARG:HH21	59:CD:1102:PRO:HA	1.75	0.51
25:BA:2287:A:C8	25:BA:2289:G:C8	2.99	0.51
58:CC:632:ASP:N	58:CC:632:ASP:OD1	2.39	0.51
58:CC:1083:GLU:CD	58:CC:1083:GLU:H	2.13	0.51
1:AA:1029:U:N3	1:AA:1033:G:C2	2.79	0.51
12:AL:81:LEU:HB3	12:AL:98:VAL:CG1	2.41	0.51
25:BA:1593:A:H2'	25:BA:1594:U:C6	2.45	0.51
45:BW:21:ARG:NH2	45:BW:87:GLN:O	2.37	0.51
58:CC:274:ILE:HA	58:CC:277:LEU:HD12	1.93	0.51
59:CD:366:CYS:O	59:CD:439:PRO:HA	2.11	0.51
1:AA:958:A:OP1	19:AS:55:ARG:NH1	2.43	0.50
24:AX:51:U:H3	24:AX:63:G:H1	1.59	0.50
25:BA:1528:A:N6	25:BA:1543:G:O2'	2.44	0.50
25:BA:2689:U:OP2	25:BA:2719:G:N2	2.39	0.50
27:BC:251:GLN:OE1	27:BC:255:LYS:HB2	2.11	0.50
30:BF:143:TYR:O	30:BF:146:VAL:HG12	2.11	0.50
58:CC:392:GLU:H	58:CC:392:GLU:CD	2.12	0.50
58:CC:855:PRO:HG3	58:CC:913:VAL:HG23	1.93	0.50
1:AA:690:G:O6	11:AK:53:ARG:NH1	2.43	0.50
14:AN:46:LEU:O	14:AN:50:THR:HG23	2.10	0.50
25:BA:357:C:H2'	25:BA:358:U:C6	2.46	0.50
25:BA:568:U:H1'	25:BA:2030:6MZ:H9C1	1.94	0.50
25:BA:686:U:O4	52:B4:12:ARG:HB2	2.12	0.50
25:BA:910:A:C6	36:BN:13:HIS:CE1	2.99	0.50
30:BF:43:ALA:HA	30:BF:46:ASP:O	2.11	0.50
49:B1:12:SER:HB3	49:B1:32:ILE:HD11	1.93	0.50
59:CD:326:SER:O	59:CD:329:ASP:N	2.43	0.50
1:AA:4:U:O2'	1:AA:5:U:P	2.69	0.50
8:AH:30:SER:O	8:AH:34:VAL:HG13	2.10	0.50
19:AS:32:ARG:HH11	19:AS:34:TRP:HH2	1.59	0.50
25:BA:400:G:N7	47:BY:57:ARG:NH1	2.56	0.50
25:BA:1141:U:H4'	25:BA:1142:A:O4'	2.11	0.50
26:BB:49:C:OP1	38:BP:101:GLY:HA3	2.10	0.50
29:BE:108:ILE:O	29:BE:112:LEU:HD13	2.11	0.50
41:BS:77:PHE:HD1	41:BS:84:ARG:HB3	1.76	0.50
55:CN:27:DA:C6	55:CN:28:DA:C6	3.00	0.50
57:CA:68:TYR:CD1	57:CA:68:TYR:N	2.79	0.50
58:CC:726:TYR:CD1	58:CC:726:TYR:C	2.84	0.50
59:CD:504:GLN:HG3	59:CD:505:ASP:N	2.25	0.50
1:AA:71:A:H2'	1:AA:72:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1006:G:N2	1:AA:1023:U:O2	2.44	0.50
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.47	0.50
20:AT:8:LYS:O	20:AT:12:ILE:HG13	2.11	0.50
25:BA:543:A:C6	25:BA:551:G:C6	2.99	0.50
25:BA:585:G:N7	40:BR:6:ARG:NH1	2.59	0.50
25:BA:1591:A:H2'	25:BA:1592:C:C6	2.46	0.50
25:BA:1871:A:O2'	25:BA:1872:A:C8	2.65	0.50
25:BA:2136:G:C6	25:BA:2156:G:H1'	2.46	0.50
25:BA:2291:U:H2'	25:BA:2292:U:H6	1.75	0.50
27:BC:4:VAL:HG13	27:BC:18:LYS:HB2	1.94	0.50
42:BT:25:ARG:HG3	42:BT:74:ILE:HG22	1.93	0.50
59:CD:137:ARG:HG3	59:CD:142:GLU:HB2	1.94	0.50
1:AA:604:G:H2'	1:AA:605:U:O4'	2.12	0.50
3:AC:71:ALA:HA	3:AC:106:VAL:HB	1.93	0.50
3:AC:79:LYS:H	3:AC:79:LYS:HD2	1.75	0.50
7:AG:22:LEU:HD21	7:AG:66:LEU:HD12	1.94	0.50
18:AR:34:THR:HG22	18:AR:38:LYS:H	1.76	0.50
25:BA:677:A:O2'	25:BA:2071:A:H5'	2.12	0.50
45:BW:7:GLU:HB2	45:BW:41:GLU:HG2	1.94	0.50
56:CT:18:DC:O2	56:CT:19:DG:C8	2.64	0.50
59:CD:175:GLU:CD	59:CD:175:GLU:H	2.15	0.50
1:AA:72:A:C6	1:AA:73:C:C5	2.99	0.50
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.76	0.50
1:AA:1530:G:N7	21:AU:46:LYS:HE2	2.27	0.50
10:AJ:26:VAL:O	10:AJ:30:LYS:HG2	2.11	0.50
25:BA:1022:G:O6	33:BK:68:LYS:NZ	2.34	0.50
25:BA:1378:A:O2'	25:BA:1380:G:N7	2.45	0.50
25:BA:1529:G:H2'	25:BA:1530:G:C8	2.46	0.50
25:BA:2106:U:H2'	25:BA:2107:G:C8	2.42	0.50
33:BK:96:ARG:HE	33:BK:99:ARG:HG2	1.76	0.50
53:B5:62:LEU:HB3	53:B5:65:ALA:HB3	1.93	0.50
59:CD:961:SER:HB2	59:CD:981:GLU:HB2	1.94	0.50
1:AA:50:A:O2'	1:AA:360:G:N2	2.45	0.50
2:AB:14:VAL:HB	2:AB:213:TYR:OH	2.12	0.50
23:AW:17:C:C2	23:AW:17(A):U:H5	2.29	0.50
25:BA:1590:A:H2'	25:BA:1591:A:H8	1.73	0.50
50:B2:31:ASP:O	50:B2:35:GLY:CA	2.60	0.50
1:AA:88:U:H3'	1:AA:89:G:C8	2.47	0.50
26:BB:16:G:N2	26:BB:69:G:H1'	2.27	0.50
27:BC:205:LEU:HB3	27:BC:210:ALA:HB3	1.94	0.50
35:BM:9:ALA:O	35:BM:12:SER:OG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:949:A:N7	13:AM:105:ASN:ND2	2.60	0.50
6:AF:44:ARG:O	6:AF:45:ARG:NH2	2.45	0.50
14:AN:80:SER:O	14:AN:84:VAL:HG13	2.11	0.50
25:BA:686:U:H6	25:BA:788:A:N1	2.09	0.50
30:BF:42:GLU:HB3	30:BF:49:LEU:HD23	1.94	0.50
33:BK:36:LEU:O	33:BK:51:GLY:HA3	2.12	0.50
35:BM:57:LEU:HD22	53:B5:54:ASP:HB3	1.93	0.50
59:CD:530:PRO:O	59:CD:533:ALA:HB3	2.12	0.50
1:AA:4:U:HO2'	1:AA:5:U:P	2.35	0.49
1:AA:296:U:O2'	1:AA:556:C:O2	2.30	0.49
1:AA:1140:C:HO2'	1:AA:1141:C:C5'	2.25	0.49
22:AV:48:C:H2'	22:AV:49:G:C1'	2.41	0.49
25:BA:1068:G:C2	25:BA:1096:A:H5'	2.47	0.49
55:CN:28:DA:H2"	55:CN:29:DG:C8	2.46	0.49
57:CA:102:LEU:HD23	57:CA:103:ASN:N	2.27	0.49
58:CC:494:ASN:C	58:CC:494:ASN:HD22	2.08	0.49
7:AG:15:ASP:OD1	7:AG:20:SER:N	2.31	0.49
16:AP:6:LEU:CD2	16:AP:19:VAL:HG22	2.42	0.49
22:AV:47:G:C4	22:AV:48:C:C5	3.00	0.49
25:BA:647:G:N2	25:BA:2350:C:O2'	2.43	0.49
25:BA:768:G:N2	25:BA:1379:U:O2'	2.46	0.49
42:BT:17:VAL:HG12	42:BT:76:VAL:HG21	1.93	0.49
53:B5:14:PHE:C	53:B5:15:LYS:HZ2	2.15	0.49
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.39	0.49
25:BA:64:A:H2'	25:BA:65:U:H6	1.76	0.49
25:BA:851:C:H2'	25:BA:852:U:C6	2.47	0.49
35:BM:81:ASP:OD1	35:BM:84:LYS:HE2	2.11	0.49
38:BP:36:TYR:HA	38:BP:52:SER:HB3	1.94	0.49
56:CT:9:DC:H2'	56:CT:10:DT:H71	1.93	0.49
56:CT:17:DG:C6	56:CT:18:DC:C5	3.00	0.49
1:AA:339:C:P	34:BL:13:ASN:HD22	2.35	0.49
1:AA:371:A:H2'	1:AA:372:C:O4'	2.13	0.49
1:AA:978:A:C5	1:AA:1319:A:C2	3.00	0.49
9:AI:55:VAL:O	9:AI:57:MET:N	2.45	0.49
10:AJ:28:THR:O	10:AJ:32:THR:HG22	2.12	0.49
25:BA:1069:A:N1	25:BA:1096:A:H5"	2.27	0.49
50:B2:43:ILE:HG22	50:B2:49:TYR:HB2	1.94	0.49
1:AA:451:A:H1'	1:AA:452:A:C2	2.47	0.49
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.48	0.49
1:AA:1183:U:H3'	1:AA:1184:G:C5'	2.42	0.49
1:AA:1246:A:C6	1:AA:1292:G:C6	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:28:LYS:HA	2:AB:31:ILE:HD12	1.94	0.49
24:AX:18:G:O2'	24:AX:57:G:N2	2.28	0.49
25:BA:396:G:OP2	47:BY:10:LYS:NZ	2.45	0.49
25:BA:1056:G:O2'	25:BA:1086:A:O2'	2.15	0.49
25:BA:1178:C:H2'	25:BA:1179:G:H8	1.71	0.49
25:BA:1199:U:H1'	40:BR:4:VAL:HG22	1.93	0.49
30:BF:31:VAL:HA	30:BF:158:THR:HG22	1.93	0.49
34:BL:70:ARG:HH12	34:BL:74:GLY:HA2	1.78	0.49
38:BP:40:ILE:HG12	38:BP:47:VAL:HG22	1.94	0.49
57:CB:34:GLY:N	57:CB:199:ASP:OD2	2.46	0.49
59:CD:813:ASP:OD1	59:CD:883:ARG:NH2	2.35	0.49
7:AG:129:GLU:CD	7:AG:131:LYS:H	2.15	0.49
17:AQ:25:ILE:O	17:AQ:25:ILE:HG22	2.13	0.49
22:AV:47:G:C2	22:AV:48:C:C4	3.00	0.49
51:B3:11:LEU:HD23	51:B3:51:GLU:HB2	1.95	0.49
57:CB:28:LEU:HD22	57:CB:28:LEU:N	2.27	0.49
58:CC:516:ASP:O	58:CC:518:ASN:N	2.41	0.49
1:AA:1022:A:C6	1:AA:1023:U:C4	3.01	0.49
1:AA:1244:G:C6	1:AA:1294:G:C6	3.01	0.49
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.60	0.49
3:AC:32:ASN:HB3	3:AC:59:ARG:NH2	2.28	0.49
3:AC:64:ILE:HG13	3:AC:99:ALA:HA	1.94	0.49
8:AH:18:GLN:HG3	8:AH:72:VAL:CG1	2.42	0.49
24:AX:20:H2U:O2	24:AX:20:H2U:H2'	2.12	0.49
30:BF:47:LYS:HA	30:BF:47:LYS:HE3	1.95	0.49
30:BF:57:LEU:HD12	30:BF:87:CYS:SG	2.52	0.49
39:BQ:33:VAL:O	39:BQ:33:VAL:HG12	2.13	0.49
40:BR:13:ARG:HH21	40:BR:13:ARG:HB3	1.78	0.49
58:CC:261:VAL:HG21	58:CC:264:GLU:HG2	1.94	0.49
59:CD:67:ASP:N	59:CD:67:ASP:OD1	2.43	0.49
1:AA:76:G:H1	1:AA:93:U:H3	1.60	0.49
1:AA:201:G:H2'	1:AA:202:G:H8	1.76	0.49
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.46	0.49
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.47	0.49
4:AD:121:LYS:HB3	4:AD:129:VAL:HG21	1.95	0.49
13:AM:65:VAL:HG22	13:AM:66:GLU:H	1.77	0.49
17:AQ:77:ARG:HD2	17:AQ:77:ARG:N	2.28	0.49
25:BA:1263:U:O2'	50:B2:8:PRO:HD2	2.12	0.49
25:BA:2162:G:H3'	25:BA:2164:C:H5	1.78	0.49
25:BA:2743:U:H2'	25:BA:2744:G:O4'	2.13	0.49
32:BH:6:LEU:HD13	32:BH:37:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:66:ASN:C	32:BH:66:ASN:HD22	2.15	0.49
58:CC:617:ALA:HB2	58:CC:650:VAL:HG21	1.93	0.49
1:AA:269:C:H2'	1:AA:270:A:C8	2.48	0.49
3:AC:109:PRO:CG	58:CC:859:GLU:OE2	2.59	0.49
4:AD:19:LEU:HD22	4:AD:64:ILE:HG13	1.95	0.49
4:AD:54:GLN:HG2	4:AD:199:LEU:HD22	1.95	0.49
7:AG:69:VAL:HG13	7:AG:100:ALA:HB1	1.95	0.49
10:AJ:56:HIS:CE1	10:AJ:57:VAL:HG13	2.48	0.49
23:AW:16:C:C2'	23:AW:17:C:H5'	2.42	0.49
25:BA:652:U:O2	25:BA:652:U:H3'	2.13	0.49
25:BA:868:U:O2	36:BN:8:LYS:NZ	2.42	0.49
25:BA:992:C:OP1	40:BR:47:TYR:OH	2.25	0.49
25:BA:1056:G:H4'	25:BA:1086:A:C8	2.47	0.49
25:BA:2125:G:OP2	25:BA:2125:G:H8	1.96	0.49
25:BA:2286:G:H22	51:B3:25:LYS:HA	1.77	0.49
26:BB:5:U:OP1	26:BB:61:G:O2'	2.26	0.49
27:BC:142:HIS:HD2	27:BC:193:GLY:O	1.95	0.49
30:BF:57:LEU:O	30:BF:61:SER:OG	2.20	0.49
55:CN:23:DT:H1'	55:CN:24:DC:C4	2.47	0.49
58:CC:1239:VAL:HG13	58:CC:1240:ASP:N	2.27	0.49
1:AA:35:G:H2'	1:AA:36:C:C6	2.48	0.49
1:AA:927:G:C2'	1:AA:928:G:H5'	2.42	0.49
3:AC:62:LYS:HE3	3:AC:62:LYS:H	1.77	0.49
13:AM:41:GLU:OE1	13:AM:41:GLU:N	2.34	0.49
24:AX:65:G:H2'	24:AX:66:U:C6	2.48	0.49
25:BA:1068:G:N2	25:BA:1096:A:H5'	2.28	0.49
25:BA:2315:G:O2'	25:BA:2316:G:O4'	2.31	0.49
25:BA:2646:C:OP2	25:BA:2732:G:O2'	2.24	0.49
25:BA:2805:C:H2'	25:BA:2806:C:O4'	2.13	0.49
28:BD:9:VAL:O	28:BD:197:THR:HG23	2.12	0.49
28:BD:129:THR:HG23	28:BD:130:GLN:O	2.13	0.49
55:CN:32:DA:H5'	55:CN:32:DA:H8	1.76	0.49
59:CD:767:LEU:HD12	59:CD:767:LEU:N	2.28	0.49
1:AA:1431:A:H2	1:AA:1469:C:H41	1.58	0.48
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.95	0.48
9:AI:63:LEU:HD12	9:AI:65:ILE:HD11	1.94	0.48
15:AO:26:GLU:OE2	15:AO:77:ARG:NE	2.35	0.48
25:BA:2346:A:H4'	25:BA:2347:C:OP2	2.13	0.48
29:BE:144:GLU:HG2	29:BE:145:ASP:H	1.78	0.48
30:BF:36:LEU:HD22	30:BF:152:LEU:HD12	1.95	0.48
1:AA:1383:C:O2'	1:AA:1384:C:H5'	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:7:PRO:HA	3:AC:10:ILE:HG22	1.94	0.48
25:BA:137:U:HO2'	25:BA:138:U:P	2.34	0.48
25:BA:1063:G:O2'	25:BA:1064:C:H5'	2.13	0.48
25:BA:1408:G:H2'	25:BA:1409:U:C6	2.48	0.48
27:BC:141:VAL:HG12	27:BC:192:LEU:HD13	1.95	0.48
28:BD:149:ASN:OD1	28:BD:150:MEQ:N	2.45	0.48
30:BF:40:VAL:C	30:BF:42:GLU:H	2.17	0.48
30:BF:55:ALA:O	30:BF:59:ALA:CA	2.60	0.48
50:B2:40:ARG:HG3	50:B2:41:HIS:ND1	2.28	0.48
56:CT:9:DC:H2'	56:CT:10:DT:C5	2.48	0.48
56:CT:20:DC:H2'	56:CT:21:DG:C8	2.47	0.48
58:CC:696:ASP:CG	58:CC:697:LYS:N	2.67	0.48
59:CD:805:GLN:OE1	59:CD:1348:LYS:HB2	2.13	0.48
59:CD:907:HIS:ND1	59:CD:908:ILE:O	2.36	0.48
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.78	0.48
7:AG:72:THR:HA	7:AG:96:ARG:HH11	1.78	0.48
20:AT:71:LYS:HG3	20:AT:74:ARG:HH21	1.79	0.48
24:AX:10:G:H2'	24:AX:11:C:C6	2.47	0.48
25:BA:63:A:H2	43:BU:70:HIS:CD2	2.32	0.48
25:BA:495:G:N3	42:BT:61:ASN:ND2	2.58	0.48
25:BA:1063:G:O2'	25:BA:1064:C:O4'	2.31	0.48
28:BD:32:ASN:HD22	28:BD:32:ASN:N	2.10	0.48
31:BG:105:LEU:HD11	31:BG:148:LEU:HD22	1.94	0.48
35:BM:79:LEU:HB3	35:BM:116:VAL:HB	1.94	0.48
42:BT:41:LYS:HE3	50:B2:22:LEU:HD11	1.95	0.48
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.48	0.48
3:AC:78:GLY:O	58:CC:943:LYS:CD	2.41	0.48
18:AR:34:THR:HG23	18:AR:36:SER:H	1.78	0.48
25:BA:1386:C:H2'	25:BA:1387:A:C8	2.48	0.48
25:BA:2185:U:C4	25:BA:2186:G:N7	2.81	0.48
35:BM:132:ARG:HG3	35:BM:142:ILE:HD12	1.94	0.48
39:BQ:8:LEU:O	39:BQ:11:GLU:HG2	2.14	0.48
57:CB:11:PRO:O	57:CB:12:ARG:HD2	2.12	0.48
57:CB:61:ILE:HD12	57:CB:142:MET:HB3	1.96	0.48
12:AL:81:LEU:HB3	12:AL:98:VAL:HG12	1.94	0.48
13:AM:71:ARG:HD3	30:BF:113:ASP:OD2	2.14	0.48
25:BA:545:A:C2	25:BA:549:C:N3	2.82	0.48
25:BA:940:G:H5"	25:BA:941:A:OP2	2.13	0.48
25:BA:1930:G:O2'	25:BA:1968:G:O6	2.26	0.48
25:BA:2557:G:H2'	25:BA:2558:C:C6	2.49	0.48
28:BD:34:VAL:O	28:BD:93:GLY:CA	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BD:186:LEU:HD21	39:BQ:4:ILE:HG12	1.94	0.48
47:BY:74:ARG:HD2	47:BY:76:GLU:HG2	1.94	0.48
55:CN:28:DA:C6	55:CN:29:DG:C6	3.01	0.48
56:CT:19:DG:C4	56:CT:20:DC:C6	3.01	0.48
56:CT:22:DC:C2	56:CT:23:DC:C5	3.01	0.48
58:CC:576:SER:OG	58:CC:577:VAL:N	2.47	0.48
1:AA:160:A:H2'	1:AA:161:A:O4'	2.13	0.48
4:AD:194:ASP:CA	59:CD:74:LYS:NZ	2.76	0.48
25:BA:742:A:H2'	25:BA:743:A:C8	2.49	0.48
25:BA:2099:U:O4	25:BA:2190:G:O6	2.31	0.48
25:BA:2314:A:H2'	25:BA:2315:G:H8	1.79	0.48
28:BD:37:VAL:HG22	28:BD:48:ILE:HG22	1.96	0.48
32:BH:133:GLN:HG3	32:BH:139:PHE:HE1	1.79	0.48
39:BQ:99:TYR:O	39:BQ:103:ARG:HG2	2.14	0.48
56:CT:19:DG:C5	56:CT:20:DC:C4	3.02	0.48
59:CD:830:ASP:OD1	59:CD:832:LYS:NZ	2.43	0.48
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.95	0.48
1:AA:1147:C:O2'	9:AI:7:TYR:OH	2.28	0.48
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.48	0.48
9:AI:26:GLY:N	9:AI:59:GLU:O	2.47	0.48
18:AR:41:PRO:HG2	18:AR:44:ILE:HB	1.95	0.48
25:BA:1394:U:H4'	25:BA:1603:A:H4'	1.95	0.48
25:BA:2118:U:OP1	25:BA:2149:U:H5'	2.13	0.48
25:BA:2804:U:HO2'	25:BA:2805:C:H6	1.61	0.48
30:BF:40:VAL:O	30:BF:42:GLU:N	2.38	0.48
30:BF:55:ALA:O	30:BF:59:ALA:CB	2.61	0.48
42:BT:41:LYS:O	42:BT:44:ALA:HB3	2.13	0.48
55:CN:32:DA:H1'	55:CN:33:DT:O4'	2.14	0.48
59:CD:1159:ILE:O	59:CD:1206:ARG:N	2.43	0.48
1:AA:652:U:O4	1:AA:752:G:O2'	2.23	0.48
1:AA:1228:C:H5'	13:AM:114:LYS:O	2.13	0.48
2:AB:47:VAL:HG13	2:AB:48:PRO:CD	2.42	0.48
5:AE:106:ILE:HB	5:AE:124:LEU:HD23	1.95	0.48
8:AH:13:ARG:NH1	8:AH:26:THR:O	2.46	0.48
22:AV:45:G:H5"	58:CC:540:ARG:HH22	1.79	0.48
25:BA:191:A:H2'	25:BA:192:C:C6	2.49	0.48
25:BA:1063:G:C4	25:BA:1064:C:C6	3.01	0.48
25:BA:2111:U:H5'	25:BA:2112:G:OP2	2.13	0.48
25:BA:2233:U:H2'	25:BA:2234:G:C8	2.49	0.48
1:AA:768:A:N3	1:AA:1512:U:O2'	2.47	0.48
25:BA:875:G:C6	25:BA:876:C:C4	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1932:A:H2'	25:BA:1933:G:O4'	2.14	0.48
25:BA:2812:G:H2'	25:BA:2813:A:O4'	2.13	0.48
26:BB:48:U:H2'	26:BB:49:C:C6	2.49	0.48
32:BH:50:ARG:HH12	32:BH:51:ARG:HE	1.62	0.48
58:CC:529:ARG:NH2	58:CC:562:GLU:OE2	2.46	0.48
58:CC:1238:LEU:N	58:CC:1238:LEU:HD23	2.29	0.48
1:AA:996:A:C4	1:AA:997:U:C5	3.02	0.48
1:AA:1320:C:N3	19:AS:36:ARG:NH1	2.62	0.48
4:AD:7:PRO:HB2	4:AD:10:LYS:CB	2.43	0.48
4:AD:188:ARG:NH2	4:AD:195:ILE:O	2.47	0.48
7:AG:69:VAL:HG11	7:AG:104:ILE:HD11	1.95	0.48
25:BA:910:A:N3	25:BA:2264:C:O2'	2.35	0.48
33:BK:9:GLU:OE1	33:BK:9:GLU:N	2.45	0.48
1:AA:17:U:H2'	1:AA:18:C:C6	2.49	0.47
1:AA:996:A:C6	1:AA:997:U:C4	3.02	0.47
1:AA:1367:C:OP1	10:AJ:62:ARG:NH2	2.47	0.47
2:AB:20:THR:HG22	2:AB:37:LYS:HG2	1.95	0.47
2:AB:196:VAL:HG21	2:AB:199:VAL:HG13	1.96	0.47
10:AJ:53:ILE:HD11	10:AJ:63:ASP:N	2.29	0.47
25:BA:1581:G:C6	25:BA:1582:C:C4	3.02	0.47
25:BA:1595:C:H2'	25:BA:1596:A:H8	1.77	0.47
25:BA:2244:U:H2'	25:BA:2245:U:C6	2.49	0.47
30:BF:8:TYR:HA	30:BF:12:VAL:HB	1.95	0.47
37:BO:20:MET:HG3	37:BO:21:PHE:N	2.28	0.47
41:BS:28:ALA:HB3	41:BS:31:GLU:OE1	2.14	0.47
55:CN:27:DA:C2	55:CN:28:DA:C4	3.02	0.47
58:CC:596:ASP:OD1	58:CC:597:GLY:N	2.38	0.47
33:BK:3:THR:HG21	40:BR:61:TRP:HE1	1.78	0.47
58:CC:234:ASP:HB3	58:CC:238:GLN:NE2	2.29	0.47
59:CD:301:GLU:OE1	59:CD:312:ARG:NE	2.46	0.47
59:CD:746:LEU:HD23	59:CD:758:PRO:HB3	1.96	0.47
1:AA:837:U:C2	1:AA:849:G:O6	2.67	0.47
1:AA:1261:A:N6	1:AA:1274:A:HO2'	2.10	0.47
27:BC:119:GLY:O	27:BC:130:LEU:HB3	2.14	0.47
31:BG:38:ASN:HB3	31:BG:41:VAL:HG13	1.96	0.47
58:CC:138:ILE:HA	58:CC:138:ILE:HD13	1.53	0.47
58:CC:267:ARG:HH22	58:CC:273:HIS:CE1	2.31	0.47
59:CD:1292:LEU:HD11	59:CD:1297:LYS:HB2	1.95	0.47
7:AG:72:THR:HA	7:AG:96:ARG:NH1	2.28	0.47
8:AH:18:GLN:OE1	8:AH:18:GLN:HA	2.14	0.47
25:BA:463:G:N2	25:BA:466:A:OP2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1040:A:N6	25:BA:1115:G:C6	2.80	0.47
25:BA:1503:A:OP1	25:BA:1503:A:H4'	2.15	0.47
25:BA:2448:A:H3'	25:BA:2449:H2U:H61	1.96	0.47
30:BF:60:ILE:HG12	30:BF:141:ILE:HG12	1.95	0.47
57:CA:79:LEU:HD23	57:CA:79:LEU:O	2.15	0.47
58:CC:530:ILE:HD13	58:CC:530:ILE:HA	1.65	0.47
58:CC:699:LEU:HA	58:CC:699:LEU:HD23	1.61	0.47
58:CC:1333:LEU:C	58:CC:1335:ILE:H	2.18	0.47
59:CD:849:LEU:HA	59:CD:856:ILE:HA	1.96	0.47
5:AE:83:HIS:NE2	5:AE:147:MET:HG3	2.29	0.47
10:AJ:42:LEU:HB2	10:AJ:71:LEU:CB	2.43	0.47
25:BA:1580:A:H5"	25:BA:1580:A:H8	1.78	0.47
25:BA:2273:A:H2'	25:BA:2274:A:C8	2.49	0.47
38:BP:55:GLU:CD	38:BP:81:ARG:HH22	2.18	0.47
40:BR:88:VAL:HG22	41:BS:51:VAL:HG12	1.96	0.47
56:CT:21:DG:H2'	56:CT:22:DC:C6	2.50	0.47
58:CC:1292:THR:OG1	58:CC:1293:VAL:N	2.47	0.47
59:CD:26:SER:HB3	59:CD:236:TRP:CZ2	2.49	0.47
1:AA:88:U:H3'	1:AA:89:G:H8	1.79	0.47
1:AA:657:U:O2	15:AO:22:THR:OG1	2.32	0.47
1:AA:685:G:N2	1:AA:704:A:OP2	2.40	0.47
20:AT:39:ILE:HD11	20:AT:83:ILE:HD12	1.96	0.47
21:AU:17:ARG:O	21:AU:21:ARG:HG3	2.15	0.47
24:AX:23:A:H2'	24:AX:24:G:C8	2.50	0.47
24:AX:57:G:OP2	36:BN:59:ARG:NH1	2.48	0.47
25:BA:2164:C:O2	25:BA:2164:C:H2'	2.14	0.47
25:BA:2521:C:O2'	25:BA:2564:A:N3	2.41	0.47
29:BE:109:LEU:HA	29:BE:109:LEU:HD23	1.71	0.47
59:CD:393:THR:HG23	59:CD:395:LYS:H	1.80	0.47
1:AA:159:G:H1'	1:AA:162:A:N6	2.29	0.47
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.50	0.47
1:AA:1255:G:O2'	1:AA:1258:G:N3	2.35	0.47
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.47	0.47
3:AC:124:LEU:HA	3:AC:124:LEU:HD23	1.74	0.47
6:AF:45:ARG:HD3	6:AF:45:ARG:HA	1.71	0.47
19:AS:48:THR:HG22	19:AS:61:PHE:HB2	1.96	0.47
25:BA:839:U:H2'	25:BA:840:C:C6	2.50	0.47
25:BA:1916:A:H2'	25:BA:1917:PSU:H6	1.75	0.47
25:BA:2104:C:H5	25:BA:2186:G:H21	1.61	0.47
25:BA:2635:A:O2'	28:BD:81:GLU:HG3	2.15	0.47
25:BA:2803:G:H2'	25:BA:2804:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2830:C:H3'	28:BD:59:ARG:NH2	2.30	0.47
26:BB:42:C:C5	30:BF:66:LEU:HD22	2.49	0.47
35:BM:33:ARG:NH2	35:BM:40:SER:O	2.48	0.47
40:BR:78:LYS:HE2	40:BR:117:LEU:HD13	1.97	0.47
45:BW:7:GLU:O	45:BW:40:ILE:HA	2.15	0.47
58:CC:1333:LEU:O	58:CC:1335:ILE:N	2.48	0.47
59:CD:158:GLN:NE2	59:CD:158:GLN:O	2.46	0.47
1:AA:195:A:C2'	1:AA:196:A:H5'	2.44	0.47
1:AA:966:2MG:O2'	9:AI:129:LYS:O	2.33	0.47
1:AA:1408:A:H2'	1:AA:1409:C:H6	1.79	0.47
10:AJ:18:ILE:HD12	10:AJ:18:ILE:HA	1.66	0.47
14:AN:27:LEU:O	14:AN:30:ILE:HG23	2.15	0.47
25:BA:1796:U:O2'	27:BC:254:GLY:N	2.34	0.47
25:BA:2029:G:N1	25:BA:2033:A:OP2	2.35	0.47
58:CC:129:LEU:HD23	58:CC:129:LEU:HA	1.68	0.47
1:AA:860:A:H2'	1:AA:861:G:O4'	2.14	0.47
1:AA:1167:A:C5	1:AA:1169:A:C6	3.03	0.47
1:AA:1527:U:H5	21:AU:42:THR:HG21	1.80	0.47
13:AM:75:MET:SD	13:AM:78:LYS:HE2	2.55	0.47
25:BA:877:A:C6	25:BA:899:A:C6	3.03	0.47
25:BA:1064:C:HO2'	25:BA:1065:U:C1'	2.28	0.47
26:BB:2:G:C6	26:BB:119:A:C6	3.02	0.47
26:BB:118:C:C2	26:BB:119:A:C8	3.02	0.47
31:BG:52:PHE:CZ	31:BG:72:LEU:HD22	2.50	0.47
42:BT:36:LEU:HD13	42:BT:48:LYS:HA	1.96	0.47
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.95	0.47
25:BA:1062:G:C8	25:BA:1088:A:C8	3.03	0.47
25:BA:1177:G:O2'	25:BA:1178:C:O4'	2.32	0.47
25:BA:2006:C:O2'	25:BA:2823:A:N3	2.47	0.47
25:BA:2901:C:N3	25:BA:2902:C:N4	2.63	0.47
32:BH:97:ARG:HB3	32:BH:112:LYS:HD3	1.95	0.47
34:BL:13:ASN:HB3	34:BL:100:PHE:HE1	1.80	0.47
39:BQ:89:ARG:HB2	39:BQ:113:ARG:NH1	2.30	0.47
58:CC:269:ILE:HD12	58:CC:269:ILE:N	2.29	0.47
59:CD:664:ILE:HG22	59:CD:678:ARG:HG2	1.97	0.47
59:CD:1249:ASN:OD1	59:CD:1250:ASP:N	2.48	0.47
1:AA:464:U:O2	1:AA:466:A:H3'	2.16	0.46
1:AA:1033:G:C2	1:AA:1034:G:C4	3.03	0.46
1:AA:1088:G:H1'	21:AU:71:TYR:HB3	1.97	0.46
1:AA:1424:U:H2'	1:AA:1425:U:O4'	2.15	0.46
20:AT:55:GLN:O	20:AT:58:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:721:A:H2'	25:BA:722:A:C8	2.50	0.46
25:BA:866:A:C8	25:BA:914:G:C6	3.04	0.46
25:BA:1056:G:C2'	25:BA:1103:A:H61	2.28	0.46
25:BA:1065:U:O2'	25:BA:1066:U:O5'	2.31	0.46
25:BA:2186:G:H2'	25:BA:2187:U:C6	2.50	0.46
25:BA:2469:A:H4'	36:BN:55:ARG:HD2	1.98	0.46
33:BK:30:THR:HG22	33:BK:31:GLU:N	2.31	0.46
59:CD:488:ASN:N	59:CD:488:ASN:OD1	2.48	0.46
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.16	0.46
3:AC:73:PRO:O	3:AC:76:VAL:N	2.48	0.46
10:AJ:24:GLU:OE1	10:AJ:92:LEU:HD12	2.15	0.46
15:AO:70:LEU:HD12	15:AO:70:LEU:HA	1.68	0.46
21:AU:60:LEU:O	21:AU:64:ASN:HB2	2.15	0.46
25:BA:929:U:H1'	49:B1:26:GLY:O	2.14	0.46
25:BA:957:C:HO2'	25:BA:959:A:H8	1.62	0.46
25:BA:989:G:OP2	49:B1:12:SER:HB2	2.15	0.46
25:BA:2149:U:H2'	25:BA:2150:C:C6	2.50	0.46
34:BL:64:ARG:NH1	34:BL:102:PRO:O	2.43	0.46
38:BP:27:VAL:HG21	38:BP:40:ILE:HD12	1.98	0.46
1:AA:212:G:C2	1:AA:213:G:C8	3.03	0.46
3:AC:20:SER:OG	3:AC:40:ARG:NH2	2.48	0.46
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.44	0.46
8:AH:103:VAL:HG22	8:AH:126:ILE:HB	1.96	0.46
9:AI:32:GLN:OE1	9:AI:64:TYR:OH	2.32	0.46
11:AK:109:ASN:OD1	11:AK:110:ILE:N	2.48	0.46
13:AM:41:GLU:H	13:AM:41:GLU:CD	2.16	0.46
15:AO:5:THR:O	15:AO:8:THR:OG1	2.26	0.46
25:BA:806:C:HO2'	25:BA:2445:2MG:HO2'	1.54	0.46
25:BA:1723:G:H3'	25:BA:1724:G:H8	1.81	0.46
25:BA:1852:U:O2	25:BA:1890:A:N6	2.48	0.46
25:BA:2743:U:OP1	54:B6:34:LYS:NZ	2.33	0.46
27:BC:13:ARG:HH22	27:BC:18:LYS:HE3	1.80	0.46
58:CC:766:ASN:O	58:CC:766:ASN:CG	2.53	0.46
59:CD:255:LEU:HG	59:CD:256:ASP:H	1.80	0.46
9:AI:9:THR:HG23	9:AI:85:ARG:HH11	1.81	0.46
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.97	0.46
24:AX:25:C:C2	24:AX:26:A:C8	3.03	0.46
25:BA:274:C:H3'	25:BA:275:C:H6	1.80	0.46
25:BA:2124:G:H2'	25:BA:2125:G:O4'	2.14	0.46
45:BW:80:HIS:ND1	45:BW:83:LYS:HB2	2.31	0.46
54:B6:23:ILE:HB	54:B6:37:GLN:CB	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CA:179:PRO:HA	57:CA:208:ASN:ND2	2.30	0.46
59:CD:416:ILE:O	59:CD:416:ILE:HG23	2.15	0.46
1:AA:148:G:O2'	1:AA:149:A:C5'	2.64	0.46
1:AA:956:U:H2'	1:AA:957:U:O4'	2.16	0.46
7:AG:4:ARG:HH11	7:AG:5:ARG:NH2	2.13	0.46
9:AI:12:ARG:O	9:AI:15:SER:N	2.48	0.46
28:BD:188:LEU:HD21	39:BQ:8:LEU:HD21	1.98	0.46
30:BF:58:ALA:HA	30:BF:63:GLN:O	2.16	0.46
59:CD:265:LEU:O	59:CD:268:LEU:N	2.45	0.46
3:AC:124:LEU:HD13	3:AC:196:ILE:CD1	2.46	0.46
20:AT:35:VAL:HG21	20:AT:54:MET:HG2	1.97	0.46
25:BA:550:U:C2	25:BA:551:G:N7	2.83	0.46
25:BA:1413:A:H2'	25:BA:1414:C:O4'	2.14	0.46
25:BA:1693:U:O2'	27:BC:14:ARG:NH2	2.43	0.46
25:BA:2315:G:O2'	25:BA:2316:G:H8	1.98	0.46
25:BA:2514:U:H2'	25:BA:2515:C:C6	2.51	0.46
25:BA:2747:G:O6	25:BA:2755:C:H5"	2.15	0.46
26:BB:27:C:OP1	38:BP:34:HIS:NE2	2.40	0.46
32:BH:72:ILE:HG22	32:BH:108:VAL:HG22	1.97	0.46
49:B1:23:THR:HG23	49:B1:47:MET:HG2	1.98	0.46
59:CD:62:PHE:O	59:CD:101:ARG:NH2	2.46	0.46
59:CD:247:PRO:HA	59:CD:250:ARG:CZ	2.45	0.46
1:AA:1320:C:C2	19:AS:72:GLY:HA3	2.50	0.46
3:AC:79:LYS:HE3	3:AC:79:LYS:HB3	1.56	0.46
6:AF:85:ILE:HG13	6:AF:86:ARG:H	1.81	0.46
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.34	0.46
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.56	0.46
12:AL:39:THR:HG22	12:AL:51:LYS:HD3	1.98	0.46
22:AV:48:C:H2'	22:AV:49:G:O4'	2.16	0.46
24:AX:24:G:H2'	24:AX:25:C:C6	2.51	0.46
25:BA:1847:A:H1'	25:BA:1848:A:N7	2.31	0.46
58:CC:705:GLU:OE1	58:CC:705:GLU:N	2.41	0.46
1:AA:158:G:C6	1:AA:159:G:C5	3.03	0.46
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.51	0.46
5:AE:57:PRO:O	5:AE:61:GLN:NE2	2.48	0.46
6:AF:73:GLU:HG3	6:AF:74:LEU:N	2.31	0.46
7:AG:17:LYS:HE2	7:AG:17:LYS:HB3	1.61	0.46
7:AG:109:ARG:CG	7:AG:109:ARG:HH11	2.29	0.46
11:AK:33:THR:HG22	11:AK:44:TRP:CB	2.46	0.46
25:BA:280:U:O4	25:BA:361:G:N2	2.49	0.46
25:BA:1744:A:H3'	25:BA:1745:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2314:A:H1'	30:BF:155:THR:HG21	1.97	0.46
41:BS:1:MET:HA	41:BS:42:ALA:O	2.15	0.46
41:BS:34:GLU:HG2	41:BS:60:LYS:HG2	1.97	0.46
54:B6:2:LYS:HE2	54:B6:32:LYS:O	2.15	0.46
1:AA:203:G:N2	1:AA:215:C:C2	2.84	0.46
1:AA:1023:U:H2'	1:AA:1024:G:O4'	2.16	0.46
3:AC:78:GLY:C	58:CC:943:LYS:HD2	2.32	0.46
25:BA:102:U:O4	48:BZ:2:LYS:N	2.49	0.46
25:BA:2572:A:N6	28:BD:150:MEQ:HE1	2.30	0.46
25:BA:2884:U:C5	50:B2:40:ARG:HD2	2.51	0.46
29:BE:37:ALA:HA	29:BE:40:ARG:HG3	1.98	0.46
33:BK:117:ALA:HA	33:BK:120:ARG:NH2	2.31	0.46
39:BQ:40:LEU:HD12	39:BQ:40:LEU:HA	1.80	0.46
58:CC:696:ASP:OD1	58:CC:696:ASP:N	2.45	0.46
59:CD:513:MET:HG3	59:CD:544:LEU:HD21	1.98	0.46
1:AA:6:G:N2	5:AE:103:THR:OG1	2.49	0.46
1:AA:1088:G:H21	1:AA:1167:A:N6	2.14	0.46
1:AA:1408:A:H2'	1:AA:1409:C:C6	2.51	0.46
21:AU:55:ARG:HD3	21:AU:55:ARG:HA	1.74	0.46
25:BA:1073:A:H2'	25:BA:1074:G:O4'	2.16	0.46
25:BA:1078:U:H5"	25:BA:1079:C:OP1	2.16	0.46
25:BA:2314:A:O2'	25:BA:2315:G:H5'	2.16	0.46
28:BD:150:MEQ:HE21	28:BD:150:MEQ:HB3	1.45	0.46
29:BE:4:VAL:HA	29:BE:11:ALA:HA	1.97	0.46
30:BF:103:LEU:HA	30:BF:107:ALA:HB3	1.97	0.46
39:BQ:99:TYR:HD1	39:BQ:103:ARG:HD2	1.81	0.46
42:BT:17:VAL:HG11	42:BT:103:ILE:HG12	1.98	0.46
59:CD:891:ASP:OD1	59:CD:1286:LYS:NZ	2.49	0.46
59:CD:1309:ILE:HG13	59:CD:1310:THR:N	2.31	0.46
1:AA:1032:G:N2	1:AA:1033:G:H4'	2.31	0.45
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.48	0.45
6:AF:5:GLU:OE2	18:AR:24:LYS:NZ	2.44	0.45
25:BA:804:A:H2'	25:BA:806:C:C4	2.51	0.45
25:BA:833:A:H2'	25:BA:834:G:C8	2.52	0.45
27:BC:159:GLY:HA2	27:BC:195:VAL:O	2.16	0.45
33:BK:40:HIS:CE1	33:BK:41:LYS:HG2	2.51	0.45
35:BM:77:VAL:O	35:BM:111:ILE:HG12	2.16	0.45
1:AA:401:C:O2'	1:AA:621:A:N3	2.44	0.45
1:AA:473:U:C2	1:AA:474:G:C8	3.04	0.45
3:AC:107:ARG:HE	58:CC:863:SER:CA	2.29	0.45
22:AV:47:G:C2	22:AV:48:C:C5	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:21:A:N6	24:AX:48:C:O4'	2.48	0.45
25:BA:747:5MU:O2	25:BA:2014:A:H1'	2.17	0.45
27:BC:251:GLN:NE2	27:BC:252:THR:O	2.49	0.45
28:BD:14:ILE:HD13	39:BQ:12:GLN:HE22	1.82	0.45
28:BD:152:PRO:HG3	28:BD:156:PHE:CZ	2.52	0.45
32:BH:131:SER:OG	32:BH:141:LYS:NZ	2.50	0.45
57:CB:66:HIS:O	57:CB:66:HIS:ND1	2.44	0.45
13:AM:5:ALA:HB1	13:AM:65:VAL:HG21	1.98	0.45
25:BA:1385:A:O2'	25:BA:1396:U:O2	2.31	0.45
32:BH:75:LEU:HD12	32:BH:77:THR:O	2.16	0.45
37:BO:100:CYS:O	37:BO:110:MET:HB2	2.16	0.45
43:BU:14:PRO:HD3	48:BZ:30:MET:SD	2.56	0.45
45:BW:27:PRO:O	45:BW:88:HIS:HA	2.16	0.45
55:CN:10:DG:H2"	55:CN:11:DT:H72	1.97	0.45
58:CC:514:PHE:CE1	58:CC:760:ASN:HB3	2.51	0.45
58:CC:1291:LEU:HD21	59:CD:1351:VAL:HG13	1.97	0.45
2:AB:122:GLN:HG3	2:AB:123:ASP:N	2.32	0.45
3:AC:31:ASP:OD1	14:AN:65:ARG:NH1	2.42	0.45
10:AJ:80:THR:O	10:AJ:84:VAL:HG12	2.17	0.45
18:AR:42:SER:OG	18:AR:47:THR:O	2.34	0.45
25:BA:67:U:C2	25:BA:68:G:C8	3.04	0.45
25:BA:475:C:N3	25:BA:479:A:N7	2.64	0.45
25:BA:2532:G:O2'	25:BA:2657:A:N1	2.50	0.45
25:BA:2742:G:OP2	54:B6:24:ARG:NH1	2.43	0.45
25:BA:2745:C:C4	25:BA:2746:U:C4	3.04	0.45
31:BG:4:VAL:HG12	31:BG:69:ARG:HD3	1.97	0.45
35:BM:70:LYS:NZ	35:BM:70:LYS:HB2	2.31	0.45
43:BU:5:GLU:H	43:BU:5:GLU:HG3	1.43	0.45
58:CC:38:PHE:CZ	58:CC:49:LEU:HD21	2.51	0.45
58:CC:563:THR:OG1	58:CC:564:PRO:HD2	2.16	0.45
59:CD:363:LEU:HA	59:CD:363:LEU:HD12	1.73	0.45
59:CD:1075:ARG:NH2	59:CD:1102:PRO:HA	2.31	0.45
1:AA:739:C:OP1	6:AF:2:ARG:NH1	2.50	0.45
1:AA:1122:U:H2'	1:AA:1123:U:C6	2.52	0.45
6:AF:38:ARG:NH2	6:AF:63:ASN:OD1	2.50	0.45
13:AM:9:ILE:HG23	13:AM:18:ALA:HB1	1.98	0.45
21:AU:40:LYS:O	21:AU:43:THR:OG1	2.28	0.45
25:BA:111:A:C6	25:BA:112:U:C4	3.04	0.45
25:BA:133:U:H2'	25:BA:134:G:O4'	2.17	0.45
25:BA:1306:C:N4	25:BA:1606:C:H2'	2.31	0.45
25:BA:2000:C:OP1	37:BO:5:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2178:C:H2'	25:BA:2179:C:H5	1.80	0.45
27:BC:176:LEU:O	27:BC:179:GLY:N	2.40	0.45
33:BK:141:ASP:O	33:BK:142:ILE:HD13	2.16	0.45
34:BL:76:VAL:HG12	39:BQ:73:VAL:HB	1.98	0.45
1:AA:911:U:H2'	1:AA:912:C:C6	2.52	0.45
1:AA:1130:A:O2'	9:AI:5:GLN:OE1	2.34	0.45
3:AC:70:THR:HG21	3:AC:76:VAL:HG21	1.99	0.45
6:AF:15:SER:HA	6:AF:18:VAL:HG23	1.99	0.45
9:AI:12:ARG:CD	9:AI:74:GLY:HA2	2.46	0.45
9:AI:41:ARG:NH1	9:AI:41:ARG:HB2	2.32	0.45
25:BA:1751:U:H2'	25:BA:1752:C:C6	2.52	0.45
26:BB:48:U:P	38:BP:30:ARG:HH22	2.39	0.45
30:BF:175:PHE:HB3	30:BF:177:PHE:CE2	2.51	0.45
32:BH:11:ASN:O	32:BH:11:ASN:ND2	2.47	0.45
33:BK:99:ARG:HD2	33:BK:99:ARG:HA	1.81	0.45
35:BM:63:LYS:HG2	53:B5:13:ARG:HD3	1.98	0.45
35:BM:89:VAL:HG11	35:BM:123:ARG:HH21	1.81	0.45
47:BY:33:LEU:HD13	47:BY:50:ARG:HG2	1.98	0.45
47:BY:39:TRP:HZ2	47:BY:44:LYS:HD3	1.81	0.45
56:CT:4:DT:H2"	56:CT:5:DG:H8	1.82	0.45
57:CB:66:HIS:CG	57:CB:68:TYR:HB3	2.52	0.45
58:CC:28:LEU:HD23	58:CC:28:LEU:HA	1.54	0.45
59:CD:119:SER:OG	59:CD:120:LEU:N	2.50	0.45
59:CD:120:LEU:HB3	59:CD:121:PRO:CD	2.47	0.45
59:CD:478:LEU:HD23	59:CD:478:LEU:HA	1.63	0.45
59:CD:1332:LEU:HA	59:CD:1332:LEU:HD12	1.73	0.45
1:AA:211:G:C5	1:AA:212:G:H1'	2.52	0.45
1:AA:278:G:OP2	17:AQ:43:LYS:NZ	2.35	0.45
3:AC:59:ARG:HB3	3:AC:64:ILE:HG22	1.98	0.45
11:AK:84:VAL:HG11	11:AK:97:ILE:HG22	1.99	0.45
22:AV:39:A:OP2	58:CC:1250:SER:OG	2.22	0.45
25:BA:2131:U:O2	25:BA:2131:U:H3'	2.17	0.45
30:BF:136:ILE:HG12	30:BF:143:TYR:CD1	2.50	0.45
34:BL:40:LYS:HE3	34:BL:57:VAL:HG12	1.99	0.45
58:CC:1043:ALA:O	58:CC:1046:VAL:HG22	2.17	0.45
58:CC:1204:LEU:HD23	58:CC:1204:LEU:HA	1.69	0.45
59:CD:850:LYS:N	59:CD:855:ASP:O	2.33	0.45
1:AA:1037:C:H2'	1:AA:1038:C:C6	2.52	0.45
1:AA:1299:A:O2'	1:AA:1301:U:O4'	2.29	0.45
5:AE:90:THR:OG1	5:AE:135:ASN:OD1	2.25	0.45
7:AG:122:ASN:O	7:AG:125:SER:OG	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:26:ILE:O	18:AR:30:LYS:N	2.37	0.45
24:AX:14:A:N1	24:AX:22:G:H1'	2.32	0.45
59:CD:213:LYS:O	59:CD:213:LYS:HD3	2.17	0.45
59:CD:952:VAL:HG13	59:CD:1014:GLY:H	1.81	0.45
1:AA:970:C:N4	9:AI:130:ARG:OXT	2.41	0.45
1:AA:1305:G:N2	1:AA:1331:G:O2'	2.44	0.45
3:AC:85:GLU:OE2	3:AC:88:ARG:NH2	2.38	0.45
9:AI:130:ARG:NH2	23:AW:33:U:OP2	2.48	0.45
12:AL:87:VAL:O	12:AL:87:VAL:HG12	2.17	0.45
25:BA:1869:G:C2	25:BA:1873:G:C6	3.04	0.45
27:BC:76:ALA:HB2	27:BC:96:TYR:CD2	2.52	0.45
36:BN:3:GLN:HE21	36:BN:92:TRP:HE1	1.65	0.45
54:B6:14:CYS:O	54:B6:15:LYS:HD3	2.17	0.45
55:CN:26:DG:C4	55:CN:27:DA:N7	2.85	0.45
1:AA:36:C:H2'	1:AA:37:U:O4'	2.17	0.45
1:AA:590:U:H2'	1:AA:591:U:C6	2.52	0.45
1:AA:1029:U:O4	1:AA:1031:C:H1'	2.16	0.45
1:AA:1118:U:H2'	1:AA:1119:C:H6	1.81	0.45
5:AE:13:GLU:CB	5:AE:39:VAL:HG12	2.46	0.45
13:AM:92:ARG:CB	25:BA:888:C:H5'	2.45	0.45
15:AO:7:ALA:O	15:AO:11:ILE:HD13	2.17	0.45
25:BA:39:G:H2'	25:BA:40:U:C6	2.52	0.45
25:BA:614:A:C8	25:BA:614:A:OP2	2.70	0.45
25:BA:626:A:H2'	35:BM:78:ARG:NH2	2.32	0.45
25:BA:2537:U:H2'	25:BA:2538:C:C6	2.51	0.45
48:BZ:10:SER:OG	48:BZ:11:VAL:N	2.50	0.45
53:B5:55:LEU:O	53:B5:58:VAL:HG12	2.17	0.45
58:CC:176:ILE:HG21	58:CC:176:ILE:HD13	1.67	0.45
58:CC:616:ILE:HA	58:CC:652:TYR:O	2.17	0.45
58:CC:836:LEU:HA	58:CC:836:LEU:HD23	1.83	0.45
59:CD:317:THR:HG21	59:CD:321:LYS:HA	1.99	0.45
1:AA:1152:A:H2'	1:AA:1153:G:O4'	2.17	0.44
6:AF:22:ILE:CG2	6:AF:39:LEU:HD21	2.47	0.44
10:AJ:76:ILE:CG1	10:AJ:79:PRO:HG3	2.48	0.44
25:BA:289:G:H2'	25:BA:290:U:C6	2.53	0.44
25:BA:1656:C:H2'	25:BA:1657:U:H6	1.82	0.44
31:BG:76:VAL:O	31:BG:79:VAL:HG12	2.16	0.44
42:BT:58:ALA:O	42:BT:62:ASP:HB3	2.17	0.44
57:CB:107:ILE:HD11	57:CB:136:GLU:HA	2.00	0.44
58:CC:145:ILE:CG2	58:CC:456:VAL:HG22	2.47	0.44
59:CD:903:LEU:HA	59:CD:903:LEU:HD13	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:587:G:OP1	8:AH:84:ARG:NH2	2.50	0.44
1:AA:590:U:H2'	1:AA:591:U:H6	1.83	0.44
1:AA:677:U:H3	1:AA:713:G:H22	1.65	0.44
1:AA:1007:U:OP1	14:AN:19:LYS:HE3	2.17	0.44
2:AB:226:SER:O	2:AB:227:GLN:HB2	2.17	0.44
25:BA:44:A:H2'	25:BA:45:G:O4'	2.17	0.44
25:BA:271:G:C4	25:BA:272:A:C8	3.06	0.44
25:BA:359:G:C5	25:BA:360:U:C5	3.06	0.44
25:BA:593:U:H2'	25:BA:594:U:C6	2.52	0.44
25:BA:888:C:H1'	25:BA:889:C:C1'	2.46	0.44
25:BA:1063:G:C5	25:BA:1064:C:C5	3.05	0.44
25:BA:1071:G:H1'	25:BA:1089:A:H2'	1.99	0.44
25:BA:2109:U:N3	25:BA:2110:G:O6	2.50	0.44
43:BU:3:ARG:HD3	43:BU:3:ARG:HA	1.76	0.44
58:CC:936:ARG:HH22	58:CC:1044:PRO:HA	1.82	0.44
58:CC:1257:GLN:NE2	59:CD:345:LYS:HD3	2.32	0.44
1:AA:147:G:H2'	1:AA:148:G:C8	2.52	0.44
1:AA:1088:G:H21	1:AA:1167:A:H62	1.65	0.44
3:AC:72:ARG:O	3:AC:75:ILE:HG22	2.16	0.44
7:AG:24:ALA:O	7:AG:27:VAL:HG22	2.17	0.44
23:AW:17(A):U:OP2	23:AW:61:C:H5'	2.17	0.44
25:BA:2012:G:OP1	42:BT:98:LYS:NZ	2.50	0.44
25:BA:2100:G:C5	25:BA:2190:G:C2	3.06	0.44
25:BA:2349:G:C6	25:BA:2369:A:C6	3.05	0.44
25:BA:2522:U:O2'	25:BA:2647:U:OP1	2.24	0.44
32:BH:115:VAL:HG12	32:BH:117:LEU:HD12	1.99	0.44
36:BN:67:VAL:HG21	36:BN:96:ILE:HD11	1.99	0.44
43:BU:6:ARG:HH22	43:BU:37:ASP:CG	2.20	0.44
43:BU:25:GLU:HG3	43:BU:26:LYS:N	2.31	0.44
58:CC:363:LEU:HA	58:CC:363:LEU:HD23	1.73	0.44
58:CC:571:LEU:HD23	58:CC:571:LEU:HA	1.47	0.44
58:CC:1076:ILE:O	58:CC:1076:ILE:HG13	2.15	0.44
1:AA:261:U:C5	20:AT:74:ARG:NH1	2.86	0.44
1:AA:1384:C:H2'	1:AA:1385:G:C8	2.53	0.44
4:AD:193:ALA:C	59:CD:74:LYS:HE2	2.38	0.44
23:AW:74:C:H5'	25:BA:2602:A:C5'	2.47	0.44
25:BA:78:U:OP1	48:BZ:7:ARG:NH2	2.51	0.44
25:BA:301:G:OP2	44:BV:82:ARG:NH1	2.51	0.44
25:BA:1408:G:H2'	25:BA:1409:U:H6	1.83	0.44
27:BC:246:THR:OG1	27:BC:250:VAL:HG13	2.17	0.44
28:BD:8:LYS:HB2	28:BD:201:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:5:LEU:O	32:BH:6:LEU:HD12	2.16	0.44
35:BM:17:LYS:HE2	35:BM:27:LEU:HD11	1.99	0.44
52:B4:41:ARG:HB2	52:B4:41:ARG:CZ	2.47	0.44
59:CD:424:ASN:O	59:CD:424:ASN:ND2	2.50	0.44
59:CD:425:ARG:HE	59:CD:464:ASP:CG	2.21	0.44
4:AD:188:ARG:NH1	59:CD:86:GLU:OE2	2.41	0.44
11:AK:40:ASN:OD1	11:AK:40:ASN:N	2.51	0.44
14:AN:41:ARG:NH2	19:AS:6:LYS:O	2.50	0.44
17:AQ:8:LEU:HD23	17:AQ:25:ILE:HG21	1.99	0.44
25:BA:1069:A:C2	25:BA:1096:A:H5"	2.52	0.44
25:BA:1796:U:H2'	25:BA:1797:G:H8	1.83	0.44
29:BE:18:THR:HG21	29:BE:197:GLU:HG3	1.99	0.44
31:BG:69:ARG:HG2	31:BG:69:ARG:HH11	1.82	0.44
37:BO:54:LEU:HD21	37:BO:65:LEU:HB3	1.99	0.44
41:BS:36:ALA:HA	41:BS:58:VAL:HG23	2.00	0.44
41:BS:37:GLU:HA	41:BS:37:GLU:OE1	2.17	0.44
58:CC:1327:LEU:HD23	58:CC:1327:LEU:HA	1.70	0.44
1:AA:71:A:H2'	1:AA:72:A:H8	1.83	0.44
1:AA:946:A:H2'	1:AA:947:G:H8	1.81	0.44
1:AA:1026:G:H1	1:AA:1035:A:H61	1.65	0.44
2:AB:43:LEU:HA	2:AB:46:THR:HB	1.99	0.44
3:AC:66:VAL:HG13	3:AC:101:ILE:HA	1.98	0.44
3:AC:108:LYS:HA	58:CC:859:GLU:CB	2.48	0.44
9:AI:8:GLY:O	9:AI:19:VAL:HG12	2.18	0.44
20:AT:10:ARG:HD3	20:AT:10:ARG:HA	1.82	0.44
21:AU:29:LEU:O	21:AU:32:VAL:HG22	2.18	0.44
25:BA:1794:A:H2'	25:BA:1795:C:C6	2.52	0.44
25:BA:2102:G:N1	25:BA:2187:U:N3	2.65	0.44
25:BA:2308:G:N2	25:BA:2311:A:OP2	2.50	0.44
26:BB:2:G:H2'	26:BB:3:C:C6	2.53	0.44
38:BP:92:PHE:CZ	38:BP:107:ALA:HB2	2.52	0.44
56:CT:4:DT:C2	56:CT:5:DG:N7	2.86	0.44
1:AA:562:U:C2	12:AL:13:ALA:O	2.71	0.44
1:AA:620:C:C2	4:AD:132:ILE:HG13	2.53	0.44
1:AA:1176:A:H2'	1:AA:1177:G:O4'	2.17	0.44
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.33	0.44
10:AJ:49:PHE:O	10:AJ:64:GLN:HA	2.18	0.44
11:AK:85:MET:HE3	11:AK:113:VAL:HG11	1.99	0.44
19:AS:12:ASP:OD1	19:AS:35:SER:OG	2.32	0.44
25:BA:927:A:O2'	49:B1:39:GLU:OE2	2.32	0.44
25:BA:1060:U:H4'	25:BA:1061:U:O5'	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2867:G:O2'	25:BA:2868:A:OP2	2.35	0.44
34:BL:21:CYS:HA	34:BL:41:ILE:HG22	1.99	0.44
52:B4:24:THR:HG23	52:B4:27:GLY:H	1.83	0.44
55:CN:28:DA:C4	55:CN:29:DG:C5	3.06	0.44
58:CC:569:ILE:O	58:CC:571:LEU:N	2.51	0.44
58:CC:1212:LEU:HA	58:CC:1212:LEU:HD23	1.66	0.44
58:CC:1278:LEU:HD23	58:CC:1278:LEU:HA	1.49	0.44
59:CD:789:LYS:HE2	59:CD:789:LYS:HB3	1.62	0.44
1:AA:1134:G:N1	1:AA:1141:C:C4	2.86	0.44
1:AA:1140:C:O2'	1:AA:1141:C:O5'	2.32	0.44
2:AB:18:HIS:NE2	2:AB:188:ASP:OD2	2.51	0.44
4:AD:15:GLU:OE2	4:AD:63:ARG:NH1	2.50	0.44
6:AF:2:ARG:NH2	6:AF:68:GLN:OE1	2.50	0.44
25:BA:1049:C:C2'	25:BA:1050:A:H5'	2.47	0.44
25:BA:2183:A:H2'	25:BA:2184:A:H8	1.83	0.44
25:BA:2591:C:H2'	25:BA:2592:G:C8	2.53	0.44
33:BK:41:LYS:NZ	33:BK:50:THR:O	2.51	0.44
58:CC:1238:LEU:N	58:CC:1238:LEU:CD2	2.81	0.44
59:CD:238:ILE:HD12	59:CD:238:ILE:HG23	1.71	0.44
1:AA:562:U:O2	12:AL:13:ALA:N	2.51	0.44
1:AA:1026:G:H1	1:AA:1035:A:N6	2.16	0.44
6:AF:73:GLU:O	6:AF:76:THR:OG1	2.31	0.44
7:AG:2:PRO:HG2	7:AG:5:ARG:HB2	2.00	0.44
7:AG:58:GLU:OE2	7:AG:59:LEU:N	2.46	0.44
9:AI:19:VAL:HG11	9:AI:82:GLY:C	2.38	0.44
23:AW:18:G:H8	23:AW:18:G:OP1	2.01	0.44
58:CC:196:VAL:HG21	58:CC:209:ILE:HD11	2.00	0.44
58:CC:680:LEU:HD23	58:CC:680:LEU:C	2.38	0.44
58:CC:794:LEU:HA	58:CC:794:LEU:HD12	1.71	0.44
58:CC:1276:TRP:CE2	59:CD:801:VAL:HG21	2.52	0.44
59:CD:770:LEU:HD13	59:CD:770:LEU:HA	1.69	0.44
1:AA:193:C:H2'	1:AA:194:C:C6	2.53	0.43
1:AA:384:G:H2'	1:AA:385:C:C6	2.53	0.43
1:AA:721:G:H4'	1:AA:722:G:O4'	2.18	0.43
1:AA:1321:U:O2'	19:AS:78:ARG:NH2	2.51	0.43
2:AB:69:PHE:HB3	2:AB:80:VAL:HG13	2.00	0.43
5:AE:10:GLU:CB	59:CD:78:LEU:HB2	2.47	0.43
14:AN:83:LYS:HA	14:AN:83:LYS:HD3	1.83	0.43
23:AW:74:C:H5'	25:BA:2602:A:H5'	2.00	0.43
25:BA:277:G:H8	25:BA:361:G:C5	2.35	0.43
25:BA:464:U:O3'	52:B4:12:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:651:G:C6	25:BA:652:U:H5	2.36	0.43
25:BA:2060:A:OP2	29:BE:66:GLY:HA2	2.18	0.43
44:BV:18:ASP:HA	44:BV:21:LYS:NZ	2.33	0.43
56:CT:5:DG:H2'	56:CT:6:DA:C8	2.53	0.43
58:CC:528:ARG:HH11	58:CC:528:ARG:HD2	1.63	0.43
58:CC:1096:ILE:HD13	58:CC:1096:ILE:HG21	1.65	0.43
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.53	0.43
1:AA:1135:U:H2'	1:AA:1137:C:C4	2.53	0.43
4:AD:91:LEU:HD23	4:AD:91:LEU:HA	1.73	0.43
23:AW:15:G:C6	23:AW:48:C:O2	2.71	0.43
24:AX:5:G:H2'	24:AX:6:G:H8	1.83	0.43
25:BA:245:G:O6	53:B5:8:ARG:NH1	2.51	0.43
25:BA:594:U:H2'	25:BA:595:C:C6	2.54	0.43
25:BA:784:G:H5'	25:BA:785:G:OP1	2.18	0.43
25:BA:1063:G:HO2'	25:BA:1064:C:H6	1.65	0.43
25:BA:1301:A:C2	25:BA:1626:A:H2	2.35	0.43
25:BA:1542:U:H2'	25:BA:1543:G:O4'	2.18	0.43
36:BN:36:VAL:O	36:BN:98:PRO:HB3	2.18	0.43
55:CN:30:DA:C6	55:CN:31:DG:C6	3.07	0.43
58:CC:493:ILE:C	58:CC:493:ILE:HD12	2.39	0.43
59:CD:108:ALA:HB3	59:CD:279:LEU:HD23	2.00	0.43
59:CD:340:GLN:HG3	59:CD:341:ASN:OD1	2.18	0.43
59:CD:500:ILE:O	59:CD:500:ILE:HG22	2.18	0.43
1:AA:1006:G:C5	1:AA:1007:U:C5	3.06	0.43
3:AC:109:PRO:HD3	58:CC:859:GLU:CD	2.36	0.43
10:AJ:31:ARG:C	10:AJ:33:GLY:H	2.22	0.43
25:BA:2788:C:H2'	25:BA:2789:C:C6	2.53	0.43
26:BB:8:C:H5"	38:BP:15:ARG:NH2	2.33	0.43
27:BC:78:VAL:HG21	27:BC:110:LEU:HD21	2.01	0.43
30:BF:73:SER:OG	30:BF:80:ARG:HA	2.18	0.43
56:CT:10:DT:H2"	56:CT:11:DC:C6	2.53	0.43
56:CT:19:DG:C6	56:CT:20:DC:N4	2.87	0.43
57:CA:213:PRO:HA	57:CA:216:ALA:HB3	2.00	0.43
58:CC:69:GLN:OE1	58:CC:101:ARG:NE	2.44	0.43
58:CC:131:THR:HG22	58:CC:132:ASP:N	2.34	0.43
1:AA:73:C:O2'	1:AA:74:A:H5'	2.19	0.43
1:AA:519:C:H2'	1:AA:520:A:O4'	2.18	0.43
2:AB:175:GLU:O	2:AB:179:LEU:HD22	2.19	0.43
4:AD:94:LEU:HD23	4:AD:94:LEU:HA	1.85	0.43
4:AD:102:VAL:HG13	4:AD:114:ALA:HB1	1.99	0.43
6:AF:85:ILE:HG13	6:AF:86:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:7:TYR:CG	9:AI:8:GLY:N	2.87	0.43
25:BA:499:U:H5"	44:BV:43:LYS:HE2	1.99	0.43
25:BA:651:G:C6	25:BA:652:U:C5	3.07	0.43
25:BA:1009:A:N3	25:BA:1153:C:O2'	2.44	0.43
25:BA:1070:A:C8	25:BA:1097:U:H4'	2.52	0.43
25:BA:1494:A:H2'	25:BA:1495:A:H8	1.83	0.43
25:BA:1868:C:H2'	25:BA:1869:G:H8	1.83	0.43
25:BA:2266:A:H4'	25:BA:2267:A:N3	2.33	0.43
31:BG:16:ASP:N	31:BG:16:ASP:OD1	2.52	0.43
31:BG:23:VAL:HA	31:BG:36:THR:HA	1.99	0.43
36:BN:117:PHE:HD2	36:BN:130:PHE:CD1	2.37	0.43
37:BO:2:ARG:HG2	37:BO:5:LYS:HB2	2.00	0.43
37:BO:101:GLY:O	37:BO:109:PRO:HA	2.18	0.43
58:CC:127:ILE:O	58:CC:127:ILE:HG13	2.18	0.43
58:CC:1058:ARG:HH21	58:CC:1240:ASP:CG	2.20	0.43
59:CD:149:GLY:HA2	59:CD:176:PHE:HB2	1.98	0.43
1:AA:908:A:H2'	1:AA:909:A:C8	2.52	0.43
1:AA:947:G:H5"	13:AM:107:ARG:HB2	2.01	0.43
1:AA:996:A:N7	1:AA:1046:A:O2'	2.51	0.43
1:AA:1026:G:H2'	1:AA:1027:C:C5	2.54	0.43
3:AC:11:ARG:NH2	3:AC:175:LEU:O	2.44	0.43
11:AK:33:THR:HG22	11:AK:44:TRP:HB3	2.00	0.43
25:BA:1187:G:H8	25:BA:1187:G:O5'	2.01	0.43
30:BF:44:ILE:HG21	30:BF:79:ILE:HG22	2.01	0.43
45:BW:11:GLU:HG3	45:BW:16:ALA:HB1	2.00	0.43
53:B5:27:ALA:O	53:B5:28:ASN:HB2	2.18	0.43
55:CN:29:DG:H2"	55:CN:30:DA:O5'	2.18	0.43
56:CT:6:DA:C2	56:CT:7:DA:C5	3.07	0.43
58:CC:771:VAL:H	58:CC:771:VAL:HG22	1.61	0.43
59:CD:1143:ASP:C	59:CD:1143:ASP:OD1	2.57	0.43
1:AA:473:U:N3	1:AA:474:G:N7	2.66	0.43
1:AA:874:G:C6	1:AA:875:U:C4	3.07	0.43
3:AC:58:GLU:OE1	3:AC:65:ARG:HD2	2.19	0.43
16:AP:69:ASP:N	16:AP:69:ASP:OD1	2.50	0.43
25:BA:1177:G:O2'	25:BA:1178:C:H6	2.01	0.43
25:BA:1295:C:C2	25:BA:1296:G:C8	3.06	0.43
25:BA:2064:C:H2'	25:BA:2065:C:C6	2.53	0.43
25:BA:2747:G:O2'	31:BG:67:THR:HG23	2.18	0.43
28:BD:84:LEU:HD22	28:BD:88:GLU:O	2.19	0.43
33:BK:78:THR:HG21	33:BK:85:LYS:HE2	2.01	0.43
51:B3:40:ASP:HB3	51:B3:43:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CD:317:THR:OG1	59:CD:322:ARG:O	2.20	0.43
59:CD:1248:ILE:HD13	59:CD:1248:ILE:HG21	1.82	0.43
1:AA:1039:G:H2'	1:AA:1040:U:H6	1.84	0.43
1:AA:1041:G:H2'	1:AA:1042:A:C8	2.54	0.43
1:AA:1382:C:C2	1:AA:1383:C:C5	3.07	0.43
18:AR:65:LEU:O	18:AR:66:SER:OG	2.31	0.43
22:AV:41:C:H6	22:AV:41:C:H2'	1.45	0.43
25:BA:139:U:C4	43:BU:1:MET:HG2	2.54	0.43
25:BA:277:G:H8	25:BA:361:G:C6	2.36	0.43
25:BA:848:C:H2'	25:BA:849:A:H8	1.83	0.43
25:BA:1799:G:OP1	27:BC:258:ARG:HD2	2.18	0.43
25:BA:2120:G:N1	25:BA:2179:C:N4	2.66	0.43
25:BA:2552:OMU:HM22	25:BA:2553:G:N7	2.34	0.43
36:BN:17:ASN:O	36:BN:38:ARG:NH1	2.52	0.43
58:CC:668:ILE:HD13	58:CC:668:ILE:HG21	1.69	0.43
59:CD:319:SER:O	59:CD:321:LYS:N	2.46	0.43
1:AA:1382:C:H2'	1:AA:1383:C:H5'	2.00	0.43
4:AD:99:ASP:O	4:AD:102:VAL:HG13	2.18	0.43
15:AO:26:GLU:HG3	15:AO:81:LEU:HD22	2.01	0.43
25:BA:1533:C:H2'	25:BA:1534:U:C6	2.54	0.43
25:BA:1720:U:H2'	25:BA:1721:G:O4'	2.19	0.43
25:BA:2104:C:C5	25:BA:2186:G:N2	2.85	0.43
25:BA:2655:G:O2'	25:BA:2664:G:O6	2.31	0.43
29:BE:145:ASP:HA	29:BE:166:LYS:HB3	2.01	0.43
32:BH:1:MET:O	32:BH:20:ASN:HA	2.19	0.43
43:BU:51:PHE:HD1	43:BU:93:LEU:HD11	1.84	0.43
43:BU:67:VAL:HA	43:BU:76:ARG:HA	2.00	0.43
45:BW:59:GLU:OE1	45:BW:59:GLU:N	2.51	0.43
58:CC:1133:LYS:O	58:CC:1135:GLN:NE2	2.47	0.43
59:CD:175:GLU:CD	59:CD:175:GLU:N	2.72	0.43
59:CD:576:ARG:HD3	59:CD:593:ASN:HA	2.00	0.43
1:AA:158:G:C5	1:AA:164:G:C6	3.07	0.43
1:AA:1064:G:H1'	1:AA:1190:G:N2	2.34	0.43
1:AA:1450:U:O2'	1:AA:1453:G:O6	2.31	0.43
3:AC:6:HIS:CE1	3:AC:8:ASN:HB3	2.54	0.43
5:AE:13:GLU:HB2	5:AE:39:VAL:HG12	2.00	0.43
25:BA:1059:G:C8	25:BA:1060:U:H2'	2.54	0.43
25:BA:1060:U:H1'	25:BA:1062:G:H5'	2.01	0.43
25:BA:2225:A:O2'	25:BA:2226:C:OP2	2.31	0.43
32:BH:50:ARG:CZ	32:BH:51:ARG:HE	2.31	0.43
55:CN:36:DA:H2"	55:CN:37:DG:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CC:1105:SER:HB2	59:CD:731:ARG:HB3	2.00	0.43
1:AA:1006:G:C4	1:AA:1007:U:C5	3.07	0.43
2:AB:9:MET:O	2:AB:14:VAL:HG13	2.19	0.43
6:AF:42:TRP:HZ2	6:AF:61:LEU:HD22	1.84	0.43
24:AX:27:G:C2	24:AX:44:G:C2	3.07	0.43
25:BA:1265:A:H4'	25:BA:1266:G:H4'	2.00	0.43
30:BF:50:LEU:HD21	30:BF:67:ILE:HG23	2.01	0.43
39:BQ:34:GLU:CD	39:BQ:39:ARG:HD3	2.40	0.43
40:BR:24:TYR:O	40:BR:29:SER:HB3	2.17	0.43
41:BS:41:ILE:HG13	41:BS:54:VAL:HG11	2.00	0.43
47:BY:32:ASN:OD1	47:BY:34:HIS:NE2	2.51	0.43
58:CC:473:ARG:HH11	58:CC:473:ARG:HG3	1.83	0.43
58:CC:1098:LEU:N	58:CC:1098:LEU:HD12	2.29	0.43
59:CD:482:ALA:O	59:CD:488:ASN:ND2	2.50	0.43
59:CD:1256:ILE:HD12	59:CD:1256:ILE:HG23	1.60	0.43
1:AA:381:C:H2'	1:AA:382:A:O4'	2.19	0.42
1:AA:1492:A:OP1	12:AL:44:LYS:HA	2.19	0.42
9:AI:27:LYS:HE3	9:AI:27:LYS:HB2	1.89	0.42
25:BA:201:C:OP1	47:BY:18:ARG:NH1	2.46	0.42
25:BA:207:A:H2'	25:BA:208:C:O4'	2.18	0.42
25:BA:1868:C:H2'	25:BA:1869:G:C8	2.54	0.42
31:BG:117:LEU:HD11	31:BG:123:ALA:HB2	2.00	0.42
32:BH:19:VAL:HG13	32:BH:21:VAL:HG13	2.01	0.42
56:CT:12:DT:H6	56:CT:12:DT:H2'	1.66	0.42
59:CD:357:VAL:HG13	59:CD:357:VAL:O	2.18	0.42
59:CD:1172:LYS:HE3	59:CD:1191:PRO:HA	2.01	0.42
1:AA:676:A:H2'	1:AA:677:U:H6	1.84	0.42
1:AA:837:U:O2	1:AA:849:G:C6	2.72	0.42
1:AA:1107:C:C4	1:AA:1108:G:C8	3.07	0.42
1:AA:1239:A:H62	1:AA:1299:A:N6	2.15	0.42
23:AW:44:A:H2'	23:AW:45:G:O4'	2.18	0.42
23:AW:56:C:O5'	23:AW:56:C:H6	2.03	0.42
61:AX:101:PHE:HA	25:BA:2585:U:O4	2.19	0.42
25:BA:811:U:H2'	35:BM:21:ARG:HA	2.01	0.42
25:BA:988:A:C5	49:B1:14:ILE:HG21	2.55	0.42
25:BA:2455:G:H2'	25:BA:2456:C:C6	2.54	0.42
27:BC:142:HIS:HD1	27:BC:143:ASN:HB2	1.84	0.42
30:BF:56:ASP:O	30:BF:60:ILE:CB	2.62	0.42
36:BN:16:ARG:HA	36:BN:16:ARG:HD3	1.67	0.42
43:BU:2:ILE:HG23	43:BU:7:LEU:HD21	2.00	0.42
51:B3:21:TYR:OH	51:B3:39:PHE:O	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CT:10:DT:H2"	56:CT:11:DC:C5	2.54	0.42
58:CC:549:ASP:OD1	58:CC:550:VAL:N	2.52	0.42
1:AA:674:G:N2	1:AA:717:U:O2	2.50	0.42
1:AA:690:G:H2'	1:AA:691:G:O4'	2.20	0.42
1:AA:1329:A:C5	1:AA:1330:U:C5	3.07	0.42
1:AA:1410:A:H2'	1:AA:1411:C:C6	2.54	0.42
10:AJ:53:ILE:HG12	10:AJ:62:ARG:HA	1.99	0.42
20:AT:44:LYS:NZ	20:AT:86:LEU:HB3	2.34	0.42
25:BA:1410:G:C6	25:BA:1411:U:C4	3.07	0.42
25:BA:2228:G:H2'	25:BA:2229:U:C6	2.55	0.42
25:BA:2600:A:H2'	25:BA:2601:C:C6	2.54	0.42
31:BG:54:PRO:HG2	31:BG:62:TRP:CE2	2.55	0.42
40:BR:9:ILE:H	40:BR:9:ILE:HD12	1.83	0.42
56:CT:17:DG:C4	56:CT:18:DC:C6	3.07	0.42
58:CC:962:GLU:O	58:CC:966:ILE:HD13	2.20	0.42
58:CC:1195:ILE:HG21	58:CC:1195:ILE:HD13	1.77	0.42
59:CD:826:ILE:HG23	59:CD:831:VAL:HG12	2.01	0.42
1:AA:150:U:C4	1:AA:170:U:C4	3.08	0.42
1:AA:410:G:H2'	1:AA:429:U:C5	2.54	0.42
3:AC:151:VAL:HG23	3:AC:200:VAL:HG22	2.01	0.42
4:AD:33:LYS:HD3	4:AD:36:GLN:HG3	2.00	0.42
10:AJ:4:GLN:N	10:AJ:103:GLY:OXT	2.52	0.42
22:AV:43:G:C6	22:AV:44:C:C4	3.07	0.42
24:AX:18:G:H21	24:AX:57:G:H2'	1.84	0.42
25:BA:693:A:O2'	25:BA:1353:A:N3	2.46	0.42
25:BA:886:A:H1'	25:BA:887:U:H5"	2.02	0.42
25:BA:1917:PSU:H2'	25:BA:1918:A:O4'	2.20	0.42
25:BA:2093:G:H21	25:BA:2198:A:N6	2.16	0.42
25:BA:2285:C:P	51:B3:26:ASN:HD22	2.42	0.42
25:BA:2902:C:C2'	25:BA:2903:U:H5'	2.50	0.42
53:B5:26:HIS:NE2	53:B5:48:ALA:HB2	2.34	0.42
55:CN:26:DG:C4	55:CN:27:DA:C5	3.07	0.42
58:CC:204:LEU:HD21	58:CC:369:MET:SD	2.59	0.42
58:CC:1014:LEU:HD12	58:CC:1017:GLN:HB3	2.00	0.42
58:CC:1339:LEU:HD22	59:CD:17:PHE:CG	2.55	0.42
59:CD:548:VAL:HG22	59:CD:549:LYS:N	2.35	0.42
1:AA:1151:A:O2'	1:AA:1152:A:O4'	2.38	0.42
1:AA:1315:U:H2'	1:AA:1316:G:O4'	2.19	0.42
3:AC:2:GLY:O	3:AC:4:LYS:NZ	2.41	0.42
6:AF:72:ASP:O	6:AF:76:THR:HG23	2.19	0.42
7:AG:129:GLU:OE1	7:AG:131:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:130:ARG:HH22	23:AW:33:U:P	2.41	0.42
19:AS:41:PHE:N	19:AS:44:MET:SD	2.89	0.42
25:BA:414:C:H2'	25:BA:415:A:C8	2.54	0.42
25:BA:752:A:P	52:B4:1:MET:HE1	2.60	0.42
25:BA:1469:A:H2'	25:BA:1470:A:H8	1.81	0.42
30:BF:44:ILE:HG22	30:BF:83:TYR:HD2	1.84	0.42
38:BP:67:ASN:ND2	38:BP:69:ASP:OD1	2.52	0.42
48:BZ:6:LEU:HD23	48:BZ:9:LYS:HD2	2.00	0.42
52:B4:21:ARG:O	52:B4:27:GLY:HA3	2.19	0.42
55:CN:27:DA:C5	55:CN:28:DA:N7	2.88	0.42
58:CC:196:VAL:HG22	58:CC:197:ARG:N	2.34	0.42
58:CC:1217:THR:HG1	58:CC:1219:GLU:CD	2.21	0.42
59:CD:213:LYS:HZ3	59:CD:216:LYS:HG3	1.85	0.42
1:AA:426:U:OP1	4:AD:33:LYS:HD2	2.20	0.42
1:AA:478:A:P	1:AA:478:A:H8	2.43	0.42
1:AA:792:A:H1'	1:AA:794:A:N7	2.35	0.42
3:AC:23:PHE:CD2	10:AJ:97:ASP:HB2	2.55	0.42
5:AE:10:GLU:CB	59:CD:78:LEU:HD13	2.43	0.42
25:BA:274:C:H2'	25:BA:275:C:O4'	2.20	0.42
25:BA:580:U:O3'	40:BR:31:VAL:HG13	2.20	0.42
25:BA:2183:A:C2	25:BA:2184:A:C5	3.07	0.42
25:BA:2200:C:OP1	47:BY:37:ARG:HG3	2.19	0.42
25:BA:2225:A:H4'	25:BA:2226:C:O5'	2.20	0.42
25:BA:2646:C:O5'	25:BA:2646:C:H6	2.01	0.42
25:BA:2801:G:C2	25:BA:2802:A:C8	3.07	0.42
26:BB:117:G:C6	26:BB:118:C:N4	2.87	0.42
28:BD:18:ASP:OD1	28:BD:19:GLY:N	2.53	0.42
29:BE:40:ARG:HH12	29:BE:92:HIS:CE1	2.37	0.42
30:BF:115:ARG:HB2	30:BF:178:ARG:HH21	1.84	0.42
37:BO:38:LEU:HB3	37:BO:39:PRO:HD3	2.00	0.42
39:BQ:19:SER:O	39:BQ:19:SER:OG	2.30	0.42
43:BU:3:ARG:NH1	43:BU:5:GLU:OE2	2.47	0.42
53:B5:28:ASN:HD22	53:B5:40:ARG:HH11	1.67	0.42
58:CC:521:LEU:HA	58:CC:521:LEU:HD12	1.74	0.42
58:CC:1336:ASN:HB2	59:CD:25:ALA:HB2	2.01	0.42
59:CD:416:ILE:HD13	59:CD:416:ILE:HG21	1.58	0.42
1:AA:165:G:H2'	1:AA:166:U:H6	1.84	0.42
1:AA:613:C:H2'	1:AA:614:C:C6	2.54	0.42
3:AC:130:PHE:CG	3:AC:131:ARG:N	2.88	0.42
3:AC:147:LYS:HB3	3:AC:147:LYS:HE3	1.59	0.42
10:AJ:34:ALA:HB1	10:AJ:76:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:54:GLY:N	11:AK:57:LYS:HG2	2.35	0.42
21:AU:69:ARG:H	21:AU:69:ARG:HG3	1.55	0.42
24:AX:40:C:H2'	24:AX:41:C:C6	2.55	0.42
25:BA:358:U:H2'	25:BA:359:G:C8	2.53	0.42
25:BA:365:U:H2'	25:BA:366:C:O4'	2.20	0.42
25:BA:1168:G:C6	25:BA:1169:A:C6	3.08	0.42
25:BA:2015:A:C6	50:B2:3:VAL:HG23	2.54	0.42
25:BA:2162:G:P	25:BA:2164:C:H41	2.36	0.42
25:BA:2473:U:C4	25:BA:2474:U:C5	3.07	0.42
30:BF:54:ALA:O	30:BF:55:ALA:C	2.57	0.42
30:BF:179:LYS:HE2	30:BF:179:LYS:HB2	1.92	0.42
43:BU:12:ARG:HD3	43:BU:12:ARG:HA	1.74	0.42
57:CA:180:VAL:HG12	57:CA:207:THR:HG22	2.02	0.42
57:CB:43:LEU:HD23	57:CB:43:LEU:HA	1.85	0.42
58:CC:210:LEU:HD23	58:CC:210:LEU:HA	1.60	0.42
59:CD:35:PHE:CZ	59:CD:101:ARG:HD2	2.55	0.42
59:CD:636:GLY:O	59:CD:638:SER:N	2.49	0.42
1:AA:562:U:H1'	12:AL:12:ARG:HB3	2.02	0.42
1:AA:876:C:H1'	8:AH:12:THR:HG21	2.00	0.42
1:AA:1012:A:C6	1:AA:1018:G:C6	3.08	0.42
1:AA:1140:C:O2'	1:AA:1141:C:H6	2.02	0.42
1:AA:1143:G:N3	1:AA:1144:G:C8	2.88	0.42
2:AB:105:LYS:H	2:AB:105:LYS:HG3	1.67	0.42
13:AM:43:VAL:HG21	13:AM:48:LEU:HD21	2.02	0.42
15:AO:12:VAL:O	15:AO:16:GLY:HA3	2.20	0.42
17:AQ:81:LYS:H	17:AQ:81:LYS:HG3	1.59	0.42
25:BA:468:G:N7	52:B4:39:ARG:NH2	2.60	0.42
25:BA:848:C:H2'	25:BA:849:A:C8	2.54	0.42
26:BB:2:G:C6	26:BB:3:C:C4	3.08	0.42
30:BF:91:LEU:C	30:BF:96:MET:HB2	2.40	0.42
30:BF:118:SER:OG	30:BF:119:ALA:N	2.50	0.42
31:BG:52:PHE:CE2	31:BG:72:LEU:HD22	2.55	0.42
31:BG:69:ARG:HG2	31:BG:69:ARG:NH1	2.34	0.42
56:CT:2:DT:H2"	56:CT:3:DC:H5	1.85	0.42
58:CC:217:THR:HG23	58:CC:351:LEU:HD21	2.02	0.42
58:CC:1211:ARG:NH1	58:CC:1220:GLN:OE1	2.52	0.42
59:CD:264:ASP:OD1	59:CD:264:ASP:N	2.51	0.42
1:AA:141:G:N2	1:AA:142:G:H1'	2.35	0.42
1:AA:696:A:H1'	1:AA:786:G:O2'	2.20	0.42
1:AA:1120:C:H2'	1:AA:1121:U:C6	2.54	0.42
6:AF:11:HIS:CE1	6:AF:54:LEU:HD22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:63:ARG:HD3	18:AR:70:TYR:CD1	2.55	0.42
25:BA:829:A:N7	25:BA:2248:C:H5'	2.34	0.42
25:BA:879:G:N1	25:BA:899:A:H1'	2.34	0.42
25:BA:1106:G:C4	25:BA:1107:G:C8	3.07	0.42
25:BA:2096:C:C2	25:BA:2097:A:C8	3.07	0.42
25:BA:2419:U:OP2	53:B5:33:LEU:HD13	2.20	0.42
25:BA:2757:A:C2	25:BA:2758:A:C8	3.07	0.42
29:BE:176:ASP:O	29:BE:179:SER:OG	2.30	0.42
34:BL:11:ALA:O	34:BL:100:PHE:HD1	2.02	0.42
42:BT:23:LEU:HD11	50:B2:24:ALA:N	2.34	0.42
43:BU:51:PHE:CD1	43:BU:93:LEU:HD21	2.55	0.42
48:BZ:5:GLU:O	48:BZ:8:GLU:HG2	2.19	0.42
58:CC:456:VAL:H	58:CC:456:VAL:HG23	1.53	0.42
58:CC:1176:LEU:HA	58:CC:1176:LEU:HD23	1.79	0.42
1:AA:884:U:H6	1:AA:884:U:H2'	1.50	0.42
1:AA:1125:U:OP1	10:AJ:37:ARG:NE	2.53	0.42
1:AA:1174:G:C2'	1:AA:1175:G:H5'	2.47	0.42
1:AA:1385:G:H2'	1:AA:1386:G:O4'	2.20	0.42
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.19	0.42
4:AD:105:MET:HG2	4:AD:173:VAL:HG13	2.01	0.42
9:AI:41:ARG:HB2	9:AI:41:ARG:HH11	1.84	0.42
10:AJ:53:ILE:HD11	10:AJ:63:ASP:CB	2.49	0.42
13:AM:23:TYR:HD1	13:AM:66:GLU:HA	1.84	0.42
25:BA:1167:C:C2	25:BA:1168:G:C8	3.08	0.42
25:BA:1333:G:C2	25:BA:1334:G:C8	3.08	0.42
25:BA:1596:A:O2'	25:BA:1597:A:C5'	2.68	0.42
25:BA:2026:U:H2'	25:BA:2027:G:O4'	2.20	0.42
25:BA:2815:C:C2	25:BA:2816:G:C8	3.07	0.42
28:BD:173:GLN:OE1	28:BD:208:LYS:HE3	2.19	0.42
30:BF:53:ALA:HB2	30:BF:150:ARG:NH1	2.34	0.42
55:CN:27:DA:H1'	55:CN:28:DA:H5'	2.01	0.42
58:CC:84:GLU:OE2	58:CC:1032:LYS:NZ	2.48	0.42
58:CC:530:ILE:HG23	58:CC:530:ILE:HD12	1.63	0.42
58:CC:746:ALA:HB2	58:CC:967:LEU:HD21	2.02	0.42
59:CD:72:CYS:HB2	59:CD:87:LYS:HD3	2.01	0.42
1:AA:6:G:O2'	1:AA:7:A:H8	2.03	0.41
1:AA:844:G:H3'	1:AA:844:G:N3	2.35	0.41
1:AA:1121:U:C2	1:AA:1122:U:C5	3.08	0.41
2:AB:111:ILE:HG22	2:AB:148:LEU:HD13	2.02	0.41
18:AR:20:GLU:OE1	18:AR:20:GLU:N	2.53	0.41
19:AS:70:LYS:O	19:AS:73:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1588:G:C2	25:BA:1589:U:C4	3.08	0.41
25:BA:1652:A:OP1	37:BO:8:ARG:HD3	2.20	0.41
25:BA:2111:U:O2	25:BA:2111:U:H2'	2.19	0.41
25:BA:2364:C:H2'	25:BA:2365:G:O4'	2.20	0.41
32:BH:15:LEU:HD13	32:BH:15:LEU:O	2.20	0.41
38:BP:74:VAL:HG13	38:BP:106:LEU:HD12	2.01	0.41
49:B1:45:ARG:NH1	49:B1:59:GLU:OE2	2.53	0.41
57:CA:205:MET:SD	57:CA:213:PRO:HG3	2.60	0.41
57:CB:154:PRO:C	57:CB:156:SER:H	2.24	0.41
58:CC:524:ILE:HG21	58:CC:524:ILE:HD13	1.76	0.41
58:CC:817:LEU:HA	58:CC:817:LEU:HD12	1.70	0.41
59:CD:1175:LEU:HB2	59:CD:1190:ILE:HD12	2.01	0.41
1:AA:606:G:N2	1:AA:632:U:OP1	2.44	0.41
1:AA:738:C:OP1	6:AF:91:ARG:HD2	2.20	0.41
1:AA:877:G:H2'	1:AA:878:A:H8	1.85	0.41
1:AA:878:A:C2	1:AA:879:C:C2	3.08	0.41
1:AA:1134:G:C8	1:AA:1135:U:C5	3.08	0.41
1:AA:1368:A:OP1	9:AI:113:ARG:NH2	2.53	0.41
7:AG:5:ARG:HB3	7:AG:7:ILE:HG23	2.03	0.41
13:AM:25:VAL:HG13	13:AM:29:ARG:HB3	2.01	0.41
14:AN:73:PHE:HE1	14:AN:75:ARG:HA	1.85	0.41
25:BA:58:G:O2'	25:BA:73:A:N1	2.41	0.41
25:BA:529:A:OP2	33:BK:116:ARG:NH2	2.45	0.41
25:BA:851:C:H2'	25:BA:852:U:H6	1.84	0.41
25:BA:1482:G:C6	25:BA:1508:A:N6	2.88	0.41
25:BA:1800:C:OP2	27:BC:182:ARG:NH1	2.53	0.41
25:BA:2344:U:H6	25:BA:2344:U:H2'	1.71	0.41
26:BB:75:G:H2'	26:BB:76:G:O4'	2.20	0.41
34:BL:108:ARG:HA	34:BL:116:ILE:HG13	2.02	0.41
48:BZ:14:LEU:HD22	48:BZ:53:VAL:HG13	2.02	0.41
58:CC:213:LEU:HA	58:CC:213:LEU:HD23	1.73	0.41
58:CC:569:ILE:HD13	58:CC:569:ILE:HG21	1.60	0.41
58:CC:1014:LEU:HD12	58:CC:1014:LEU:HA	1.87	0.41
58:CC:1251:TYR:CE1	58:CC:1301:ARG:CZ	3.03	0.41
59:CD:139:LEU:HD23	59:CD:139:LEU:HA	1.68	0.41
1:AA:553:A:H5"	12:AL:21:VAL:HG21	2.02	0.41
1:AA:600:A:H5'	8:AH:121:LEU:HA	2.02	0.41
1:AA:841:C:O2'	1:AA:842:U:O5'	2.39	0.41
1:AA:1022:A:C2	1:AA:1023:U:C2	3.08	0.41
1:AA:1034:G:H2'	1:AA:1035:A:H8	1.84	0.41
3:AC:51:SER:O	3:AC:51:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:81:LEU:HD23	5:AE:81:LEU:HA	1.82	0.41
8:AH:39:VAL:O	8:AH:42:GLU:HG2	2.20	0.41
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.84	0.41
10:AJ:15:HIS:O	10:AJ:18:ILE:HG22	2.20	0.41
10:AJ:52:LEU:HD23	10:AJ:62:ARG:HD3	2.02	0.41
15:AO:64:ARG:NH1	15:AO:68:ASP:OD1	2.53	0.41
25:BA:18:U:OP1	40:BR:30:ARG:NH2	2.40	0.41
25:BA:1587:G:H2'	25:BA:1588:G:H8	1.85	0.41
29:BE:58:LYS:NZ	29:BE:70:SER:O	2.52	0.41
31:BG:160:LYS:HB3	31:BG:160:LYS:HE2	1.73	0.41
32:BH:50:ARG:NH2	32:BH:51:ARG:HE	2.17	0.41
34:BL:123:LEU:HD13	34:BL:123:LEU:HA	1.94	0.41
56:CT:20:DC:C2	56:CT:21:DG:N7	2.88	0.41
57:CA:85:LEU:HD23	57:CA:85:LEU:HA	1.84	0.41
57:CB:66:HIS:CE1	57:CB:68:TYR:HD1	2.39	0.41
58:CC:1141:LEU:HD12	58:CC:1141:LEU:HA	1.84	0.41
59:CD:541:LEU:HD23	59:CD:541:LEU:HA	1.84	0.41
1:AA:156:C:H2'	1:AA:157:U:O4'	2.19	0.41
1:AA:996:A:N6	1:AA:1046:A:O4'	2.53	0.41
1:AA:1060:U:H2'	1:AA:1061:G:H8	1.85	0.41
2:AB:187:VAL:CG1	2:AB:199:VAL:HG12	2.41	0.41
3:AC:108:LYS:HB3	3:AC:111:LEU:HD13	2.02	0.41
7:AG:58:GLU:OE2	7:AG:58:GLU:N	2.53	0.41
9:AI:28:ILE:HG13	9:AI:63:LEU:HD21	2.02	0.41
18:AR:65:LEU:HD23	18:AR:65:LEU:HA	1.85	0.41
25:BA:27:G:O2'	25:BA:28:A:OP2	2.35	0.41
25:BA:1355:G:C2	25:BA:1356:G:C8	3.08	0.41
25:BA:1380:G:O2'	25:BA:1569:A:N6	2.54	0.41
25:BA:1877:A:H2'	25:BA:1878:G:O4'	2.21	0.41
25:BA:2125:G:H2'	25:BA:2173:A:H61	1.84	0.41
25:BA:2822:G:O5'	25:BA:2822:G:H8	2.03	0.41
27:BC:107:PRO:HG2	27:BC:127:GLY:HA2	2.02	0.41
27:BC:144:VAL:HG21	27:BC:162:VAL:HG21	2.02	0.41
32:BH:55:GLU:HA	32:BH:58:LEU:HD12	2.02	0.41
55:CN:28:DA:C4	55:CN:29:DG:N7	2.89	0.41
56:CT:20:DC:O2	56:CT:21:DG:C8	2.73	0.41
58:CC:45:GLY:O	58:CC:51:ALA:HB2	2.19	0.41
58:CC:1251:TYR:CE1	58:CC:1301:ARG:NH1	2.88	0.41
59:CD:311:ARG:HH11	59:CD:311:ARG:HD3	1.72	0.41
59:CD:424:ASN:ND2	59:CD:424:ASN:C	2.73	0.41
59:CD:572:THR:HG23	59:CD:573:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CD:1350:ASN:ND2	59:CD:1358:PRO:HD3	2.34	0.41
1:AA:767:A:H2'	1:AA:768:A:O4'	2.21	0.41
1:AA:844:G:N2	1:AA:846:G:C4	2.88	0.41
1:AA:1251:A:H2'	1:AA:1252:A:O4'	2.21	0.41
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	2.03	0.41
4:AD:57:GLU:OE1	4:AD:200:ILE:HG13	2.19	0.41
5:AE:10:GLU:HB2	59:CD:78:LEU:CD1	2.49	0.41
8:AH:18:GLN:HE21	8:AH:72:VAL:HG12	1.85	0.41
10:AJ:32:THR:CG2	10:AJ:83:THR:HG23	2.50	0.41
19:AS:48:THR:HA	19:AS:61:PHE:HA	2.03	0.41
20:AT:5:LYS:HB2	20:AT:5:LYS:HE3	1.53	0.41
21:AU:36:GLU:OE1	21:AU:36:GLU:HA	2.20	0.41
25:BA:52:A:H2'	25:BA:53:A:C8	2.55	0.41
25:BA:550:U:O2	25:BA:551:G:C8	2.73	0.41
25:BA:984:A:H2'	25:BA:984:A:N3	2.36	0.41
25:BA:1405:U:H2'	25:BA:1406:U:C5	2.56	0.41
25:BA:2071:A:H2'	25:BA:2072:C:H6	1.83	0.41
25:BA:2901:C:C2	25:BA:2902:C:C4	3.08	0.41
35:BM:27:LEU:HD23	35:BM:27:LEU:HA	1.89	0.41
44:BV:88:GLU:C	44:BV:90:GLY:H	2.23	0.41
58:CC:1223:ARG:HA	58:CC:1224:PRO:HD3	1.92	0.41
59:CD:554:GLU:OE1	59:CD:588:PRO:HA	2.20	0.41
59:CD:1310:THR:O	59:CD:1310:THR:HG22	2.20	0.41
59:CD:1342:ASP:C	59:CD:1342:ASP:OD1	2.58	0.41
2:AB:214:LEU:HD23	2:AB:214:LEU:HA	1.97	0.41
5:AE:81:LEU:HD11	5:AE:96:MET:HG3	2.02	0.41
25:BA:263:G:H2'	25:BA:264:C:O4'	2.21	0.41
25:BA:638:G:H2'	25:BA:639:U:O4'	2.21	0.41
25:BA:1056:G:H1'	25:BA:1103:A:H61	1.85	0.41
25:BA:1528:A:H2'	25:BA:1529:G:O4'	2.20	0.41
25:BA:2303:G:O6	25:BA:2314:A:N6	2.54	0.41
25:BA:2576:G:H5'	25:BA:2578:G:N7	2.35	0.41
25:BA:2901:C:C4	25:BA:2902:C:N4	2.89	0.41
27:BC:232:HIS:HA	27:BC:242:LYS:HE3	2.03	0.41
30:BF:178:ARG:O	30:BF:179:LYS:HD3	2.21	0.41
38:BP:55:GLU:OE1	38:BP:81:ARG:NH2	2.47	0.41
43:BU:29:THR:OG1	43:BU:30:ILE:N	2.52	0.41
51:B3:43:VAL:HG21	51:B3:45:GLN:HE21	1.85	0.41
56:CT:4:DT:H2"	56:CT:5:DG:C8	2.55	0.41
58:CC:1248:THR:HG22	58:CC:1249:GLY:N	2.36	0.41
59:CD:331:ILE:HD13	59:CD:331:ILE:HG21	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CD:872:LEU:HD22	59:CD:877:VAL:HG21	2.02	0.41
1:AA:495:A:C2	1:AA:496:A:C6	3.08	0.41
4:AD:9:LEU:HD13	4:AD:32:CYS:SG	2.61	0.41
5:AE:55:GLU:N	5:AE:55:GLU:OE2	2.53	0.41
23:AW:53:G:C5	23:AW:54:5MU:H72	2.55	0.41
25:BA:1:G:N2	25:BA:2903:U:O2	2.54	0.41
25:BA:167:A:C2	25:BA:168:G:H1'	2.55	0.41
25:BA:613:A:H8	25:BA:613:A:O5'	2.03	0.41
25:BA:896:A:O2'	25:BA:897:C:O4'	2.32	0.41
25:BA:1231:U:H2'	25:BA:1232:G:H8	1.85	0.41
25:BA:2187:U:O5'	25:BA:2187:U:H6	2.03	0.41
25:BA:2210:U:H4'	25:BA:2211:G:C5'	2.51	0.41
25:BA:2298:A:H61	25:BA:2318:G:H1'	1.85	0.41
30:BF:57:LEU:HA	30:BF:57:LEU:HD23	1.83	0.41
43:BU:6:ARG:HA	43:BU:6:ARG:HD2	1.85	0.41
45:BW:48:MET:O	45:BW:51:GLN:HG3	2.21	0.41
58:CC:1105:SER:OG	59:CD:731:ARG:NE	2.51	0.41
58:CC:1235:LEU:HA	58:CC:1235:LEU:HD23	1.75	0.41
58:CC:1336:ASN:HD22	58:CC:1336:ASN:C	2.22	0.41
59:CD:157:GLN:CG	59:CD:158:GLN:H	2.34	0.41
59:CD:290:ILE:H	59:CD:290:ILE:HD12	1.85	0.41
1:AA:94:G:N2	1:AA:97:G:O6	2.53	0.41
1:AA:1183:U:H3'	1:AA:1184:G:H5"	2.02	0.41
1:AA:1326:U:H2'	1:AA:1327:C:H6	1.86	0.41
1:AA:1467:C:H2'	1:AA:1468:A:C8	2.56	0.41
1:AA:1492:A:N6	12:AL:47:SER:OG	2.54	0.41
1:AA:1527:U:C5	21:AU:42:THR:HG21	2.56	0.41
5:AE:144:LEU:HD23	5:AE:144:LEU:HA	1.79	0.41
13:AM:92:ARG:HH11	25:BA:888:C:H3'	1.85	0.41
15:AO:67:LEU:HD23	15:AO:67:LEU:HA	1.69	0.41
18:AR:34:THR:N	18:AR:38:LYS:O	2.51	0.41
25:BA:118:A:C8	25:BA:119:A:C8	3.08	0.41
25:BA:543:A:N1	25:BA:551:G:C6	2.89	0.41
25:BA:1063:G:O2'	25:BA:1064:C:H6	2.04	0.41
25:BA:1802:A:H2'	25:BA:1803:A:C8	2.56	0.41
25:BA:2532:G:N2	25:BA:2663:G:O2'	2.54	0.41
27:BC:105:LEU:O	27:BC:107:PRO:HD3	2.20	0.41
36:BN:134:THR:HG21	45:BW:79:ARG:CZ	2.51	0.41
37:BO:49:GLU:O	37:BO:53:THR:HG23	2.20	0.41
42:BT:36:LEU:HD23	42:BT:36:LEU:HA	1.93	0.41
57:CA:58:GLU:OE1	57:CA:170:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:CD:80:HIS:O	59:CD:83:VAL:HG22	2.21	0.41
59:CD:160:LEU:HD23	59:CD:160:LEU:N	2.34	0.41
59:CD:416:ILE:O	59:CD:418:GLU:N	2.53	0.41
1:AA:413:G:H21	1:AA:428:G:H1'	1.86	0.41
1:AA:868:C:H2'	1:AA:869:G:O4'	2.21	0.41
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.56	0.41
1:AA:1443:C:H2'	1:AA:1444:U:O4'	2.20	0.41
3:AC:114:LYS:HE2	3:AC:185:ASN:OD1	2.21	0.41
4:AD:5:LEU:HD23	4:AD:5:LEU:HA	1.78	0.41
5:AE:12:GLN:CD	59:CD:79:LYS:HD2	2.41	0.41
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.54	0.41
9:AI:4:ASN:HB3	9:AI:6:TYR:CE1	2.56	0.41
17:AQ:54:GLY:N	17:AQ:57:ASP:OD2	2.47	0.41
25:BA:274:C:H3'	25:BA:275:C:C6	2.55	0.41
25:BA:404:A:H5"	25:BA:405:U:OP1	2.21	0.41
25:BA:1078:U:O2	25:BA:1088:A:H2'	2.20	0.41
25:BA:1182:G:H2'	25:BA:1183:U:O4'	2.20	0.41
25:BA:1794:A:H2'	25:BA:1795:C:H6	1.86	0.41
25:BA:2125:G:H1	25:BA:2171:A:P	2.44	0.41
25:BA:2313:C:N3	25:BA:2314:A:N7	2.69	0.41
25:BA:2314:A:C2	25:BA:2315:G:C5	3.09	0.41
25:BA:2345:G:N3	25:BA:2381:A:H2'	2.36	0.41
25:BA:2500:U:O2'	25:BA:2504:PSU:OP1	2.37	0.41
25:BA:2685:G:OP1	34:BL:78:ARG:NH2	2.53	0.41
25:BA:2898:U:C2	25:BA:2899:A:N7	2.89	0.41
27:BC:225:MET:HB3	27:BC:229:ASP:HB2	2.02	0.41
30:BF:171:ALA:O	30:BF:174:ASP:N	2.43	0.41
33:BK:60:ASP:CG	33:BK:61:LYS:HZ3	2.24	0.41
40:BR:83:LEU:HD22	40:BR:88:VAL:HB	2.02	0.41
45:BW:75:GLN:HB2	45:BW:92:VAL:HG13	2.03	0.41
45:BW:80:HIS:CE1	45:BW:83:LYS:HD2	2.54	0.41
46:BX:54:GLY:O	46:BX:57:HIS:N	2.53	0.41
50:B2:34:SER:OG	50:B2:36:GLU:HG2	2.21	0.41
55:CN:26:DG:C8	55:CN:26:DG:H5"	2.56	0.41
55:CN:27:DA:C4	55:CN:28:DA:N7	2.89	0.41
56:CT:5:DG:H2'	56:CT:6:DA:O4'	2.21	0.41
57:CB:66:HIS:ND1	57:CB:68:TYR:HB3	2.36	0.41
58:CC:145:ILE:N	58:CC:145:ILE:HD12	2.36	0.41
58:CC:615:VAL:O	58:CC:615:VAL:HG13	2.20	0.41
58:CC:660:VAL:HG13	58:CC:661:VAL:HG13	2.02	0.41
58:CC:753:LEU:HD23	58:CC:753:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:CC:1104:PRO:HA	59:CD:740:LEU:HD11	2.03	0.41
59:CD:201:LEU:HD23	59:CD:221:ILE:HG22	2.03	0.41
59:CD:327:LEU:O	59:CD:330:MET:N	2.51	0.41
59:CD:619:ILE:HD12	59:CD:619:ILE:HA	1.86	0.41
1:AA:81:A:H2'	1:AA:82:G:O4'	2.21	0.41
1:AA:336:A:C6	1:AA:337:G:C5	3.09	0.41
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.35	0.41
1:AA:1038:C:C2	1:AA:1039:G:C8	3.09	0.41
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.44	0.41
1:AA:1277:C:C2'	1:AA:1278:G:H5"	2.51	0.41
1:AA:1370:G:C2	1:AA:1371:G:C8	3.09	0.41
4:AD:145:ILE:HD13	4:AD:145:ILE:HA	1.94	0.41
9:AI:99:ARG:HD2	9:AI:104:VAL:HG21	2.02	0.41
12:AL:81:LEU:O	12:AL:98:VAL:HG12	2.21	0.41
13:AM:3:ARG:O	13:AM:57:ARG:NH2	2.51	0.41
25:BA:1060:U:C1'	25:BA:1062:G:H5'	2.51	0.41
25:BA:1105:U:H2'	25:BA:1106:G:C8	2.53	0.41
25:BA:1495:A:H2'	25:BA:1496:A:C8	2.56	0.41
25:BA:1790:C:H2'	25:BA:1791:A:C5	2.56	0.41
25:BA:2250:G:O2'	25:BA:2497:A:OP2	2.33	0.41
25:BA:2308:G:C6	30:BF:77:PHE:CZ	3.09	0.41
25:BA:2899:A:H2'	25:BA:2900:A:H8	1.86	0.41
26:BB:2:G:O6	26:BB:119:A:N6	2.54	0.41
32:BH:64:ALA:O	32:BH:68:ARG:HG2	2.20	0.41
38:BP:49:VAL:HG12	38:BP:50:ALA:N	2.36	0.41
44:BV:42:VAL:O	44:BV:60:GLU:HA	2.21	0.41
57:CA:102:LEU:HD23	57:CA:102:LEU:C	2.41	0.41
58:CC:138:ILE:HD12	58:CC:138:ILE:HG23	1.78	0.41
58:CC:149:LEU:HA	58:CC:149:LEU:HD12	1.87	0.41
58:CC:166:SER:HB2	59:CD:1151:LYS:HE3	2.03	0.41
59:CD:249:LEU:HA	59:CD:249:LEU:HD23	1.85	0.41
59:CD:1050:THR:C	59:CD:1057:SER:HB3	2.41	0.41
1:AA:1215:G:C2	1:AA:1216:A:C8	3.09	0.40
3:AC:74:GLY:N	58:CC:867:GLU:CB	2.48	0.40
3:AC:79:LYS:H	3:AC:79:LYS:CD	2.34	0.40
7:AG:110:LYS:HA	7:AG:110:LYS:HD2	1.67	0.40
13:AM:65:VAL:HG22	13:AM:66:GLU:N	2.36	0.40
25:BA:239:C:O2'	25:BA:622:G:O2'	2.21	0.40
25:BA:389:G:C8	25:BA:2413:G:H4'	2.57	0.40
25:BA:456:C:H2'	43:BU:73:ARG:HH11	1.86	0.40
25:BA:955:PSU:H6	25:BA:955:PSU:O5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1040:A:H2'	25:BA:1041:G:O4'	2.20	0.40
25:BA:2377:A:O2'	38:BP:117:PHE:O	2.39	0.40
25:BA:2694:G:H2'	25:BA:2695:U:O4'	2.22	0.40
36:BN:25:ASP:OD1	36:BN:25:ASP:N	2.46	0.40
39:BQ:14:LYS:NZ	39:BQ:78:SER:O	2.37	0.40
47:BY:6:GLN:O	47:BY:74:ARG:NH2	2.53	0.40
58:CC:678:ARG:NH1	58:CC:681:MET:SD	2.94	0.40
58:CC:690:VAL:H	58:CC:690:VAL:HG12	1.73	0.40
58:CC:866:ASP:OD1	58:CC:866:ASP:C	2.60	0.40
58:CC:886:LYS:HB3	58:CC:916:SER:O	2.22	0.40
58:CC:1340:GLU:CD	58:CC:1341:ASP:H	2.21	0.40
59:CD:755:ILE:HG22	59:CD:757:THR:H	1.85	0.40
59:CD:871:LEU:O	59:CD:874:GLU:HB3	2.21	0.40
1:AA:1160:G:H5"	2:AB:131:LYS:NZ	2.36	0.40
1:AA:1292:G:C6	1:AA:1293:C:C4	3.09	0.40
1:AA:1408:A:C6	1:AA:1494:G:C6	3.09	0.40
1:AA:1518:MA6:O5'	1:AA:1518:MA6:H8	2.21	0.40
4:AD:106:GLY:HA2	4:AD:165:ARG:HH22	1.87	0.40
4:AD:194:ASP:CA	59:CD:74:LYS:HE2	2.47	0.40
5:AE:13:GLU:OE2	5:AE:68:ARG:NH2	2.53	0.40
5:AE:99:ALA:HB3	5:AE:103:THR:HG21	2.04	0.40
7:AG:16:PRO:HB2	9:AI:42:GLU:HG3	2.04	0.40
9:AI:32:GLN:HE21	9:AI:32:GLN:HB2	1.75	0.40
11:AK:18:ASP:HA	11:AK:81:ASN:O	2.21	0.40
12:AL:66:TYR:HB2	12:AL:87:VAL:HG21	2.03	0.40
17:AQ:38:ILE:HD12	17:AQ:40:ARG:HD2	2.03	0.40
18:AR:68:LEU:HD13	18:AR:68:LEU:HA	1.88	0.40
21:AU:29:LEU:HA	21:AU:32:VAL:HG22	2.04	0.40
23:AW:55:PSU:O5'	23:AW:55:PSU:H6	2.04	0.40
25:BA:81:G:H2'	25:BA:82:U:O4'	2.21	0.40
25:BA:638:G:C5	25:BA:651:G:C2	3.09	0.40
25:BA:711:G:C6	25:BA:721:A:C6	3.09	0.40
25:BA:1872:A:H8	25:BA:1872:A:O5'	2.04	0.40
25:BA:2175:C:H2'	25:BA:2176:A:N7	2.36	0.40
25:BA:2287:A:N7	25:BA:2289:G:C8	2.90	0.40
26:BB:12:C:H5'	26:BB:15:A:H61	1.86	0.40
27:BC:267:ILE:HG21	27:BC:270:ARG:HD2	2.03	0.40
30:BF:114:PHE:CE2	30:BF:176:PRO:HB2	2.37	0.40
47:BY:19:SER:OG	47:BY:20:HIS:N	2.54	0.40
52:B4:41:ARG:HB2	52:B4:41:ARG:NH2	2.36	0.40
59:CD:1356:LEU:HD23	59:CD:1356:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:211:G:C6	1:AA:212:G:H1'	2.56	0.40
1:AA:425:G:C6	1:AA:426:U:C4	3.10	0.40
1:AA:676:A:H2'	1:AA:677:U:C6	2.56	0.40
1:AA:947:G:C6	1:AA:948:C:C4	3.09	0.40
1:AA:981:U:OP1	14:AN:9:ARG:NH1	2.55	0.40
1:AA:1246:A:N1	1:AA:1292:G:C6	2.89	0.40
1:AA:1319:A:C8	1:AA:1323:G:C5	3.09	0.40
1:AA:1355:G:H2'	1:AA:1356:G:H8	1.86	0.40
1:AA:1480:A:H2'	1:AA:1481:U:O4'	2.21	0.40
6:AF:50:PRO:HB3	6:AF:55:HIS:CD2	2.55	0.40
23:AW:7:G:O2'	23:AW:49:G:O5'	2.27	0.40
25:BA:404:A:H4'	25:BA:405:U:H5"	2.02	0.40
25:BA:2347:C:C2	25:BA:2348:U:C5	3.10	0.40
25:BA:2375:G:N2	25:BA:2378:A:OP2	2.38	0.40
25:BA:2552:OMU:C2	25:BA:2554:U:H5"	2.51	0.40
25:BA:2797:U:H6	25:BA:2797:U:H2'	1.78	0.40
26:BB:65:U:C4	26:BB:108:A:C4	3.08	0.40
28:BD:31:ALA:O	28:BD:33:ARG:HD3	2.21	0.40
28:BD:48:ILE:O	28:BD:48:ILE:HG13	2.21	0.40
36:BN:33:LEU:HD13	36:BN:117:PHE:HB3	2.03	0.40
39:BQ:98:TYR:O	39:BQ:101:ARG:HB3	2.21	0.40
51:B3:7:GLU:HG2	51:B3:8:LYS:N	2.36	0.40
57:CB:58:GLU:OE2	57:CB:170:ARG:NE	2.44	0.40
58:CC:951:MET:O	58:CC:955:GLN:HG2	2.21	0.40
59:CD:884:SER:OG	59:CD:885:VAL:N	2.55	0.40
1:AA:176:C:C2	1:AA:177:G:C2	3.10	0.40
1:AA:213:G:C8	1:AA:214:C:C5	3.10	0.40
1:AA:663:A:H2'	1:AA:664:G:O4'	2.22	0.40
1:AA:737:C:H5"	6:AF:91:ARG:HG3	2.03	0.40
1:AA:1119:C:OP2	9:AI:11:ARG:NH2	2.54	0.40
2:AB:73:LYS:HE2	2:AB:73:LYS:HB2	1.71	0.40
8:AH:34:VAL:O	8:AH:38:ASN:ND2	2.52	0.40
12:AL:43:LYS:HG2	12:AL:44:LYS:H	1.86	0.40
25:BA:197:A:H2	25:BA:2434:A:H62	1.70	0.40
25:BA:289:G:H2'	25:BA:290:U:O4'	2.21	0.40
25:BA:2104:C:H41	25:BA:2186:G:N2	2.19	0.40
25:BA:2182:U:O2'	25:BA:2183:A:C8	2.68	0.40
26:BB:42:C:C6	30:BF:66:LEU:HB2	2.56	0.40
26:BB:45:A:C4	26:BB:46:A:C8	3.10	0.40
26:BB:94:A:H2'	26:BB:95:U:O4'	2.21	0.40
27:BC:240:PHE:O	27:BC:242:LYS:NZ	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:15:GLY:O	34:BL:47:ILE:HG23	2.22	0.40
34:BL:59:LYS:HG3	34:BL:89:ASN:HA	2.04	0.40
40:BR:18:LEU:HA	40:BR:18:LEU:HD13	1.80	0.40
44:BV:41:LEU:HB3	44:BV:60:GLU:HG2	2.03	0.40
57:CA:11:PRO:HB3	57:CA:31:LEU:HD21	2.02	0.40
58:CC:267:ARG:NH2	58:CC:268:ARG:O	2.54	0.40
58:CC:675:ASP:OD1	58:CC:676:ALA:N	2.54	0.40
58:CC:1333:LEU:HA	58:CC:1333:LEU:HD23	1.84	0.40
58:CC:1339:LEU:HA	58:CC:1339:LEU:HD23	1.88	0.40
59:CD:441:LEU:N	59:CD:441:LEU:CD2	2.84	0.40
1:AA:148:G:O2'	1:AA:149:A:P	2.79	0.40
1:AA:255:G:C2	1:AA:272:C:C2	3.10	0.40
1:AA:346:G:H4'	39:BQ:39:ARG:HH12	1.87	0.40
1:AA:459:A:H2'	1:AA:460:A:C8	2.56	0.40
1:AA:495:A:C6	1:AA:496:A:N6	2.89	0.40
1:AA:1012:A:N6	1:AA:1018:G:O6	2.54	0.40
1:AA:1054:C:C5	1:AA:1196:A:C8	3.10	0.40
1:AA:1134:G:H3'	1:AA:1135:U:C5	2.57	0.40
2:AB:207:ILE:O	2:AB:211:THR:HG23	2.21	0.40
3:AC:93:ASP:OD1	3:AC:94:ILE:HG13	2.22	0.40
13:AM:85:CYS:HB3	19:AS:74:PHE:CE1	2.56	0.40
18:AR:55:LEU:HA	18:AR:55:LEU:HD12	1.84	0.40
24:AX:8:4SU:H2'	24:AX:13:C:N4	2.36	0.40
24:AX:23:A:C2	24:AX:24:G:C5	3.10	0.40
25:BA:92:U:H2'	25:BA:93:G:O4'	2.22	0.40
25:BA:873:C:H4'	36:BN:64:TRP:CD1	2.57	0.40
25:BA:2552:OMU:H6	25:BA:2552:OMU:O5'	2.22	0.40
25:BA:2813:A:C4	25:BA:2814:A:C8	3.10	0.40
35:BM:77:VAL:HG12	35:BM:78:ARG:H	1.86	0.40
38:BP:7:ARG:HD2	38:BP:97:PHE:CZ	2.57	0.40
50:B2:53:LYS:HE3	50:B2:55:ILE:O	2.22	0.40
58:CC:130:MET:SD	58:CC:134:GLY:HA2	2.61	0.40
59:CD:421:VAL:O	59:CD:421:VAL:HG23	2.21	0.40
59:CD:1325:PHE:CD1	59:CD:1325:PHE:C	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	224/241 (93%)	208 (93%)	15 (7%)	1 (0%)	34	66
3	AC	207/233 (89%)	194 (94%)	10 (5%)	3 (1%)	11	38
4	AD	203/206 (98%)	193 (95%)	9 (4%)	1 (0%)	29	61
5	AE	154/167 (92%)	143 (93%)	10 (6%)	1 (1%)	25	57
6	AF	102/131 (78%)	95 (93%)	7 (7%)	0	100	100
7	AG	151/156 (97%)	142 (94%)	8 (5%)	1 (1%)	22	54
8	AH	127/130 (98%)	117 (92%)	9 (7%)	1 (1%)	19	51
9	AI	126/130 (97%)	115 (91%)	9 (7%)	2 (2%)	9	36
10	AJ	98/103 (95%)	88 (90%)	7 (7%)	3 (3%)	4	23
11	AK	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	48
12	AL	119/124 (96%)	109 (92%)	8 (7%)	2 (2%)	9	35
13	AM	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	17	48
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
17	AQ	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
18	AR	52/75 (69%)	50 (96%)	2 (4%)	0	100	100
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%)	66 (97%)	1 (2%)	1 (2%)	10	38
27	BC	270/273 (99%)	249 (92%)	18 (7%)	3 (1%)	14	45
28	BD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	61
29	BE	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
30	BF	176/179 (98%)	162 (92%)	14 (8%)	0	100	100
31	BG	173/177 (98%)	158 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	22	54
33	BK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
35	BM	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	11	38
36	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
37	BO	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
38	BP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	48
39	BQ	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
40	BR	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
41	BS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	46
42	BT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	BU	93/100 (93%)	88 (95%)	5 (5%)	0	100	100
44	BV	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	46
45	BW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
47	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	BZ	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
51	B3	51/55 (93%)	49 (96%)	2 (4%)	0	100	100
52	B4	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
53	B5	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	9	36
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
57	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
57	CB	215/329 (65%)	204 (95%)	10 (5%)	1 (0%)	29	61
58	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	22	54
59	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	19	51
All	All	8623/9235 (93%)	8034 (93%)	540 (6%)	49 (1%)	29	57

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AI	13	LYS

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Mol	Chain	Res	Type
9	AI	56	ASP
11	AK	93	ARG
12	AL	88	LYS
27	BC	241	GLY
58	CC	165	HIS
59	CD	1159	ILE
2	AB	165	ASP
3	AC	51	SER
10	AJ	57	VAL
21	AU	65	ALA
28	BD	149	ASN
35	BM	36	LYS
38	BP	100	HIS
53	B5	32	ILE
57	CB	155	ALA
58	CC	47	TYR
59	CD	1051	ASP
4	AD	43	ALA
7	AG	130	ASN
32	BH	120	GLY
41	BS	53	PHE
58	CC	258	ASN
58	CC	1177	ARG
59	CD	119	SER
59	CD	121	PRO
59	CD	712	GLN
59	CD	854	ALA
59	CD	1200	GLU
3	AC	14	ILE
12	AL	102	LEU
27	BC	233	GLY
27	BC	253	LYS
35	BM	99	ASN
44	BV	8	ASP
58	CC	282	VAL
58	CC	596	ASP
58	CC	1153	ALA
59	CD	586	GLY
10	AJ	78	GLU
13	AM	49	SER
59	CD	312	ARG
3	AC	60	PRO

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Mol	Chain	Res	Type
10	AJ	58	ASN
58	CC	1223	ARG
5	AE	108	GLY
8	AH	75	ILE
58	CC	1186	VAL
59	CD	500	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/199 (94%)	175 (94%)	12 (6%)	17	46
3	AC	171/190 (90%)	153 (90%)	18 (10%)	7	25
4	AD	172/173 (99%)	154 (90%)	18 (10%)	7	25
5	AE	118/126 (94%)	107 (91%)	11 (9%)	9	30
6	AF	91/112 (81%)	83 (91%)	8 (9%)	10	33
7	AG	126/129 (98%)	111 (88%)	15 (12%)	5	21
8	AH	104/105 (99%)	97 (93%)	7 (7%)	16	45
9	AI	106/107 (99%)	97 (92%)	9 (8%)	10	35
10	AJ	87/90 (97%)	75 (86%)	12 (14%)	3	16
11	AK	89/99 (90%)	85 (96%)	4 (4%)	27	58
12	AL	102/103 (99%)	90 (88%)	12 (12%)	5	21
13	AM	93/96 (97%)	86 (92%)	7 (8%)	13	39
14	AN	83/84 (99%)	77 (93%)	6 (7%)	14	41
15	AO	76/77 (99%)	67 (88%)	9 (12%)	5	21
16	AP	65/65 (100%)	63 (97%)	2 (3%)	40	67
17	AQ	73/78 (94%)	63 (86%)	10 (14%)	3	16
18	AR	47/65 (72%)	43 (92%)	4 (8%)	10	35
19	AS	72/79 (91%)	69 (96%)	3 (4%)	30	60
20	AT	65/66 (98%)	58 (89%)	7 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	60/61 (98%)	58 (97%)	2 (3%)	38	66
27	BC	217/218 (100%)	207 (95%)	10 (5%)	27	58
28	BD	163/163 (100%)	151 (93%)	12 (7%)	13	40
29	BE	165/165 (100%)	150 (91%)	15 (9%)	9	31
30	BF	149/150 (99%)	135 (91%)	14 (9%)	8	30
31	BG	136/138 (99%)	122 (90%)	14 (10%)	7	26
32	BH	114/114 (100%)	100 (88%)	14 (12%)	4	20
33	BK	116/116 (100%)	108 (93%)	8 (7%)	15	44
34	BL	104/104 (100%)	96 (92%)	8 (8%)	13	38
35	BM	103/103 (100%)	92 (89%)	11 (11%)	6	25
36	BN	108/108 (100%)	103 (95%)	5 (5%)	27	58
37	BO	100/103 (97%)	95 (95%)	5 (5%)	24	55
38	BP	87/87 (100%)	80 (92%)	7 (8%)	12	37
39	BQ	99/100 (99%)	91 (92%)	8 (8%)	11	36
40	BR	89/90 (99%)	84 (94%)	5 (6%)	21	52
41	BS	84/84 (100%)	78 (93%)	6 (7%)	14	42
42	BT	93/93 (100%)	88 (95%)	5 (5%)	22	53
43	BU	82/84 (98%)	73 (89%)	9 (11%)	6	24
44	BV	84/85 (99%)	81 (96%)	3 (4%)	35	63
45	BW	78/78 (100%)	72 (92%)	6 (8%)	13	38
46	BX	58/63 (92%)	55 (95%)	3 (5%)	23	54
47	BY	67/68 (98%)	66 (98%)	1 (2%)	65	81
48	BZ	54/55 (98%)	52 (96%)	2 (4%)	34	63
49	B1	48/49 (98%)	41 (85%)	7 (15%)	3	14
50	B2	47/48 (98%)	42 (89%)	5 (11%)	6	25
51	B3	48/49 (98%)	46 (96%)	2 (4%)	30	60
52	B4	38/38 (100%)	36 (95%)	2 (5%)	22	53
53	B5	51/52 (98%)	50 (98%)	1 (2%)	55	76
54	B6	34/44 (77%)	34 (100%)	0	100	100
57	CA	197/286 (69%)	193 (98%)	4 (2%)	55	76
57	CB	187/286 (65%)	177 (95%)	10 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	CC	1139/1157 (98%)	1096 (96%)	43 (4%)	33	62
59	CD	1118/1168 (96%)	1097 (98%)	21 (2%)	57	77
All	All	7244/7650 (95%)	6802 (94%)	442 (6%)	22	48

All (442) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	5	SER
2	AB	14	VAL
2	AB	23	TRP
2	AB	47	VAL
2	AB	113	ARG
2	AB	129	LEU
2	AB	132	LYS
2	AB	169	GLU
2	AB	188	ASP
2	AB	192	ASP
2	AB	199	VAL
2	AB	220	THR
3	AC	3	GLN
3	AC	21	THR
3	AC	35	SER
3	AC	59	ARG
3	AC	62	LYS
3	AC	66	VAL
3	AC	79	LYS
3	AC	83	ASP
3	AC	89	LYS
3	AC	134	MET
3	AC	139	GLN
3	AC	154	SER
3	AC	172	ARG
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	196	ILE
3	AC	208	LEU
4	AD	21	LEU
4	AD	34	ILE
4	AD	50	ASP
4	AD	57	GLU

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Mol	Chain	Res	Type
4	AD	58	LYS
4	AD	95	GLU
4	AD	102	VAL
4	AD	104	ARG
4	AD	116	GLN
4	AD	138	SER
4	AD	143	VAL
4	AD	146	ARG
4	AD	147	GLU
4	AD	148	LYS
4	AD	179	GLU
4	AD	190	ASP
4	AD	197	GLU
4	AD	206	LYS
5	AE	15	LEU
5	AE	18	VAL
5	AE	61	GLN
5	AE	65	GLU
5	AE	69	ARG
5	AE	71	MET
5	AE	76	LEU
5	AE	114	VAL
5	AE	123	VAL
5	AE	138	ARG
5	AE	141	ILE
6	AF	24	ARG
6	AF	38	ARG
6	AF	44	ARG
6	AF	45	ARG
6	AF	54	LEU
6	AF	72	ASP
6	AF	73	GLU
6	AF	86	ARG
7	AG	4	ARG
7	AG	6	VAL
7	AG	7	ILE
7	AG	13	LEU
7	AG	17	LYS
7	AG	27	VAL
7	AG	58	GLU
7	AG	60	GLU
7	AG	78	ARG

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Mol	Chain	Res	Type
7	AG	80	VAL
7	AG	89	VAL
7	AG	90	GLU
7	AG	123	GLU
7	AG	143	ARG
7	AG	146	GLU
8	AH	25	VAL
8	AH	30	SER
8	AH	61	LEU
8	AH	73	GLU
8	AH	77	ARG
8	AH	96	MET
8	AH	121	LEU
9	AI	3	GLU
9	AI	9	THR
9	AI	12	ARG
9	AI	22	LYS
9	AI	32	GLN
9	AI	61	LEU
9	AI	63	LEU
9	AI	118	LEU
9	AI	123	ARG
10	AJ	5	ARG
10	AJ	7	ARG
10	AJ	17	LEU
10	AJ	18	ILE
10	AJ	24	GLU
10	AJ	27	GLU
10	AJ	37	ARG
10	AJ	44	THR
10	AJ	76	ILE
10	AJ	85	ASP
10	AJ	96	VAL
10	AJ	102	LEU
11	AK	15	GLN
11	AK	37	ARG
11	AK	69	ARG
11	AK	76	GLU
12	AL	4	VAL
12	AL	5	ASN
12	AL	10	LYS
12	AL	16	VAL

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Mol	Chain	Res	Type
12	AL	19	SER
12	AL	24	LEU
12	AL	47	SER
12	AL	64	THR
12	AL	72	HIS
12	AL	74	LEU
12	AL	90	LEU
12	AL	123	LYS
13	AM	11	ASP
13	AM	27	LYS
13	AM	89	LEU
13	AM	92	ARG
13	AM	93	ARG
13	AM	96	PRO
13	AM	104	THR
14	AN	30	ILE
14	AN	46	LEU
14	AN	52	PRO
14	AN	89	MET
14	AN	92	GLU
14	AN	100	SER
15	AO	11	ILE
15	AO	22	THR
15	AO	39	LEU
15	AO	40	GLN
15	AO	57	LEU
15	AO	61	SER
15	AO	64	ARG
15	AO	72	ARG
15	AO	83	GLU
16	AP	1	MET
16	AP	21	VAL
17	AQ	5	ILE
17	AQ	27	ARG
17	AQ	33	ILE
17	AQ	40	ARG
17	AQ	41	THR
17	AQ	42	THR
17	AQ	53	CYS
17	AQ	57	ASP
17	AQ	75	LEU
17	AQ	77	ARG

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Mol	Chain	Res	Type
18	AR	35	GLU
18	AR	44	ILE
18	AR	55	LEU
18	AR	68	LEU
19	AS	20	GLU
19	AS	49	ILE
19	AS	51	VAL
20	AT	6	SER
20	AT	15	GLU
20	AT	25	ARG
20	AT	43	ASP
20	AT	54	MET
20	AT	58	VAL
20	AT	83	ILE
21	AU	4	ILE
21	AU	69	ARG
27	BC	3	VAL
27	BC	4	VAL
27	BC	52	ARG
27	BC	88	SER
27	BC	120	VAL
27	BC	125	LYS
27	BC	130	LEU
27	BC	195	VAL
27	BC	203	ARG
27	BC	250	VAL
28	BD	13	ARG
28	BD	17	GLU
28	BD	18	ASP
28	BD	32	ASN
28	BD	33	ARG
28	BD	43	ASP
28	BD	59	ARG
28	BD	89	GLU
28	BD	110	THR
28	BD	118	PHE
28	BD	129	THR
28	BD	157	LYS
29	BE	2	GLU
29	BE	3	LEU
29	BE	21	ARG
29	BE	40	ARG

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Mol	Chain	Res	Type
29	BE	57	LYS
29	BE	65	THR
29	BE	69	ARG
29	BE	73	ILE
29	BE	77	ILE
29	BE	88	ARG
29	BE	111	GLU
29	BE	119	ILE
29	BE	123	LYS
29	BE	152	GLU
29	BE	184	ASP
30	BF	13	VAL
30	BF	47	LYS
30	BF	48	LYS
30	BF	56	ASP
30	BF	57	LEU
30	BF	80	ARG
30	BF	98	GLU
30	BF	115	ARG
30	BF	123	ASP
30	BF	134	GLU
30	BF	140	GLU
30	BF	141	ILE
30	BF	152	LEU
30	BF	164	GLU
31	BG	16	ASP
31	BG	32	GLU
31	BG	39	ASP
31	BG	41	VAL
31	BG	69	ARG
31	BG	84	THR
31	BG	110	SER
31	BG	111	HIS
31	BG	114	ASP
31	BG	125	CYS
31	BG	127	THR
31	BG	155	GLU
31	BG	167	GLU
31	BG	173	GLU
32	BH	4	ILE
32	BH	11	ASN
32	BH	12	LEU

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Mol	Chain	Res	Type
32	BH	37	VAL
32	BH	48	GLU
32	BH	60	GLU
32	BH	66	ASN
32	BH	70	GLU
32	BH	75	LEU
32	BH	89	LYS
32	BH	97	ARG
32	BH	101	ASP
32	BH	112	LYS
32	BH	144	VAL
33	BK	1	MET
33	BK	30	THR
33	BK	31	GLU
33	BK	57	LEU
33	BK	108	MET
33	BK	123	LYS
33	BK	129	GLU
33	BK	142	ILE
34	BL	17	ARG
34	BL	18	ARG
34	BL	35	VAL
34	BL	41	ILE
34	BL	58	LEU
34	BL	67	LYS
34	BL	99	ILE
34	BL	111	LYS
35	BM	2	ARG
35	BM	30	THR
35	BM	33	ARG
35	BM	40	SER
35	BM	67	THR
35	BM	76	GLU
35	BM	78	ARG
35	BM	84	LYS
35	BM	115	GLU
35	BM	120	VAL
35	BM	129	LYS
36	BN	18	ARG
36	BN	78	LEU
36	BN	110	GLU
36	BN	115	GLU

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Mol	Chain	Res	Type
36	BN	127	LYS
37	BO	2	ARG
37	BO	13	ASN
37	BO	20	MET
37	BO	65	LEU
37	BO	69	ARG
38	BP	2	ASP
38	BP	13	ARG
38	BP	52	SER
38	BP	60	GLU
38	BP	89	ASP
38	BP	103	VAL
38	BP	116	GLN
39	BQ	26	VAL
39	BQ	80	VAL
39	BQ	88	ARG
39	BQ	104	THR
39	BQ	111	LYS
39	BQ	113	ARG
39	BQ	114	LEU
39	BQ	115	ASN
40	BR	11	ARG
40	BR	13	ARG
40	BR	51	ARG
40	BR	52	GLN
40	BR	91	ASP
41	BS	10	LYS
41	BS	39	LEU
41	BS	46	GLU
41	BS	48	LYS
41	BS	79	ARG
41	BS	86	GLN
42	BT	59	GLU
42	BT	65	ASP
42	BT	83	LYS
42	BT	109	ASP
42	BT	110	ARG
43	BU	5	GLU
43	BU	7	LEU
43	BU	12	ARG
43	BU	16	VAL
43	BU	24	MET

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Mol	Chain	Res	Type
43	BU	29	THR
43	BU	67	VAL
43	BU	70	HIS
43	BU	89	GLU
44	BV	9	ASP
44	BV	24	LYS
44	BV	88	GLU
45	BW	1	MET
45	BW	20	LEU
45	BW	34	LYS
45	BW	40	ILE
45	BW	45	ASP
45	BW	58	SER
46	BX	11	ARG
46	BX	55	ARG
46	BX	70	GLU
47	BY	60	ASP
48	BZ	5	GLU
48	BZ	7	ARG
49	B1	4	THR
49	B1	10	THR
49	B1	11	ARG
49	B1	19	LYS
49	B1	31	ARG
49	B1	37	GLU
49	B1	45	ARG
50	B2	9	THR
50	B2	12	LYS
50	B2	28	LEU
50	B2	40	ARG
50	B2	55	ILE
51	B3	5	ILE
51	B3	25	LYS
52	B4	22	MET
52	B4	25	LYS
53	B5	31	HIS
57	CA	13	LEU
57	CA	74	VAL
57	CA	101	THR
57	CA	166	ARG
57	CB	17	GLU
57	CB	41	ASN

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Mol	Chain	Res	Type
57	CB	48	LEU
57	CB	66	HIS
57	CB	72	GLU
57	CB	76	GLU
57	CB	83	LEU
57	CB	170	ARG
57	CB	174	ASP
57	CB	191	ARG
58	CC	47	TYR
58	CC	65	ASN
58	CC	108	GLU
58	CC	116	ASP
58	CC	150	HIS
58	CC	193	ASN
58	CC	262	TYR
58	CC	267	ARG
58	CC	369	MET
58	CC	494	ASN
58	CC	524	ILE
58	CC	529	ARG
58	CC	562	GLU
58	CC	568	ASN
58	CC	569	ILE
58	CC	575	LEU
58	CC	657	THR
58	CC	726	TYR
58	CC	745	GLU
58	CC	772	SER
58	CC	822	VAL
58	CC	830	THR
58	CC	843	THR
58	CC	844	LYS
58	CC	856	ASN
58	CC	867	GLU
58	CC	888	THR
58	CC	1002	LEU
58	CC	1005	GLU
58	CC	1022	LYS
58	CC	1080	ASN
58	CC	1158	LYS
58	CC	1223	ARG
58	CC	1240	ASP

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Mol	Chain	Res	Type
58	CC	1247	SER
58	CC	1250	SER
58	CC	1274	GLU
58	CC	1287	LEU
58	CC	1291	LEU
58	CC	1298	VAL
58	CC	1304	MET
58	CC	1336	ASN
58	CC	1340	GLU
59	CD	68	TYR
59	CD	99	ARG
59	CD	113	HIS
59	CD	158	GLN
59	CD	196	GLN
59	CD	255	LEU
59	CD	275	ARG
59	CD	281	ARG
59	CD	418	GLU
59	CD	505	ASP
59	CD	700	ASN
59	CD	709	ARG
59	CD	802	ASP
59	CD	826	ILE
59	CD	839	VAL
59	CD	1046	ILE
59	CD	1165	PHE
59	CD	1167	LYS
59	CD	1195	GLN
59	CD	1237	VAL
59	CD	1261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	70	ASN
6	AF	11	HIS
9	AI	31	ASN
39	BQ	115	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	288 (18%)	32 (2%)
22	AV	28/57 (49%)	12 (42%)	1 (3%)
23	AW	76/77 (98%)	21 (27%)	6 (7%)
24	AX	73/76 (96%)	18 (24%)	0
25	BA	2895/2904 (99%)	552 (19%)	66 (2%)
26	BB	119/120 (99%)	15 (12%)	0
All	All	4720/4776 (98%)	906 (19%)	105 (2%)

All (906) 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	74	A
1	AA	76	G
1	AA	80	C
1	AA	83	C
1	AA	84	U
1	AA	86	G
1	AA	87	C
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	121	U
1	AA	122	G

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Mol	Chain	Res	Type
1	AA	131	A
1	AA	141	G
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	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	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
1	AA	373	A

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Mol	Chain	Res	Type
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	467	U
1	AA	468	A
1	AA	469	C
1	AA	479	U
1	AA	480	U
1	AA	481	G
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
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	572	A
1	AA	573	A

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Mol	Chain	Res	Type
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	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	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	849	G
1	AA	874	G
1	AA	887	G
1	AA	902	G
1	AA	914	A
1	AA	916	U

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Mol	Chain	Res	Type
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	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	1009	U
1	AA	1017	U
1	AA	1018	G
1	AA	1020	G
1	AA	1021	A
1	AA	1024	G
1	AA	1026	G
1	AA	1028	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	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

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Mol	Chain	Res	Type
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	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1151	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1167	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
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

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Mol	Chain	Res	Type
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	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	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	1398	A
1	AA	1404	C
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	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1503	A

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Mol	Chain	Res	Type
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	AV	15	C
22	AV	16	A
22	AV	19	U
22	AV	24	A
22	AV	25	U
22	AV	26	A
22	AV	27	C
22	AV	40	A
22	AV	41	C
22	AV	42	G
22	AV	45	G
22	AV	49	G
23	AW	6	G
23	AW	14	A
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	47	U
23	AW	48	C
23	AW	49	G
23	AW	57	A
23	AW	59	A
23	AW	69	C
23	AW	74	C
23	AW	75	C
23	AW	76	A
24	AX	8	4SU
24	AX	9	A
24	AX	10	G
24	AX	14	A
24	AX	16	H2U

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Mol	Chain	Res	Type
24	AX	17	C
24	AX	18	G
24	AX	19	G
24	AX	20	H2U
24	AX	21	A
24	AX	22	G
24	AX	23	A
24	AX	33	U
24	AX	48	C
24	AX	49	C
24	AX	58	A
24	AX	71	G
24	AX	74	C
25	BA	10	A
25	BA	14	A
25	BA	23	G
25	BA	34	U
25	BA	35	G
25	BA	45	G
25	BA	46	G
25	BA	58	G
25	BA	60	G
25	BA	62	U
25	BA	63	A
25	BA	71	A
25	BA	74	A
25	BA	75	G
25	BA	83	A
25	BA	84	A
25	BA	85	G
25	BA	99	U
25	BA	101	A
25	BA	102	U
25	BA	110	G
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	122	G
25	BA	131	A
25	BA	136	G
25	BA	138	U
25	BA	139	U

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Mol	Chain	Res	Type
25	BA	140	C
25	BA	141	G
25	BA	142	A
25	BA	144	A
25	BA	149	A
25	BA	163	C
25	BA	165	A
25	BA	181	A
25	BA	196	A
25	BA	215	G
25	BA	216	A
25	BA	221	A
25	BA	222	A
25	BA	248	G
25	BA	249	C
25	BA	250	G
25	BA	264	C
25	BA	265	A
25	BA	266	G
25	BA	270	A
25	BA	271	G
25	BA	272	A
25	BA	275	C
25	BA	276	U
25	BA	277	G
25	BA	278	A
25	BA	285	G
25	BA	302	C
25	BA	311	A
25	BA	327	G
25	BA	329	G
25	BA	330	A
25	BA	353	C
25	BA	361	G
25	BA	362	A
25	BA	371	A
25	BA	386	G
25	BA	396	G
25	BA	403	U
25	BA	405	U
25	BA	411	G
25	BA	412	A

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Mol	Chain	Res	Type
25	BA	424	G
25	BA	435	C
25	BA	451	U
25	BA	456	C
25	BA	477	A
25	BA	480	A
25	BA	481	G
25	BA	491	G
25	BA	501	A
25	BA	503	A
25	BA	504	A
25	BA	505	A
25	BA	508	A
25	BA	509	C
25	BA	531	C
25	BA	532	A
25	BA	533	G
25	BA	544	G
25	BA	545	A
25	BA	563	A
25	BA	569	U
25	BA	573	U
25	BA	574	A
25	BA	575	A
25	BA	586	A
25	BA	603	A
25	BA	609	A
25	BA	613	A
25	BA	614	A
25	BA	615	U
25	BA	616	A
25	BA	618	G
25	BA	627	A
25	BA	637	A
25	BA	645	C
25	BA	647	G
25	BA	651	G
25	BA	654	A
25	BA	655	A
25	BA	668	A
25	BA	686	U
25	BA	696	G

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Mol	Chain	Res	Type
25	BA	717	C
25	BA	724	U
25	BA	730	A
25	BA	738	G
25	BA	746	PSU
25	BA	747	5MU
25	BA	757	G
25	BA	764	A
25	BA	765	C
25	BA	775	G
25	BA	776	G
25	BA	782	A
25	BA	783	A
25	BA	784	G
25	BA	785	G
25	BA	788	A
25	BA	789	A
25	BA	790	U
25	BA	805	G
25	BA	812	C
25	BA	827	U
25	BA	828	U
25	BA	846	U
25	BA	858	G
25	BA	859	G
25	BA	869	G
25	BA	878	A
25	BA	881	G
25	BA	883	G
25	BA	884	U
25	BA	885	C
25	BA	887	U
25	BA	888	C
25	BA	890	C
25	BA	891	G
25	BA	892	A
25	BA	893	C
25	BA	895	U
25	BA	896	A
25	BA	897	C
25	BA	899	A
25	BA	910	A

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Mol	Chain	Res	Type
25	BA	914	G
25	BA	915	C
25	BA	931	U
25	BA	933	A
25	BA	940	G
25	BA	941	A
25	BA	946	C
25	BA	953	G
25	BA	961	C
25	BA	974	G
25	BA	983	A
25	BA	984	A
25	BA	985	C
25	BA	996	A
25	BA	999	U
25	BA	1005	C
25	BA	1012	U
25	BA	1013	C
25	BA	1023	U
25	BA	1026	G
25	BA	1033	U
25	BA	1040	A
25	BA	1043	C
25	BA	1045	C
25	BA	1046	A
25	BA	1047	G
25	BA	1050	A
25	BA	1055	G
25	BA	1060	U
25	BA	1061	U
25	BA	1063	G
25	BA	1064	C
25	BA	1065	U
25	BA	1067	A
25	BA	1068	G
25	BA	1069	A
25	BA	1070	A
25	BA	1073	A
25	BA	1074	G
25	BA	1083	U
25	BA	1087	G
25	BA	1088	A

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Mol	Chain	Res	Type
25	BA	1090	A
25	BA	1101	U
25	BA	1107	G
25	BA	1111	A
25	BA	1112	G
25	BA	1119	U
25	BA	1122	G
25	BA	1130	U
25	BA	1132	U
25	BA	1134	A
25	BA	1135	C
25	BA	1142	A
25	BA	1170	C
25	BA	1171	G
25	BA	1173	U
25	BA	1174	U
25	BA	1176	U
25	BA	1177	G
25	BA	1178	C
25	BA	1179	G
25	BA	1180	U
25	BA	1186	G
25	BA	1212	G
25	BA	1236	G
25	BA	1238	G
25	BA	1248	G
25	BA	1253	A
25	BA	1256	G
25	BA	1265	A
25	BA	1271	G
25	BA	1272	A
25	BA	1273	U
25	BA	1301	A
25	BA	1302	A
25	BA	1321	A
25	BA	1345	C
25	BA	1352	U
25	BA	1365	A
25	BA	1368	G
25	BA	1378	A
25	BA	1379	U
25	BA	1380	G

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Mol	Chain	Res	Type
25	BA	1383	A
25	BA	1395	A
25	BA	1405	U
25	BA	1406	U
25	BA	1407	G
25	BA	1408	G
25	BA	1409	U
25	BA	1414	C
25	BA	1416	G
25	BA	1417	C
25	BA	1420	A
25	BA	1428	C
25	BA	1434	A
25	BA	1435	G
25	BA	1452	G
25	BA	1453	A
25	BA	1455	G
25	BA	1458	U
25	BA	1460	U
25	BA	1478	G
25	BA	1482	G
25	BA	1483	G
25	BA	1490	A
25	BA	1493	C
25	BA	1495	A
25	BA	1497	U
25	BA	1503	A
25	BA	1508	A
25	BA	1509	A
25	BA	1510	G
25	BA	1515	A
25	BA	1529	G
25	BA	1534	U
25	BA	1535	A
25	BA	1536	C
25	BA	1537	G
25	BA	1554	U
25	BA	1558	C
25	BA	1559	U
25	BA	1566	A
25	BA	1569	A
25	BA	1578	U

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Mol	Chain	Res	Type
25	BA	1580	A
25	BA	1581	G
25	BA	1583	A
25	BA	1584	U
25	BA	1585	C
25	BA	1586	A
25	BA	1589	U
25	BA	1590	A
25	BA	1592	C
25	BA	1593	A
25	BA	1594	U
25	BA	1595	C
25	BA	1596	A
25	BA	1597	A
25	BA	1608	A
25	BA	1609	A
25	BA	1610	A
25	BA	1613	G
25	BA	1619	G
25	BA	1630	A
25	BA	1647	U
25	BA	1648	U
25	BA	1649	G
25	BA	1651	G
25	BA	1674	G
25	BA	1677	A
25	BA	1703	G
25	BA	1713	A
25	BA	1714	U
25	BA	1715	G
25	BA	1718	G
25	BA	1729	U
25	BA	1730	C
25	BA	1732	C
25	BA	1738	G
25	BA	1742	U
25	BA	1750	G
25	BA	1755	A
25	BA	1758	U
25	BA	1761	C
25	BA	1764	C
25	BA	1773	A

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Mol	Chain	Res	Type
25	BA	1791	A
25	BA	1800	C
25	BA	1801	A
25	BA	1808	A
25	BA	1811	G
25	BA	1816	C
25	BA	1829	A
25	BA	1833	C
25	BA	1848	A
25	BA	1858	A
25	BA	1859	U
25	BA	1862	G
25	BA	1864	U
25	BA	1869	G
25	BA	1870	C
25	BA	1872	A
25	BA	1905	C
25	BA	1906	G
25	BA	1907	G
25	BA	1912	A
25	BA	1913	A
25	BA	1914	C
25	BA	1917	PSU
25	BA	1918	A
25	BA	1919	A
25	BA	1929	G
25	BA	1930	G
25	BA	1931	U
25	BA	1936	A
25	BA	1938	A
25	BA	1939	5MU
25	BA	1955	U
25	BA	1960	A
25	BA	1965	C
25	BA	1966	A
25	BA	1967	C
25	BA	1970	A
25	BA	1971	U
25	BA	1972	G
25	BA	1987	A
25	BA	1991	U
25	BA	1992	G

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Mol	Chain	Res	Type
25	BA	1993	U
25	BA	1997	C
25	BA	2002	G
25	BA	2022	U
25	BA	2023	C
25	BA	2026	U
25	BA	2031	A
25	BA	2033	A
25	BA	2043	C
25	BA	2051	A
25	BA	2052	A
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2063	C
25	BA	2069	G7M
25	BA	2093	G
25	BA	2097	A
25	BA	2099	U
25	BA	2100	G
25	BA	2101	A
25	BA	2108	A
25	BA	2110	G
25	BA	2111	U
25	BA	2112	G
25	BA	2113	U
25	BA	2115	G
25	BA	2116	G
25	BA	2117	A
25	BA	2118	U
25	BA	2120	G
25	BA	2122	U
25	BA	2124	G
25	BA	2125	G
25	BA	2126	A
25	BA	2127	G
25	BA	2128	G
25	BA	2131	U
25	BA	2132	U
25	BA	2133	G

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Mol	Chain	Res	Type
25	BA	2134	A
25	BA	2139	U
25	BA	2141	G
25	BA	2146	C
25	BA	2147	A
25	BA	2154	A
25	BA	2157	G
25	BA	2158	A
25	BA	2159	G
25	BA	2162	G
25	BA	2163	A
25	BA	2164	C
25	BA	2165	C
25	BA	2169	A
25	BA	2171	A
25	BA	2172	U
25	BA	2178	C
25	BA	2182	U
25	BA	2183	A
25	BA	2185	U
25	BA	2188	U
25	BA	2190	G
25	BA	2197	U
25	BA	2198	A
25	BA	2199	A
25	BA	2203	U
25	BA	2204	G
25	BA	2211	G
25	BA	2212	A
25	BA	2213	U
25	BA	2225	A
25	BA	2226	C
25	BA	2229	U
25	BA	2238	G
25	BA	2239	G
25	BA	2245	U
25	BA	2246	G
25	BA	2250	G
25	BA	2251	OMG
25	BA	2252	G
25	BA	2268	A
25	BA	2278	A

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Mol	Chain	Res	Type
25	BA	2283	C
25	BA	2287	A
25	BA	2294	G
25	BA	2297	A
25	BA	2305	U
25	BA	2308	G
25	BA	2309	A
25	BA	2315	G
25	BA	2322	A
25	BA	2325	G
25	BA	2333	A
25	BA	2335	A
25	BA	2336	A
25	BA	2347	C
25	BA	2350	C
25	BA	2372	U
25	BA	2376	A
25	BA	2383	G
25	BA	2385	C
25	BA	2402	U
25	BA	2403	C
25	BA	2406	A
25	BA	2410	G
25	BA	2423	U
25	BA	2424	C
25	BA	2425	A
25	BA	2426	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U
25	BA	2435	A
25	BA	2441	U
25	BA	2445	2MG
25	BA	2448	A
25	BA	2470	G
25	BA	2474	U
25	BA	2476	A
25	BA	2478	A
25	BA	2491	U
25	BA	2498	OMC
25	BA	2502	G
25	BA	2504	PSU

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Mol	Chain	Res	Type
25	BA	2505	G
25	BA	2512	C
25	BA	2513	A
25	BA	2518	A
25	BA	2520	C
25	BA	2525	G
25	BA	2529	G
25	BA	2535	G
25	BA	2547	A
25	BA	2552	OMU
25	BA	2554	U
25	BA	2566	A
25	BA	2567	G
25	BA	2573	C
25	BA	2574	G
25	BA	2585	U
25	BA	2586	U
25	BA	2602	A
25	BA	2603	G
25	BA	2609	U
25	BA	2610	C
25	BA	2613	U
25	BA	2629	U
25	BA	2630	G
25	BA	2663	G
25	BA	2671	G
25	BA	2682	A
25	BA	2689	U
25	BA	2690	U
25	BA	2714	G
25	BA	2716	C
25	BA	2726	A
25	BA	2744	G
25	BA	2748	A
25	BA	2757	A
25	BA	2762	C
25	BA	2777	G
25	BA	2778	A
25	BA	2791	G
25	BA	2797	U
25	BA	2798	U
25	BA	2799	G

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Mol	Chain	Res	Type
25	BA	2800	A
25	BA	2801	G
25	BA	2818	U
25	BA	2820	A
25	BA	2821	A
25	BA	2825	G
25	BA	2849	U
25	BA	2859	G
25	BA	2861	U
25	BA	2867	G
25	BA	2872	A
25	BA	2879	A
25	BA	2880	C
25	BA	2883	A
25	BA	2884	U
25	BA	2885	G
25	BA	2891	U
25	BA	2902	C
25	BA	2903	U
26	BB	9	G
26	BB	13	G
26	BB	16	G
26	BB	17	C
26	BB	35	C
26	BB	36	C
26	BB	45	A
26	BB	56	G
26	BB	64	G
26	BB	66	A
26	BB	88	C
26	BB	89	U
26	BB	90	C
26	BB	99	A
26	BB	109	A

All (105) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	70	U
1	AA	147	G

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Mol	Chain	Res	Type
1	AA	148	G
1	AA	181	A
1	AA	182	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	873	A
1	AA	961	U
1	AA	991	U
1	AA	992	U
1	AA	1129	C
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
1	AA	1396	A
1	AA	1447	A
22	AV	39	A
23	AW	15	G
23	AW	16	C
23	AW	18	G
23	AW	19	G
23	AW	47	U
23	AW	60	U
25	BA	33	C
25	BA	62	U
25	BA	71	A
25	BA	101	A
25	BA	137	U
25	BA	138	U
25	BA	140	C

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Mol	Chain	Res	Type
25	BA	196	A
25	BA	199	A
25	BA	271	G
25	BA	310	A
25	BA	404	A
25	BA	503	A
25	BA	685	A
25	BA	764	A
25	BA	776	G
25	BA	784	G
25	BA	883	G
25	BA	884	U
25	BA	892	A
25	BA	984	A
25	BA	1045	C
25	BA	1060	U
25	BA	1064	C
25	BA	1067	A
25	BA	1069	A
25	BA	1109	C
25	BA	1111	A
25	BA	1128	G
25	BA	1173	U
25	BA	1300	G
25	BA	1320	C
25	BA	1344	U
25	BA	1395	A
25	BA	1405	U
25	BA	1407	G
25	BA	1408	G
25	BA	1434	A
25	BA	1490	A
25	BA	1494	A
25	BA	1509	A
25	BA	1596	A
25	BA	1608	A
25	BA	1913	A
25	BA	1918	A
25	BA	2062	A
25	BA	2146	C
25	BA	2162	G
25	BA	2168	G

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Mol	Chain	Res	Type
25	BA	2197	U
25	BA	2198	A
25	BA	2210	U
25	BA	2212	A
25	BA	2225	A
25	BA	2250	G
25	BA	2296	U
25	BA	2308	G
25	BA	2425	A
25	BA	2573	C
25	BA	2585	U
25	BA	2601	C
25	BA	2610	C
25	BA	2756	U
25	BA	2797	U
25	BA	2798	U
25	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	$\#\|Z\| > 2$
1	4OC	AA	1402	1,60	20,23,24	3.29	9 (45%)	26,32,35	1.05	3 (11%)
25	PSU	BA	746	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.04	6 (27%)
1	G7M	AA	527	1	20,26,27	2.24	8 (40%)	17,39,42	1.31	2 (11%)
24	H2U	AX	20	24	18,21,22	3.21	5 (27%)	21,30,33	1.90	5 (23%)
25	5MU	BA	747	25	19,22,23	1.41	4 (21%)	28,32,35	2.25	6 (21%)
25	G7M	BA	2069	25	20,26,27	2.21	8 (40%)	17,39,42	1.24	1 (5%)
24	PSU	AX	39	24	18,21,22	1.11	2 (11%)	22,30,33	1.86	4 (18%)
25	PSU	BA	2457	25	18,21,22	1.06	2 (11%)	22,30,33	2.09	6 (27%)
24	3AU	AX	47	24	18,21,29	3.41	8 (44%)	26,30,43	1.66	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	H2U	AX	16	24	18,21,22	2.99	5 (27%)	21,30,33	1.94	5 (23%)
23	H2U	AW	20	23	18,21,22	3.05	5 (27%)	21,30,33	2.03	4 (19%)
1	5MC	AA	1407	1	18,22,23	3.75	7 (38%)	26,32,35	1.03	1 (3%)
25	5MC	BA	1962	25	18,22,23	3.70	7 (38%)	26,32,35	1.11	1 (3%)
25	PSU	BA	2580	25	18,21,22	1.09	2 (11%)	22,30,33	2.27	8 (36%)
1	MA6	AA	1518	1	18,26,27	1.40	3 (16%)	19,38,41	3.96	2 (10%)
24	PSU	AX	32	24	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
24	7MG	AX	46	24	20,25,27	3.16	10 (50%)	27,37,42	2.05	7 (25%)
23	4SU	AW	8	23	18,21,22	4.08	8 (44%)	26,30,33	2.21	5 (19%)
25	2MG	BA	2445	29,25	18,26,27	2.18	7 (38%)	16,38,41	1.63	4 (25%)
1	MA6	AA	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.51	2 (10%)
1	2MG	AA	1516	1	18,26,27	2.20	7 (38%)	16,38,41	1.65	4 (25%)
25	OMU	BA	2552	25	19,22,23	2.80	6 (31%)	26,31,34	1.85	5 (19%)
1	PSU	AA	516	1,60	18,21,22	1.03	2 (11%)	22,30,33	2.04	7 (31%)
1	2MG	AA	966	1	18,25,27	2.54	8 (44%)	19,37,41	1.69	5 (26%)
1	5MC	AA	967	1	18,22,23	3.85	7 (38%)	26,32,35	1.11	2 (7%)
28	MEQ	BD	150	28	8,9,10	0.94	0	5,10,12	0.97	1 (20%)
25	6MZ	BA	1618	25	18,25,26	1.96	3 (16%)	16,36,39	2.19	3 (18%)
25	PSU	BA	2604	25	18,21,22	1.04	2 (11%)	22,30,33	1.90	5 (22%)
23	OMC	AW	32	23	19,22,23	2.90	8 (42%)	26,31,34	0.82	0
12	D2T	AL	89	12	6,7,10	1.02	0	5,8,13	1.07	0
25	PSU	BA	2605	25	18,21,22	1.08	2 (11%)	22,30,33	1.88	3 (13%)
25	3TD	BA	1915	25	18,22,23	4.39	10 (55%)	22,32,35	2.04	4 (18%)
24	PSU	AX	55	24	18,21,22	1.01	1 (5%)	22,30,33	1.94	5 (22%)
24	4SU	AX	8	24	18,21,22	4.03	8 (44%)	26,30,33	2.20	4 (15%)
23	PSU	AW	55	23	18,21,22	1.03	1 (5%)	22,30,33	1.96	5 (22%)
25	5MU	BA	1939	25,60	19,22,23	1.45	3 (15%)	28,32,35	2.36	6 (21%)
25	PSU	BA	2504	25,60	18,21,22	1.12	3 (16%)	22,30,33	2.11	6 (27%)
25	2MG	BA	1835	25	18,26,27	2.23	7 (38%)	16,38,41	1.57	4 (25%)
36	4D4	BN	81	36	9,11,12	2.47	3 (33%)	8,13,15	0.84	0
25	OMC	BA	2498	25,60	19,22,23	2.69	7 (36%)	26,31,34	0.84	1 (3%)
25	OMG	BA	2251	25,23	18,26,27	2.54	8 (44%)	19,38,41	1.48	4 (21%)
1	2MG	AA	1207	1	18,25,27	2.49	8 (44%)	19,37,41	1.66	5 (26%)
25	1MG	BA	745	25	18,26,27	2.55	4 (22%)	19,39,42	1.52	4 (21%)
25	6MZ	BA	2030	25	18,25,26	1.95	3 (16%)	16,36,39	2.61	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	PSU	BA	1917	25	18,21,22	1.00	3 (16%)	22,30,33	1.90	5 (22%)
1	UR3	AA	1498	1	19,22,23	2.40	6 (31%)	26,32,35	1.29	1 (3%)
25	PSU	BA	955	25,36	18,21,22	1.17	3 (16%)	22,30,33	1.94	5 (22%)
25	PSU	BA	1911	25	18,21,22	1.11	2 (11%)	22,30,33	1.87	4 (18%)
24	MIA	AX	37	24	18,24,32	1.48	3 (16%)	18,35,47	1.53	2 (11%)
25	H2U	BA	2449	25	18,21,22	2.74	5 (27%)	21,30,33	2.10	5 (23%)
24	5MU	AX	54	24	19,22,23	1.37	4 (21%)	28,32,35	2.11	6 (21%)
25	2MA	BA	2503	25,60	17,25,26	2.58	6 (35%)	17,37,40	1.45	4 (23%)
23	5MU	AW	54	23	19,22,23	1.38	5 (26%)	28,32,35	2.20	8 (28%)

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
1	4OC	AA	1402	1,60	-	0/9/29/30	0/2/2/2
25	PSU	BA	746	25,60	-	1/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
24	H2U	AX	20	24	-	5/7/38/39	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
24	3AU	AX	47	24	-	0/7/25/35	0/2/2/2
24	H2U	AX	16	24	-	1/7/38/39	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
25	5MC	BA	1962	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	3/7/29/30	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	4/7/34/38	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	2MG	BA	2445	29,25	-	2/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	6/7/29/30	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
25	OMU	BA	2552	25	-	2/9/27/28	0/2/2/2
1	PSU	AA	516	1,60	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	966	1	-	2/3/25/28	0/3/3/3
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
28	MEQ	BD	150	28	-	3/8/9/11	-
25	6MZ	BA	1618	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2604	25	-	0/7/25/26	0/2/2/2
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
12	D2T	AL	89	12	-	1/5/6/14	-
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
25	3TD	BA	1915	25	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	2/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	1/7/25/26	0/2/2/2
25	5MU	BA	1939	25,60	-	2/7/25/26	0/2/2/2
25	PSU	BA	2504	25,60	-	0/7/25/26	0/2/2/2
25	2MG	BA	1835	25	-	0/5/27/28	0/3/3/3
36	4D4	BN	81	36	-	7/11/12/14	-
25	OMC	BA	2498	25,60	-	2/9/27/28	0/2/2/2
25	OMG	BA	2251	25,23	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	2/3/25/28	0/3/3/3
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	1917	25	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
25	PSU	BA	955	25,36	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/3/25/34	0/3/3/3
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	2MA	BA	2503	25,60	-	2/3/25/26	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2

All (255) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.44	1.48	1.35
24	AX	20	H2U	C2-N1	10.34	1.50	1.35
25	BA	1915	3TD	C2-N1	9.65	1.49	1.37
23	AW	20	H2U	C2-N1	9.55	1.49	1.35
1	AA	967	5MC	C6-C5	9.49	1.50	1.34
1	AA	1407	5MC	C6-C5	9.43	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	8	4SU	C4-N3	9.20	1.47	1.37
23	AW	8	4SU	C4-N3	9.20	1.47	1.37
24	AX	16	H2U	C2-N1	9.13	1.48	1.35
25	BA	1962	5MC	C6-C5	9.08	1.49	1.34
25	BA	2449	H2U	C2-N1	7.99	1.47	1.35
24	AX	8	4SU	C2-N1	7.51	1.50	1.38
24	AX	47	3AU	C2-N1	7.51	1.50	1.38
23	AW	8	4SU	C2-N1	7.48	1.50	1.38
25	BA	745	1MG	C2-N3	7.32	1.48	1.34
1	AA	967	5MC	C4-N3	7.15	1.46	1.34
25	BA	1962	5MC	C4-N3	7.10	1.46	1.34
25	BA	2503	2MA	C2-N3	7.10	1.46	1.31
24	AX	47	3AU	C6-C5	7.01	1.51	1.35
1	AA	1407	5MC	C4-N3	6.76	1.45	1.34
1	AA	967	5MC	C2-N3	6.56	1.49	1.36
1	AA	1402	4OC	C4-N3	6.55	1.44	1.32
24	AX	47	3AU	C2-N3	6.46	1.49	1.38
25	BA	2552	OMU	C2-N3	6.43	1.49	1.38
25	BA	1618	6MZ	C6-N6	6.41	1.45	1.35
1	AA	1407	5MC	C2-N3	6.38	1.49	1.36
24	AX	20	H2U	C2-N3	6.36	1.49	1.38
23	AW	8	4SU	C2-N3	6.34	1.49	1.38
1	AA	1402	4OC	C6-C5	6.31	1.49	1.35
24	AX	16	H2U	C2-N3	6.31	1.49	1.38
25	BA	2030	6MZ	C6-N6	6.31	1.45	1.35
25	BA	1962	5MC	C2-N3	6.30	1.49	1.36
23	AW	20	H2U	C2-N3	6.27	1.49	1.38
24	AX	8	4SU	C2-N3	6.25	1.49	1.38
23	AW	32	OMC	C2-N3	6.20	1.48	1.36
23	AW	8	4SU	C6-C5	6.02	1.49	1.35
1	AA	966	2MG	C2-N3	5.94	1.47	1.33
25	BA	1915	3TD	C6-N1	5.92	1.46	1.36
24	AX	8	4SU	C6-C5	5.90	1.48	1.35
23	AW	32	OMC	C6-C5	5.82	1.48	1.35
1	AA	1498	UR3	C6-C5	5.77	1.48	1.35
24	AX	46	7MG	C4-N3	5.75	1.47	1.34
25	BA	2552	OMU	C6-C5	5.74	1.48	1.35
24	AX	46	7MG	C2-N3	5.73	1.47	1.33
24	AX	8	4SU	C4-S4	-5.71	1.57	1.68
25	BA	2449	H2U	C2-N3	5.68	1.48	1.38
36	BN	81	4D4	CZ-NE	5.66	1.44	1.33
1	AA	1207	2MG	C2-N3	5.60	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2498	OMC	C2-N3	5.56	1.47	1.36
23	AW	8	4SU	C4-S4	-5.50	1.58	1.68
23	AW	8	4SU	C5-C4	5.49	1.49	1.42
25	BA	2498	OMC	C6-C5	5.49	1.47	1.35
1	AA	1498	UR3	C2-N1	5.48	1.46	1.38
1	AA	1402	4OC	C2-N3	5.46	1.47	1.36
25	BA	1915	3TD	C1'-C5	-5.42	1.37	1.50
1	AA	967	5MC	C4-N4	5.31	1.47	1.34
25	BA	1962	5MC	C4-N4	5.31	1.47	1.34
1	AA	1402	4OC	O2-C2	-5.22	1.14	1.23
24	AX	46	7MG	C4-N9	5.21	1.43	1.37
1	AA	1407	5MC	C4-N4	5.16	1.47	1.34
25	BA	2503	2MA	C4-N3	5.13	1.49	1.37
24	AX	47	3AU	C4-N3	5.09	1.47	1.38
25	BA	2251	OMG	C2-N2	5.07	1.46	1.34
25	BA	745	1MG	C2-N2	4.96	1.43	1.34
25	BA	2251	OMG	C4-N3	4.91	1.49	1.37
24	AX	8	4SU	C5-C4	4.90	1.48	1.42
24	AX	16	H2U	C4-N3	4.89	1.45	1.37
25	BA	2552	OMU	C2-N1	4.88	1.46	1.38
23	AW	32	OMC	C4-N3	4.87	1.44	1.34
25	BA	2251	OMG	C2-N3	4.87	1.45	1.33
1	AA	967	5MC	C6-N1	4.86	1.46	1.38
24	AX	20	H2U	C4-N3	4.82	1.45	1.37
1	AA	1402	4OC	C4-N4	4.80	1.45	1.35
1	AA	1407	5MC	C6-N1	4.73	1.46	1.38
1	AA	527	G7M	C2-N3	4.73	1.44	1.33
23	AW	32	OMC	C4-N4	4.72	1.45	1.33
23	AW	20	H2U	C4-N3	4.72	1.45	1.37
24	AX	46	7MG	C2-N2	4.66	1.45	1.34
25	BA	1915	3TD	C2-N3	4.61	1.48	1.38
1	AA	967	5MC	C2-N1	4.58	1.49	1.40
25	BA	2069	G7M	C2-N3	4.57	1.44	1.33
1	AA	527	G7M	C2-N2	4.52	1.44	1.34
25	BA	2498	OMC	C4-N4	4.51	1.44	1.33
25	BA	1962	5MC	C6-N1	4.51	1.45	1.38
25	BA	745	1MG	C4-N3	4.40	1.48	1.37
25	BA	2498	OMC	C4-N3	4.40	1.43	1.34
25	BA	2069	G7M	C2-N2	4.33	1.44	1.34
25	BA	2069	G7M	C4-N3	4.32	1.47	1.37
25	BA	1835	2MG	C2-N2	4.28	1.42	1.33
1	AA	1407	5MC	C2-N1	4.25	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	G7M	C4-N3	4.18	1.47	1.37
1	AA	1402	4OC	C5-C4	4.17	1.49	1.40
25	BA	2449	H2U	C4-N3	4.17	1.44	1.37
1	AA	1516	2MG	C2-N2	4.15	1.42	1.33
24	AX	46	7MG	C5-C4	4.15	1.43	1.37
23	AW	32	OMC	C2-N1	4.13	1.49	1.40
1	AA	966	2MG	C2-N2	4.09	1.43	1.34
24	AX	46	7MG	C2-N1	4.09	1.47	1.37
25	BA	2445	2MG	C2-N2	4.07	1.42	1.33
24	AX	46	7MG	C5-C6	4.05	1.52	1.42
24	AX	37	MIA	C6-N6	4.05	1.48	1.34
25	BA	2552	OMU	O4-C4	-4.05	1.16	1.24
1	AA	1498	UR3	C2-N3	4.02	1.46	1.39
1	AA	966	2MG	C4-N3	3.98	1.47	1.37
1	AA	1207	2MG	C2-N2	3.93	1.43	1.34
25	BA	1962	5MC	C2-N1	3.86	1.48	1.40
1	AA	1207	2MG	C6-N1	3.80	1.43	1.37
25	BA	1835	2MG	C6-N1	3.76	1.43	1.37
1	AA	966	2MG	C6-N1	3.75	1.43	1.37
1	AA	1402	4OC	C2-N1	3.75	1.48	1.40
1	AA	1516	2MG	C6-N1	3.72	1.43	1.37
1	AA	1516	2MG	C2-N1	3.70	1.42	1.36
1	AA	1207	2MG	C4-N3	3.69	1.46	1.37
25	BA	1835	2MG	C4-N3	3.68	1.46	1.37
25	BA	2445	2MG	C2-N1	3.65	1.42	1.36
25	BA	2251	OMG	C6-N1	3.63	1.43	1.37
25	BA	2552	OMU	C4-N3	3.63	1.45	1.38
25	BA	2445	2MG	O6-C6	-3.59	1.16	1.23
24	AX	46	7MG	O6-C6	-3.52	1.16	1.23
25	BA	2445	2MG	C6-N1	3.52	1.43	1.37
1	AA	1207	2MG	O6-C6	-3.52	1.16	1.23
25	BA	2498	OMC	C2-N1	3.52	1.47	1.40
25	BA	1835	2MG	O6-C6	-3.52	1.16	1.23
25	BA	1835	2MG	C2-N1	3.49	1.42	1.36
1	AA	1402	4OC	CM4-N4	3.48	1.51	1.45
25	BA	2445	2MG	C4-N3	3.45	1.45	1.37
25	BA	1939	5MU	C4-N3	-3.42	1.32	1.38
1	AA	966	2MG	O6-C6	-3.40	1.16	1.23
1	AA	1516	2MG	C4-N3	3.39	1.45	1.37
25	BA	2552	OMU	O2-C2	-3.39	1.16	1.23
1	AA	1516	2MG	O6-C6	-3.38	1.16	1.23
24	AX	46	7MG	C6-N1	3.37	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	39	PSU	C6-C5	3.33	1.39	1.35
25	BA	747	5MU	C4-N3	-3.32	1.32	1.38
24	AX	47	3AU	C6-N1	3.32	1.46	1.38
25	BA	1939	5MU	C6-N1	-3.29	1.32	1.38
23	AW	8	4SU	O2-C2	-3.29	1.17	1.23
25	BA	2251	OMG	C5-C4	-3.24	1.34	1.43
36	BN	81	4D4	CZ-NH2	3.23	1.45	1.32
25	BA	2498	OMC	O2-C2	-3.23	1.17	1.23
25	BA	2069	G7M	C6-N1	3.17	1.42	1.37
1	AA	527	G7M	C6-N1	3.17	1.42	1.37
25	BA	2030	6MZ	C5-C4	-3.17	1.32	1.40
24	AX	8	4SU	O2-C2	-3.16	1.17	1.23
1	AA	1519	MA6	C5-C4	-3.16	1.32	1.40
23	AW	8	4SU	C6-N1	3.13	1.45	1.38
1	AA	1518	MA6	C5-C4	-3.11	1.32	1.40
25	BA	2445	2MG	C5-C4	-3.08	1.35	1.43
25	BA	2503	2MA	C5-C4	-3.07	1.35	1.43
1	AA	1207	2MG	C5-C4	-3.04	1.35	1.43
1	AA	1518	MA6	C2-N3	3.03	1.37	1.32
25	BA	1835	2MG	C5-C4	-3.03	1.35	1.43
25	BA	2503	2MA	C6-N1	3.03	1.44	1.38
25	BA	1911	PSU	C6-C5	3.03	1.38	1.35
24	AX	46	7MG	C5-N7	3.02	1.44	1.35
1	AA	1516	2MG	C5-C4	-3.02	1.35	1.43
25	BA	1618	6MZ	C5-C4	-3.01	1.33	1.40
24	AX	32	PSU	C6-C5	3.00	1.38	1.35
25	BA	1939	5MU	C2-N3	-2.99	1.32	1.38
24	AX	8	4SU	C6-N1	2.98	1.45	1.38
24	AX	47	3AU	O4-C4	-2.96	1.18	1.24
25	BA	747	5MU	C6-N1	-2.95	1.33	1.38
23	AW	32	OMC	O2-C2	-2.94	1.18	1.23
25	BA	1915	3TD	O2-C2	-2.91	1.17	1.23
23	AW	55	PSU	C6-C5	2.90	1.38	1.35
1	AA	966	2MG	C5-C4	-2.89	1.35	1.43
24	AX	47	3AU	C5-C4	2.89	1.50	1.43
23	AW	32	OMC	C6-N1	2.87	1.44	1.38
25	BA	1915	3TD	C4-N3	2.82	1.46	1.40
25	BA	2498	OMC	C6-N1	2.80	1.44	1.38
1	AA	1498	UR3	O2-C2	-2.78	1.17	1.22
24	AX	54	5MU	C4-N3	-2.77	1.33	1.38
25	BA	1962	5MC	O2-C2	-2.77	1.18	1.23
25	BA	1915	3TD	O4-C4	-2.75	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	55	PSU	C6-C5	2.74	1.38	1.35
25	BA	2449	H2U	O2-C2	-2.73	1.18	1.23
1	AA	1518	MA6	C10-N6	2.71	1.51	1.45
25	BA	746	PSU	O4'-C1'	-2.71	1.40	1.43
25	BA	747	5MU	C2-N3	-2.68	1.33	1.38
1	AA	966	2MG	C5-C6	2.67	1.52	1.47
1	AA	1402	4OC	C6-N1	2.66	1.44	1.38
1	AA	527	G7M	C5-C6	2.66	1.52	1.45
25	BA	1915	3TD	C10-N3	2.65	1.51	1.47
1	AA	1519	MA6	C2-N3	2.64	1.36	1.32
1	AA	1207	2MG	C5-C6	2.63	1.52	1.47
24	AX	37	MIA	C5-C4	-2.60	1.34	1.40
23	AW	54	5MU	C4-N3	-2.59	1.34	1.38
1	AA	1516	2MG	C5-C6	2.58	1.52	1.47
1	AA	527	G7M	O6-C6	-2.57	1.18	1.23
25	BA	2503	2MA	CM2-C2	2.57	1.56	1.49
1	AA	1519	MA6	C10-N6	2.56	1.51	1.45
25	BA	2069	G7M	O6-C6	-2.54	1.18	1.23
1	AA	1407	5MC	O2-C2	-2.53	1.19	1.23
23	AW	20	H2U	O2-C2	-2.53	1.18	1.23
1	AA	967	5MC	O2-C2	-2.51	1.19	1.23
24	AX	54	5MU	C6-N1	-2.51	1.33	1.38
24	AX	47	3AU	O2-C2	-2.50	1.18	1.23
25	BA	2504	PSU	C6-C5	2.49	1.38	1.35
25	BA	2069	G7M	C5-C6	2.49	1.51	1.45
1	AA	516	PSU	C6-C5	2.48	1.38	1.35
23	AW	54	5MU	C6-N1	-2.48	1.33	1.38
1	AA	1498	UR3	O4-C4	-2.48	1.18	1.23
25	BA	745	1MG	C5-C4	-2.47	1.36	1.43
1	AA	1498	UR3	C6-N1	2.46	1.43	1.38
23	AW	54	5MU	C4-C5	2.46	1.48	1.44
25	BA	2251	OMG	C5-C6	2.45	1.52	1.47
24	AX	54	5MU	C6-C5	2.45	1.38	1.34
25	BA	2449	H2U	O4-C4	-2.42	1.18	1.23
25	BA	955	PSU	C4-C5	-2.39	1.37	1.44
36	BN	81	4D4	CZ-NH1	-2.36	1.25	1.34
1	AA	527	G7M	C2-N1	2.35	1.43	1.37
25	BA	2251	OMG	C2-N1	2.35	1.43	1.37
24	AX	20	H2U	O2-C2	-2.34	1.18	1.23
25	BA	955	PSU	C6-C5	2.32	1.38	1.35
25	BA	1835	2MG	C5-C6	2.31	1.52	1.47
25	BA	2251	OMG	O6-C6	-2.30	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2503	2MA	C2-N1	2.29	1.43	1.36
25	BA	2504	PSU	O4'-C1'	-2.29	1.40	1.43
25	BA	2580	PSU	C4-C5	-2.28	1.37	1.44
25	BA	2605	PSU	C6-C5	2.28	1.38	1.35
23	AW	54	5MU	C6-C5	2.28	1.38	1.34
24	AX	16	H2U	O2-C2	-2.27	1.18	1.23
24	AX	20	H2U	O4-C4	-2.27	1.18	1.23
25	BA	2604	PSU	C4-C5	-2.27	1.37	1.44
25	BA	2069	G7M	C2-N1	2.26	1.43	1.37
1	AA	527	G7M	C5-C4	-2.24	1.34	1.39
24	AX	54	5MU	C2-N3	-2.24	1.34	1.38
25	BA	1915	3TD	O4'-C1'	-2.22	1.40	1.43
23	AW	32	OMC	C5-C4	2.22	1.48	1.42
25	BA	746	PSU	C4-C5	-2.22	1.37	1.44
25	BA	2580	PSU	C6-C5	2.22	1.37	1.35
23	AW	54	5MU	C2-N3	-2.21	1.34	1.38
25	BA	2604	PSU	C6-C5	2.20	1.37	1.35
24	AX	16	H2U	O4-C4	-2.20	1.18	1.23
25	BA	2069	G7M	C5-C4	-2.19	1.34	1.39
25	BA	1917	PSU	O4'-C1'	-2.18	1.40	1.43
24	AX	37	MIA	C2-N3	2.17	1.35	1.32
25	BA	1917	PSU	C4-C5	-2.17	1.38	1.44
25	BA	1618	6MZ	C2-N3	2.15	1.35	1.32
23	AW	20	H2U	O4-C4	-2.15	1.18	1.23
25	BA	2504	PSU	C4-C5	-2.14	1.38	1.44
25	BA	2457	PSU	C6-C5	2.14	1.37	1.35
25	BA	2457	PSU	C4-C5	-2.13	1.38	1.44
25	BA	1911	PSU	O4'-C1'	-2.11	1.40	1.43
25	BA	2445	2MG	C5-C6	2.11	1.51	1.47
25	BA	1917	PSU	C6-C5	2.10	1.37	1.35
1	AA	516	PSU	C4-C5	-2.10	1.38	1.44
25	BA	2030	6MZ	C6-N1	-2.09	1.31	1.34
25	BA	746	PSU	C6-C5	2.09	1.37	1.35
1	AA	1207	2MG	C2-N1	2.07	1.42	1.37
25	BA	2605	PSU	C4-C5	-2.07	1.38	1.44
1	AA	966	2MG	C2-N1	2.05	1.42	1.37
25	BA	955	PSU	C2'-C1'	-2.02	1.51	1.53
24	AX	39	PSU	C4-C5	-2.02	1.38	1.44
25	BA	747	5MU	C6-C5	2.02	1.37	1.34

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-18.57	97.51	117.06
1	AA	1518	MA6	N1-C6-N6	-16.24	99.97	117.06
23	AW	8	4SU	C4-N3-C2	-7.77	119.79	127.34
24	AX	8	4SU	C4-N3-C2	-7.50	120.05	127.34
25	BA	2030	6MZ	C9-N6-C6	-7.37	116.52	122.87
25	BA	2449	H2U	C4-N3-C2	-7.12	119.89	125.79
23	AW	20	H2U	C4-N3-C2	-7.00	119.98	125.79
24	AX	46	7MG	C5-C4-N3	-6.80	120.78	127.80
24	AX	16	H2U	C4-N3-C2	-6.74	120.20	125.79
24	AX	20	H2U	C4-N3-C2	-6.50	120.40	125.79
25	BA	1915	3TD	N1-C2-N3	6.22	121.05	116.14
25	BA	1939	5MU	C4-N3-C2	-5.94	119.66	127.35
24	AX	8	4SU	C5-C4-N3	5.81	120.08	114.69
25	BA	2552	OMU	C4-N3-C2	-5.80	118.92	126.58
25	BA	747	5MU	C4-N3-C2	-5.80	119.84	127.35
1	AA	1519	MA6	N3-C2-N1	-5.73	119.72	128.68
25	BA	2030	6MZ	N3-C2-N1	-5.70	119.76	128.68
25	BA	1618	6MZ	N3-C2-N1	-5.50	120.09	128.68
23	AW	8	4SU	C5-C4-N3	5.48	119.77	114.69
24	AX	37	MIA	N3-C2-N1	-5.48	120.11	128.68
25	BA	1939	5MU	N3-C2-N1	5.42	122.09	114.89
25	BA	1618	6MZ	C9-N6-C6	-5.34	118.27	122.87
24	AX	54	5MU	C4-N3-C2	-5.31	120.47	127.35
25	BA	747	5MU	N3-C2-N1	5.29	121.92	114.89
23	AW	54	5MU	C4-N3-C2	-5.28	120.51	127.35
25	BA	2457	PSU	C4-N3-C2	-5.23	118.81	126.34
25	BA	2504	PSU	N1-C2-N3	5.23	121.05	115.13
1	AA	1518	MA6	N3-C2-N1	-5.21	120.54	128.68
25	BA	2580	PSU	N1-C2-N3	5.17	120.99	115.13
25	BA	2580	PSU	C4-N3-C2	-5.14	118.94	126.34
24	AX	54	5MU	N3-C2-N1	5.09	121.65	114.89
25	BA	2605	PSU	C4-N3-C2	-5.06	119.06	126.34
24	AX	55	PSU	C4-N3-C2	-5.02	119.10	126.34
25	BA	955	PSU	C4-N3-C2	-4.99	119.14	126.34
25	BA	2504	PSU	C4-N3-C2	-4.99	119.15	126.34
24	AX	47	3AU	C4-N3-C2	-4.97	120.02	126.58
23	AW	54	5MU	C5-C4-N3	4.94	119.53	115.31
25	BA	2604	PSU	C4-N3-C2	-4.93	119.24	126.34
25	BA	747	5MU	C5-C4-N3	4.89	119.49	115.31
25	BA	1939	5MU	C5-C4-N3	4.88	119.47	115.31
25	BA	955	PSU	N1-C2-N3	4.85	120.62	115.13
1	AA	1498	UR3	C4-N3-C2	-4.84	120.01	124.56
25	BA	2457	PSU	N1-C2-N3	4.82	120.59	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	55	PSU	N1-C2-N3	4.78	120.54	115.13
1	AA	516	PSU	C4-N3-C2	-4.72	119.54	126.34
25	BA	1911	PSU	N1-C2-N3	4.72	120.47	115.13
24	AX	39	PSU	N1-C2-N3	4.71	120.47	115.13
25	BA	1939	5MU	C5-C6-N1	-4.70	118.50	123.34
23	AW	55	PSU	C4-N3-C2	-4.68	119.60	126.34
25	BA	2604	PSU	N1-C2-N3	4.65	120.40	115.13
25	BA	1911	PSU	C4-N3-C2	-4.65	119.64	126.34
25	BA	1917	PSU	N1-C2-N3	4.63	120.37	115.13
25	BA	1917	PSU	C4-N3-C2	-4.62	119.68	126.34
24	AX	39	PSU	C4-N3-C2	-4.61	119.70	126.34
25	BA	746	PSU	C4-N3-C2	-4.60	119.71	126.34
25	BA	2605	PSU	N1-C2-N3	4.52	120.25	115.13
24	AX	32	PSU	C4-N3-C2	-4.50	119.85	126.34
23	AW	54	5MU	N3-C2-N1	4.48	120.84	114.89
25	BA	746	PSU	N1-C2-N3	4.46	120.19	115.13
24	AX	54	5MU	C5-C4-N3	4.42	119.08	115.31
25	BA	747	5MU	C5-C6-N1	-4.38	118.83	123.34
23	AW	55	PSU	N1-C2-N3	4.32	120.03	115.13
25	BA	1939	5MU	O4-C4-C5	-4.26	119.96	124.90
24	AX	54	5MU	O4-C4-C5	-4.26	119.96	124.90
25	BA	1915	3TD	C4-N3-C2	-4.25	120.00	124.61
24	AX	32	PSU	N1-C2-N3	4.20	119.89	115.13
24	AX	46	7MG	C2-N3-C4	4.20	119.78	112.30
25	BA	1962	5MC	C5-C6-N1	-4.11	119.11	123.34
25	BA	745	1MG	C5-C6-N1	4.10	120.07	113.90
1	AA	516	PSU	N1-C2-N3	4.08	119.75	115.13
25	BA	1939	5MU	O2-C2-N1	-4.01	117.46	122.79
25	BA	2552	OMU	N3-C2-N1	3.99	120.19	114.89
23	AW	8	4SU	N3-C2-N1	3.91	120.08	114.89
24	AX	47	3AU	N3-C2-N1	3.87	120.03	114.89
24	AX	8	4SU	C5-C4-S4	-3.87	119.48	124.47
25	BA	2503	2MA	C5-C6-N1	3.84	120.65	114.02
1	AA	1516	2MG	CM2-N2-C2	-3.83	115.39	123.86
23	AW	54	5MU	O4-C4-C5	-3.83	120.46	124.90
23	AW	54	5MU	C5-C6-N1	-3.81	119.42	123.34
25	BA	1915	3TD	C6-C5-C4	3.80	120.85	118.22
24	AX	54	5MU	C5-C6-N1	-3.70	119.54	123.34
1	AA	1207	2MG	C5-C6-N1	3.68	120.45	113.95
25	BA	747	5MU	O4-C4-C5	-3.68	120.64	124.90
25	BA	2552	OMU	C5-C4-N3	3.65	120.30	114.84
25	BA	2030	6MZ	C2-N1-C6	3.63	119.70	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	966	2MG	C5-C6-N1	3.60	120.31	113.95
25	BA	747	5MU	O2-C2-N1	-3.56	118.05	122.79
23	AW	20	H2U	N3-C2-N1	3.53	120.38	116.65
1	AA	1407	5MC	C5-C6-N1	-3.52	119.71	123.34
25	BA	1835	2MG	C5-C6-N1	3.48	120.10	113.95
25	BA	2449	H2U	N3-C2-N1	3.45	120.30	116.65
25	BA	2445	2MG	C5-C6-N1	3.44	120.03	113.95
25	BA	1618	6MZ	C2-N1-C6	3.43	119.53	116.59
25	BA	2445	2MG	CM2-N2-C2	-3.43	116.29	123.86
1	AA	1516	2MG	C5-C6-N1	3.42	119.99	113.95
1	AA	967	5MC	C5-C6-N1	-3.39	119.85	123.34
24	AX	47	3AU	C5-C4-N3	3.38	119.90	114.84
25	BA	2251	OMG	C5-C6-N1	3.37	119.91	113.95
24	AX	8	4SU	N3-C2-N1	3.26	119.22	114.89
25	BA	1917	PSU	O2-C2-N1	-3.25	119.21	122.79
25	BA	1911	PSU	O2-C2-N1	-3.22	119.24	122.79
23	AW	8	4SU	C5-C4-S4	-3.22	120.32	124.47
25	BA	2552	OMU	O4-C4-C5	-3.15	119.62	125.16
24	AX	46	7MG	O6-C6-C5	-3.15	120.02	127.24
1	AA	1207	2MG	C2-N1-C6	-3.14	119.31	125.10
25	BA	2449	H2U	O2-C2-N1	-3.04	119.29	123.11
1	AA	527	G7M	C2-N1-C6	-3.04	119.50	125.10
1	AA	966	2MG	C2-N1-C6	-3.03	119.52	125.10
1	AA	516	PSU	O2-C2-N1	-3.00	119.49	122.79
23	AW	54	5MU	C5M-C5-C4	2.98	122.05	118.77
24	AX	20	H2U	C5-C4-N3	2.97	119.99	116.65
25	BA	955	PSU	O2-C2-N1	-2.96	119.53	122.79
25	BA	2504	PSU	O2-C2-N1	-2.95	119.54	122.79
25	BA	2604	PSU	O2-C2-N1	-2.95	119.55	122.79
25	BA	1917	PSU	C6-N1-C2	-2.90	119.72	122.68
25	BA	1835	2MG	CM2-N2-C2	-2.90	117.45	123.86
24	AX	46	7MG	C2-N1-C6	-2.90	119.81	125.10
24	AX	47	3AU	O4-C4-C5	-2.90	120.06	125.16
1	AA	516	PSU	O4'-C1'-C2'	2.90	109.23	105.14
25	BA	746	PSU	O2-C2-N1	-2.89	119.61	122.79
25	BA	2580	PSU	O2-C2-N1	-2.89	119.61	122.79
25	BA	2503	2MA	C8-N7-C5	2.86	108.44	102.99
25	BA	2251	OMG	C2-N1-C6	-2.86	119.83	125.10
24	AX	20	H2U	C5-C6-N1	2.85	121.01	111.61
25	BA	2069	G7M	C2-N1-C6	-2.85	119.86	125.10
24	AX	16	H2U	C5-C4-N3	2.82	119.82	116.65
25	BA	2251	OMG	C8-N7-C5	2.81	108.34	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	2580	PSU	O4'-C1'-C2'	2.79	109.08	105.14
1	AA	1207	2MG	C8-N7-C5	2.79	108.31	102.99
24	AX	55	PSU	O2-C2-N1	-2.79	119.72	122.79
24	AX	16	H2U	N3-C2-N1	2.77	119.59	116.65
23	AW	20	H2U	C5-C4-N3	2.77	119.76	116.65
23	AW	20	H2U	C5-C6-N1	2.76	120.72	111.61
25	BA	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64
25	BA	2449	H2U	C5-C4-N3	2.74	119.73	116.65
24	AX	39	PSU	O2-C2-N1	-2.74	119.78	122.79
25	BA	2580	PSU	C6-N1-C2	-2.71	119.92	122.68
1	AA	966	2MG	C8-N7-C5	2.68	108.10	102.99
1	AA	516	PSU	C3'-C2'-C1'	2.66	104.74	101.64
25	BA	745	1MG	C8-N7-C5	2.66	108.06	102.99
24	AX	20	H2U	N3-C2-N1	2.66	119.47	116.65
25	BA	746	PSU	C6-C5-C4	2.65	120.05	118.20
24	AX	32	PSU	O2-C2-N1	-2.65	119.88	122.79
24	AX	16	H2U	C5-C6-N1	2.65	120.33	111.61
25	BA	1911	PSU	C6-N1-C2	-2.65	119.98	122.68
25	BA	2449	H2U	C5-C6-N1	2.64	120.30	111.61
24	AX	39	PSU	C6-N1-C2	-2.63	120.00	122.68
25	BA	746	PSU	O2'-C2'-C3'	2.62	120.28	111.82
25	BA	2457	PSU	O2-C2-N1	-2.61	119.91	122.79
25	BA	2445	2MG	O6-C6-C5	-2.59	119.31	124.37
25	BA	2504	PSU	C6-N1-C2	-2.59	120.03	122.68
25	BA	745	1MG	O6-C6-C5	-2.58	119.63	124.19
25	BA	1835	2MG	O6-C6-C5	-2.53	119.43	124.37
1	AA	1402	4OC	C6-C5-C4	2.52	120.04	116.96
23	AW	54	5MU	O2-C2-N1	-2.51	119.44	122.79
24	AX	55	PSU	C6-C5-C4	2.49	119.94	118.20
23	AW	55	PSU	C3'-C2'-C1'	2.49	104.53	101.64
24	AX	46	7MG	C5-C6-N1	2.48	119.71	112.31
23	AW	55	PSU	O2'-C2'-C3'	2.48	119.86	111.82
24	AX	46	7MG	N9-C4-N3	2.48	129.18	125.47
24	AX	54	5MU	O2-C2-N1	-2.48	119.49	122.79
1	AA	1207	2MG	N2-C2-N1	2.48	121.99	116.71
25	BA	2504	PSU	C6-C5-C4	2.46	119.92	118.20
25	BA	1835	2MG	C8-N7-C5	2.45	107.66	102.99
25	BA	955	PSU	C6-N1-C2	-2.45	120.18	122.68
1	AA	1516	2MG	C8-N7-C5	2.44	107.64	102.99
1	AA	527	G7M	N2-C2-N1	2.43	121.90	116.71
24	AX	46	7MG	C5-C4-N9	2.41	110.04	106.68
25	BA	1915	3TD	O4'-C1'-C2'	2.41	108.54	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	2445	2MG	C8-N7-C5	2.41	107.57	102.99
1	AA	1402	4OC	CM4-N4-C4	-2.40	117.76	122.45
25	BA	2604	PSU	C6-C5-C4	2.35	119.84	118.20
1	AA	1516	2MG	O6-C6-C5	-2.34	119.79	124.37
25	BA	2498	OMC	O3'-C3'-C2'	2.33	117.79	111.17
25	BA	2251	OMG	O6-C6-C5	-2.31	119.86	124.37
25	BA	2457	PSU	C6-C5-C4	2.31	119.81	118.20
1	AA	516	PSU	O2'-C2'-C3'	2.30	119.25	111.82
25	BA	2457	PSU	O4'-C1'-C2'	2.28	108.36	105.14
25	BA	746	PSU	C6-N1-C2	-2.27	120.36	122.68
24	AX	16	H2U	O2-C2-N1	-2.25	120.28	123.11
23	AW	54	5MU	C5M-C5-C6	-2.21	119.89	122.85
1	AA	966	2MG	O6-C6-C5	-2.21	120.05	124.37
25	BA	2552	OMU	O2-C2-N1	-2.21	119.84	122.79
25	BA	2580	PSU	C6-C5-C4	2.21	119.74	118.20
25	BA	1917	PSU	O4'-C1'-C2'	2.21	108.26	105.14
24	AX	55	PSU	C6-N1-C2	-2.16	120.47	122.68
25	BA	2504	PSU	O2'-C2'-C3'	2.16	118.81	111.82
24	AX	20	H2U	O2-C2-N3	-2.15	117.50	121.50
25	BA	2604	PSU	C6-N1-C2	-2.15	120.49	122.68
25	BA	745	1MG	CM1-N1-C6	2.14	120.48	117.55
28	BD	150	MEQ	CB-CG-CD	-2.14	108.25	113.04
1	AA	516	PSU	C6-N1-C2	-2.14	120.50	122.68
25	BA	2503	2MA	N1-C2-N3	-2.13	119.53	123.06
23	AW	55	PSU	C6-N1-C2	-2.13	120.51	122.68
25	BA	2605	PSU	O2-C2-N1	-2.12	120.46	122.79
25	BA	2503	2MA	CM2-C2-N1	2.12	120.95	116.23
1	AA	967	5MC	CM5-C5-C6	-2.12	120.02	122.85
1	AA	1207	2MG	O6-C6-C5	-2.12	120.24	124.37
25	BA	955	PSU	O2'-C2'-C3'	2.12	118.67	111.82
1	AA	966	2MG	O3'-C3'-C4'	2.11	117.16	111.05
23	AW	8	4SU	O2-C2-N1	-2.11	119.98	122.79
25	BA	2457	PSU	O2'-C2'-C3'	2.08	118.54	111.82
25	BA	2580	PSU	O2'-C2'-C3'	2.07	118.52	111.82
1	AA	1402	4OC	O2-C2-N3	-2.06	118.98	122.33
24	AX	32	PSU	C6-N1-C2	-2.06	120.58	122.68
25	BA	2030	6MZ	C4-C5-N7	-2.02	107.29	109.40
24	AX	37	MIA	C5-C6-N6	2.00	123.40	120.35

There are no chirality outliers.

All (70) 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	1518	MA6	C5-C6-N6-C9
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C5-C6-N6-C9
1	AA	1519	MA6	C5-C6-N6-C10
24	AX	20	H2U	O4'-C4'-C5'-O5'
24	AX	20	H2U	C3'-C4'-C5'-O5'
36	BN	81	4D4	C-CA-CB-OB
36	BN	81	4D4	C-CA-CB-CG
36	BN	81	4D4	N-CA-CB-OB
36	BN	81	4D4	N-CA-CB-CG
36	BN	81	4D4	OB-CB-CG-CD
23	AW	20	H2U	O4'-C4'-C5'-O5'
23	AW	20	H2U	C3'-C4'-C5'-O5'
23	AW	20	H2U	O4'-C1'-N1-C2
23	AW	20	H2U	O4'-C1'-N1-C6
25	BA	1618	6MZ	O4'-C4'-C5'-O5'
25	BA	1618	6MZ	C3'-C4'-C5'-O5'
25	BA	2552	OMU	O4'-C4'-C5'-O5'
24	AX	20	H2U	C2'-C1'-N1-C2
1	AA	967	5MC	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
25	BA	1917	PSU	C3'-C4'-C5'-O5'
25	BA	1917	PSU	O4'-C4'-C5'-O5'
25	BA	2503	2MA	O4'-C4'-C5'-O5'
25	BA	2552	OMU	C3'-C4'-C5'-O5'
1	AA	516	PSU	C3'-C4'-C5'-O5'
1	AA	967	5MC	C3'-C4'-C5'-O5'
1	AA	1207	2MG	O4'-C4'-C5'-O5'
25	BA	2498	OMC	C3'-C4'-C5'-O5'
25	BA	2503	2MA	C3'-C4'-C5'-O5'
1	AA	1518	MA6	N1-C6-N6-C10
1	AA	1519	MA6	N1-C6-N6-C10
24	AX	20	H2U	C2'-C1'-N1-C6
23	AW	20	H2U	C2'-C1'-N1-C6
28	BD	150	MEQ	NE2-CD-CG-CB
28	BD	150	MEQ	OE1-CD-CG-CB
25	BA	2445	2MG	C3'-C4'-C5'-O5'
25	BA	2498	OMC	O4'-C4'-C5'-O5'
24	AX	16	H2U	C4'-C5'-O5'-P
23	AW	20	H2U	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
36	BN	81	4D4	CA-CB-CG-CD
24	AX	46	7MG	O4'-C1'-N9-C4
23	AW	20	H2U	C2'-C1'-N1-C2
25	BA	2445	2MG	O4'-C4'-C5'-O5'
24	AX	20	H2U	C4'-C5'-O5'-P
24	AX	46	7MG	C4'-C5'-O5'-P
25	BA	1911	PSU	O4'-C4'-C5'-O5'
25	BA	2030	6MZ	O4'-C4'-C5'-O5'
24	AX	46	7MG	C2'-C1'-N9-C8
25	BA	1939	5MU	O4'-C4'-C5'-O5'
28	BD	150	MEQ	CA-CB-CG-CD
1	AA	527	G7M	C4'-C5'-O5'-P
25	BA	2069	G7M	C4'-C5'-O5'-P
24	AX	46	7MG	O4'-C1'-N9-C8
24	AX	55	PSU	O4'-C1'-C5-C4
1	AA	516	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C4'-C5'-O5'-P
1	AA	1207	2MG	C3'-C4'-C5'-O5'
23	AW	55	PSU	C3'-C4'-C5'-O5'
25	BA	1939	5MU	C3'-C4'-C5'-O5'
24	AX	55	PSU	O4'-C1'-C5-C6
25	BA	746	PSU	O4'-C1'-C5-C6
25	BA	2069	G7M	O4'-C4'-C5'-O5'
25	BA	2030	6MZ	C3'-C4'-C5'-O5'
36	BN	81	4D4	O-C-CA-CB
12	AL	89	D2T	CA-CB-CG-OD2
1	AA	967	5MC	C4'-C5'-O5'-P

There are no ring outliers.

26 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	2	0
24	AX	20	H2U	2	0
25	BA	747	5MU	1	0
25	BA	2069	G7M	1	0
24	AX	16	H2U	1	0
1	AA	1518	MA6	2	0
24	AX	46	7MG	1	0
25	BA	2445	2MG	1	0
1	AA	1519	MA6	1	0
1	AA	1516	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BA	2552	OMU	3	0
1	AA	966	2MG	2	0
1	AA	967	5MC	1	0
28	BD	150	MEQ	3	0
25	BA	1915	3TD	3	0
24	AX	8	4SU	2	0
23	AW	55	PSU	1	0
25	BA	2504	PSU	1	0
1	AA	1207	2MG	2	0
25	BA	2030	6MZ	1	0
25	BA	1917	PSU	3	0
1	AA	1498	UR3	1	0
25	BA	955	PSU	1	0
24	AX	37	MIA	2	0
25	BA	2449	H2U	2	0
23	AW	54	5MU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 425 ligands modelled in this entry, 424 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	$\#\|Z\| > 2$
61	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.24	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
61	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
61	AX	101	PHE	CA-CB-CG-CD1
61	AX	101	PHE	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AX	101	PHE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	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-11420. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.