Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:06 AM EDT

PDB ID	:	4V9H
Title	:	Crystal structure of the ribosome bound to elongation factor G in the guanosine triphosphatase state
Authors	:	Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2013-03-25
Resolution	:	2.86 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

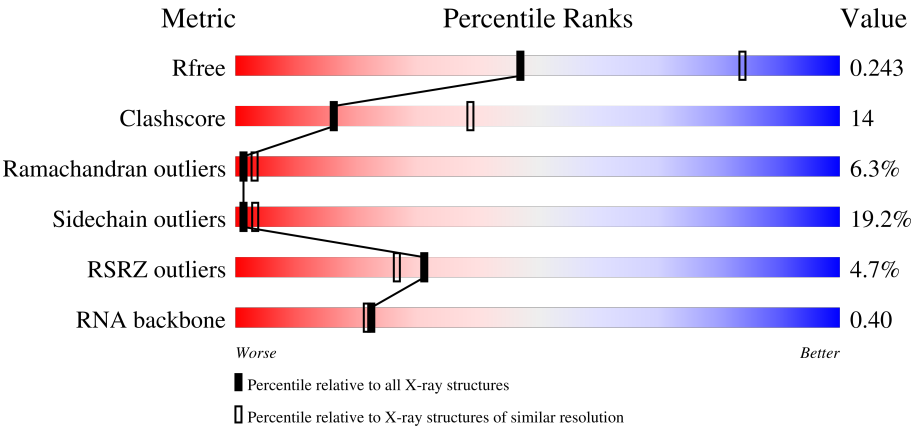
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1516	3% 51% 36% 10% •
2	AV	76	% 42% 26% 24% 5% •
3	AX	25	4% 16% 8% 76%
4	AJ	98	3% 58% 28% 14%

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Mol	Chain	Length	Quality of chain
5	AK	119	3% 57% 36% 7%
6	AL	124	2% 65% 27% 7%
7	AM	124	10% 45% 44% 10%
8	AN	60	3% 53% 37% 10%
9	AO	88	68% 25% 6%
10	AP	83	75% 19% 5%
11	AQ	99	64% 32%
12	AR	70	71% 23% 6%
13	AS	78	9% 50% 37% 10%
14	AT	99	4% 59% 29% 10%
15	AB	234	6% 55% 38% 7%
16	AC	206	58% 33% 7%
17	AD	208	2% 63% 25% 8%
18	AE	150	69% 23% 7%
19	AF	101	69% 27%
20	AG	155	6% 69% 26% 5%
21	AH	138	61% 33% 7%
22	AI	127	2% 61% 27% 12%
23	AY	680	52% 31% 8% 9%
24	AU	24	4% 54% 38% 8%
25	BA	2915	2% 45% 36% 14%
26	BB	122	39% 41% 17%
27	BN	140	3% 45% 38% 13%
28	BO	122	56% 38% 7%
29	BP	150	10% 34% 27% 29% 8%

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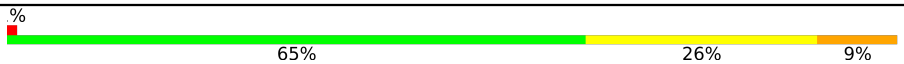
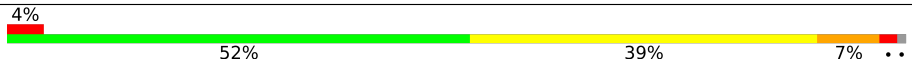
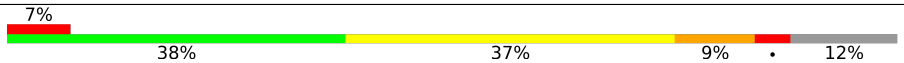
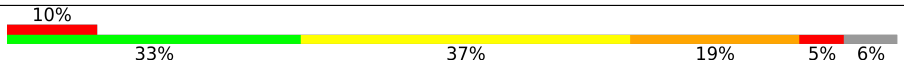
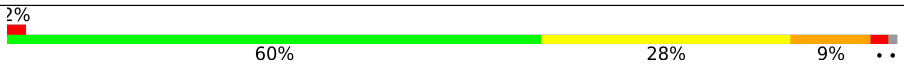
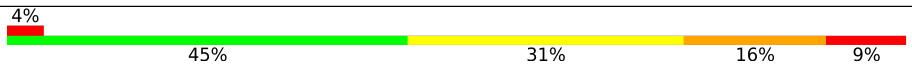
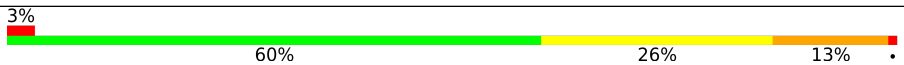
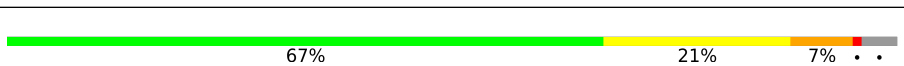
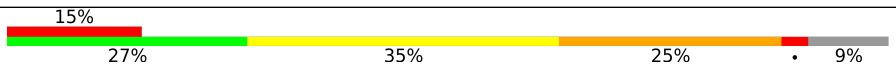
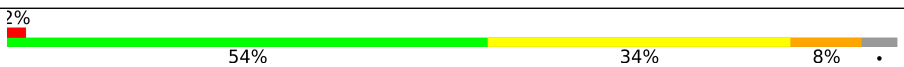
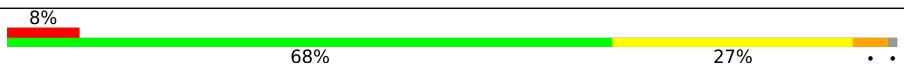
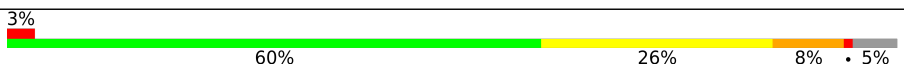
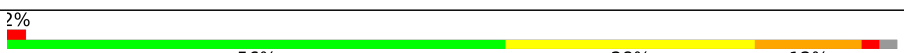
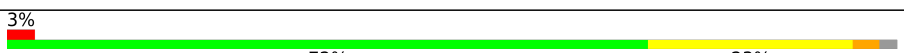
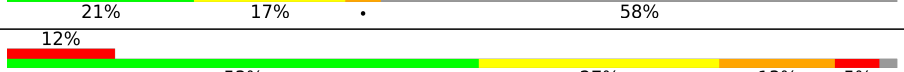
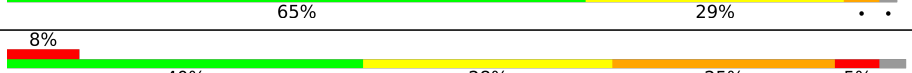
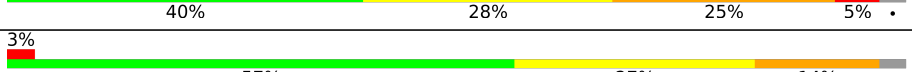
Mol	Chain	Length	Quality of chain
30	BQ	141	
31	BR	118	
32	BS	112	
33	BT	146	
34	BU	118	
35	BV	101	
36	BW	113	
37	BX	96	
38	BY	110	
39	BZ	206	
40	B0	85	
41	B1	98	
42	B2	72	
43	BD	276	
44	B3	60	
45	B4	71	
46	B5	60	
47	B6	54	
48	B7	49	
49	B8	65	
50	B9	37	
51	BC	229	
52	BE	206	
53	BF	210	
54	BG	182	

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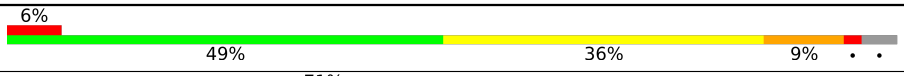
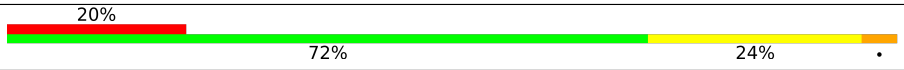
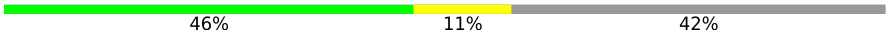
Mol	Chain	Length	Quality of chain
55	BH	180	
56	BK	147	
57	BJ	130	
58	BL	125	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1514	32529	14480	6018	10518	1513	0	0	0

- Molecule 2 is a RNA chain called PE hybrid state tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AV	74	1579	705	285	516	73	0	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AX	6	125	56	19	44	6	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AJ	98	795	499	156	139	1	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AK	119	885	549	168	165	3	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AL	124	971	611	195	164	1	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 8 is a protein called 30S ribosomal protein S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 14 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 15 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 17 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 18 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

- Molecule 19 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 20 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 21 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 22 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	622	Total	C	N	O	S	0	0	0
			4877	3097	837	924	19			

- Molecule 24 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2859	Total	C	N	O	P	0	0	0
			61580	27407	11519	19796	2858			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BZ	198	Total	C	N	O	S	0	0	0
			1508	960	274	272	2			

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 43 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BC	225	Total	C	N	O	S	0	0	0
			1718	1085	315	316	2			

- Molecule 52 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 53 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BH	173	Total	C	N	O	S	0	0	0
			1303	824	244	234	1			

- Molecule 56 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	127	Total	C	N	O	S	0	0	0
			936	598	161	172	5			

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

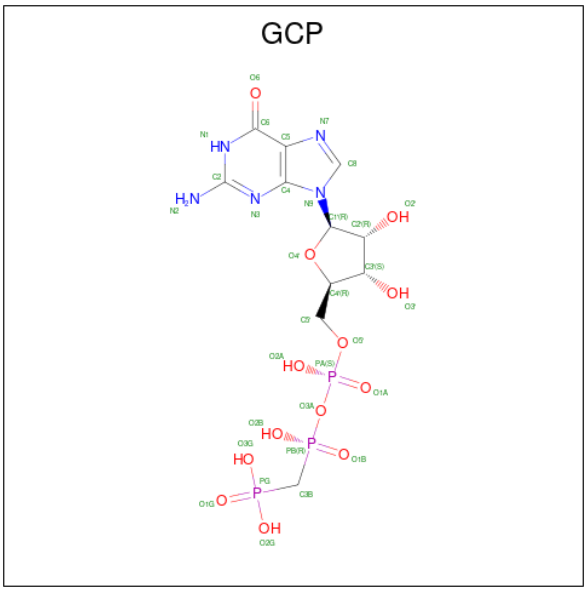
- Molecule 58 is a protein called 50S ribosomal protein L12 CTD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BL	72	Total	C	N	O	0	0	1
			356	213	72	71			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	45	Total	Mg	0	0
			45	45		
59	AY	1	Total	Mg	0	0
			1	1		
59	BA	88	Total	Mg	0	0
			88	88		
59	BD	1	Total	Mg	0	0
			1	1		
59	B8	1	Total	Mg	0	0
			1	1		
59	BE	1	Total	Mg	0	0
			1	1		
59	BF	1	Total	Mg	0	0
			1	1		

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 61 is water.

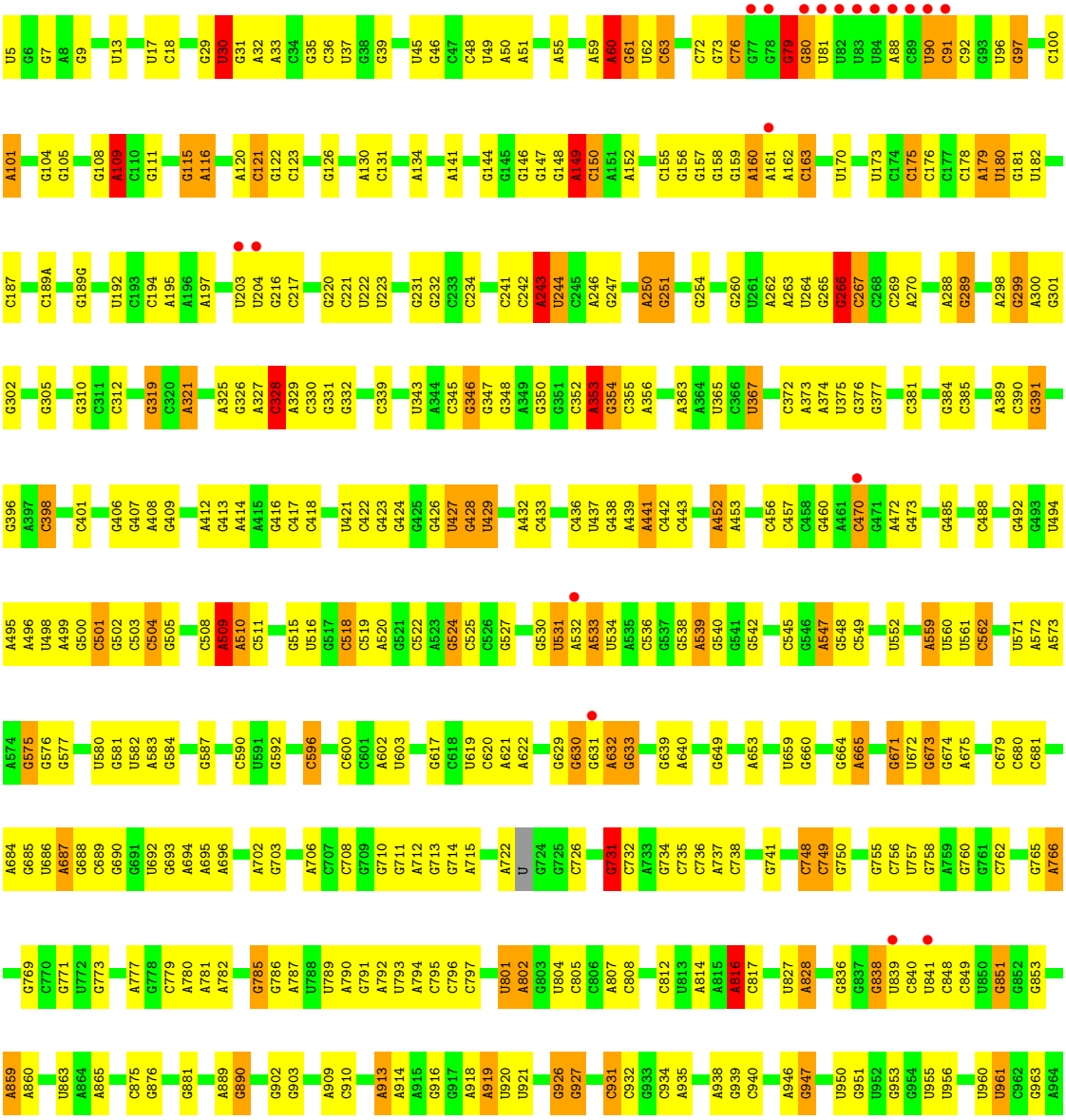
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	4	Total	O	0	0
			4	4		

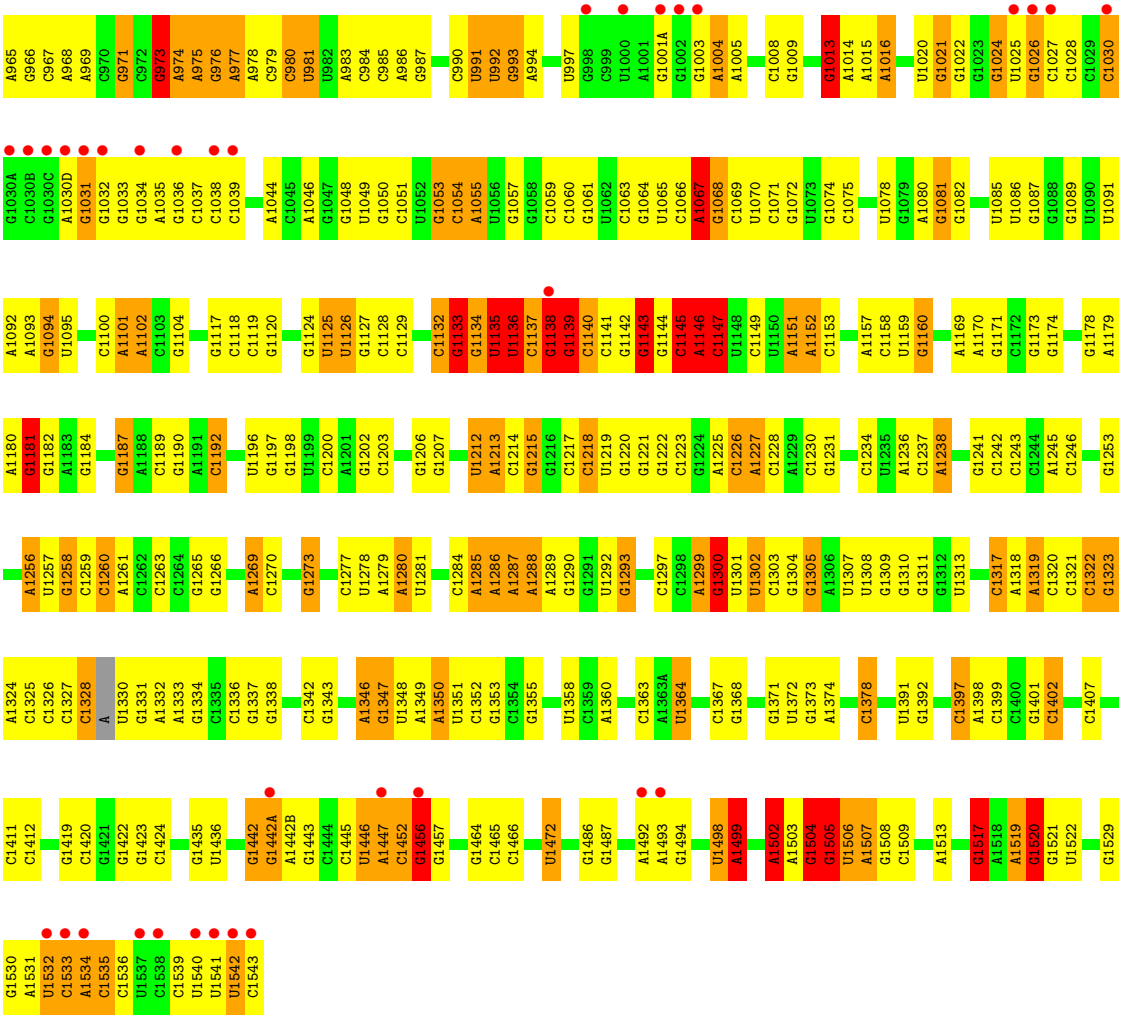
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

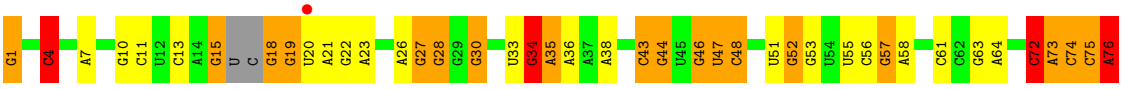
- Molecule 1: 16S ribosomal RNA

Chain AA: 



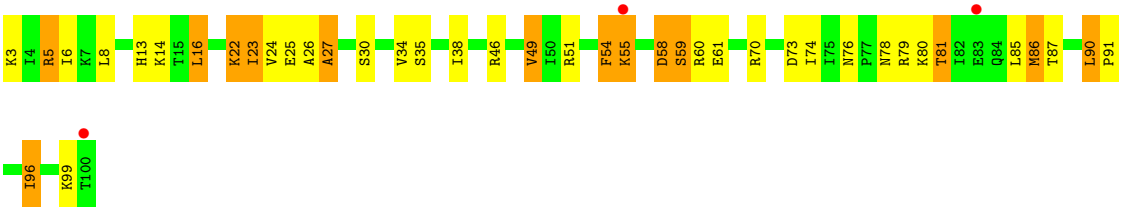


• Molecule 2: PE hybrid state tRNA Phe



• Molecule 3: mRNA

• Molecule 4: 30S ribosomal protein S10

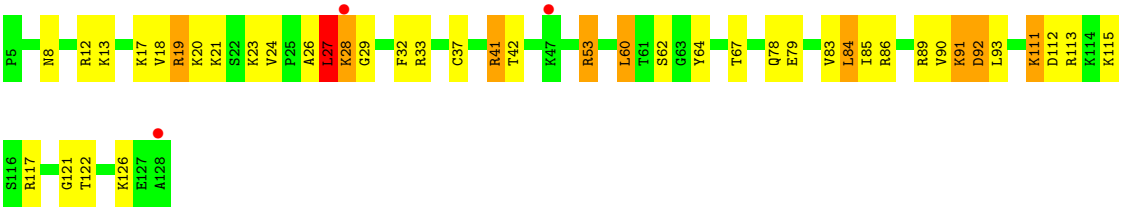


• Molecule 5: 30S ribosomal protein S11

Chain AK:

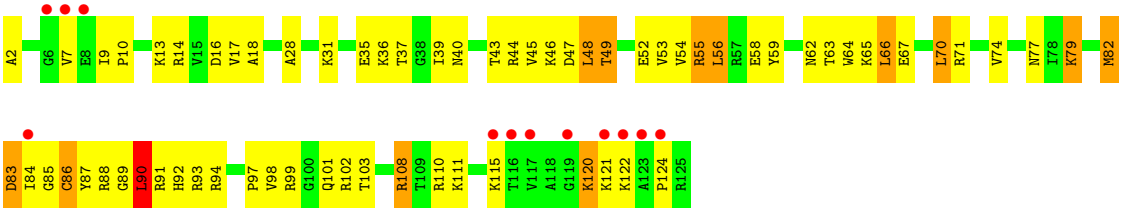
• Molecule 6: 30S ribosomal protein S12

Chain AL:



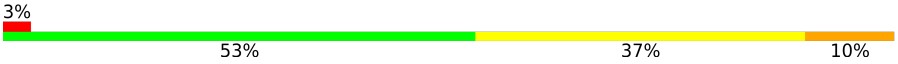
• Molecule 7: 30S ribosomal protein S13

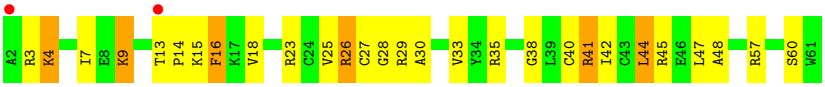
Chain AM:



• Molecule 8: 30S ribosomal protein S14 TYPE Z

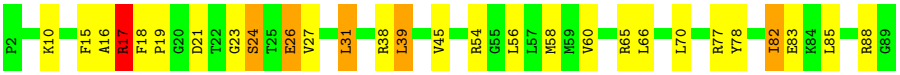
Chain AN:



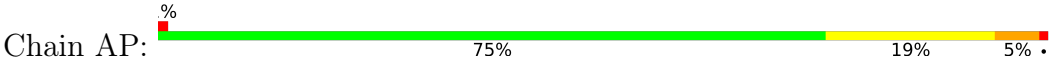


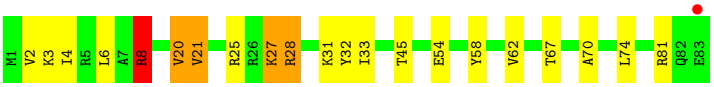
• Molecule 9: 30S ribosomal protein S15

Chain AO:

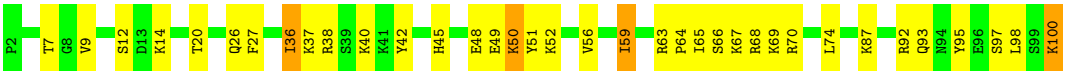


• Molecule 10: 30S ribosomal protein S16

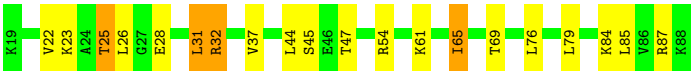




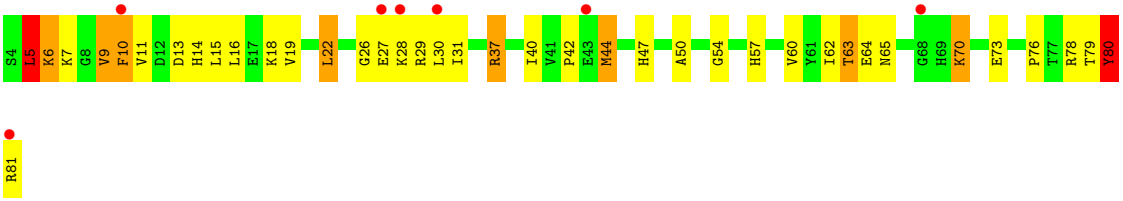
• Molecule 11: 30S ribosomal protein S17



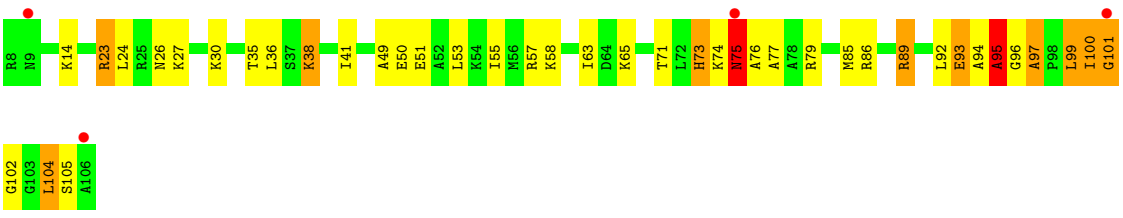
• Molecule 12: 30S ribosomal protein S18



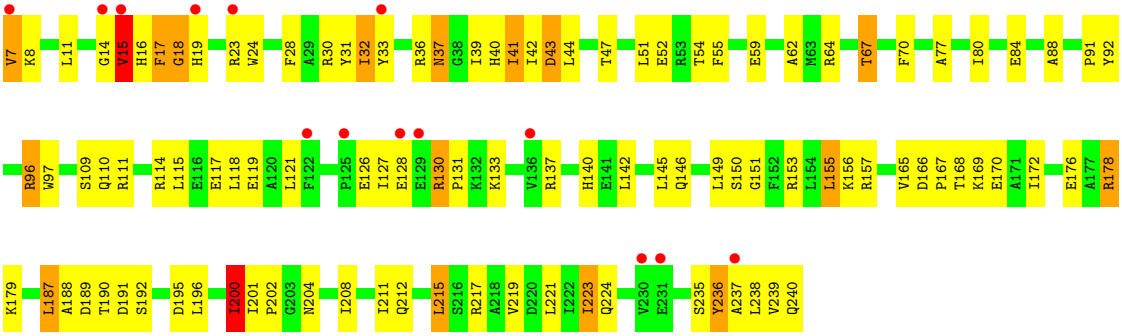
• Molecule 13: 30S ribosomal protein S19



• Molecule 14: 30S ribosomal protein S20



• Molecule 15: 30S ribosomal protein S2

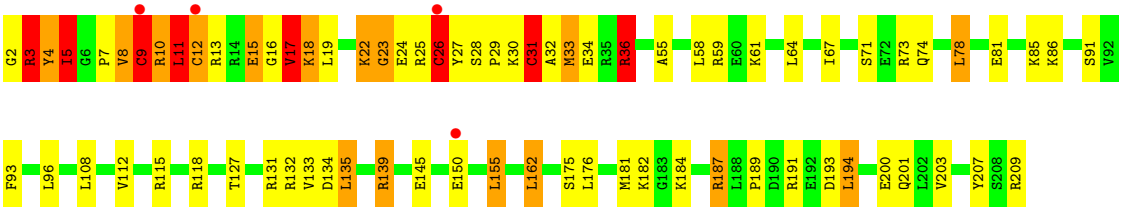


• Molecule 16: 30S ribosomal protein S3

Chain AC:

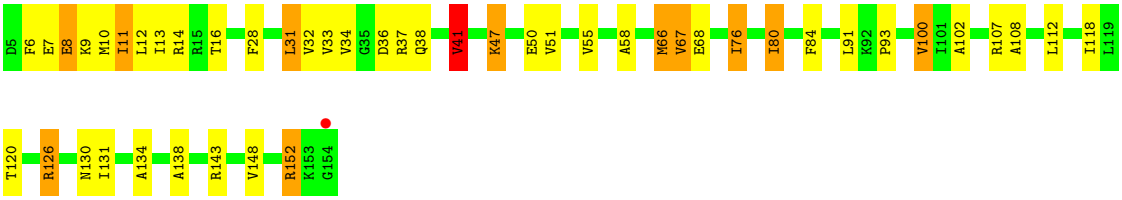
• Molecule 17: 30S ribosomal protein S4

Chain AD:



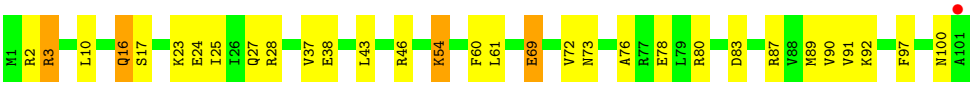
• Molecule 18: 30S ribosomal protein S5

Chain AE:

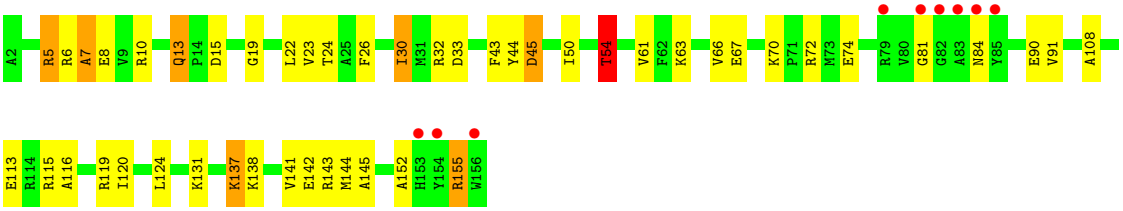


• Molecule 19: 30S ribosomal protein S6

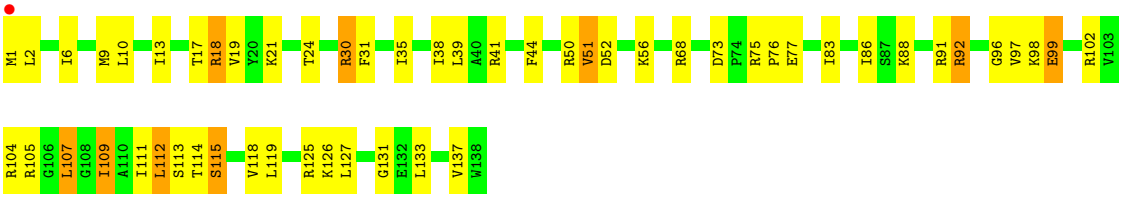
Chain AF:



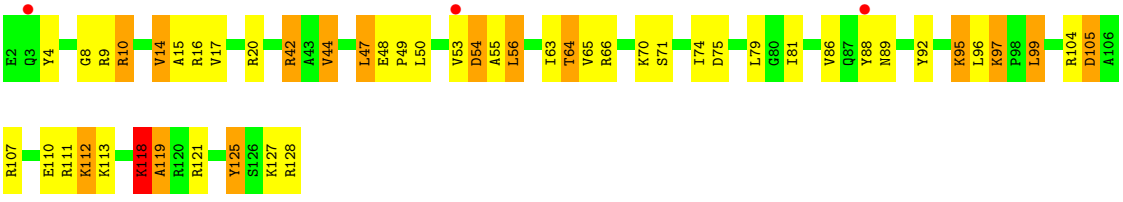
• Molecule 20: 30S ribosomal protein S7



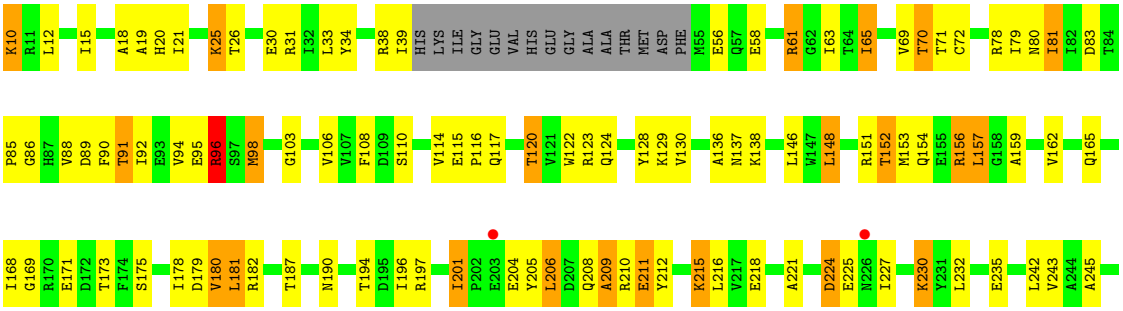
• Molecule 21: 30S ribosomal protein S8

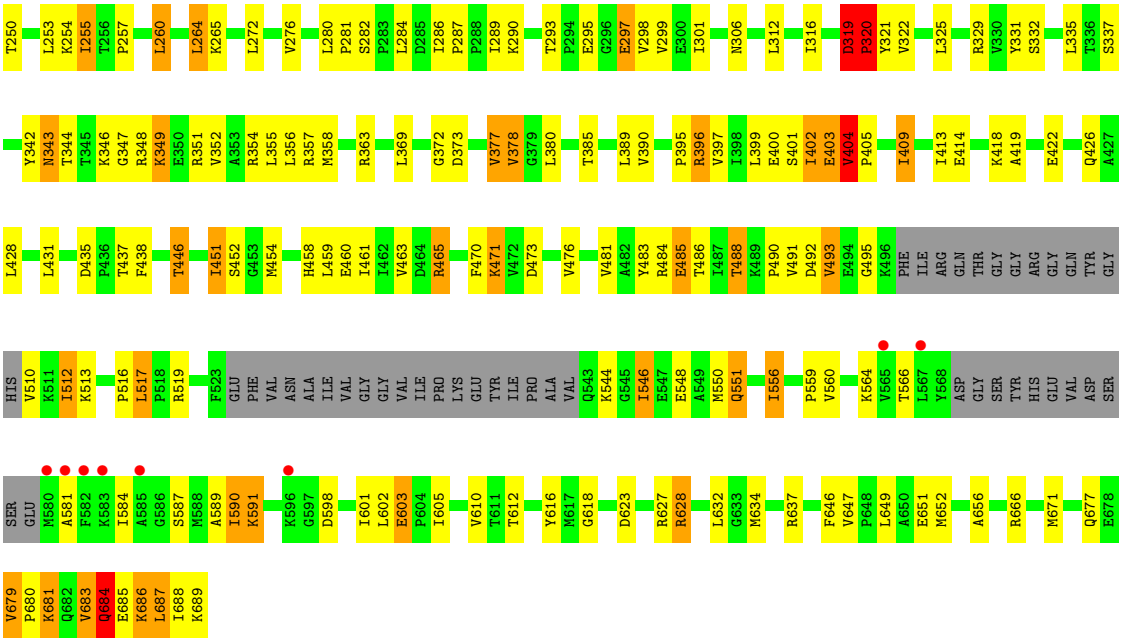


• Molecule 22: 30S ribosomal protein S9



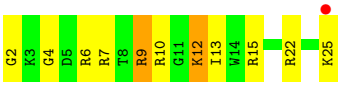
• Molecule 23: Elongation factor G





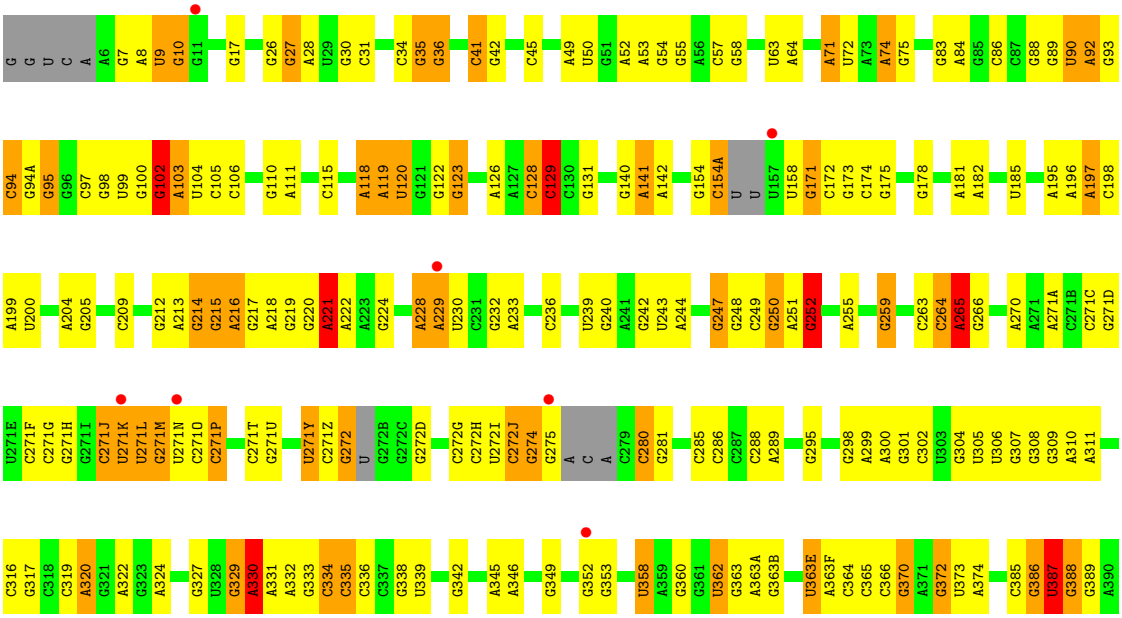
• Molecule 24: 30S ribosomal protein THX

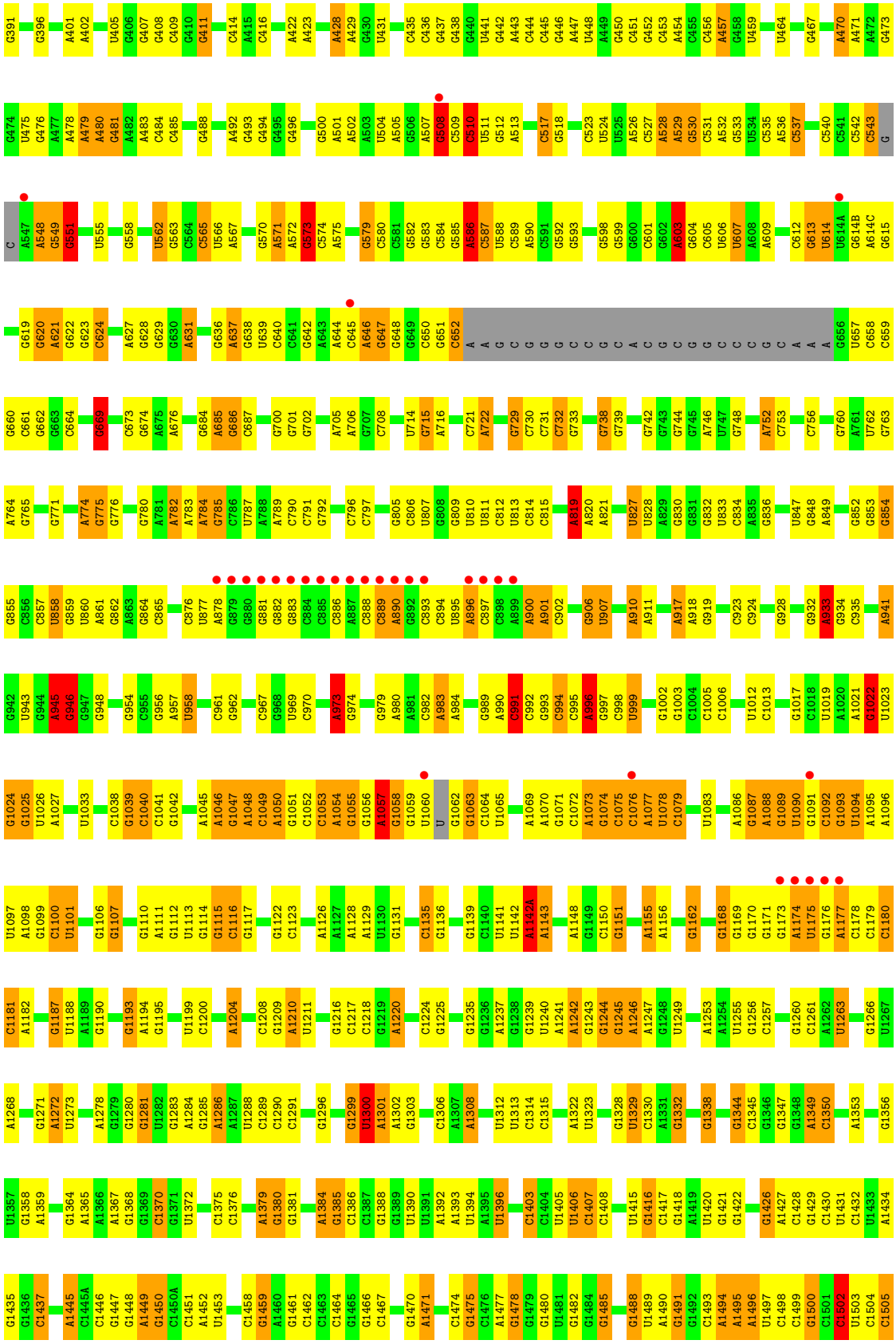
Chain AU:

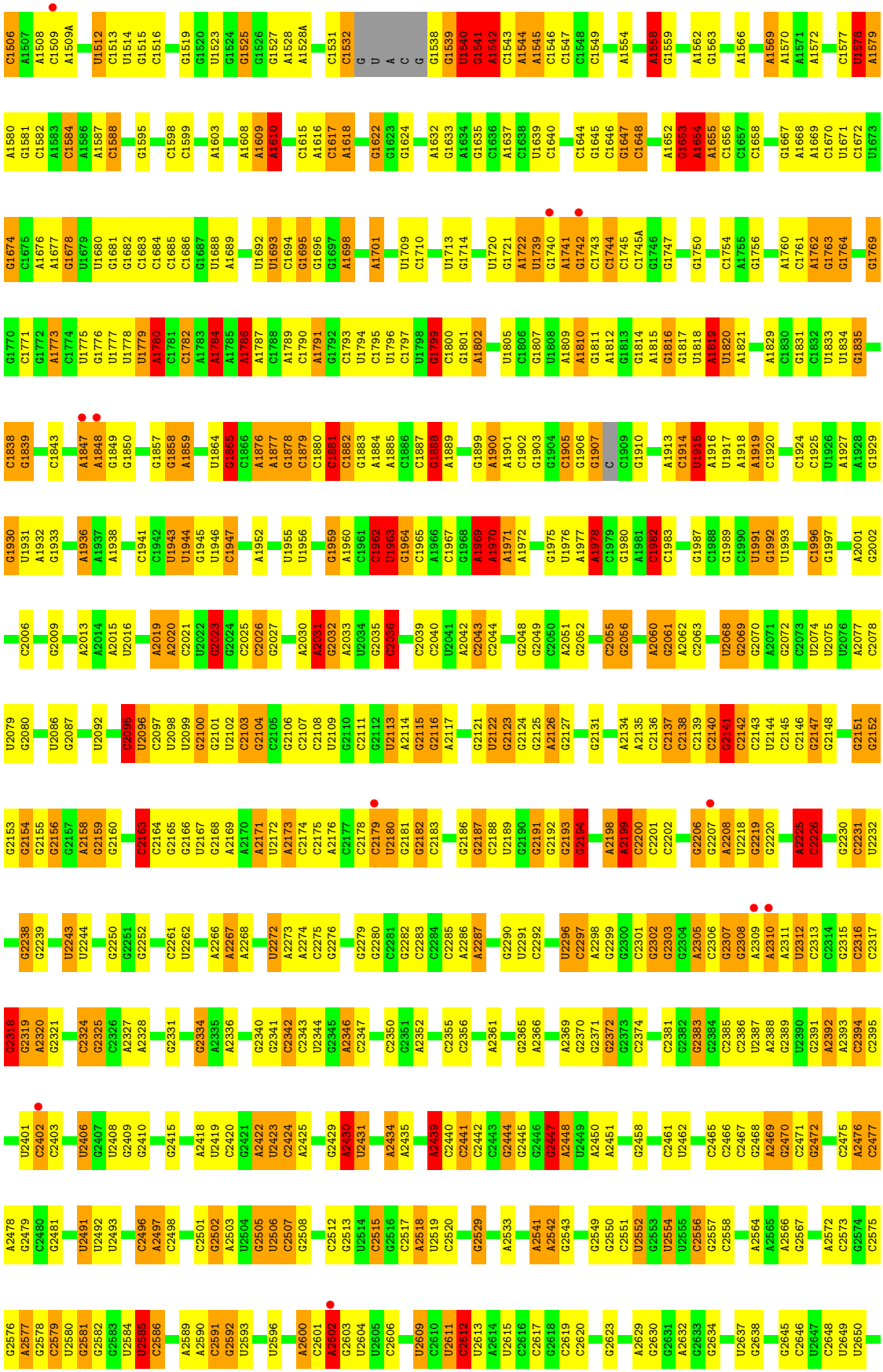


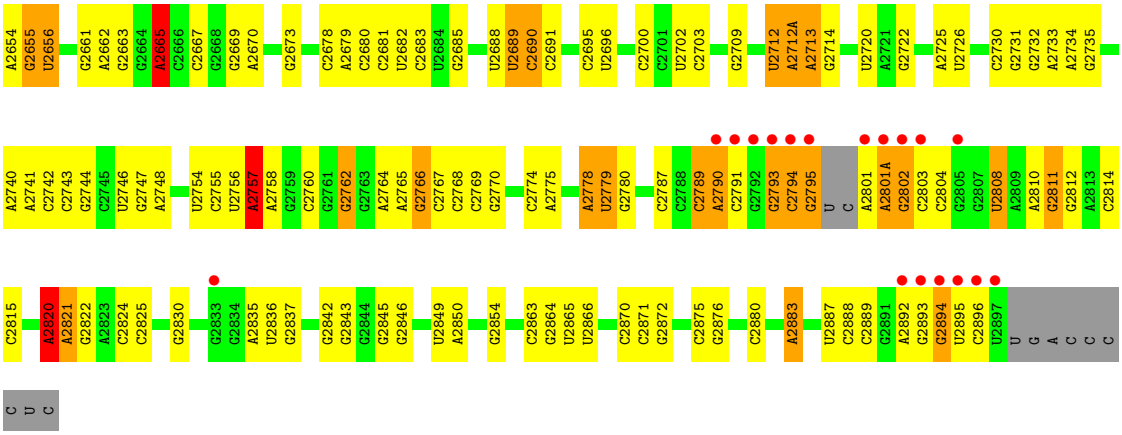
• Molecule 25: 23S ribosomal RNA

Chain BA:



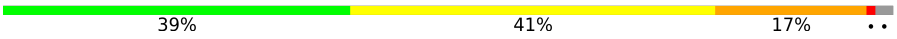


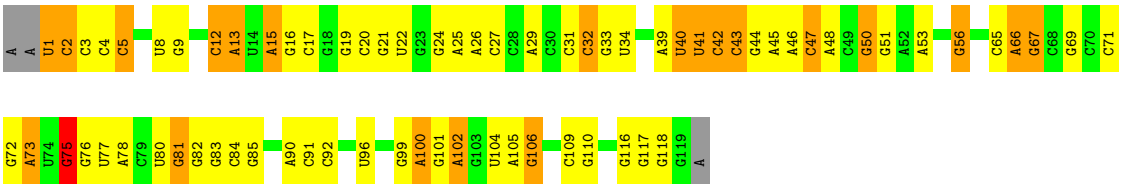

C1506 A1507 A1508 C1509 A1509A U1512 C1513 U1514 G1515 C1516 G1519 G1520 U1523 G1524 G1525 G1526 G1527 A1528 A1528A C1531 C1532 G U A C G G1538 G1539 U1540 G1541 A1542 C1543 A1544 A1545 C1546 C1547 C1548 C1549 A1554 A1558 G1559 A1562 G1563 A1566 A1569 A1570 A1571 A1572 C1577 U1578 A1579
A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 G1595 C1598 C1599 A1603 A1608 A1609 A1610 C1615 A1616 C1617 A1618 G1622 G1623 G1624 A1632 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640 C1644 G1645 C1646 G1647 C1648 A1652 G1653 A1654 A1655 C1656 C1657 C1658 G1667 A1668 A1669 C1670 U1671 C1672 U1673
G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1683 C1684 C1685 C1686 G1687 U1688 A1689 U1692 U1693 C1694 G1695 G1696 G1697 A1698 A1701 U1709 C1710 U1713 G1714 U1720 G1721 A1722 U1739 G1740 A1741 G1742 C1743 C1744 C1745 C1745A G1746 G1747 G1750 C1754 A1755 G1756 A1760 C1761 A1762 G1763 G1764 G1769
G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 U1805 C1806 G1807 U1808 A1809 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 A1829 C1830 G1831 C1832 U1833 U1834 G1835
C1838 G1839 C1843 A1847 A1848 G1849 G1850 G1857 G1858 A1859 U1864 G1865 C1866 A1876 A1877 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C G1909 G1910 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 C1924 C1925 U1926 A1927 A1928 G1929
G1930 U1931 A1932 G1933 A1936 A1937 A1938 C1941 C1942 U1943 U1944 G1945 U1946 C1947 A1952 U1955 U1956 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1975 U1976 A1977 A1978 C1979 G1980 A1981 C1982 C1983 G1987 C1988 G1989 C1990 U1991 G1992 U1993 C1996 G1997 A2001 G2002
C2006 G2009 A2013 A2014 A2015 U2016 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 A2030 A2031 G2032 A2033 U2034 G2035 C2036 C2039 C2040 U2041 A2042 C2043 C2044 G2048 G2049 C2050 A2051 G2052 C2055 G2056 A2060 G2061 A2062 C2063 U2068 G2069 G2070 A2071 G2072 C2073 U2074 U2075 U2076 A2077 C2078
U2079 G2080 U2086 G2087 U2092 C2095 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 C2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2131 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 U2143 U2144 C2145 C2146 G2147 G2148 G2151 G2152
G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 A2198 A2199 C2200 C2201 C2202 G2206 G2207 A2208 U2218 G2219 G2220 A2225 C2226 G2230 C2231 U2232
G2238 G2239 U2243 U2244 G2250 G2251 G2252 C2261 U2262 A2266 A2267 A2268 U2272 A2273 A2274 C2275 G2276 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 G2290 U2291 C2292 U2296 C2297 A2298 G2299 G2300 C2301 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 C2316 C2317
G2318 G2319 A2320 G2321 C2324 G2325 C2326 A2327 A2328 G2331 G2334 A2335 A2336 G2340 G2341 C2342 C2343 U2344 G2345 A2346 C2347 C2350 G2351 A2352 C2355 C2356 A2361 G2365 A2366 A2369 G2370 G2371 G2372 G2373 C2374 C2381 G2382 G2383 G2384 C2385 C2386 U2387 A2388 G2389 U2390 G2391 A2392 A2393 C2394 C2395
U2401 C2402 C2403 U2406 G2407 U2408 G2409 G2410 G2415 A2418 U2419 C2420 G2421 A2422 U2423 C2424 A2425 G2429 A2430 U2431 A2434 A2435 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 U2449 A2450 A2451 G2458 C2461 U2462 C2465 C2466 C2467 G2468 A2469 G2470 C2471 G2472 C2475 A2476 C2477
A2478 G2479 C2480 G2481 U2491 U2492 U2493 C2496 A2497 C2498 C2501 G2502 A2503 U2504 G2505 U2506 C2507 G2508 C2512 G2513 U2514 C2515 G2516 C2517 A2518 U2519 C2520 G2529 A2533 A2541 A2542 G2543 G2549 G2550 C2551 U2552 G2553 U2554 U2555 C2556 G2557 C2558 A2564 A2565 A2566 G2567 A2572 C2573 G2574 C2575
G2576 A2577 G2578 C2579 U2580 G2581 G2582 G2583 U2584 U2585 C2586 A2589 A2590 G2591 G2592 U2593 U2596 A2600 C2601 A2602 G2603 U2604 U2605 C2606 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 C2617 G2618 C2619 C2620 G2623 A2629 G2630 G2631 A2632 G2633 G2634 U2637 G2638 G2645 C2646 U2647 C2648 U2649 U2650



• Molecule 26: 5S ribosomal RNA

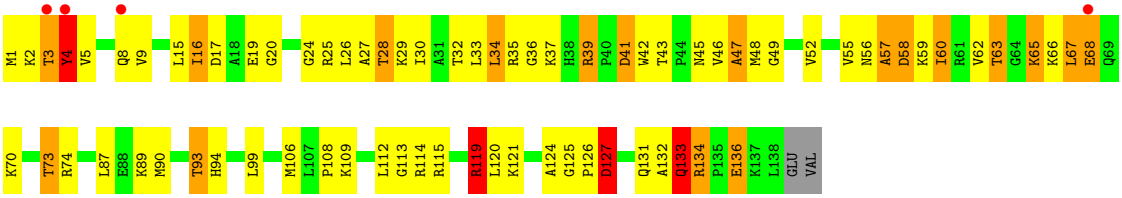
Chain BB:





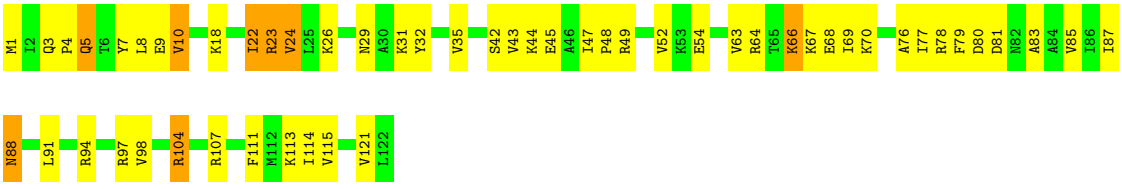
• Molecule 27: 50S ribosomal protein L13

Chain BN:



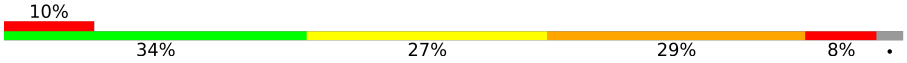
• Molecule 28: 50S ribosomal protein L14

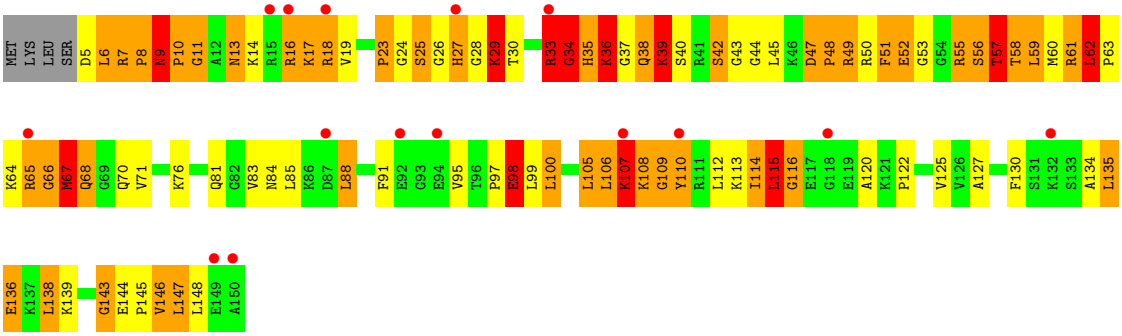
Chain BO:



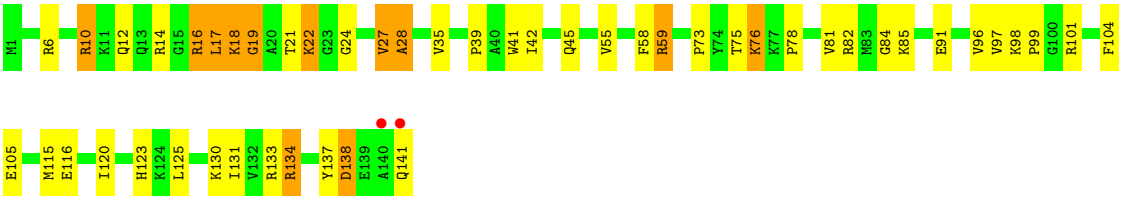
• Molecule 29: 50S ribosomal protein L15

Chain BP:

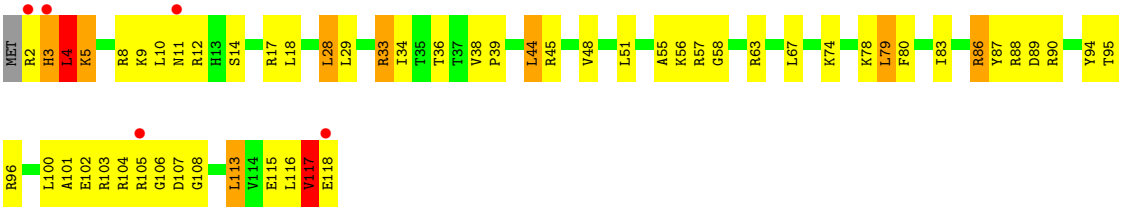




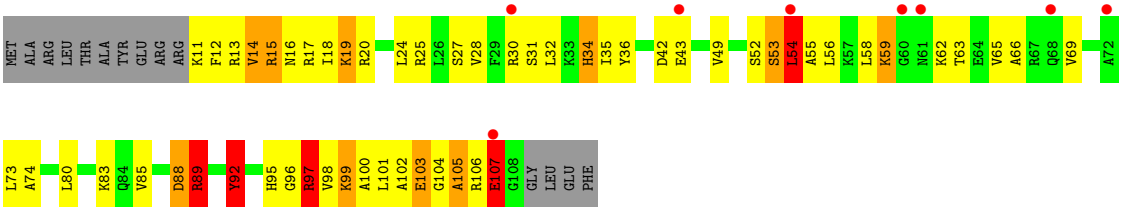
• Molecule 30: 50S ribosomal protein L16



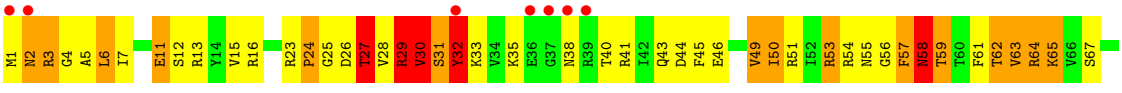
• Molecule 31: 50S ribosomal protein L17

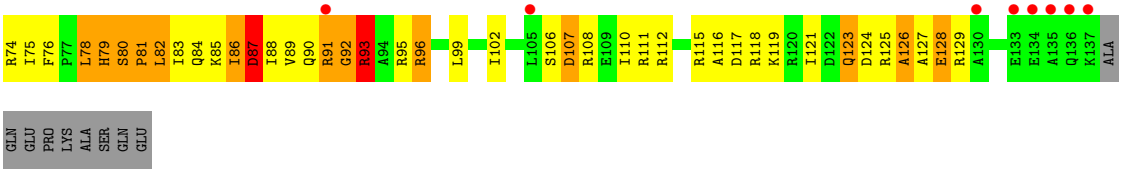


• Molecule 32: 50S ribosomal protein L18

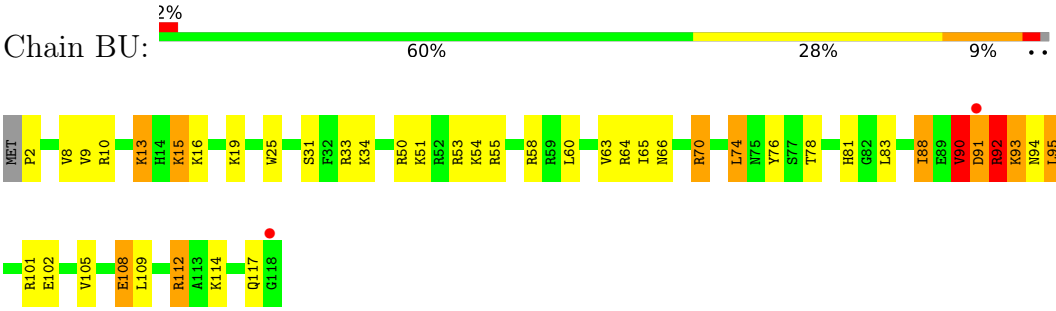


• Molecule 33: 50S ribosomal protein L19

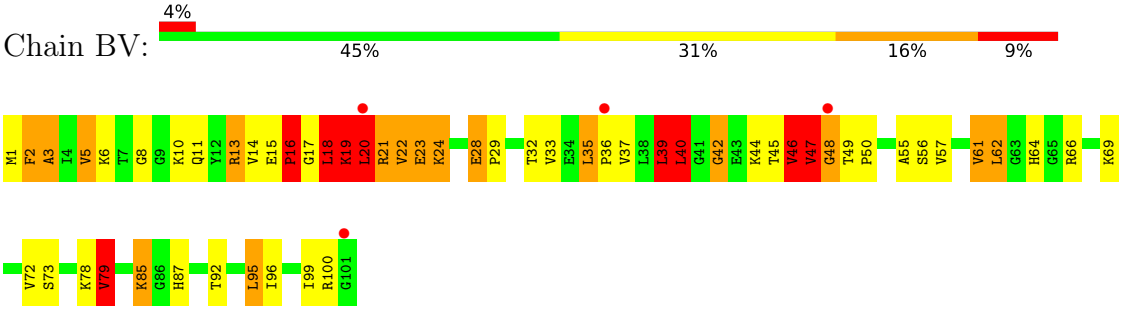




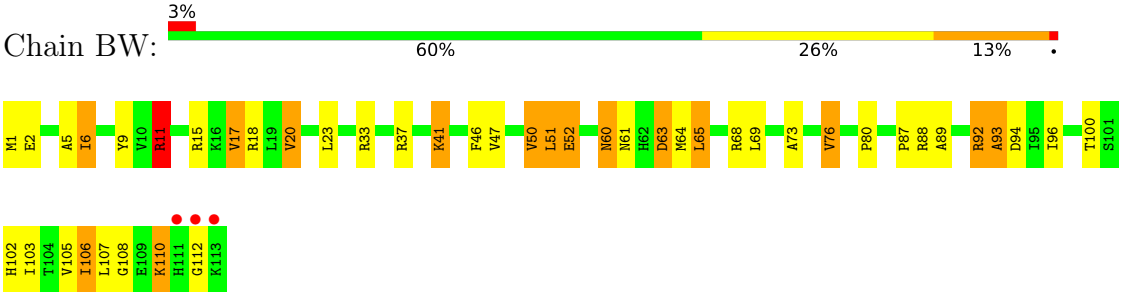
• Molecule 34: 50S ribosomal protein L20



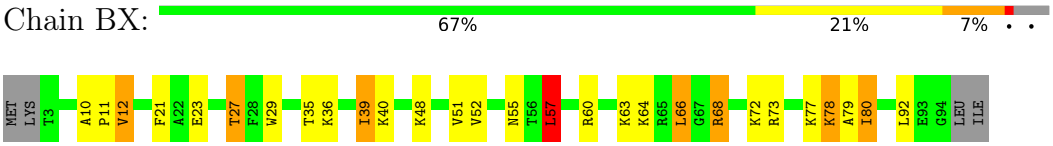
• Molecule 35: 50S ribosomal protein L21



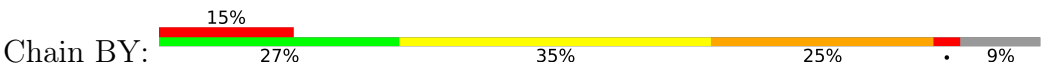
• Molecule 36: 50S ribosomal protein L22

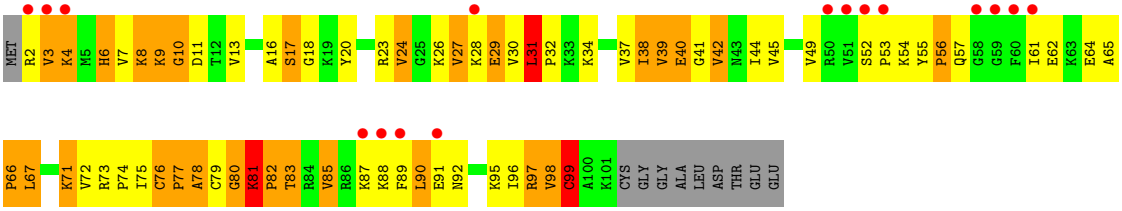


• Molecule 37: 50S ribosomal protein L23

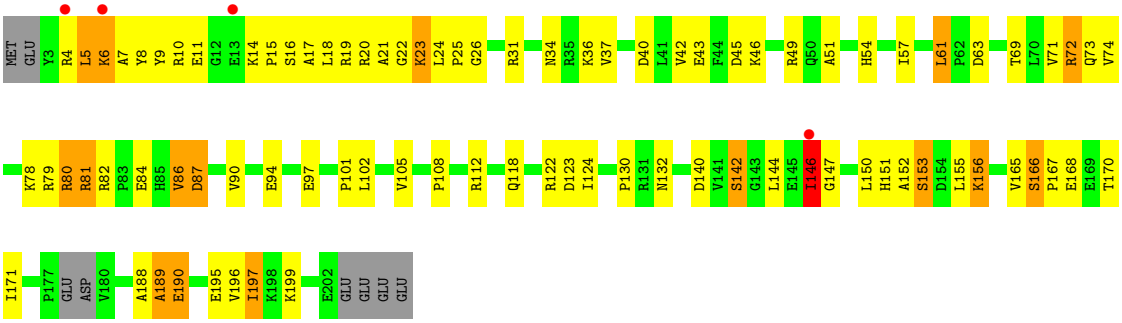


• Molecule 38: 50S ribosomal protein L24

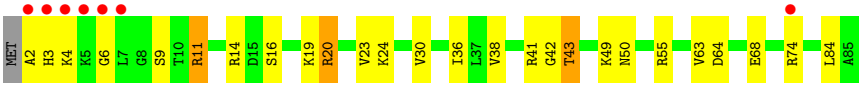




• Molecule 39: 50S ribosomal protein L25

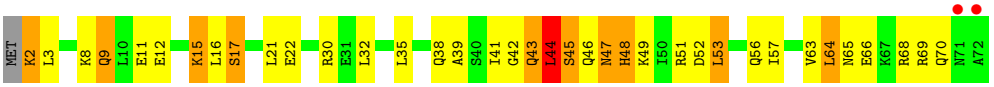


• Molecule 40: 50S ribosomal protein L27

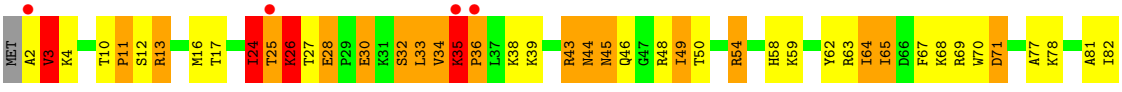


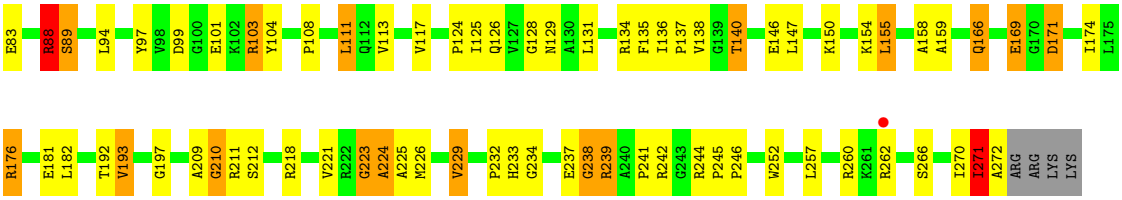
• Molecule 41: 50S ribosomal protein L28

• Molecule 42: 50S ribosomal protein L29

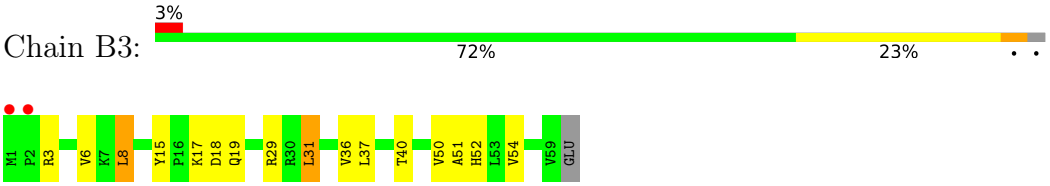


• Molecule 43: 50S ribosomal protein L2

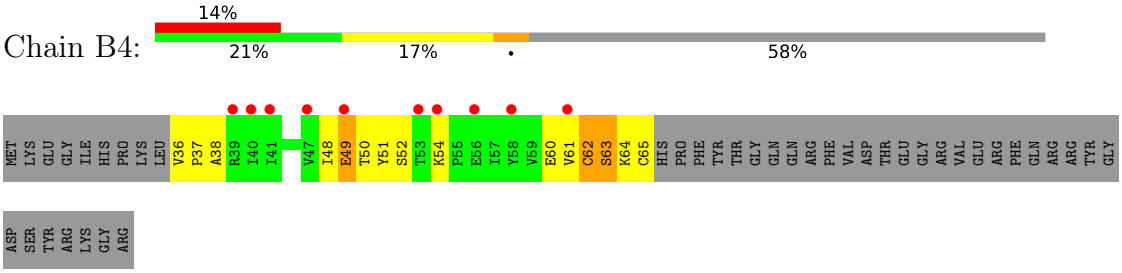




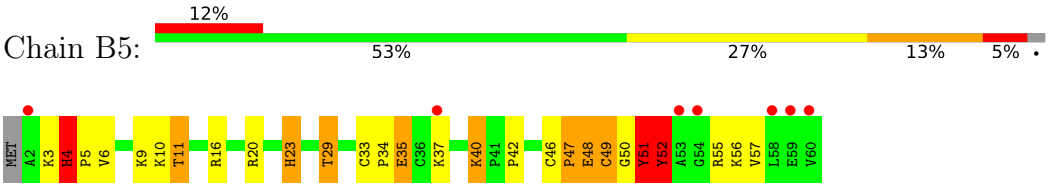
• Molecule 44: 50S ribosomal protein L30



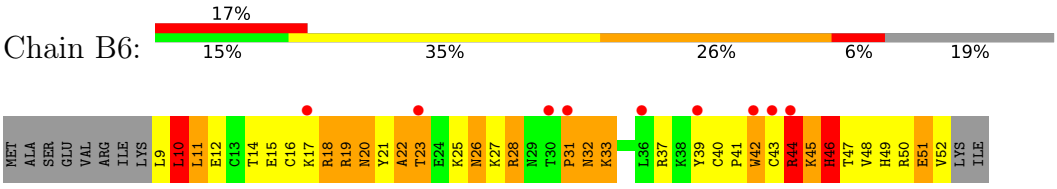
• Molecule 45: 50S ribosomal protein L31



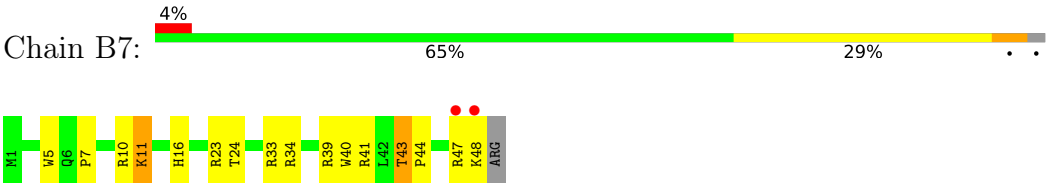
• Molecule 46: 50S ribosomal protein L32



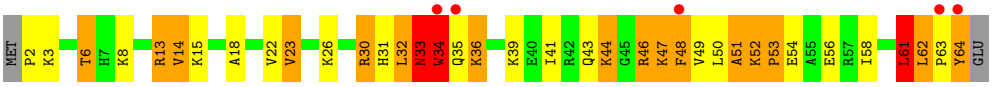
• Molecule 47: 50S ribosomal protein L33



• Molecule 48: 50S ribosomal protein L34



• Molecule 49: 50S ribosomal protein L35

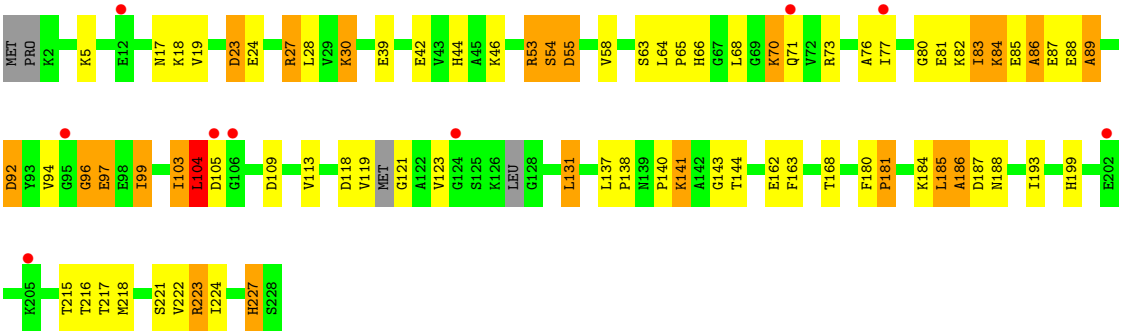


• Molecule 50: 50S ribosomal protein L36

Chain B9:

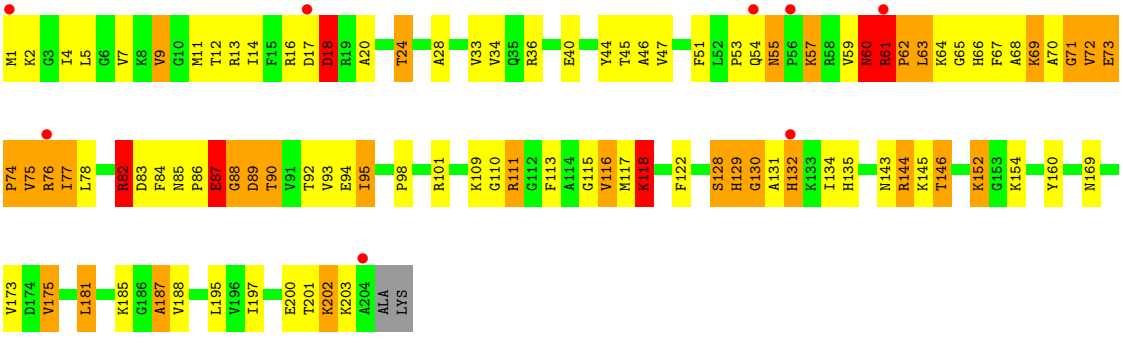
• Molecule 51: 50S ribosomal protein L1

Chain BC:



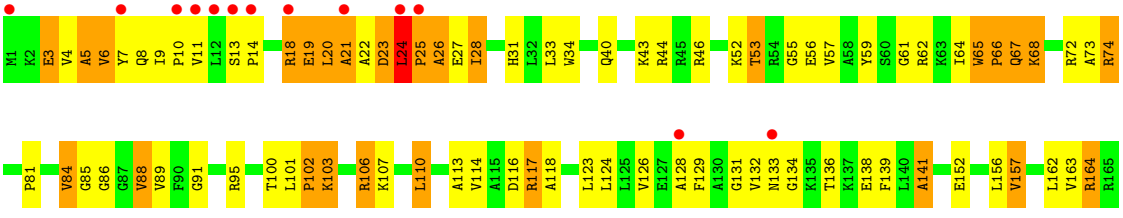
• Molecule 52: 50S ribosomal protein L3

Chain BE:



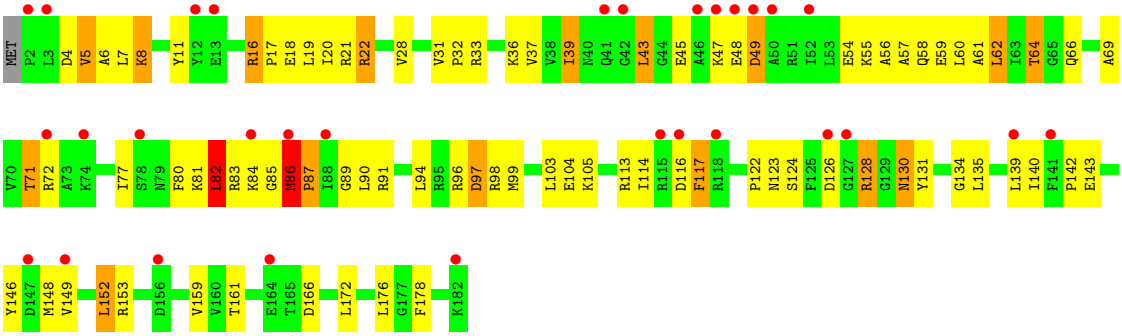
• Molecule 53: 50S ribosomal protein L4

Chain BF:



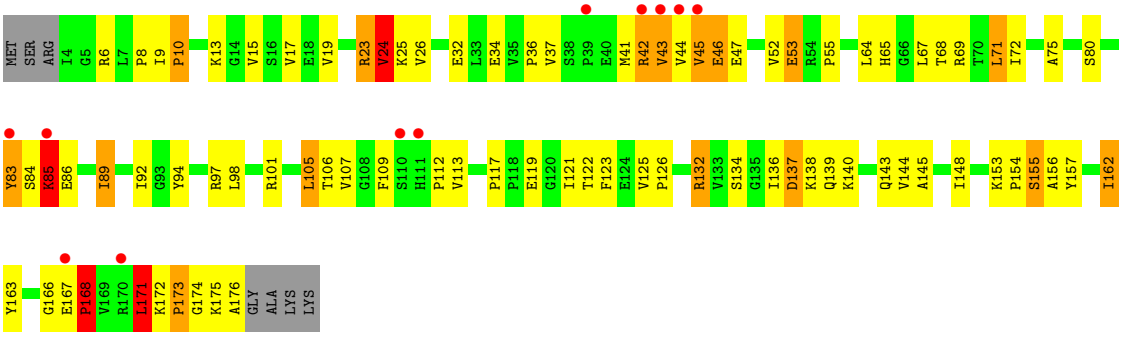
• Molecule 54: 50S ribosomal protein L5

Chain BG:



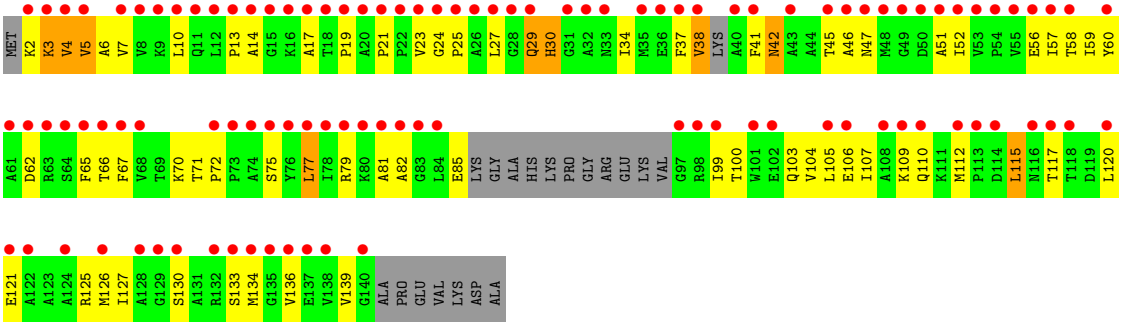
• Molecule 55: 50S ribosomal protein L6

Chain BH:



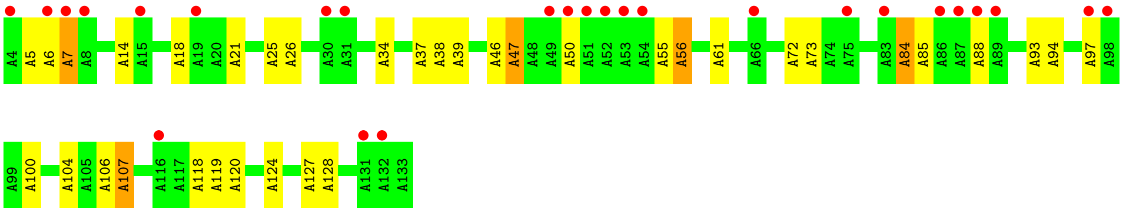
• Molecule 56: 50S ribosomal protein L11

Chain BK:



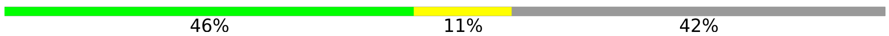
• Molecule 57: 50S ribosomal protein L10

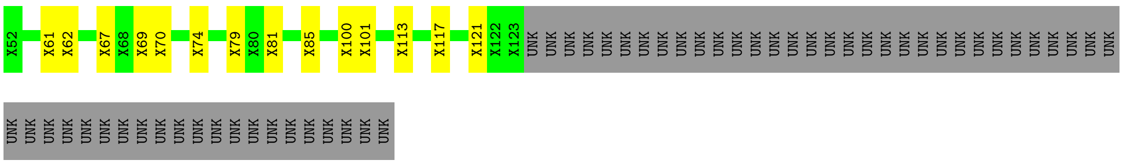
Chain BJ:



• Molecule 58: 50S ribosomal protein L12 CTD

Chain BL:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	201.58Å 241.65Å 305.80Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	39.60 – 2.86 39.59 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-2.86) 98.5 (39.59-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.250 0.201 , 0.243	Depositor DCC
R_{free} test set	32790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	151831	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GCP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.54	8/36408 (0.0%)	0.90	98/56818 (0.2%)
2	AV	0.49	1/1764 (0.1%)	0.96	11/2747 (0.4%)
3	AX	0.50	0/138	0.79	0/212
4	AJ	0.66	0/808	0.96	0/1085
5	AK	0.59	0/900	0.86	0/1213
6	AL	0.67	0/987	1.03	1/1320 (0.1%)
7	AM	0.54	0/999	0.89	0/1336
8	AN	0.61	0/501	1.08	2/664 (0.3%)
9	AO	0.61	0/745	0.94	1/992 (0.1%)
10	AP	0.59	0/717	0.92	2/963 (0.2%)
11	AQ	0.68	0/837	0.89	1/1117 (0.1%)
12	AR	0.60	0/579	0.84	0/768
13	AS	0.58	0/643	0.91	1/865 (0.1%)
14	AT	0.61	0/765	0.90	0/1007
15	AB	0.56	0/1936	0.83	1/2609 (0.0%)
16	AC	0.64	0/1637	0.93	3/2205 (0.1%)
17	AD	0.63	2/1733 (0.1%)	0.97	8/2318 (0.3%)
18	AE	0.71	0/1163	0.93	3/1564 (0.2%)
19	AF	0.55	0/856	0.78	0/1154
20	AG	0.54	0/1276	0.82	0/1709
21	AH	0.64	0/1136	0.95	1/1527 (0.1%)
22	AI	0.57	0/1029	0.92	0/1378
23	AY	0.53	0/4961	0.81	3/6710 (0.0%)
24	AU	0.58	0/213	0.92	0/277
25	BA	0.61	43/68964 (0.1%)	0.95	224/107644 (0.2%)
26	BB	0.40	0/2853	0.84	4/4451 (0.1%)
27	BN	0.74	1/1131 (0.1%)	1.07	5/1525 (0.3%)
28	BO	0.67	0/943	0.98	2/1269 (0.2%)
29	BP	0.86	0/1131	1.29	8/1504 (0.5%)
30	BQ	0.64	0/1143	0.92	0/1527
31	BR	0.70	0/974	1.01	1/1302 (0.1%)
32	BS	0.55	0/778	0.87	0/1036

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BT	0.70	0/1155	1.15	5/1542 (0.3%)
34	BU	0.75	0/975	1.02	1/1297 (0.1%)
35	BV	0.69	0/790	0.99	1/1057 (0.1%)
36	BW	0.67	0/907	1.02	3/1216 (0.2%)
37	BX	0.69	0/739	0.90	1/993 (0.1%)
38	BY	0.81	0/788	1.08	1/1051 (0.1%)
39	BZ	0.56	0/1539	0.87	0/2093
40	B0	0.57	0/671	0.86	0/892
41	B1	0.69	0/738	0.95	0/981
42	B2	0.57	0/600	0.86	0/793
43	BD	0.87	3/2154 (0.1%)	1.08	5/2905 (0.2%)
44	B3	0.55	0/472	0.80	0/634
45	B4	0.54	0/228	0.71	0/309
46	B5	0.85	0/473	1.22	5/639 (0.8%)
47	B6	0.94	0/387	1.36	3/518 (0.6%)
48	B7	0.74	0/426	0.85	0/561
49	B8	0.79	0/515	1.22	3/679 (0.4%)
50	B9	0.69	0/302	1.05	1/397 (0.3%)
51	BC	0.56	1/1747 (0.1%)	1.01	4/2351 (0.2%)
52	BE	0.75	0/1596	1.01	3/2153 (0.1%)
53	BF	0.69	0/1658	0.93	2/2244 (0.1%)
54	BG	0.48	0/1499	0.78	2/2016 (0.1%)
55	BH	0.59	0/1327	0.93	2/1794 (0.1%)
56	BK	0.41	0/951	0.60	0/1290
57	BJ	0.51	0/650	0.62	0/907
All	All	0.61	59/163935 (0.0%)	0.93	422/244128 (0.2%)

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
4	AJ	0	1
6	AL	0	1
8	AN	0	1
14	AT	0	2
17	AD	0	2
23	AY	0	4
27	BN	0	2
29	BP	0	15
30	BQ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BR	0	2
32	BS	0	1
33	BT	0	6
34	BU	0	3
35	BV	0	3
38	BY	0	6
41	B1	0	2
43	BD	0	4
46	B5	0	2
47	B6	0	3
51	BC	0	2
52	BE	0	5
53	BF	0	1
55	BH	0	1
58	BL	0	1
All	All	0	72

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2506	U	O3'-P	12.63	1.76	1.61
25	BA	1695	G	O3'-P	-9.03	1.50	1.61
27	BN	127	ASP	CB-CG	8.59	1.69	1.51
25	BA	1299	G	O3'-P	-7.33	1.52	1.61
25	BA	1300	U	O3'-P	-6.92	1.52	1.61
2	AV	72	C	O3'-P	-6.78	1.53	1.61
25	BA	1779	U	O3'-P	-6.73	1.53	1.61
1	AA	1145	C	O3'-P	-6.69	1.53	1.61
25	BA	2591	C	O3'-P	-6.58	1.53	1.61
25	BA	330	A	O3'-P	-6.47	1.53	1.61
25	BA	1370	C	O3'-P	-6.37	1.53	1.61
51	BC	27	ARG	CG-CD	-6.32	1.36	1.51
25	BA	2592	G	O3'-P	-6.25	1.53	1.61
43	BD	30	GLU	CG-CD	6.08	1.61	1.51
25	BA	1694	C	O3'-P	-6.08	1.53	1.61
25	BA	126	A	O3'-P	-5.92	1.54	1.61
25	BA	1819	A	O3'-P	-5.78	1.54	1.61
1	AA	1517	G	O3'-P	-5.73	1.54	1.61
25	BA	2031	A	O3'-P	-5.72	1.54	1.61
43	BD	237	GLU	CG-CD	5.71	1.60	1.51
25	BA	2080	G	O3'-P	-5.70	1.54	1.61
25	BA	2194	G	O3'-P	-5.70	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1498	C	O3'-P	-5.69	1.54	1.61
17	AD	26	CYS	CB-SG	5.67	1.91	1.82
25	BA	1216	G	O3'-P	-5.66	1.54	1.61
17	AD	26	CYS	CA-CB	5.63	1.66	1.53
25	BA	447	A	O3'-P	-5.62	1.54	1.61
1	AA	675	A	O3'-P	-5.58	1.54	1.61
25	BA	1769	G	O3'-P	-5.58	1.54	1.61
25	BA	2198	A	O3'-P	-5.58	1.54	1.61
43	BD	237	GLU	CD-OE1	5.54	1.31	1.25
25	BA	2280	G	O3'-P	-5.54	1.54	1.61
25	BA	1793	C	O3'-P	-5.51	1.54	1.61
25	BA	1332	G	O3'-P	-5.47	1.54	1.61
25	BA	973	A	P-OP2	5.42	1.58	1.49
25	BA	2068	U	O3'-P	-5.42	1.54	1.61
25	BA	1970	A	O3'-P	-5.40	1.54	1.61
1	AA	1363	C	O3'-P	-5.39	1.54	1.61
25	BA	1350	C	O3'-P	-5.36	1.54	1.61
25	BA	2072	G	O3'-P	-5.36	1.54	1.61
25	BA	1802	A	O3'-P	-5.34	1.54	1.61
1	AA	1502	A	O3'-P	5.33	1.67	1.61
25	BA	209	C	O3'-P	-5.30	1.54	1.61
25	BA	1300	U	P-OP2	-5.27	1.40	1.49
25	BA	1773	A	O3'-P	-5.21	1.54	1.61
25	BA	1432	C	O3'-P	-5.20	1.54	1.61
25	BA	1831	G	O3'-P	-5.19	1.54	1.61
25	BA	129	C	O3'-P	-5.17	1.54	1.61
25	BA	1257	C	O3'-P	-5.14	1.54	1.61
25	BA	1693	U	O3'-P	-5.14	1.54	1.61
25	BA	1963	U	O3'-P	5.14	1.67	1.61
25	BA	1978	A	O3'-P	-5.14	1.54	1.61
1	AA	932	C	O3'-P	-5.13	1.54	1.61
25	BA	2549	G	O3'-P	-5.13	1.54	1.61
25	BA	756	C	O3'-P	-5.09	1.55	1.61
25	BA	232	G	O3'-P	-5.08	1.55	1.61
25	BA	1970	A	P-OP1	5.08	1.57	1.49
1	AA	875	C	O3'-P	-5.08	1.55	1.61
1	AA	504	C	O3'-P	-5.06	1.55	1.61

All (422) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	BC	27	ARG	NE-CZ-NH2	-24.39	108.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	996	A	O5'-P-OP1	-17.66	89.51	110.70
1	AA	1499	A	O5'-P-OP1	-14.95	92.25	105.70
25	BA	946	G	O5'-P-OP1	-14.17	92.95	105.70
25	BA	2502	G	O5'-P-OP1	-13.94	93.15	105.70
25	BA	1647	G	O5'-P-OP1	-13.70	93.37	105.70
25	BA	1300	U	P-O3'-C3'	13.62	136.04	119.70
25	BA	1970	A	O5'-P-OP2	-13.05	93.95	105.70
1	AA	1081	G	O5'-P-OP2	-12.52	94.44	105.70
1	AA	1498	U	C2'-C3'-O3'	12.37	136.71	109.50
25	BA	1648	C	O5'-P-OP1	-12.05	94.85	105.70
25	BA	2439	A	O5'-P-OP2	-11.61	95.25	105.70
1	AA	1067	A	C2'-C3'-O3'	11.53	134.88	109.50
17	AD	9	CYS	CA-CB-SG	11.21	134.19	114.00
25	BA	2577	A	O5'-P-OP2	-11.07	95.73	105.70
17	AD	26	CYS	CA-CB-SG	11.06	133.91	114.00
1	AA	1520	G	O5'-P-OP2	-10.82	95.96	105.70
1	AA	1198	G	O5'-P-OP1	-10.62	96.14	105.70
1	AA	1499	A	O5'-P-OP2	10.62	123.44	110.70
25	BA	1617	C	O5'-P-OP1	-10.57	96.19	105.70
1	AA	328	C	C2'-C3'-O3'	10.43	132.44	109.50
25	BA	1799	G	C2'-C3'-O3'	10.32	132.21	109.50
51	BC	27	ARG	CD-NE-CZ	-10.31	109.17	123.60
25	BA	996	A	O5'-P-OP2	10.27	123.02	110.70
25	BA	2554	U	O5'-P-OP1	-10.20	96.52	105.70
25	BA	819	A	O5'-P-OP1	-10.17	96.54	105.70
25	BA	2506	U	C2'-C3'-O3'	10.15	131.84	109.50
13	AS	5	LEU	CA-CB-CG	10.00	138.30	115.30
17	AD	12	CYS	CA-CB-SG	9.92	131.86	114.00
25	BA	732	C	O5'-P-OP2	-9.76	96.92	105.70
25	BA	2430	A	O5'-P-OP1	-9.67	97.00	105.70
1	AA	1145	C	C2'-C3'-O3'	-9.66	88.25	109.50
25	BA	510	C	O5'-P-OP2	-9.65	97.01	105.70
25	BA	1784	A	O5'-P-OP1	-9.62	97.05	105.70
1	AA	353	A	O5'-P-OP2	-9.54	97.11	105.70
1	AA	299	G	O5'-P-OP1	-9.38	97.26	105.70
25	BA	1782	C	O5'-P-OP2	-9.37	97.27	105.70
25	BA	1992	G	C2'-C3'-O3'	9.32	130.00	109.50
25	BA	1647	G	O5'-P-OP2	9.30	121.86	110.70
25	BA	1622	G	O5'-P-OP2	-9.28	97.35	105.70
1	AA	828	A	O5'-P-OP2	-9.20	97.42	105.70
25	BA	2141	G	C2'-C3'-O3'	9.16	129.65	109.50
1	AA	708	C	O5'-P-OP2	-9.11	97.50	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	2577	A	O5'-P-OP1	9.06	121.57	110.70
25	BA	1786	A	N9-C1'-C2'	9.03	125.74	114.00
8	AN	40	CYS	CA-CB-SG	9.00	130.20	114.00
1	AA	30	U	C2'-C3'-O3'	8.96	129.22	109.50
25	BA	2225	A	C2'-C3'-O3'	8.92	129.13	109.50
1	AA	353	A	O5'-P-OP1	8.76	121.21	110.70
25	BA	2491	U	O5'-P-OP1	-8.71	97.86	105.70
17	AD	31	CYS	CA-CB-SG	-8.69	98.36	114.00
25	BA	1332	G	O5'-P-OP2	-8.67	97.90	105.70
2	AV	34	G	C2'-C3'-O3'	8.45	128.08	109.50
25	BA	2272	U	O5'-P-OP2	-8.43	98.12	105.70
1	AA	1181	G	O5'-P-OP2	-8.39	98.15	105.70
25	BA	752	A	C4'-C3'-O3'	-8.34	91.89	109.40
25	BA	1622	G	O5'-P-OP1	8.31	120.67	110.70
25	BA	387	U	C2'-C3'-O3'	8.21	127.56	109.50
25	BA	787	U	O5'-P-OP1	8.15	120.48	110.70
51	BC	27	ARG	CB-CG-CD	8.13	132.73	111.60
50	B9	27	CYS	CA-CB-SG	8.01	128.41	114.00
29	BP	7	ARG	NE-CZ-NH1	8.00	124.30	120.30
25	BA	1784	A	O5'-P-OP2	7.99	120.28	110.70
25	BA	752	A	C2'-C3'-O3'	7.98	127.05	109.50
25	BA	945	A	O5'-P-OP1	7.95	120.23	110.70
25	BA	2430	A	O5'-P-OP2	7.94	120.23	110.70
1	AA	1143	G	C2'-C3'-O3'	7.92	126.92	109.50
2	AV	72	C	C4'-C3'-O3'	7.91	128.82	113.00
25	BA	2479	G	O5'-P-OP2	-7.90	98.59	105.70
33	BT	93	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	AA	115	G	C2'-C3'-O3'	7.79	126.65	109.50
25	BA	2439	A	O5'-P-OP1	7.79	120.04	110.70
25	BA	2444	G	O5'-P-OP2	-7.77	98.70	105.70
25	BA	1653	G	C2'-C3'-O3'	7.75	126.55	109.50
25	BA	2318	G	C2'-C3'-O3'	7.67	126.37	109.50
1	AA	1520	G	O5'-P-OP1	7.67	119.90	110.70
25	BA	1314	C	O5'-P-OP2	-7.66	98.81	105.70
1	AA	1102	A	O5'-P-OP1	-7.63	98.83	105.70
25	BA	1780	A	O5'-P-OP1	7.63	119.86	110.70
1	AA	687	A	C2'-C3'-O3'	7.59	126.19	109.50
25	BA	1541	G	C2'-C3'-O3'	7.55	126.11	109.50
1	AA	1082	G	O5'-P-OP2	-7.53	98.92	105.70
25	BA	1610	A	O5'-P-OP2	-7.50	98.95	105.70
25	BA	1693	U	P-O3'-C3'	7.50	128.70	119.70
46	B5	51	TYR	CA-CB-CG	7.50	127.65	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B6	45	LYS	N-CA-C	7.50	131.24	111.00
1	AA	562	C	O5'-P-OP1	-7.49	98.96	105.70
25	BA	115	C	O5'-P-OP1	-7.47	98.97	105.70
25	BA	1819	A	C2'-C3'-O3'	7.45	125.89	109.50
1	AA	1133	G	N9-C1'-C2'	-7.44	103.81	112.00
1	AA	726	C	O5'-P-OP1	-7.43	99.02	105.70
9	AO	17	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	AA	1145	C	C4'-C3'-O3'	-7.39	93.87	109.40
25	BA	579	G	O5'-P-OP1	-7.38	99.05	105.70
25	BA	2778	A	O5'-P-OP2	-7.38	99.06	105.70
1	AA	916	G	O5'-P-OP2	-7.37	99.06	105.70
1	AA	1138	G	O4'-C1'-N9	7.37	114.10	108.20
25	BA	2200	C	C2'-C3'-O3'	7.34	125.65	109.50
1	AA	785	G	C2'-C3'-O3'	7.33	125.63	109.50
25	BA	1671	U	O5'-P-OP1	-7.32	99.12	105.70
29	BP	59	LEU	CA-CB-CG	7.31	132.10	115.30
25	BA	2191	G	C2'-C3'-O3'	7.28	125.51	109.50
25	BA	2447	G	C4'-C3'-O3'	-7.26	94.15	109.40
36	BW	92	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	AA	1133	G	C2'-C3'-O3'	7.24	125.43	109.50
25	BA	272	G	C2'-C3'-O3'	7.24	125.42	109.50
25	BA	787	U	O5'-P-OP2	-7.22	99.20	105.70
25	BA	1541	G	C4'-C3'-O3'	-7.21	94.25	109.40
25	BA	1542	A	O5'-P-OP1	-7.20	99.22	105.70
25	BA	1648	C	O5'-P-OP2	7.19	119.32	110.70
25	BA	1812	A	O5'-P-OP2	-7.18	99.24	105.70
25	BA	1022	G	C2'-C3'-O3'	7.15	125.23	109.50
36	BW	92	ARG	NE-CZ-NH2	-7.15	116.72	120.30
27	BN	127	ASP	CB-CG-OD1	7.14	124.73	118.30
1	AA	1504	G	O5'-P-OP1	-7.14	99.27	105.70
21	AH	92	ARG	NE-CZ-NH1	7.13	123.86	120.30
25	BA	1502	C	C2'-C3'-O3'	7.13	125.18	109.50
29	BP	60	MET	CG-SD-CE	7.12	111.59	100.20
25	BA	603	A	C2'-C3'-O3'	7.12	125.15	109.50
25	BA	2507	C	O5'-P-OP2	-7.10	99.31	105.70
25	BA	2581	G	O4'-C1'-N9	7.09	113.87	108.20
1	AA	266	G	P-O3'-C3'	7.08	128.20	119.70
25	BA	2199	A	C2'-C3'-O3'	7.06	125.04	109.50
25	BA	2031	A	O5'-P-OP2	-7.05	99.35	105.70
28	BO	78	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	AV	28	G	C2'-C3'-O3'	6.98	124.87	113.70
10	AP	8	ARG	NE-CZ-NH1	6.97	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	299	G	O5'-P-OP2	6.97	119.06	110.70
25	BA	2036	C	O5'-P-OP1	6.96	119.05	110.70
43	BD	99	ASP	CB-CA-C	-6.92	96.55	110.40
17	AD	12	CYS	N-CA-C	-6.89	92.39	111.00
1	AA	1505	G	O5'-P-OP2	6.89	118.96	110.70
1	AA	243	A	C2'-C3'-O3'	6.88	124.70	113.70
25	BA	2585	U	C2'-C3'-O3'	6.86	124.67	113.70
1	AA	1138	G	C1'-O4'-C4'	-6.84	104.43	109.90
25	BA	990	A	C4'-C3'-O3'	-6.84	95.04	109.40
1	AA	79	G	C2'-C3'-O3'	6.81	124.60	113.70
25	BA	2541	A	C2'-C3'-O3'	6.76	124.51	113.70
1	AA	1504	G	P-O3'-C3'	6.74	127.79	119.70
43	BD	88	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	AV	72	C	N1-C1'-C2'	-6.67	104.66	112.00
25	BA	2199	A	O5'-P-OP2	6.67	118.70	110.70
25	BA	945	A	C2'-C3'-O3'	-6.67	94.83	109.50
1	AA	771	G	O5'-P-OP2	-6.64	99.72	105.70
1	AA	1519	A	O5'-P-OP2	-6.62	99.74	105.70
1	AA	913	A	C2'-C3'-O3'	6.60	124.26	113.70
1	AA	533	A	C2'-C3'-O3'	6.58	124.23	113.70
23	AY	320	PRO	N-CA-C	-6.54	95.08	112.10
25	BA	2403	C	O5'-P-OP1	-6.52	99.83	105.70
1	AA	377	G	O5'-P-OP2	-6.47	99.87	105.70
1	AA	267	C	P-O5'-C5'	-6.46	110.57	120.90
25	BA	74	A	C2'-C3'-O3'	6.44	124.00	113.70
29	BP	7	ARG	NE-CZ-NH2	-6.44	117.08	120.30
29	BP	116	GLY	N-CA-C	6.43	129.17	113.10
36	BW	11	ARG	NE-CZ-NH1	6.39	123.50	120.30
25	BA	1970	A	C4'-C3'-O3'	-6.39	95.99	109.40
1	AA	180	U	O5'-P-OP1	-6.38	99.95	105.70
25	BA	1349	A	O4'-C4'-C3'	-6.38	97.62	104.00
23	AY	260	LEU	CA-CB-CG	6.37	129.95	115.30
1	AA	1139	G	C3'-C2'-O2'	-6.37	94.83	113.30
18	AE	41	VAL	CB-CA-C	-6.37	99.30	111.40
25	BA	1970	A	C1'-O4'-C4'	-6.36	104.81	109.90
17	AD	12	CYS	CB-CA-C	6.32	123.03	110.40
27	BN	119	ARG	NE-CZ-NH1	6.30	123.45	120.30
53	BF	7	TYR	CA-CB-CG	6.29	125.35	113.40
25	BA	1698	A	O4'-C1'-C2'	-6.28	99.52	105.80
25	BA	982	C	O5'-P-OP2	-6.27	100.05	105.70
25	BA	1618	A	O5'-P-OP1	-6.26	100.07	105.70
28	BO	78	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	827	U	C2'-C3'-O3'	-6.24	95.78	109.50
25	BA	1255	U	O5'-P-OP2	-6.23	100.09	105.70
25	BA	722	A	C2'-C3'-O3'	6.22	123.66	113.70
25	BA	906	G	C2'-C3'-O3'	6.22	123.66	113.70
25	BA	2830	G	C2'-C3'-O3'	6.22	123.66	113.70
25	BA	701	G	C2'-C3'-O3'	6.22	123.65	113.70
25	BA	948	G	O5'-P-OP1	6.19	118.12	110.70
25	BA	2023	G	O5'-P-OP1	-6.18	100.13	105.70
25	BA	512	G	O4'-C1'-N9	6.18	113.14	108.20
25	BA	2579	C	O5'-P-OP2	-6.17	100.15	105.70
25	BA	1300	U	O3'-P-O5'	6.16	115.71	104.00
25	BA	732	C	O5'-P-OP1	6.15	118.08	110.70
25	BA	1516	C	O5'-P-OP1	-6.15	100.17	105.70
25	BA	2346	A	O4'-C1'-N9	6.15	113.12	108.20
1	AA	1502	A	N9-C1'-C2'	6.13	121.97	114.00
25	BA	967	C	O5'-P-OP2	-6.13	100.18	105.70
1	AA	1181	G	C4'-C3'-O3'	-6.13	96.53	109.40
1	AA	509	A	C2'-C3'-O3'	6.13	123.51	113.70
25	BA	1017	G	C2'-C3'-O3'	6.12	123.50	113.70
25	BA	1024	G	O5'-P-OP1	-6.12	100.19	105.70
16	AC	11	ARG	NE-CZ-NH1	6.12	123.36	120.30
25	BA	834	C	O5'-P-OP2	-6.12	100.19	105.70
1	AA	681	C	O5'-P-OP2	-6.11	100.20	105.70
1	AA	1300	G	O5'-P-OP2	6.10	118.03	110.70
25	BA	2722	G	O5'-P-OP1	-6.08	100.22	105.70
37	BX	57	LEU	CA-CB-CG	6.08	129.28	115.30
26	BB	75	G	C2'-C3'-O3'	6.08	123.42	113.70
25	BA	2722	G	O5'-P-OP2	6.07	117.98	110.70
1	AA	524	G	O5'-P-OP2	-6.06	100.24	105.70
43	BD	88	ARG	NE-CZ-NH1	6.04	123.32	120.30
46	B5	52	TYR	N-CA-C	-6.02	94.74	111.00
1	AA	1472	U	O5'-P-OP2	-6.01	100.29	105.70
25	BA	2163	C	C2'-C3'-O3'	6.00	123.30	113.70
23	AY	88	VAL	CB-CA-C	-5.97	100.05	111.40
25	BA	2015	A	O5'-P-OP2	-5.96	100.34	105.70
25	BA	1780	A	O5'-P-OP2	-5.95	100.34	105.70
25	BA	1962	C	C1'-C2'-O2'	-5.95	92.74	110.60
52	BE	88	GLY	N-CA-C	5.95	127.96	113.10
25	BA	54	G	C2'-C3'-O3'	5.93	123.19	113.70
51	BC	104	LEU	CA-CB-CG	5.93	128.95	115.30
1	AA	194	C	O5'-P-OP2	-5.93	100.36	105.70
25	BA	2612	C	O5'-P-OP2	-5.93	100.36	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	945	A	N9-C1'-C2'	5.91	121.68	114.00
8	AN	44	LEU	CA-CB-CG	5.89	128.85	115.30
1	AA	1147	C	C2'-C3'-O3'	5.88	123.11	113.70
25	BA	1970	A	C5'-C4'-O4'	5.87	116.15	109.10
25	BA	2600	A	O5'-P-OP2	5.86	117.73	110.70
25	BA	2031	A	C5'-C4'-C3'	-5.86	106.62	116.00
25	BA	1540	U	P-O5'-C5'	-5.85	111.54	120.90
1	AA	1330	U	O5'-P-OP2	-5.84	100.45	105.70
46	B5	3	LYS	C-N-CA	5.84	136.29	121.70
25	BA	774	A	O5'-P-OP2	-5.83	100.45	105.70
1	AA	1420	C	O5'-P-OP2	5.83	117.70	110.70
25	BA	1882	C	C2'-C3'-O3'	5.83	123.03	113.70
25	BA	1057	A	C2'-C3'-O3'	5.83	123.02	113.70
1	AA	244	U	O5'-P-OP1	-5.82	100.46	105.70
1	AA	260	G	O5'-P-OP1	-5.82	100.46	105.70
54	BG	89	GLY	N-CA-C	-5.81	98.57	113.10
55	BH	10	PRO	N-CA-CB	5.81	110.27	103.30
25	BA	1982	C	O5'-P-OP2	-5.80	100.47	105.70
2	AV	1	G	C5'-C4'-O4'	5.79	116.05	109.10
25	BA	2006	C	O5'-P-OP1	5.79	117.65	110.70
1	AA	1013	G	C2'-C3'-O3'	5.79	122.96	113.70
25	BA	2346	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	AA	391	G	O5'-P-OP2	-5.79	100.49	105.70
25	BA	2506	U	C4'-C3'-O3'	-5.78	97.26	109.40
25	BA	2346	A	O4'-C1'-C2'	-5.76	100.04	105.80
2	AV	4	C	C2'-C3'-O3'	5.75	122.91	113.70
38	BY	31	LEU	C-N-CD	-5.75	107.95	120.60
25	BA	991	C	O5'-P-OP2	5.75	117.60	110.70
1	AA	762	C	O5'-P-OP1	-5.75	100.53	105.70
1	AA	828	A	O5'-P-OP1	5.74	117.59	110.70
25	BA	1959	G	C2'-C3'-O3'	5.73	122.87	113.70
17	AD	31	CYS	N-CA-CB	5.73	120.92	110.60
25	BA	252	G	O5'-P-OP2	-5.71	100.56	105.70
25	BA	1888	G	O4'-C4'-C3'	-5.71	98.29	104.00
43	BD	54	ARG	NE-CZ-NH2	-5.71	117.44	120.30
26	BB	19	G	C2'-C3'-O3'	5.70	122.83	113.70
25	BA	669	G	O5'-P-OP1	5.69	117.53	110.70
33	BT	30	VAL	N-CA-C	5.69	126.36	111.00
25	BA	739	G	C2'-C3'-O3'	-5.69	96.98	109.50
25	BA	1838	C	C4'-C3'-O3'	-5.68	97.47	109.40
25	BA	2596	U	O5'-P-OP1	-5.68	100.59	105.70
11	AQ	68	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AC	94	LEU	CA-CB-CG	5.67	128.34	115.30
25	BA	2095	C	C2'-C3'-O3'	5.67	122.78	113.70
25	BA	102	G	N9-C1'-C2'	5.67	121.37	114.00
25	BA	510	C	O5'-P-OP1	5.66	117.49	110.70
29	BP	36	LYS	CD-CE-NZ	5.65	124.69	111.70
49	B8	48	PHE	CB-CA-C	-5.65	99.11	110.40
25	BA	1865	G	O5'-P-OP1	-5.64	100.62	105.70
25	BA	247	G	O5'-P-OP2	-5.64	100.62	105.70
46	B5	48	GLU	N-CA-C	-5.64	95.77	111.00
1	AA	731	G	O5'-P-OP2	-5.63	100.64	105.70
25	BA	1915	U	C2'-C3'-O3'	5.63	122.70	113.70
25	BA	1782	C	O5'-P-OP1	5.62	117.45	110.70
1	AA	1081	G	O5'-P-OP1	5.62	117.45	110.70
49	B8	46	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	AA	1498	U	P-O3'-C3'	5.60	126.42	119.70
25	BA	1485	G	C2'-C3'-O3'	5.60	122.66	113.70
25	BA	2757	A	O5'-P-OP2	-5.60	100.66	105.70
25	BA	2226	C	O5'-P-OP2	-5.59	100.67	105.70
25	BA	1969	A	O5'-P-OP2	-5.59	100.67	105.70
1	AA	1420	C	O5'-P-OP1	-5.58	100.67	105.70
29	BP	27	HIS	N-CA-C	5.57	126.05	111.00
25	BA	789	A	O5'-P-OP1	-5.57	100.69	105.70
17	AD	36	ARG	NE-CZ-NH1	5.57	123.08	120.30
25	BA	2048	G	O5'-P-OP1	5.57	117.38	110.70
31	BR	4	LEU	CB-CG-CD1	5.57	120.46	111.00
25	BA	744	G	O5'-P-OP2	-5.56	100.69	105.70
25	BA	1204	A	O4'-C1'-C2'	-5.55	100.25	105.80
25	BA	1500	G	C2'-C3'-O3'	5.55	122.58	113.70
25	BA	994	C	O5'-P-OP2	-5.55	100.71	105.70
1	AA	175	C	O5'-P-OP1	-5.54	100.71	105.70
29	BP	62	LEU	CB-CG-CD1	5.54	120.42	111.00
25	BA	586	A	O5'-P-OP2	-5.54	100.71	105.70
25	BA	1807	G	N9-C1'-C2'	-5.54	105.91	112.00
33	BT	87	ASP	CB-CG-OD1	-5.54	113.32	118.30
25	BA	1426	G	C2'-C3'-O3'	5.53	122.54	113.70
1	AA	149	A	N9-C1'-C2'	-5.51	105.93	112.00
53	BF	46	ARG	CG-CD-NE	-5.51	100.23	111.80
25	BA	2198	A	C2'-C3'-O3'	-5.50	97.40	109.50
1	AA	189(A)	C	O5'-P-OP2	-5.50	100.75	105.70
25	BA	2031	A	C2'-C3'-O3'	5.48	122.47	113.70
25	BA	1308	A	O5'-P-OP2	-5.48	100.77	105.70
25	BA	2700	C	O5'-P-OP2	-5.47	100.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BN	74	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	AA	1456	G	O5'-P-OP1	5.47	117.26	110.70
27	BN	114	ARG	NE-CZ-NH1	5.45	123.03	120.30
25	BA	1970	A	O4'-C1'-C2'	-5.44	100.36	105.80
25	BA	573	G	O5'-P-OP2	-5.44	100.81	105.70
27	BN	119	ARG	NE-CZ-NH2	-5.43	117.58	120.30
25	BA	551	G	C2'-C3'-O3'	5.43	122.39	113.70
1	AA	350	G	O5'-P-OP2	-5.43	100.81	105.70
25	BA	1142(A)	A	O5'-P-OP1	-5.43	100.81	105.70
1	AA	348	G	C2'-C3'-O3'	5.43	122.38	113.70
25	BA	537	C	C2'-C3'-O3'	5.43	122.38	113.70
52	BE	132	HIS	C-N-CA	-5.43	108.14	121.70
25	BA	1764	G	O5'-P-OP2	-5.42	100.82	105.70
25	BA	700	G	C2'-C3'-O3'	5.42	122.37	113.70
25	BA	738	G	O5'-P-OP2	-5.41	100.84	105.70
25	BA	1744	C	C2'-C3'-O3'	5.41	122.35	113.70
1	AA	1138	G	C5'-C4'-O4'	5.40	115.58	109.10
15	AB	200	ILE	CB-CA-C	-5.40	100.81	111.60
1	AA	149	A	C4'-C3'-O3'	5.39	123.78	113.00
25	BA	1193	G	O5'-P-OP2	-5.39	100.85	105.70
25	BA	2060	A	O5'-P-OP1	-5.38	100.86	105.70
1	AA	1151	A	O5'-P-OP2	-5.37	100.87	105.70
25	BA	1963	U	N1-C1'-C2'	5.37	120.98	114.00
25	BA	2820	A	C2'-C3'-O3'	-5.37	97.69	109.50
35	BV	39	LEU	CA-CB-CG	5.36	127.63	115.30
49	B8	62	LEU	CB-CG-CD1	5.36	120.11	111.00
1	AA	1261	A	O5'-P-OP1	-5.36	100.88	105.70
25	BA	508	G	C2'-C3'-O3'	-5.36	97.72	109.50
25	BA	1947	C	C2'-C3'-O3'	5.36	122.27	113.70
25	BA	1881	C	C2'-C3'-O3'	5.35	122.26	113.70
1	AA	971	G	O5'-P-OP2	-5.35	100.89	105.70
2	AV	1	G	C5'-C4'-C3'	5.35	124.56	116.00
25	BA	2497	A	C4'-C3'-O3'	-5.34	98.18	109.40
1	AA	1136	U	O4'-C1'-N1	5.34	112.47	108.20
1	AA	1506	U	O5'-P-OP1	5.33	117.10	110.70
25	BA	1558	A	C2'-C3'-O3'	5.33	122.23	113.70
25	BA	1653	G	P-O3'-C3'	5.33	126.09	119.70
33	BT	30	VAL	CB-CA-C	-5.32	101.28	111.40
47	B6	10	LEU	CA-CB-CG	5.32	127.53	115.30
25	BA	1917	U	O5'-P-OP1	-5.32	100.92	105.70
25	BA	1654	A	O5'-P-OP1	-5.31	100.92	105.70
25	BA	1970	A	C5'-C4'-C3'	5.31	124.49	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B6	46	HIS	N-CA-C	5.30	125.32	111.00
25	BA	1578	U	O5'-P-OP2	-5.30	100.93	105.70
25	BA	1879	C	C2'-C3'-O3'	5.29	122.16	113.70
25	BA	1786	A	O4'-C1'-C2'	-5.28	100.52	105.80
1	AA	973	G	C2'-C3'-O3'	5.28	122.14	113.70
18	AE	126	ARG	NE-CZ-NH2	-5.28	117.66	120.30
33	BT	93	ARG	NE-CZ-NH2	-5.28	117.66	120.30
25	BA	2778	A	O5'-P-OP1	5.28	117.03	110.70
25	BA	1388	G	C2'-C3'-O3'	5.27	122.14	113.70
25	BA	2171	A	C4'-C3'-O3'	-5.27	98.33	109.40
1	AA	427	U	O5'-P-OP2	-5.27	100.96	105.70
10	AP	8	ARG	NE-CZ-NH2	-5.27	117.67	120.30
25	BA	562	U	O5'-P-OP1	-5.25	100.97	105.70
26	BB	100	A	O5'-P-OP2	-5.23	100.99	105.70
25	BA	2682	U	O5'-P-OP2	5.23	116.98	110.70
1	AA	816	A	O5'-P-OP1	5.23	116.97	110.70
1	AA	180	U	O5'-P-OP2	5.23	116.97	110.70
25	BA	2768	C	O5'-P-OP2	-5.23	101.00	105.70
1	AA	708	C	O5'-P-OP1	5.22	116.97	110.70
1	AA	1198	G	O5'-P-OP2	5.22	116.97	110.70
2	AV	72	C	C4'-C3'-C2'	-5.21	97.39	102.60
25	BA	2665	A	O4'-C4'-C3'	-5.21	98.78	104.00
1	AA	109	A	O5'-P-OP2	-5.21	101.02	105.70
25	BA	1936	A	N9-C1'-C2'	5.20	120.76	114.00
25	BA	2655	G	O5'-P-OP1	-5.20	101.02	105.70
1	AA	321	A	O5'-P-OP2	-5.20	101.02	105.70
43	BD	71	ASP	CB-CA-C	-5.19	100.01	110.40
1	AA	1145	C	C3'-C2'-O2'	-5.19	98.24	113.30
46	B5	40	LYS	CD-CE-NZ	5.19	123.64	111.70
54	BG	152	LEU	CA-CB-CG	5.19	127.24	115.30
25	BA	102	G	O4'-C1'-C2'	-5.19	100.61	105.80
25	BA	1693	U	O3'-P-O5'	5.18	113.85	104.00
25	BA	1905	C	O5'-P-OP2	-5.17	101.05	105.70
25	BA	120	U	O5'-P-OP1	-5.17	101.05	105.70
25	BA	933	A	O4'-C4'-C3'	-5.17	98.83	104.00
2	AV	76	A	C4'-C3'-C2'	-5.16	97.44	102.60
25	BA	1545	A	C2'-C3'-O3'	5.16	121.95	113.70
26	BB	15	A	C2'-C3'-O3'	5.15	121.95	113.70
6	AL	113	ARG	NE-CZ-NH2	-5.15	117.72	120.30
25	BA	2602	A	O5'-P-OP2	5.15	116.88	110.70
25	BA	1888	G	C5'-C4'-O4'	5.14	115.27	109.10
25	BA	753	C	O5'-P-OP1	-5.14	101.08	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	60	A	C2'-C3'-O3'	5.13	121.91	113.70
25	BA	2006	C	O5'-P-OP2	-5.13	101.08	105.70
25	BA	2392	A	O4'-C4'-C3'	-5.13	98.87	104.00
1	AA	1146	A	C2'-C3'-O3'	5.13	121.91	113.70
52	BE	60	ASN	N-CA-C	5.13	124.85	111.00
1	AA	1504	G	C4'-C3'-O3'	5.12	123.24	113.00
2	AV	64	A	C2'-C3'-O3'	5.12	121.89	113.70
25	BA	935	C	C2'-C3'-O3'	5.12	121.89	113.70
25	BA	2700	C	O5'-P-OP1	5.11	116.83	110.70
1	AA	319	G	O5'-P-OP2	-5.10	101.11	105.70
1	AA	762	C	O5'-P-OP2	5.10	116.82	110.70
25	BA	619	G	O5'-P-OP1	-5.10	101.11	105.70
1	AA	1261	A	O5'-P-OP2	5.09	116.81	110.70
25	BA	265	A	N9-C1'-C2'	5.08	120.61	114.00
25	BA	2444	G	O5'-P-OP1	5.08	116.80	110.70
1	AA	7	G	C2'-C3'-O3'	-5.08	98.33	109.50
25	BA	2714	G	C5'-C4'-C3'	-5.08	107.88	116.00
25	BA	221	A	C2'-C3'-O3'	5.07	121.82	113.70
25	BA	2714	G	C2'-C3'-O3'	5.07	121.82	113.70
25	BA	2075	U	O5'-P-OP2	5.07	116.79	110.70
55	BH	8	PRO	N-CA-CB	5.07	109.39	103.30
25	BA	271(Y)	U	O4'-C1'-N1	5.07	112.26	108.20
25	BA	1525	G	O5'-P-OP2	-5.07	101.14	105.70
25	BA	2074	U	O5'-P-OP2	-5.07	101.14	105.70
18	AE	14	ARG	NE-CZ-NH2	-5.07	117.77	120.30
25	BA	1245	G	C2'-C3'-O3'	5.07	121.80	113.70
25	BA	2231	C	C2'-C3'-O3'	5.07	121.81	113.70
16	AC	196	LEU	CA-CB-CG	5.06	126.93	115.30
25	BA	1204	A	C3'-C2'-C1'	-5.06	97.45	101.50
34	BU	92	ARG	NE-CZ-NH1	5.06	122.83	120.30
25	BA	2040	C	O5'-P-OP1	-5.05	101.16	105.70
25	BA	2048	G	O5'-P-OP2	-5.05	101.16	105.70
25	BA	1162	G	C2'-C3'-O3'	5.05	121.77	113.70
1	AA	1135	U	C4'-C3'-O3'	5.04	123.09	113.00
25	BA	508	G	P-O5'-C5'	5.04	128.96	120.90
2	AV	72	C	O4'-C4'-C3'	-5.04	98.97	104.00
1	AA	931	C	C2'-C3'-O3'	5.03	121.75	113.70
25	BA	1941	C	O5'-P-OP1	-5.03	101.17	105.70
25	BA	2811	G	C2'-C3'-O3'	5.03	121.75	113.70
25	BA	2620	C	O5'-P-OP2	-5.03	101.18	105.70
25	BA	2465	C	O5'-P-OP2	-5.02	101.18	105.70
25	BA	1280	G	C2'-C3'-O3'	5.01	121.72	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	585	G	C4'-C3'-O3'	5.01	123.02	113.00

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	AD	11	LEU	Peptide
17	AD	17	VAL	Peptide
4	AJ	54	PHE	Peptide
6	AL	28	LYS	Peptide
8	AN	13	THR	Peptide
14	AT	73	HIS	Peptide
14	AT	95	ALA	Peptide
23	AY	209	ALA	Peptide
23	AY	319	ASP	Peptide
23	AY	320	PRO	Peptide
23	AY	404	VAL	Peptide
41	B1	29	GLY	Peptide
41	B1	94	LEU	Peptide
46	B5	47	PRO	Peptide
46	B5	51	TYR	Peptide
47	B6	10	LEU	Peptide
47	B6	20	ASN	Peptide
47	B6	31	PRO	Peptide
51	BC	143	GLY	Peptide
51	BC	70	LYS	Peptide
43	BD	197	GLY	Peptide
43	BD	223	GLY	Peptide
43	BD	24	ILE	Peptide
43	BD	36	PRO	Peptide
52	BE	131	ALA	Peptide
52	BE	61	ARG	Peptide
52	BE	62	PRO	Peptide
52	BE	76	ARG	Peptide
52	BE	86	PRO	Peptide
53	BF	85	GLY	Peptide
55	BH	166	GLY	Peptide
58	BL	121	UNK	Peptide
27	BN	124	ALA	Peptide
27	BN	20	GLY	Peptide
29	BP	10	PRO	Peptide
29	BP	107	LYS	Peptide

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Mol	Chain	Res	Type	Group
29	BP	115	LEU	Peptide
29	BP	143	GLY	Peptide
29	BP	29	LYS	Peptide
29	BP	33	ARG	Peptide
29	BP	34	GLY	Peptide
29	BP	37	GLY	Peptide
29	BP	40	SER	Peptide
29	BP	44	GLY	Peptide
29	BP	51	PHE	Peptide
29	BP	57	THR	Peptide
29	BP	70	GLN	Peptide
29	BP	8	PRO	Peptide
29	BP	9	ASN	Peptide
30	BQ	17	LEU	Peptide
30	BQ	19	GLY	Peptide
31	BR	117	VAL	Peptide
31	BR	5	LYS	Peptide
32	BS	11	LYS	Peptide
33	BT	29	ARG	Peptide
33	BT	30	VAL	Peptide
33	BT	58	ASN	Peptide
33	BT	79	HIS	Peptide
33	BT	92	GLY	Peptide
33	BT	93	ARG	Peptide
34	BU	90	VAL	Peptide
34	BU	95	LEU	Peptide
34	BU	96	ALA	Peptide
35	BV	1	MET	Peptide
35	BV	18	LEU	Peptide
35	BV	42	GLY	Peptide
38	BY	16	ALA	Peptide
38	BY	17	SER	Peptide
38	BY	40	GLU	Peptide
38	BY	6	HIS	Peptide
38	BY	61	ILE	Peptide
38	BY	76	CYS	Peptide

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	32529	0	16426	525	0
2	AV	1579	0	802	43	0
3	AX	125	0	64	2	0
4	AJ	795	0	840	29	0
5	AK	885	0	904	28	0
6	AL	971	0	1057	26	0
7	AM	988	0	1059	43	0
8	AN	492	0	529	21	0
9	AO	734	0	771	16	0
10	AP	701	0	720	14	0
11	AQ	824	0	891	19	0
12	AR	574	0	644	10	0
13	AS	630	0	652	25	0
14	AT	763	0	861	30	0
15	AB	1901	0	1951	86	0
16	AC	1613	0	1677	49	0
17	AD	1703	0	1763	64	0
18	AE	1147	0	1207	33	0
19	AF	843	0	857	19	0
20	AG	1257	0	1296	25	0
21	AH	1116	0	1177	27	0
22	AI	1011	0	1043	35	0
23	AY	4877	0	4964	166	0
24	AU	209	0	221	8	0
25	BA	61580	0	31049	1148	0
26	BB	2551	0	1295	55	0
27	BN	1104	0	1180	63	0
28	BO	933	0	996	35	0
29	BP	1114	0	1187	142	0
30	BQ	1122	0	1179	38	0
31	BR	960	0	1021	39	0
32	BS	770	0	832	42	0
33	BT	1141	0	1202	114	0
34	BU	958	0	1015	51	0
35	BV	779	0	852	50	0
36	BW	896	0	953	27	0
37	BX	725	0	778	15	0
38	BY	775	0	870	71	0
39	BZ	1508	0	1486	56	0
40	B0	662	0	688	22	0
41	B1	731	0	808	33	0
42	B2	598	0	653	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BD	2104	0	2182	101	0
44	B3	467	0	523	5	0
45	B4	225	0	229	10	0
46	B5	459	0	477	31	0
47	B6	380	0	390	55	0
48	B7	418	0	467	12	0
49	B8	507	0	576	58	0
50	B9	299	0	323	10	0
51	BC	1718	0	1766	54	0
52	BE	1563	0	1629	81	0
53	BF	1623	0	1677	83	0
54	BG	1474	0	1535	56	0
55	BH	1303	0	1348	55	0
56	BK	936	0	970	60	0
57	BJ	651	0	649	17	0
58	BL	356	0	75	7	0
59	AA	45	0	0	0	0
59	AY	1	0	0	0	0
59	B8	1	0	0	0	0
59	BA	88	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
60	AY	32	0	14	5	0
61	AY	4	0	0	1	0
All	All	151831	0	105250	3647	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 14.

All (3647) 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)
25:BA:2111:C:N3	25:BA:2147:G:N2	1.74	1.36
25:BA:1332:G:N2	25:BA:1609:A:O2'	1.62	1.26
47:B6:40:CYS:SG	47:B6:45:LYS:NZ	1.02	1.24
25:BA:90:U:O2'	25:BA:92:A:OP2	1.54	1.24
25:BA:1332:G:N2	25:BA:1609:A:HO2'	1.30	1.23
25:BA:2394:C:OP1	29:BP:63:PRO:HD2	1.41	1.20
23:AY:404:VAL:HG13	23:AY:405:PRO:HA	1.22	1.20
25:BA:1914:C:O2'	25:BA:1915:U:O5'	1.61	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:271(H):G:C5'	41:B1:81:LYS:HE2	1.72	1.17
25:BA:271(G):C:O2'	41:B1:81:LYS:CE	1.95	1.14
47:B6:48:VAL:HG23	47:B6:49:HIS:N	1.53	1.14
25:BA:271(H):G:H5'	41:B1:81:LYS:CE	1.78	1.14
25:BA:1048:A:N6	25:BA:1107:G:O6	1.81	1.12
29:BP:7:ARG:HD3	53:BF:188:ARG:HA	1.30	1.11
47:B6:40:CYS:SG	47:B6:45:LYS:CE	2.39	1.09
47:B6:48:VAL:HG23	47:B6:49:HIS:H	1.02	1.09
38:BY:79:CYS:SG	38:BY:80:GLY:N	2.20	1.08
29:BP:48:PRO:O	29:BP:50:ARG:N	1.88	1.05
29:BP:7:ARG:HA	29:BP:7:ARG:HH11	1.14	1.05
47:B6:37:ARG:O	47:B6:48:VAL:O	1.76	1.03
2:AV:76:A:H4'	2:AV:76:A:OP1	1.57	1.03
29:BP:7:ARG:HA	29:BP:7:ARG:NH1	1.72	1.02
25:BA:271(G):C:O2'	41:B1:81:LYS:HE3	1.59	1.02
25:BA:811:U:OP2	29:BP:30:THR:O	1.78	1.02
25:BA:2419:U:O4	49:B8:30:ARG:CZ	2.08	1.01
25:BA:1540:U:H6	25:BA:1540:U:H5'	1.23	1.00
35:BV:24:LYS:HA	35:BV:92:THR:HG23	1.40	0.99
29:BP:64:LYS:O	29:BP:66:GLY:N	1.95	0.99
1:AA:706:A:O4'	5:AK:29:ILE:HD11	1.63	0.99
1:AA:1054:C:O2	1:AA:1054:C:H3'	1.62	0.98
25:BA:242:G:H5"	49:B8:62:LEU:HD13	1.45	0.98
25:BA:2656:U:H3	25:BA:2665:A:H2	1.09	0.98
47:B6:48:VAL:CG2	47:B6:49:HIS:H	1.77	0.98
25:BA:676:A:H8	25:BA:2069:G:H21	1.05	0.97
25:BA:1100:C:H4'	25:BA:1100:C:OP1	1.63	0.97
17:AD:9:CYS:HA	17:AD:12:CYS:HB2	1.45	0.97
47:B6:47:THR:HG22	47:B6:48:VAL:N	1.76	0.97
1:AA:90:U:HO2'	1:AA:91:C:H5	1.09	0.96
1:AA:1502:A:H2	1:AA:1505:G:H1	1.02	0.96
8:AN:23:ARG:HD2	8:AN:28:GLY:O	1.63	0.96
25:BA:1899:G:H22	25:BA:1902:C:H41	1.09	0.96
27:BN:16:ILE:HD11	27:BN:26:LEU:HD11	1.46	0.96
46:B5:4:HIS:HB3	46:B5:5:PRO:CD	1.96	0.96
23:AY:404:VAL:HG13	23:AY:405:PRO:CA	1.95	0.96
43:BD:30:GLU:HG3	43:BD:63:ARG:NH2	1.81	0.96
25:BA:250:G:OP2	49:B8:13:ARG:NH2	1.98	0.95
47:B6:47:THR:CG2	47:B6:48:VAL:N	2.30	0.95
47:B6:48:VAL:CG2	47:B6:49:HIS:N	2.29	0.95
33:BT:85:LYS:NZ	33:BT:85:LYS:HB3	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BP:56:SER:O	29:BP:58:THR:N	1.97	0.95
50:B9:29:ASN:HD21	50:B9:32:HIS:CE1	1.84	0.95
25:BA:2137:C:H3'	25:BA:2137:C:O2	1.67	0.95
29:BP:17:LYS:O	29:BP:19:VAL:N	1.99	0.95
29:BP:59:LEU:HA	29:BP:61:ARG:NH1	1.81	0.94
7:AM:65:LYS:HA	7:AM:66:LEU:HB2	1.50	0.94
25:BA:1771:C:HO2'	25:BA:1786:A:H8	0.99	0.94
52:BE:129:HIS:O	52:BE:130:GLY:O	1.86	0.94
17:AD:26:CYS:HA	17:AD:31:CYS:HB2	1.46	0.94
27:BN:58:ASP:O	27:BN:60:ILE:N	2.01	0.94
46:B5:50:GLY:O	46:B5:51:TYR:HD1	1.51	0.93
1:AA:159:G:N2	1:AA:162:A:OP2	2.00	0.93
25:BA:243:U:OP1	49:B8:6:THR:HG21	1.68	0.93
25:BA:2200:C:OP2	41:B1:50:ARG:NH2	2.02	0.93
39:BZ:19:ARG:NH1	39:BZ:84:GLU:O	2.01	0.93
23:AY:71:THR:HG22	23:AY:80:ASN:OD1	1.69	0.93
25:BA:1658:C:OP1	52:BE:132:HIS:CE1	2.22	0.93
1:AA:1277:C:HO2'	1:AA:1279:A:H8	1.16	0.93
25:BA:1779:U:H5	25:BA:1784:A:N7	1.66	0.92
39:BZ:18:LEU:H	39:BZ:18:LEU:HD12	1.31	0.92
25:BA:807:U:OP2	29:BP:39:LYS:HG3	1.69	0.92
25:BA:1494:A:H3'	25:BA:1494:A:N3	1.84	0.92
25:BA:141:A:C8	25:BA:1408:C:O2'	2.22	0.92
25:BA:271(G):C:O2'	41:B1:81:LYS:NZ	2.02	0.92
1:AA:1321:C:H3'	1:AA:1322:C:H5"	1.49	0.91
4:AJ:34:VAL:HG22	4:AJ:74:ILE:HG22	1.52	0.91
25:BA:1910:G:H1	25:BA:1920:C:H5	1.16	0.91
1:AA:1138:G:O2'	1:AA:1139:G:OP1	1.88	0.91
25:BA:1447:G:O2'	25:BA:1544:A:H8	1.52	0.91
39:BZ:9:TYR:CE1	39:BZ:61:LEU:HD12	2.04	0.91
25:BA:259:G:H21	25:BA:621:A:H8	1.13	0.91
34:BU:91:ASP:OD1	34:BU:96:ALA:N	2.04	0.91
43:BD:2:ALA:O	43:BD:3:VAL:HB	1.71	0.91
25:BA:1538:G:H2'	25:BA:1539:G:H8	1.35	0.90
25:BA:1570:A:O4'	43:BD:38:LYS:HE2	1.70	0.90
15:AB:178:ARG:HG2	15:AB:178:ARG:HH11	1.34	0.90
25:BA:2111:C:C2	25:BA:2147:G:N2	2.38	0.90
43:BD:43:ARG:NH1	43:BD:44:ASN:OD1	2.04	0.90
56:BK:77:LEU:HD12	56:BK:107:ILE:HG23	1.54	0.90
38:BY:76:CYS:SG	38:BY:77:PRO:HD2	2.12	0.90
38:BY:96:ILE:HD12	38:BY:99:CYS:SG	2.12	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BU:90:VAL:O	34:BU:92:ARG:N	2.05	0.90
46:B5:4:HIS:HB3	46:B5:5:PRO:HD3	1.52	0.90
1:AA:353:A:H8	1:AA:353:A:H5'	1.34	0.89
16:AC:154:SER:OG	16:AC:155:GLY:N	1.95	0.89
39:BZ:9:TYR:CZ	39:BZ:61:LEU:HD12	2.06	0.89
25:BA:330:A:H2	25:BA:1210:A:H2'	1.37	0.89
31:BR:11:ASN:OD1	31:BR:12:ARG:N	2.05	0.89
14:AT:73:HIS:HB3	14:AT:74:LYS:HG2	1.54	0.89
55:BH:41:MET:SD	55:BH:42:ARG:N	2.45	0.89
17:AD:9:CYS:HA	17:AD:12:CYS:CB	2.02	0.89
25:BA:1496:A:H8	25:BA:1577:C:HO2'	0.92	0.89
25:BA:1155:A:OP2	34:BU:58:ARG:NH1	2.05	0.89
25:BA:2068:U:N3	25:BA:2430:A:H2	1.70	0.89
38:BY:8:LYS:HB2	38:BY:28:LYS:NZ	1.88	0.89
47:B6:41:PRO:HD2	47:B6:46:HIS:H	1.36	0.89
50:B9:27:CYS:SG	50:B9:32:HIS:CD2	2.66	0.89
46:B5:46:CYS:SG	46:B5:47:PRO:N	2.46	0.88
17:AD:31:CYS:O	17:AD:31:CYS:SG	2.32	0.88
29:BP:64:LYS:C	29:BP:66:GLY:N	2.25	0.88
47:B6:41:PRO:HD2	47:B6:46:HIS:N	1.87	0.88
25:BA:242:G:C5'	49:B8:62:LEU:HD13	2.03	0.88
25:BA:1143:A:OP1	27:BN:25:ARG:NH2	2.07	0.88
25:BA:2068:U:H3	25:BA:2430:A:H2	1.00	0.88
25:BA:2445:G:OP1	53:BF:74:ARG:NH2	2.07	0.88
33:BT:50:ILE:HD11	33:BT:102:ILE:HD11	1.56	0.88
25:BA:2139:C:O2'	25:BA:2140:C:OP2	1.92	0.87
25:BA:993:G:OP1	34:BU:50:ARG:NH2	2.08	0.87
25:BA:1899:G:H22	25:BA:1902:C:N4	1.72	0.87
1:AA:250:A:H4'	1:AA:251:G:O5'	1.74	0.87
27:BN:2:LYS:O	27:BN:4:TYR:CZ	2.27	0.86
46:B5:33:CYS:HB2	46:B5:40:LYS:HE3	1.54	0.86
6:AL:27:LEU:O	6:AL:29:GLY:N	2.07	0.86
11:AQ:66:SER:O	11:AQ:70:ARG:NH1	2.08	0.86
47:B6:47:THR:CG2	47:B6:48:VAL:H	1.88	0.86
1:AA:1004:A:O2'	1:AA:1038:C:O2	1.91	0.86
25:BA:2394:C:OP1	29:BP:63:PRO:CD	2.23	0.86
39:BZ:102:LEU:HD11	39:BZ:124:ILE:HG12	1.56	0.86
1:AA:748:C:H4'	1:AA:749:C:O5'	1.74	0.86
47:B6:16:CYS:O	47:B6:18:ARG:NH2	2.09	0.86
49:B8:61:LEU:HD12	49:B8:62:LEU:HD12	1.58	0.86
43:BD:25:THR:O	43:BD:27:THR:N	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:B6:41:PRO:CD	47:B6:46:HIS:H	1.88	0.86
1:AA:975:A:H4'	1:AA:976:G:H5"	1.59	0.85
25:BA:141:A:H8	25:BA:1408:C:O2'	1.59	0.85
1:AA:692:U:OP1	5:AK:124:LYS:NZ	2.08	0.85
25:BA:1689:A:H62	25:BA:1698:A:H2	1.24	0.85
55:BH:19:VAL:HG11	55:BH:43:VAL:O	1.77	0.85
42:B2:22:GLU:HG3	42:B2:64:LEU:HD11	1.57	0.85
17:AD:2:GLY:O	17:AD:4:TYR:N	2.10	0.85
50:B9:27:CYS:SG	50:B9:32:HIS:HD2	1.99	0.85
36:BW:64:MET:O	36:BW:65:LEU:HB2	1.75	0.85
46:B5:50:GLY:O	46:B5:51:TYR:CD1	2.29	0.85
25:BA:1019:U:HO2'	25:BA:1021:A:H2	0.86	0.85
25:BA:1914:C:HO2'	25:BA:1915:U:P	1.98	0.85
25:BA:271(H):G:H5'	41:B1:81:LYS:HE2	0.90	0.84
25:BA:1540:U:O2'	25:BA:1541:G:H5'	1.76	0.84
25:BA:2611:U:H5'	25:BA:2611:U:H6	1.42	0.84
29:BP:58:THR:O	29:BP:61:ARG:CZ	2.25	0.84
25:BA:528:A:C2	25:BA:2043:C:H4'	2.14	0.83
2:AV:27:G:H1	2:AV:43:C:H5	1.21	0.83
4:AJ:23:ILE:HG22	4:AJ:23:ILE:O	1.77	0.83
1:AA:508:C:OP2	17:AD:209:ARG:NH2	2.11	0.83
1:AA:1539:C:H2'	1:AA:1540:U:O4'	1.77	0.83
1:AA:111:G:O6	1:AA:330:C:N4	2.12	0.83
33:BT:29:ARG:HB3	33:BT:30:VAL:HG22	1.59	0.83
33:BT:78:LEU:O	33:BT:79:HIS:CG	2.30	0.83
38:BY:2:ARG:O	38:BY:4:LYS:N	2.10	0.83
38:BY:76:CYS:SG	38:BY:77:PRO:CD	2.67	0.83
13:AS:44:MET:N	13:AS:44:MET:SD	2.51	0.82
25:BA:2187:G:H5'	25:BA:2188:C:OP2	1.79	0.82
29:BP:7:ARG:CD	53:BF:188:ARG:HA	2.08	0.82
23:AY:428:LEU:HD22	23:AY:451:ILE:HD11	1.61	0.82
25:BA:1447:G:O2'	25:BA:1544:A:C8	2.30	0.82
1:AA:1054:C:O2'	1:AA:1055:A:H5"	1.79	0.82
17:AD:8:VAL:O	17:AD:10:ARG:N	2.13	0.82
1:AA:1189:C:OP1	4:AJ:51:ARG:NH2	2.11	0.82
17:AD:30:LYS:O	17:AD:32:ALA:N	2.13	0.82
9:AO:26:GLU:OE2	9:AO:77:ARG:NH1	2.12	0.81
25:BA:2305:A:C2	25:BA:2306:C:H1'	2.15	0.81
43:BD:44:ASN:HB2	43:BD:48:ARG:O	1.79	0.81
25:BA:1022:G:H22	25:BA:1142(A):A:H2	1.24	0.81
35:BV:64:HIS:ND1	35:BV:92:THR:HG22	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:607:U:OP1	53:BF:102:PRO:HA	1.80	0.81
25:BA:714:U:O2'	25:BA:716:A:N7	2.12	0.81
38:BY:97:ARG:O	38:BY:98:VAL:HB	1.78	0.81
1:AA:1008:C:O2	1:AA:1021:G:N2	2.13	0.81
25:BA:1169:G:N2	25:BA:1181:C:O2	2.14	0.81
25:BA:1980:G:O2'	25:BA:1982:C:OP2	1.98	0.81
29:BP:6:LEU:HG	29:BP:8:PRO:O	1.81	0.81
29:BP:47:ASP:HB3	29:BP:48:PRO:O	1.81	0.81
16:AC:180:ALA:O	16:AC:205:GLY:O	1.99	0.80
1:AA:1126:U:O2	1:AA:1280:A:H2'	1.80	0.80
38:BY:8:LYS:HB2	38:BY:28:LYS:CE	2.11	0.80
1:AA:1054:C:O2	1:AA:1054:C:C3'	2.28	0.80
29:BP:58:THR:O	29:BP:61:ARG:NE	2.14	0.80
25:BA:1047:G:OP2	25:BA:1047:G:H4'	1.79	0.80
25:BA:1048:A:H4'	25:BA:1049:C:OP1	1.82	0.80
25:BA:1782:C:H1'	25:BA:2609:U:H5"	1.64	0.80
38:BY:17:SER:OG	38:BY:18:GLY:N	2.09	0.80
47:B6:20:ASN:O	47:B6:21:TYR:CG	2.35	0.80
1:AA:1117:G:O3'	22:AI:104:ARG:HD3	1.82	0.80
25:BA:1093:G:OP2	25:BA:1093:G:H8	1.65	0.80
6:AL:117:ARG:HD2	6:AL:122:THR:HG22	1.64	0.80
25:BA:1915:U:H5"	25:BA:1916:A:OP2	1.82	0.79
39:BZ:151:HIS:HB2	39:BZ:170:THR:HA	1.64	0.79
25:BA:1019:U:O2'	25:BA:1021:A:H2	1.64	0.79
26:BB:8:U:O3'	32:BS:25:ARG:NH2	2.15	0.79
25:BA:2517:C:O2'	25:BA:2542:A:N1	2.14	0.79
55:BH:41:MET:HE3	55:BH:43:VAL:HG13	1.65	0.79
29:BP:64:LYS:C	29:BP:66:GLY:H	1.85	0.79
25:BA:2808:U:O2	25:BA:2892:A:N6	2.16	0.78
57:BJ:26:ALA:HA	57:BJ:84:ALA:HA	1.65	0.78
1:AA:1134:G:C5	1:AA:1135:U:C5	2.71	0.78
15:AB:178:ARG:HH11	15:AB:178:ARG:CG	1.95	0.78
25:BA:860:U:H5	25:BA:917:A:N7	1.82	0.78
47:B6:12:GLU:HG3	47:B6:23:THR:HG22	1.64	0.78
2:AV:76:A:OP1	2:AV:76:A:C4'	2.31	0.78
25:BA:271(G):C:HO2'	41:B1:81:LYS:HE3	1.49	0.78
1:AA:1452:C:H4'	1:AA:1456:G:C2	2.19	0.78
25:BA:662:G:OP1	29:BP:18:ARG:HD2	1.84	0.78
25:BA:956:G:OP2	30:BQ:14:ARG:NH2	2.17	0.78
28:BO:4:PRO:O	28:BO:5:GLN:HB2	1.83	0.78
53:BF:24:LEU:HB3	53:BF:25:PRO:HD2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BD:44:ASN:HB3	43:BD:49:ILE:HA	1.66	0.77
55:BH:121:ILE:HD11	55:BH:140:LYS:HB3	1.66	0.77
13:AS:40:ILE:HG21	13:AS:62:ILE:HD11	1.66	0.77
25:BA:243:U:OP1	49:B8:6:THR:CG2	2.31	0.77
25:BA:1502:C:C6	25:BA:1502:C:H5"	2.20	0.77
43:BD:44:ASN:CB	43:BD:49:ILE:HA	2.15	0.77
25:BA:1022:G:N2	25:BA:1142(A):A:C2	2.50	0.77
23:AY:15:ILE:HA	23:AY:103:GLY:O	1.85	0.77
40:B0:23:VAL:HG22	40:B0:38:VAL:HG22	1.65	0.77
5:AK:84:VAL:HG11	5:AK:95:ILE:HD11	1.66	0.77
25:BA:881:G:N1	25:BA:895:U:O2	2.17	0.77
29:BP:84:ASN:HA	29:BP:115:LEU:O	1.84	0.77
35:BV:17:GLY:HA2	35:BV:96:ILE:O	1.84	0.77
25:BA:1539:G:C2'	25:BA:1540:U:H5"	2.15	0.77
33:BT:38:ASN:ND2	33:BT:40:THR:OG1	2.17	0.77
25:BA:2632:A:N3	52:BE:61:ARG:NH1	2.33	0.76
1:AA:254:G:OP1	11:AQ:67:LYS:O	2.02	0.76
1:AA:1368:G:OP2	22:AI:112:LYS:HD3	1.85	0.76
1:AA:426:G:OP1	17:AD:36:ARG:NH1	2.17	0.76
17:AD:8:VAL:C	17:AD:10:ARG:H	1.88	0.76
25:BA:1300:U:H4'	25:BA:1301:A:H5'	1.68	0.76
43:BD:181:GLU:HA	43:BD:272:ALA:HB3	1.68	0.76
52:BE:117:MET:O	52:BE:118:LYS:HB2	1.84	0.76
43:BD:137:PRO:O	43:BD:140:THR:OG1	2.03	0.76
52:BE:57:LYS:HD3	52:BE:57:LYS:N	2.01	0.76
25:BA:1063:G:N1	25:BA:1075:C:N4	2.34	0.76
23:AY:205:TYR:O	23:AY:209:ALA:N	2.18	0.76
35:BV:19:LYS:HG3	35:BV:20:LEU:N	1.99	0.76
43:BD:69:ARG:NH2	43:BD:128:GLY:O	2.19	0.76
55:BH:41:MET:CE	55:BH:43:VAL:HG13	2.16	0.76
1:AA:353:A:H5'	1:AA:353:A:C8	2.20	0.76
33:BT:85:LYS:HB3	33:BT:85:LYS:HZ2	1.49	0.76
25:BA:2287:A:N1	25:BA:2346:A:C2	2.54	0.75
46:B5:40:LYS:HE2	46:B5:46:CYS:HB3	1.66	0.75
25:BA:2392:A:H2	25:BA:2424:C:H42	1.31	0.75
1:AA:673:G:H2'	1:AA:674:G:C8	2.21	0.75
1:AA:632:A:H3'	1:AA:633:G:H5"	1.68	0.75
39:BZ:72:ARG:NH2	39:BZ:97:GLU:O	2.18	0.75
1:AA:1217:C:OP1	8:AN:9:LYS:NZ	2.19	0.75
25:BA:1089:G:H4'	25:BA:1090:U:OP1	1.85	0.75
47:B6:48:VAL:O	47:B6:49:HIS:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AB:54:THR:HG21	15:AB:201:ILE:HD11	1.69	0.75
23:AY:437:THR:HB	23:AY:454:MET:HE3	1.66	0.75
25:BA:2420:C:P	49:B8:33:ASN:O	2.45	0.75
11:AQ:95:TYR:HA	11:AQ:98:LEU:HD12	1.67	0.74
15:AB:17:PHE:O	15:AB:18:GLY:O	2.06	0.74
15:AB:67:THR:HG21	15:AB:155:LEU:HD21	1.69	0.74
25:BA:1540:U:H5'	25:BA:1540:U:C6	2.15	0.74
56:BK:30:HIS:HA	56:BK:59:ILE:HD12	1.69	0.74
1:AA:390:C:O3'	10:AP:28:ARG:NH2	2.20	0.74
1:AA:1138:G:H1'	1:AA:1139:G:OP1	1.88	0.74
25:BA:2068:U:N3	25:BA:2430:A:C2	2.47	0.74
43:BD:210:GLY:O	43:BD:212:SER:N	2.20	0.74
56:BK:99:ILE:HD12	56:BK:103:GLN:HB3	1.69	0.74
2:AV:34:G:H2'	2:AV:35:A:H5"	1.69	0.74
49:B8:61:LEU:CD1	49:B8:62:LEU:HD12	2.17	0.74
25:BA:528:A:N1	25:BA:2042:A:H2'	2.03	0.74
53:BF:22:ALA:O	53:BF:26:ALA:HB2	1.87	0.74
6:AL:26:ALA:O	6:AL:27:LEU:O	2.05	0.74
25:BA:774:A:O2'	25:BA:775:G:OP2	2.04	0.74
4:AJ:8:LEU:HD23	4:AJ:96:ILE:HG22	1.70	0.74
33:BT:89:VAL:C	33:BT:91:ARG:H	1.91	0.74
38:BY:8:LYS:HB2	38:BY:28:LYS:HZ3	1.53	0.74
55:BH:41:MET:SD	55:BH:53:GLU:O	2.46	0.74
56:BK:106:GLU:HA	56:BK:109:LYS:HD3	1.68	0.74
39:BZ:151:HIS:CB	39:BZ:170:THR:HA	2.18	0.73
53:BF:167:ALA:HB1	53:BF:173:VAL:HG11	1.67	0.73
56:BK:100:THR:HA	56:BK:139:VAL:HB	1.68	0.73
9:AO:17:ARG:HH11	9:AO:17:ARG:HG3	1.54	0.73
41:B1:51:VAL:O	41:B1:57:GLU:O	2.06	0.73
23:AY:210:ARG:O	23:AY:212:TYR:N	2.18	0.73
25:BA:2849:U:OP2	33:BT:95:ARG:NH1	2.22	0.73
4:AJ:49:VAL:HG22	8:AN:41:ARG:HB2	1.69	0.73
25:BA:1091:G:O6	25:BA:1100:C:N4	2.15	0.73
31:BR:87:TYR:O	31:BR:89:ASP:N	2.22	0.73
6:AL:8:ASN:O	6:AL:12:ARG:HG3	1.89	0.73
25:BA:1899:G:N2	25:BA:1902:C:H5	1.86	0.73
52:BE:60:ASN:HD22	52:BE:60:ASN:N	1.85	0.73
23:AY:264:LEU:HB2	60:AY:702:GCP:C6	2.19	0.72
25:BA:1899:G:N2	25:BA:1902:C:C5	2.57	0.72
1:AA:1446:U:O2'	1:AA:1447:A:H3'	1.89	0.72
25:BA:1786:A:C2	25:BA:2606:C:H1'	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2079:U:OP1	41:B1:21:ARG:NH1	2.19	0.72
1:AA:1305:G:OP2	24:AU:2:GLY:N	2.22	0.72
38:BY:74:PRO:O	38:BY:80:GLY:HA3	1.88	0.72
25:BA:1064:C:H2'	25:BA:1065:U:O4'	1.89	0.72
43:BD:3:VAL:HG13	43:BD:17:THR:HB	1.70	0.72
2:AV:74:C:O2'	2:AV:75:C:OP2	2.06	0.72
25:BA:2810:A:H2'	52:BE:61:ARG:NH2	2.05	0.72
43:BD:10:THR:OG1	43:BD:13:ARG:HB2	1.89	0.72
33:BT:7:ILE:HG23	52:BE:181:LEU:HD21	1.72	0.72
27:BN:56:ASN:C	27:BN:57:ALA:O	2.27	0.71
29:BP:51:PHE:HB3	29:BP:52:GLU:OE2	1.89	0.71
9:AO:39:LEU:CD1	9:AO:56:LEU:HB2	2.20	0.71
15:AB:115:LEU:HD13	15:AB:145:LEU:HB3	1.71	0.71
23:AY:679:VAL:HB	23:AY:680:PRO:CD	2.20	0.71
25:BA:2137:C:O2	25:BA:2137:C:C3'	2.37	0.71
43:BD:25:THR:O	43:BD:26:LYS:C	2.28	0.71
25:BA:1899:G:N2	25:BA:1902:C:H41	1.85	0.71
33:BT:89:VAL:HG11	33:BT:91:ARG:HG3	1.72	0.71
38:BY:26:LYS:O	38:BY:27:VAL:O	2.07	0.71
39:BZ:10:ARG:NH2	39:BZ:26:GLY:O	2.23	0.71
54:BG:96:ARG:O	54:BG:99:MET:N	2.21	0.71
33:BT:23:ARG:O	33:BT:25:GLY:N	2.23	0.71
51:BC:131:LEU:HB3	51:BC:137:LEU:HD23	1.73	0.71
1:AA:633:G:H5"	1:AA:633:G:H8	1.56	0.71
6:AL:53:ARG:HG2	6:AL:93:LEU:HD11	1.73	0.71
12:AR:22:VAL:O	12:AR:25:THR:HB	1.91	0.71
25:BA:2139:C:O2'	25:BA:2140:C:P	2.48	0.71
25:BA:2180:U:C6	25:BA:2180:U:C5'	2.74	0.71
56:BK:81:ALA:HB1	56:BK:99:ILE:HD11	1.73	0.71
56:BK:99:ILE:HG23	56:BK:103:GLN:HB2	1.72	0.71
34:BU:92:ARG:NH1	34:BU:94:ASN:HD22	1.89	0.71
25:BA:259:G:N2	25:BA:621:A:H8	1.86	0.71
25:BA:1538:G:H2'	25:BA:1539:G:C8	2.25	0.71
34:BU:92:ARG:O	34:BU:94:ASN:N	2.24	0.71
53:BF:66:PRO:O	53:BF:67:GLN:CB	2.39	0.71
25:BA:1396:U:O2	25:BA:1396:U:H2'	1.89	0.70
43:BD:13:ARG:HD2	43:BD:16:MET:HE3	1.73	0.70
1:AA:953:G:H5'	1:AA:965:A:H61	1.56	0.70
25:BA:1847:A:N3	25:BA:1847:A:H2'	2.06	0.70
25:BA:1887:C:H2'	25:BA:1888:G:H5'	1.73	0.70
25:BA:613:G:H5"	25:BA:613:G:H8	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2317:C:H2'	25:BA:2318:G:H5'	1.72	0.70
25:BA:271(J):C:H5'	25:BA:271(K):U:OP2	1.90	0.70
51:BC:42:GLU:CG	51:BC:215:THR:HG23	2.21	0.70
1:AA:1144:G:O2'	1:AA:1145:C:H5'	1.92	0.70
1:AA:1533:C:H2'	1:AA:1534:A:O4'	1.92	0.70
23:AY:25:LYS:NZ	60:AY:702:GCP:O3G	2.25	0.70
25:BA:662:G:OP1	29:BP:18:ARG:NH1	2.24	0.70
42:B2:42:GLY:O	42:B2:44:LEU:N	2.25	0.70
13:AS:42:PRO:O	13:AS:44:MET:SD	2.50	0.70
23:AY:212:TYR:HA	23:AY:215:LYS:HB3	1.72	0.70
25:BA:330:A:C2	25:BA:1210:A:H2'	2.25	0.70
2:AV:33:U:H5	2:AV:36:A:OP2	1.75	0.70
25:BA:943:U:OP2	29:BP:38:GLN:CD	2.30	0.70
33:BT:16:ARG:NH2	33:BT:82:LEU:O	2.21	0.70
1:AA:1136:U:H3'	1:AA:1137:C:H5"	1.74	0.69
25:BA:2317:C:C2'	25:BA:2318:G:H5'	2.22	0.69
47:B6:41:PRO:HD3	47:B6:46:HIS:HA	1.74	0.69
1:AA:975:A:H5'	1:AA:975:A:H8	1.56	0.69
25:BA:1079:C:H41	25:BA:1088:A:H5"	1.56	0.69
25:BA:2683:C:OP1	33:BT:53:ARG:NH2	2.25	0.69
1:AA:1133:G:C8	1:AA:1133:G:H3'	2.27	0.69
14:AT:73:HIS:O	14:AT:76:ALA:HB3	1.92	0.69
25:BA:1092:C:H2'	25:BA:1093:G:H5'	1.75	0.69
47:B6:47:THR:HG23	47:B6:48:VAL:H	1.54	0.69
1:AA:1392:G:N2	1:AA:1502:A:H8	1.90	0.69
23:AY:162:VAL:HG21	23:AY:255:ILE:HG12	1.74	0.69
51:BC:185:LEU:O	51:BC:188:ASN:N	2.25	0.69
23:AY:61:ARG:NH2	23:AY:460:GLU:OE2	2.25	0.69
10:AP:8:ARG:HG2	10:AP:8:ARG:HH11	1.58	0.69
25:BA:2646:C:OP2	25:BA:2732:G:O2'	2.08	0.69
29:BP:47:ASP:HB3	29:BP:48:PRO:C	2.13	0.69
1:AA:460:G:O6	1:AA:470:C:H5'	1.93	0.69
1:AA:979:C:H2'	1:AA:980:C:H5'	1.73	0.69
25:BA:1100:C:C5'	25:BA:1100:C:H6	2.06	0.69
25:BA:2167:U:H3	25:BA:2171:A:H2	1.41	0.69
37:BX:11:PRO:HB3	37:BX:92:LEU:HD21	1.75	0.69
45:B4:60:GLU:O	54:BG:113:ARG:NH2	2.26	0.69
7:AM:90:LEU:O	7:AM:92:HIS:N	2.26	0.69
23:AY:19:ALA:HB3	23:AY:25:LYS:HE3	1.75	0.69
25:BA:587:C:OP2	29:BP:33:ARG:NH2	2.26	0.69
25:BA:1918:A:HO2'	25:BA:1919:A:H2	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BN:2:LYS:O	27:BN:4:TYR:CE1	2.45	0.69
29:BP:7:ARG:HB2	29:BP:8:PRO:HD2	1.75	0.69
1:AA:62:U:H2'	1:AA:63:C:H5"	1.75	0.68
1:AA:1138:G:C2'	1:AA:1139:G:OP1	2.41	0.68
15:AB:195:ASP:O	21:AH:68:ARG:NH2	2.26	0.68
25:BA:1093:G:OP2	25:BA:1093:G:C8	2.46	0.68
26:BB:50:G:OP1	32:BS:63:THR:HG23	1.93	0.68
46:B5:46:CYS:SG	46:B5:47:PRO:CD	2.81	0.68
25:BA:2476:A:N1	25:BA:2477:C:C6	2.61	0.68
51:BC:42:GLU:HG3	51:BC:215:THR:HG23	1.75	0.68
1:AA:1293:G:H8	1:AA:1293:G:H5"	1.58	0.68
40:B0:43:THR:HG23	40:B0:43:THR:O	1.91	0.68
2:AV:34:G:C2'	2:AV:35:A:H5"	2.23	0.68
15:AB:88:ALA:HB2	15:AB:219:VAL:HG13	1.75	0.68
27:BN:46:VAL:O	27:BN:47:ALA:HB3	1.92	0.68
1:AA:1243:C:OP2	24:AU:10:ARG:NH2	2.27	0.68
5:AK:61:ALA:HB1	5:AK:94:ALA:HB2	1.76	0.68
25:BA:1266:G:O5'	36:BW:15:ARG:NH2	2.26	0.68
25:BA:1496:A:H8	25:BA:1577:C:O2'	1.71	0.68
52:BE:64:LYS:O	52:BE:73:GLU:OE1	2.11	0.68
55:BH:175:LYS:N	55:BH:176:ALA:HB2	2.08	0.68
1:AA:530:G:O2'	1:AA:531:U:OP1	2.10	0.68
25:BA:9:U:C5	25:BA:2629:A:N6	2.62	0.68
27:BN:3:THR:O	27:BN:5:VAL:HG12	1.93	0.68
52:BE:129:HIS:O	52:BE:130:GLY:C	2.31	0.68
56:BK:4:VAL:HG12	56:BK:5:VAL:H	1.59	0.68
29:BP:51:PHE:CB	29:BP:52:GLU:HG2	2.24	0.68
2:AV:73:A:H2'	2:AV:74:C:H5'	1.76	0.68
25:BA:847:U:OP2	25:BA:928:G:O6	2.11	0.68
55:BH:89:ILE:C	55:BH:89:ILE:HD12	2.15	0.68
25:BA:1502:C:H5"	25:BA:1502:C:H6	1.56	0.68
29:BP:16:ARG:C	29:BP:16:ARG:HD3	2.14	0.68
14:AT:73:HIS:CB	14:AT:74:LYS:HG2	2.23	0.67
25:BA:684:G:OP1	48:B7:16:HIS:HD2	1.76	0.67
33:BT:30:VAL:HG21	33:BT:84:GLN:HG3	1.74	0.67
25:BA:271(H):G:C4'	41:B1:81:LYS:HE2	2.25	0.67
35:BV:47:VAL:O	35:BV:49:THR:O	2.12	0.67
25:BA:2287:A:N1	25:BA:2346:A:H2	1.92	0.67
38:BY:7:VAL:HB	38:BY:8:LYS:CE	2.24	0.67
56:BK:57:ILE:HA	56:BK:66:THR:O	1.94	0.67
1:AA:17:U:H2'	1:AA:18:C:C6	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AM:97:PRO:HA	7:AM:110:ARG:HD3	1.76	0.67
23:AY:255:ILE:HG23	23:AY:257:PRO:HD3	1.77	0.67
25:BA:2632:A:O2'	52:BE:61:ARG:NH2	2.27	0.67
7:AM:89:GLY:C	7:AM:90:LEU:O	2.31	0.67
29:BP:9:ASN:HA	29:BP:11:GLY:H	1.60	0.67
38:BY:39:VAL:HG12	38:BY:40:GLU:H	1.59	0.67
1:AA:100:C:H2'	1:AA:101:A:C8	2.29	0.67
25:BA:517:C:OP1	46:B5:16:ARG:NH2	2.28	0.67
25:BA:2506:U:C6	25:BA:2506:U:H5'	2.30	0.67
57:BJ:34:ALA:HA	57:BJ:37:ALA:HB3	1.75	0.67
1:AA:1138:G:C1'	1:AA:1139:G:OP1	2.42	0.67
23:AY:94:VAL:O	23:AY:96:ARG:N	2.28	0.67
23:AY:404:VAL:CG1	23:AY:405:PRO:HA	2.15	0.67
25:BA:1076:C:O2'	25:BA:1077:A:O5'	2.12	0.67
25:BA:2439:A:H5'	25:BA:2439:A:C8	2.29	0.67
51:BC:66:HIS:CD2	51:BC:184:LYS:HG3	2.30	0.67
54:BG:54:GLU:HA	54:BG:57:ALA:HB3	1.77	0.67
25:BA:1053:C:H2'	25:BA:1054:A:H5"	1.75	0.67
34:BU:65:ILE:HD11	34:BU:93:LYS:HA	1.76	0.67
35:BV:21:ARG:O	35:BV:22:VAL:HG13	1.95	0.67
36:BW:73:ALA:HB3	36:BW:106:ILE:HG12	1.75	0.67
25:BA:142:A:H8	25:BA:1595:G:H21	1.44	0.66
25:BA:1858:G:O2'	25:BA:1883:G:N2	2.26	0.66
26:BB:20:C:H2'	26:BB:21:G:H5'	1.75	0.66
25:BA:2681:C:H5	25:BA:2725:A:H62	1.41	0.66
25:BA:2850:A:OP2	25:BA:2866:U:H5	1.77	0.66
56:BK:6:ALA:HB3	56:BK:59:ILE:HG22	1.77	0.66
1:AA:376:G:OP2	10:AP:67:THR:HG21	1.95	0.66
16:AC:154:SER:O	16:AC:157:ILE:HD11	1.95	0.66
17:AD:10:ARG:CG	17:AD:10:ARG:O	2.43	0.66
23:AY:357:ARG:NH1	23:AY:373:ASP:OD2	2.28	0.66
39:BZ:18:LEU:H	39:BZ:18:LEU:CD1	2.08	0.66
1:AA:1101:A:H4'	1:AA:1102:A:O5'	1.96	0.66
1:AA:1143:G:H5"	1:AA:1144:G:OP2	1.94	0.66
25:BA:943:U:OP2	29:BP:38:GLN:NE2	2.29	0.66
53:BF:65:TRP:CZ3	53:BF:73:ALA:O	2.49	0.66
55:BH:41:MET:HE2	55:BH:52:VAL:HA	1.78	0.66
56:BK:75:SER:O	56:BK:79:ARG:HG3	1.96	0.66
25:BA:1019:U:H3	25:BA:1142(A):A:H62	1.44	0.66
27:BN:126:PRO:O	27:BN:127:ASP:O	2.13	0.66
30:BQ:82:ARG:HH22	40:B0:2:ALA:HB1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AB:33:TYR:HB3	15:AB:41:ILE:HG22	1.78	0.66
38:BY:39:VAL:C	38:BY:40:GLU:OE1	2.34	0.66
15:AB:67:THR:HG21	15:AB:155:LEU:CD2	2.26	0.66
25:BA:1779:U:C5	25:BA:1784:A:N7	2.57	0.66
25:BA:1887:C:C2'	25:BA:1888:G:H5'	2.25	0.66
55:BH:83:TYR:HB3	55:BH:134:SER:HA	1.78	0.66
25:BA:661:C:O2'	29:BP:16:ARG:O	2.10	0.65
33:BT:28:VAL:HG12	33:BT:29:ARG:HD3	1.77	0.65
36:BW:5:ALA:HB3	36:BW:50:VAL:HG23	1.76	0.65
56:BK:17:ALA:HB3	56:BK:38:VAL:HG22	1.78	0.65
1:AA:975:A:H5'	1:AA:975:A:C8	2.31	0.65
14:AT:100:ILE:O	14:AT:102:GLY:N	2.29	0.65
29:BP:51:PHE:O	29:BP:52:GLU:HB2	1.95	0.65
46:B5:51:TYR:HB3	46:B5:52:TYR:O	1.97	0.65
25:BA:252:G:OP2	29:BP:50:ARG:NH1	2.24	0.65
43:BD:70:TRP:CH2	43:BD:150:LYS:HA	2.31	0.65
1:AA:328:C:O2	1:AA:328:C:H2'	1.97	0.65
15:AB:28:PHE:CD1	15:AB:190:THR:HA	2.31	0.65
17:AD:25:ARG:C	17:AD:27:TYR:H	2.00	0.65
25:BA:71:A:H5'	25:BA:71:A:C8	2.31	0.65
29:BP:7:ARG:HB2	29:BP:8:PRO:CD	2.27	0.65
33:BT:50:ILE:CD1	33:BT:102:ILE:HD11	2.27	0.65
39:BZ:94:GLU:O	39:BZ:130:PRO:HD3	1.97	0.65
1:AA:1149:C:OP1	22:AI:9:ARG:NH1	2.26	0.65
15:AB:17:PHE:HB3	15:AB:44:LEU:HD21	1.78	0.65
33:BT:54:ARG:HA	33:BT:59:THR:HB	1.79	0.65
47:B6:41:PRO:CD	47:B6:46:HIS:N	2.55	0.65
14:AT:53:LEU:HB2	14:AT:100:ILE:CG2	2.27	0.65
25:BA:1046:A:N7	57:BJ:5:ALA:HB3	2.11	0.65
25:BA:1962:C:O2'	25:BA:1964:G:OP2	2.12	0.65
29:BP:55:ARG:HG2	29:BP:56:SER:H	1.60	0.65
47:B6:19:ARG:HG3	47:B6:20:ASN:N	2.09	0.65
49:B8:63:PRO:O	49:B8:64:TYR:O	2.12	0.65
53:BF:66:PRO:O	53:BF:67:GLN:HB3	1.97	0.65
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.12	0.65
1:AA:1307:U:OP1	7:AM:101:GLN:OE1	2.14	0.65
12:AR:32:ARG:HA	12:AR:69:THR:HG21	1.77	0.65
22:AI:17:VAL:HG22	22:AI:63:ILE:HG12	1.77	0.65
47:B6:20:ASN:C	47:B6:21:TYR:CG	2.69	0.65
4:AJ:16:LEU:HD13	4:AJ:70:ARG:HG2	1.79	0.65
23:AY:10:LYS:N	23:AY:282:SER:HG	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1956:U:H1'	25:BA:2552:U:OP1	1.96	0.65
25:BA:2602:A:OP2	25:BA:2602:A:H4'	1.96	0.65
33:BT:13:ARG:NH1	33:BT:13:ARG:HA	2.11	0.65
1:AA:1004:A:OP1	1:AA:1024:G:N2	2.30	0.65
25:BA:1899:G:H21	25:BA:1902:C:H5	1.45	0.65
25:BA:896:A:C8	39:BZ:146:ILE:HD13	2.32	0.65
25:BA:1141:U:OP2	27:BN:63:THR:OG1	2.15	0.65
25:BA:2420:C:OP2	49:B8:33:ASN:O	2.15	0.65
25:BA:2787:C:O2	52:BE:61:ARG:NH1	2.30	0.65
52:BE:1:MET:HB3	52:BE:200:GLU:OE1	1.96	0.65
52:BE:132:HIS:CD2	52:BE:135:HIS:CE1	2.84	0.65
42:B2:47:ASN:O	42:B2:49:LYS:N	2.30	0.64
12:AR:26:LEU:O	19:AF:100:ASN:ND2	2.30	0.64
23:AY:603:GLU:O	23:AY:605:ILE:HD12	1.96	0.64
33:BT:78:LEU:O	33:BT:79:HIS:ND1	2.30	0.64
53:BF:28:ILE:HD13	53:BF:28:ILE:H	1.62	0.64
25:BA:548:A:O2'	25:BA:549:G:OP1	2.13	0.64
47:B6:11:LEU:HD22	47:B6:12:GLU:N	2.11	0.64
23:AY:122:TRP:CD2	23:AY:157:LEU:HD12	2.33	0.64
1:AA:975:A:H4'	1:AA:976:G:C5'	2.26	0.64
25:BA:9:U:C4	25:BA:2629:A:N6	2.65	0.64
25:BA:1058:G:H21	56:BK:126:MET:HE3	1.61	0.64
29:BP:85:LEU:HD23	29:BP:85:LEU:H	1.62	0.64
33:BT:27:THR:O	33:BT:28:VAL:HG23	1.98	0.64
43:BD:24:ILE:O	43:BD:26:LYS:N	2.31	0.64
1:AA:1013:G:N2	1:AA:1015:A:H3'	2.12	0.64
1:AA:1464:G:OP2	33:BT:111:ARG:NH2	2.31	0.64
8:AN:23:ARG:CD	8:AN:28:GLY:O	2.43	0.64
23:AY:437:THR:HB	23:AY:454:MET:CE	2.27	0.64
25:BA:118:A:N3	25:BA:178:G:H1'	2.12	0.64
25:BA:250:G:P	49:B8:13:ARG:HH22	2.21	0.64
25:BA:860:U:C5	25:BA:917:A:N7	2.65	0.64
56:BK:42:ASN:O	56:BK:46:ALA:HB2	1.98	0.64
1:AA:36:C:O2'	1:AA:501:C:OP1	2.12	0.64
1:AA:542:G:OP1	17:AD:10:ARG:NH2	2.29	0.64
25:BA:1100:C:C5'	25:BA:1100:C:C6	2.81	0.64
43:BD:11:PRO:O	43:BD:13:ARG:N	2.29	0.64
54:BG:124:SER:HB2	54:BG:131:TYR:CE1	2.33	0.64
1:AA:737:A:H1'	19:AF:73:ASN:OD1	1.98	0.64
15:AB:97:TRP:CZ3	15:AB:176:GLU:OE2	2.50	0.64
23:AY:272:LEU:O	23:AY:276:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1458:C:H4'	25:BA:1459:G:O5'	1.97	0.64
27:BN:3:THR:O	27:BN:5:VAL:N	2.31	0.64
28:BO:88:ASN:C	28:BO:88:ASN:HD22	2.01	0.64
29:BP:136:GLU:O	29:BP:139:LYS:N	2.31	0.64
30:BQ:12:GLN:HG2	30:BQ:73:PRO:HD2	1.80	0.64
32:BS:52:SER:HB2	32:BS:55:ALA:HB3	1.79	0.64
51:BC:119:VAL:HB	51:BC:123:VAL:HG23	1.79	0.64
52:BE:77:ILE:HG22	52:BE:78:LEU:H	1.62	0.64
52:BE:70:ALA:O	52:BE:72:VAL:N	2.31	0.63
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.33	0.63
4:AJ:23:ILE:O	4:AJ:23:ILE:CG2	2.46	0.63
33:BT:85:LYS:HB3	33:BT:85:LYS:HZ3	1.63	0.63
25:BA:1538:G:C4	25:BA:1539:G:C8	2.87	0.63
13:AS:40:ILE:CG2	13:AS:62:ILE:HD11	2.28	0.63
33:BT:27:THR:HA	33:BT:87:ASP:HB2	1.81	0.63
1:AA:472:A:H2'	1:AA:473:G:O4'	1.99	0.63
25:BA:2611:U:H5'	25:BA:2611:U:C6	2.31	0.63
41:B1:52:ARG:O	41:B1:56:GLN:O	2.15	0.63
43:BD:223:GLY:C	43:BD:224:ALA:O	2.33	0.63
1:AA:974:A:OP2	8:AN:41:ARG:NH1	2.32	0.63
33:BT:28:VAL:O	33:BT:29:ARG:CB	2.45	0.63
14:AT:36:LEU:HD12	14:AT:55:ILE:HG23	1.80	0.63
34:BU:88:ILE:HD13	34:BU:109:LEU:HD22	1.81	0.63
47:B6:26:ASN:ND2	47:B6:32:ASN:OD1	2.32	0.63
1:AA:1075:C:OP1	15:AB:179:LYS:NZ	2.26	0.63
25:BA:90:U:O2'	25:BA:92:A:P	2.57	0.63
25:BA:1407:C:C6	25:BA:1407:C:H5"	2.32	0.63
25:BA:2517:C:O2'	25:BA:2542:A:C2	2.48	0.63
26:BB:45:A:OP2	54:BG:96:ARG:NH2	2.32	0.63
33:BT:93:ARG:HG3	33:BT:93:ARG:HH11	1.63	0.63
43:BD:27:THR:CG2	43:BD:83:GLU:HB3	2.28	0.63
1:AA:509:A:H5'	17:AD:55:ALA:HB2	1.79	0.63
17:AD:11:LEU:C	17:AD:13:ARG:N	2.51	0.63
23:AY:616:TYR:OH	23:AY:666:ARG:NH1	2.32	0.63
25:BA:1494:A:H2'	25:BA:1495:A:H5"	1.81	0.63
33:BT:89:VAL:CG1	33:BT:91:ARG:HG3	2.28	0.63
47:B6:40:CYS:HG	47:B6:45:LYS:NZ	0.95	0.63
1:AA:452:A:HO2'	1:AA:453:A:H8	1.47	0.62
1:AA:1452:C:H4'	1:AA:1456:G:N2	2.13	0.62
25:BA:1539:G:C3'	25:BA:1540:U:H5"	2.29	0.62
28:BO:4:PRO:O	28:BO:5:GLN:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BF:24:LEU:O	53:BF:26:ALA:N	2.32	0.62
43:BD:27:THR:HG21	43:BD:83:GLU:OE2	1.99	0.62
53:BF:133:ASN:HA	53:BF:162:LEU:HD23	1.80	0.62
4:AJ:85:LEU:O	4:AJ:87:THR:N	2.32	0.62
47:B6:28:ARG:HA	47:B6:32:ASN:HB3	1.80	0.62
52:BE:87:GLU:O	52:BE:89:ASP:N	2.31	0.62
23:AY:153:MET:HA	23:AY:157:LEU:HD21	1.80	0.62
25:BA:1332:G:N2	25:BA:1610:A:H8	1.96	0.62
25:BA:1403:C:H5"	25:BA:1471:A:H1'	1.80	0.62
25:BA:2849:U:O4	33:BT:23:ARG:NH2	2.30	0.62
25:BA:2850:A:OP2	25:BA:2866:U:C5	2.52	0.62
1:AA:1401:G:C2	1:AA:1402:C:H1'	2.33	0.62
10:AP:20:VAL:HG21	10:AP:32:TYR:CD1	2.34	0.62
25:BA:1906:G:H2'	25:BA:1907:G:O4'	2.00	0.62
25:BA:2180:U:C6	25:BA:2180:U:H5"	2.34	0.62
51:BC:119:VAL:O	51:BC:121:GLY:N	2.33	0.62
13:AS:5:LEU:HG	13:AS:10:PHE:HD1	1.65	0.62
25:BA:252:G:P	29:BP:50:ARG:HH11	2.23	0.62
25:BA:806:C:P	29:BP:39:LYS:HB3	2.40	0.62
25:BA:2296:U:H4'	25:BA:2297:C:OP1	1.98	0.62
26:BB:77:U:OP1	39:BZ:19:ARG:NH2	2.32	0.62
27:BN:131:GLN:OE1	27:BN:131:GLN:HA	1.99	0.62
1:AA:1305:G:H5"	24:AU:4:GLY:HA3	1.82	0.62
25:BA:27:G:O2'	25:BA:28:A:OP2	2.16	0.62
25:BA:140:G:N3	25:BA:142:A:N1	2.47	0.62
29:BP:107:LYS:O	29:BP:109:GLY:N	2.28	0.62
14:AT:38:LYS:O	14:AT:41:ILE:HG12	2.00	0.62
25:BA:1040:C:O2'	25:BA:1041:C:OP2	2.15	0.62
38:BY:55:TYR:O	38:BY:57:GLN:O	2.17	0.62
54:BG:57:ALA:HA	54:BG:90:LEU:HD21	1.81	0.62
6:AL:115:LYS:O	6:AL:117:ARG:N	2.32	0.62
23:AY:683:VAL:O	23:AY:686:LYS:N	2.32	0.62
29:BP:146:VAL:HG13	29:BP:147:LEU:N	2.14	0.62
33:BT:30:VAL:CG2	33:BT:84:GLN:O	2.48	0.62
7:AM:14:ARG:NH2	7:AM:16:ASP:OD2	2.32	0.62
25:BA:271(H):G:H4'	41:B1:81:LYS:HG2	1.82	0.62
25:BA:2734:A:H5'	25:BA:2735:G:OP2	2.00	0.62
29:BP:24:GLY:O	29:BP:25:SER:HB3	1.99	0.62
58:BL:67:UNK:O	58:BL:69:UNK:N	2.33	0.62
1:AA:460:G:C6	1:AA:470:C:H5"	2.35	0.61
1:AA:680:C:O2'	43:BD:166:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1057:G:H5”	16:AC:154:SER:HB2	1.81	0.61
1:AA:1435:G:H2’	1:AA:1436:U:C6	2.34	0.61
2:AV:72:C:H3’	2:AV:72:C:C6	2.35	0.61
16:AC:154:SER:HG	16:AC:155:GLY:H	1.46	0.61
17:AD:189:PRO:HB2	17:AD:194:LEU:HD21	1.80	0.61
34:BU:90:VAL:O	34:BU:91:ASP:C	2.37	0.61
25:BA:2419:U:O4	49:B8:30:ARG:NH2	2.32	0.61
25:BA:2801:A:N3	25:BA:2801:A:H2’	2.14	0.61
27:BN:90:MET:O	27:BN:93:THR:O	2.18	0.61
38:BY:73:ARG:NH2	38:BY:81:LYS:HA	2.14	0.61
55:BH:144:VAL:O	55:BH:148:ILE:HG12	2.00	0.61
1:AA:967:C:H4’	22:AI:125:TYR:HE1	1.65	0.61
25:BA:2476:A:N1	25:BA:2477:C:C5	2.69	0.61
25:BA:2602:A:H2’	25:BA:2602:A:N3	2.15	0.61
34:BU:95:LEU:O	34:BU:98:LEU:HG	1.99	0.61
36:BW:60:ASN:OD1	36:BW:61:ASN:ND2	2.33	0.61
53:BF:132:VAL:O	53:BF:138:GLU:OE1	2.18	0.61
55:BH:89:ILE:HD11	55:BH:94:TYR:O	1.99	0.61
4:AJ:5:ARG:HD3	4:AJ:73:ASP:OD1	2.01	0.61
25:BA:1246:A:OP1	29:BP:16:ARG:NH2	2.33	0.61
25:BA:2163:C:O2	25:BA:2163:C:O4’	2.15	0.61
29:BP:112:LEU:CD1	29:BP:114:ILE:HG22	2.30	0.61
33:BT:13:ARG:HA	33:BT:13:ARG:CZ	2.30	0.61
45:B4:62:CYS:SG	45:B4:63:SER:N	2.73	0.61
46:B5:46:CYS:SG	46:B5:47:PRO:HD2	2.39	0.61
1:AA:1136:U:H3’	1:AA:1137:C:C5’	2.31	0.61
23:AY:683:VAL:HG23	23:AY:684:GLN:H	1.62	0.61
25:BA:910:A:H62	30:BQ:12:GLN:HA	1.65	0.61
2:AV:73:A:C2’	2:AV:74:C:H5’	2.30	0.61
23:AY:230:LYS:HG2	23:AY:235:GLU:O	2.00	0.61
38:BY:97:ARG:O	38:BY:98:VAL:CB	2.47	0.61
43:BD:209:ALA:C	43:BD:210:GLY:O	2.37	0.61
1:AA:1158:C:O2’	1:AA:1160:G:OP1	2.17	0.61
23:AY:354:ARG:HG2	23:AY:378:VAL:HG22	1.83	0.61
25:BA:996:A:O2’	34:BU:92:ARG:HG3	2.01	0.61
47:B6:9:LEU:O	47:B6:25:LYS:HB2	2.00	0.61
25:BA:1332:G:H5’	25:BA:1332:G:H8	1.66	0.61
26:BB:105:A:H2’	26:BB:106:G:O4’	2.01	0.61
18:AE:9:LYS:HB2	18:AE:112:LEU:HD11	1.83	0.61
25:BA:1952:A:OP1	28:BO:44:LYS:NZ	2.30	0.61
42:B2:38:GLN:HB3	42:B2:44:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:580:U:H2'	1:AA:581:G:O4'	2.01	0.61
1:AA:889:A:H4'	1:AA:890:G:OP1	2.00	0.61
7:AM:88:ARG:HG3	7:AM:98:VAL:HG13	1.83	0.61
17:AD:30:LYS:C	17:AD:32:ALA:H	2.03	0.61
25:BA:2168:G:H22	25:BA:2171:A:H5'	1.65	0.61
42:B2:43:GLN:O	42:B2:44:LEU:HB2	2.00	0.61
20:AG:120:ILE:O	20:AG:124:LEU:HG	2.00	0.60
23:AY:409:ILE:HG12	23:AY:656:ALA:HB3	1.82	0.60
25:BA:1263:U:H1'	46:B5:10:LYS:HG3	1.83	0.60
25:BA:1915:U:C5'	25:BA:1916:A:OP2	2.48	0.60
25:BA:2179:C:O2'	25:BA:2180:U:OP2	2.17	0.60
39:BZ:45:ASP:OD2	39:BZ:49:ARG:HD2	2.00	0.60
22:AI:118:LYS:O	22:AI:119:ALA:HB3	2.00	0.60
25:BA:607:U:N3	25:BA:621:A:C2	2.63	0.60
25:BA:2019:A:N7	46:B5:9:LYS:HE3	2.16	0.60
31:BR:102:GLU:OE1	36:BW:37:ARG:NH1	2.34	0.60
4:AJ:58:ASP:O	4:AJ:59:SER:C	2.40	0.60
7:AM:65:LYS:HA	7:AM:66:LEU:CB	2.30	0.60
18:AE:10:MET:SD	18:AE:13:ILE:HG13	2.41	0.60
20:AG:5:ARG:NH1	20:AG:5:ARG:HB2	2.15	0.60
25:BA:652:C:O2	25:BA:652:C:C2'	2.48	0.60
25:BA:860:U:O2	25:BA:860:U:O4'	2.14	0.60
25:BA:1495:A:H2'	25:BA:1495:A:N3	2.15	0.60
30:BQ:134:ARG:HA	30:BQ:137:TYR:CD1	2.36	0.60
35:BV:49:THR:HB	35:BV:50:PRO:CD	2.31	0.60
1:AA:1277:C:O2'	1:AA:1279:A:H8	1.82	0.60
14:AT:104:LEU:HD23	14:AT:104:LEU:C	2.22	0.60
17:AD:10:ARG:O	17:AD:10:ARG:HG2	1.99	0.60
25:BA:996:A:H4'	34:BU:92:ARG:NE	2.16	0.60
25:BA:1100:C:H6	25:BA:1100:C:H5"	1.66	0.60
25:BA:1504:C:O2'	25:BA:1505:C:P	2.59	0.60
25:BA:2140:C:O2	25:BA:2140:C:O4'	2.18	0.60
32:BS:14:VAL:HG12	32:BS:15:ARG:N	2.15	0.60
47:B6:20:ASN:O	47:B6:21:TYR:CD2	2.53	0.60
25:BA:2406:U:H2'	25:BA:2406:U:OP2	2.01	0.60
26:BB:2:C:O2	26:BB:2:C:H2'	2.02	0.60
26:BB:20:C:C2'	26:BB:21:G:H5'	2.31	0.60
29:BP:51:PHE:HB2	29:BP:52:GLU:HG2	1.84	0.60
25:BA:2585:U:O2	25:BA:2585:U:O4'	2.19	0.60
33:BT:89:VAL:HG21	33:BT:91:ARG:NE	2.17	0.60
43:BD:224:ALA:O	43:BD:225:ALA:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:B8:32:LEU:HB3	49:B8:36:LYS:NZ	2.17	0.60
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.18	0.60
25:BA:483:A:H5"	38:BY:49:VAL:HG22	1.84	0.60
25:BA:2690:C:OP2	31:BR:14:SER:HB2	2.02	0.60
30:BQ:27:VAL:O	30:BQ:28:ALA:HB3	2.01	0.60
1:AA:1118:C:OP1	22:AI:104:ARG:HD2	2.01	0.60
6:AL:24:VAL:O	6:AL:24:VAL:HG12	2.02	0.60
15:AB:97:TRP:HZ3	15:AB:176:GLU:OE2	1.85	0.60
16:AC:36:ASP:OD2	16:AC:59:ARG:NH2	2.34	0.60
25:BA:900:A:OP1	25:BA:900:A:H4'	2.02	0.60
25:BA:994:C:OP1	34:BU:53:ARG:NH2	2.35	0.60
25:BA:2681:C:H5	25:BA:2725:A:N6	2.00	0.60
28:BO:76:ALA:HB3	33:BT:75:ILE:HD12	1.82	0.60
43:BD:34:VAL:O	43:BD:64:ILE:HG23	2.01	0.60
43:BD:270:ILE:C	43:BD:271:ILE:HG13	2.21	0.60
1:AA:116:A:OP2	1:AA:116:A:C8	2.55	0.60
1:AA:149:A:O2'	1:AA:150:C:C6	2.55	0.60
4:AJ:30:SER:HB2	4:AJ:81:THR:OG1	2.01	0.60
9:AO:70:LEU:HD23	9:AO:78:TYR:HA	1.84	0.60
23:AY:681:LYS:C	23:AY:684:GLN:HE22	2.05	0.60
25:BA:1169:G:N2	25:BA:1181:C:C2	2.70	0.60
32:BS:104:GLY:O	32:BS:106:ARG:N	2.29	0.60
26:BB:92:C:OP1	30:BQ:19:GLY:HA2	2.01	0.60
43:BD:71:ASP:HB2	43:BD:103:ARG:HH22	1.67	0.60
52:BE:128:SER:OG	52:BE:129:HIS:N	2.35	0.60
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.37	0.59
1:AA:1346:A:O4'	1:AA:1348:U:C6	2.54	0.59
17:AD:9:CYS:HA	17:AD:12:CYS:HB3	1.83	0.59
22:AI:42:ARG:NH1	22:AI:71:SER:OG	2.34	0.59
23:AY:264:LEU:HD12	60:AY:702:GCP:C2	2.32	0.59
25:BA:247:G:H4'	25:BA:386:G:C5	2.37	0.59
25:BA:969:U:H2'	25:BA:970:C:C6	2.37	0.59
25:BA:2392:A:OP1	49:B8:32:LEU:CD2	2.50	0.59
25:BA:2590:A:OP2	43:BD:238:GLY:HA2	2.01	0.59
36:BW:20:VAL:CG2	36:BW:47:VAL:HG21	2.32	0.59
51:BC:104:LEU:N	51:BC:105:ASP:HA	2.17	0.59
55:BH:98:LEU:HD13	55:BH:125:VAL:HG23	1.82	0.59
55:BH:171:LEU:O	55:BH:173:PRO:HD3	2.02	0.59
1:AA:979:C:C3'	1:AA:980:C:H5'	2.31	0.59
23:AY:618:GLY:HA3	25:BA:1095:A:OP1	2.01	0.59
25:BA:1448:G:H1'	25:BA:1528:A:H62	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BP:47:ASP:OD2	29:BP:50:ARG:NH2	2.36	0.59
35:BV:45:THR:O	35:BV:46:VAL:HG12	2.02	0.59
39:BZ:18:LEU:HD12	39:BZ:18:LEU:N	2.12	0.59
1:AA:263:A:OP2	14:AT:79:ARG:NH1	2.35	0.59
25:BA:2092:U:C5	25:BA:2226:C:OP2	2.55	0.59
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.18	0.59
23:AY:110:SER:OG	23:AY:137:ASN:O	2.14	0.59
25:BA:994:C:OP2	34:BU:54:LYS:NZ	2.36	0.59
25:BA:1449:A:H5'	25:BA:1450:G:OP2	2.03	0.59
25:BA:2306:C:C5	25:BA:2307:G:H1'	2.37	0.59
26:BB:21:G:H2'	26:BB:22:U:O4'	2.02	0.59
27:BN:134:ARG:HD2	27:BN:134:ARG:O	2.01	0.59
42:B2:38:GLN:OE1	42:B2:44:LEU:HD22	2.02	0.59
51:BC:30:LYS:NZ	51:BC:180:PHE:O	2.27	0.59
1:AA:1138:G:H1'	1:AA:1139:G:P	2.42	0.59
25:BA:1063:G:H1	25:BA:1075:C:N4	1.98	0.59
25:BA:1217:C:OP2	34:BU:15:LYS:NZ	2.34	0.59
25:BA:1539:G:C2	25:BA:1540:U:C2	2.90	0.59
25:BA:2097:C:O2'	25:BA:2098:U:H5'	2.03	0.59
25:BA:2476:A:C2	25:BA:2477:C:C6	2.90	0.59
26:BB:71:C:H2'	26:BB:72:G:O4'	2.03	0.59
1:AA:46:G:O2'	1:AA:365:U:H1'	2.02	0.59
1:AA:375:U:C4	1:AA:376:G:N7	2.70	0.59
16:AC:64:VAL:HB	16:AC:99:VAL:HG12	1.84	0.59
18:AE:143:ARG:NH1	21:AH:77:GLU:OE2	2.34	0.59
25:BA:1239:G:H2'	25:BA:1240:U:O4'	2.03	0.59
38:BY:9:LYS:O	38:BY:11:ASP:N	2.33	0.59
9:AO:39:LEU:HD11	9:AO:56:LEU:HB2	1.84	0.59
25:BA:154(A):C:O2	25:BA:154(A):C:O4'	2.21	0.59
51:BC:70:LYS:HG2	51:BC:71:GLN:HE21	1.67	0.59
12:AR:44:LEU:HD22	12:AR:79:LEU:HD22	1.85	0.59
25:BA:881:G:H2'	25:BA:882:G:O4'	2.03	0.59
25:BA:2688:U:H5	25:BA:2720:U:OP2	1.86	0.59
25:BA:2793:G:O2'	25:BA:2794:C:OP2	2.20	0.59
31:BR:103:ARG:NH1	31:BR:108:GLY:O	2.36	0.59
14:AT:99:LEU:O	14:AT:101:GLY:N	2.36	0.59
25:BA:1742:G:H8	25:BA:1742:G:H3'	1.68	0.59
25:BA:1796:U:H2'	25:BA:1797:C:C6	2.37	0.59
28:BO:111:PHE:HB3	28:BO:114:ILE:HD13	1.83	0.59
38:BY:40:GLU:HB3	38:BY:64:GLU:OE2	2.01	0.59
53:BF:65:TRP:HZ3	53:BF:73:ALA:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1446:U:N3	1:AA:1452:C:N3	2.51	0.59
25:BA:639:U:H2'	25:BA:640:C:C6	2.37	0.59
25:BA:900:A:H3'	25:BA:901:A:H8	1.68	0.59
25:BA:1054:A:C5'	25:BA:1054:A:H8	2.16	0.59
25:BA:2138:C:H6	25:BA:2138:C:C5'	2.15	0.59
25:BA:2319:G:OP1	25:BA:2319:G:C4'	2.51	0.59
29:BP:23:PRO:O	29:BP:33:ARG:HD2	2.03	0.59
25:BA:662:G:P	29:BP:18:ARG:HD2	2.43	0.58
25:BA:2096:U:C4'	25:BA:2096:U:OP1	2.51	0.58
42:B2:45:SER:O	42:B2:46:GLN:NE2	2.36	0.58
1:AA:79:G:O2'	1:AA:80:G:O5'	2.14	0.58
1:AA:509:A:C5'	17:AD:55:ALA:HB2	2.33	0.58
1:AA:979:C:C2'	1:AA:980:C:H5'	2.32	0.58
2:AV:73:A:C3'	2:AV:74:C:H5'	2.33	0.58
25:BA:1312:U:H4'	25:BA:1313:U:O5'	2.03	0.58
25:BA:1531:C:H6	25:BA:1531:C:O5'	1.86	0.58
29:BP:64:LYS:O	29:BP:66:GLY:CA	2.50	0.58
29:BP:105:LEU:O	29:BP:106:LEU:CB	2.51	0.58
35:BV:18:LEU:HD22	35:BV:19:LYS:HA	1.84	0.58
35:BV:29:PRO:O	35:BV:61:VAL:O	2.20	0.58
40:B0:36:ILE:C	40:B0:36:ILE:HD12	2.22	0.58
52:BE:36:ARG:NH1	52:BE:85:ASN:OD1	2.35	0.58
56:BK:59:ILE:HG12	56:BK:60:TYR:N	2.18	0.58
1:AA:1013:G:C8	1:AA:1013:G:H5"	2.39	0.58
1:AA:1392:G:N2	1:AA:1502:A:C8	2.69	0.58
17:AD:26:CYS:CA	17:AD:31:CYS:HB2	2.28	0.58
25:BA:1174:A:OP1	25:BA:1175:U:OP1	2.20	0.58
25:BA:1418:G:OP1	25:BA:1588:C:O2'	2.22	0.58
25:BA:1528:A:C2	25:BA:1541:G:C2	2.91	0.58
25:BA:2422:A:H4'	25:BA:2423:U:OP1	2.02	0.58
26:BB:50:G:H2'	26:BB:51:G:O4'	2.02	0.58
29:BP:81:GLN:OE1	29:BP:106:LEU:HA	2.03	0.58
35:BV:2:PHE:O	35:BV:14:VAL:O	2.21	0.58
39:BZ:74:VAL:HG22	39:BZ:86:VAL:HG13	1.84	0.58
51:BC:185:LEU:O	51:BC:187:ASP:N	2.36	0.58
1:AA:1228:C:OP1	7:AM:108:ARG:NH2	2.36	0.58
16:AC:92:ALA:O	16:AC:95:THR:O	2.20	0.58
23:AY:683:VAL:O	23:AY:685:GLU:N	2.36	0.58
25:BA:2789:C:N3	25:BA:2894:G:O6	2.36	0.58
43:BD:77:ALA:HB2	43:BD:97:TYR:CD2	2.37	0.58
1:AA:60:A:H4'	1:AA:61:G:O5'	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:978:A:C5	1:AA:1319:A:C2	2.92	0.58
22:AI:42:ARG:NH2	22:AI:75:ASP:OD2	2.35	0.58
43:BD:26:LYS:HD3	43:BD:113:VAL:HG21	1.85	0.58
47:B6:48:VAL:O	47:B6:49:HIS:CB	2.48	0.58
1:AA:432:A:C8	1:AA:433:C:C5	2.92	0.58
16:AC:55:VAL:O	16:AC:55:VAL:HG12	2.02	0.58
30:BQ:16:ARG:C	30:BQ:17:LEU:HD23	2.24	0.58
34:BU:92:ARG:NH1	35:BV:11:GLN:O	2.36	0.58
6:AL:37:CYS:O	6:AL:79:GLU:O	2.20	0.58
15:AB:109:SER:O	15:AB:111:ARG:N	2.36	0.58
25:BA:90:U:H1'	25:BA:92:A:N7	2.19	0.58
25:BA:385:C:O2'	25:BA:388:G:N2	2.36	0.58
25:BA:662:G:H5'	29:BP:18:ARG:HA	1.86	0.58
25:BA:2681:C:C5	25:BA:2725:A:N6	2.71	0.58
38:BY:76:CYS:O	38:BY:96:ILE:CD1	2.51	0.58
1:AA:158:G:N2	1:AA:163:C:O2	2.33	0.58
1:AA:1442(A):G:N3	1:AA:1442(A):G:H2'	2.18	0.58
26:BB:1:U:O2	26:BB:1:U:H2'	2.03	0.58
28:BO:64:ARG:NH1	28:BO:81:ASP:OD2	2.37	0.58
33:BT:106:SER:C	33:BT:107:ASP:OD1	2.42	0.58
46:B5:40:LYS:CE	46:B5:46:CYS:HB3	2.33	0.58
55:BH:157:TYR:CE1	55:BH:171:LEU:HD22	2.38	0.58
25:BA:1210:A:H5'	25:BA:1210:A:H8	1.68	0.58
25:BA:1970:A:H5"	25:BA:1971:A:OP1	2.02	0.58
25:BA:2315:G:OP1	54:BG:36:LYS:NZ	2.35	0.58
25:BA:2529:G:O6	50:B9:31:LYS:NZ	2.37	0.58
25:BA:2836:U:H2'	25:BA:2837:G:C8	2.39	0.58
30:BQ:138:ASP:OD2	30:BQ:138:ASP:N	2.37	0.58
42:B2:35:LEU:HD12	42:B2:53:LEU:HD12	1.86	0.58
56:BK:103:GLN:O	56:BK:106:GLU:HG2	2.03	0.58
6:AL:53:ARG:NH1	6:AL:92:ASP:OD2	2.36	0.58
8:AN:26:ARG:NH1	8:AN:47:LEU:HD21	2.19	0.58
23:AY:428:LEU:CD2	23:AY:451:ILE:HD11	2.32	0.58
25:BA:685:A:OP1	48:B7:11:LYS:NZ	2.36	0.58
25:BA:2542:A:H2'	25:BA:2542:A:N3	2.19	0.58
25:BA:607:U:H3	25:BA:621:A:H2	1.44	0.57
33:BT:7:ILE:O	33:BT:11:GLU:OE1	2.21	0.57
33:BT:123:GLN:HA	33:BT:126:ALA:HB3	1.86	0.57
34:BU:105:VAL:HG11	35:BV:40:LEU:HD11	1.86	0.57
51:BC:39:GLU:OE1	51:BC:216:THR:HB	2.04	0.57
56:BK:14:ALA:HA	56:BK:41:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:269:C:H2'	1:AA:270:A:C8	2.39	0.57
1:AA:814:A:H2'	1:AA:816:A:H5"	1.86	0.57
25:BA:330:A:HO2'	25:BA:331:A:H8	1.51	0.57
25:BA:705:A:H2'	25:BA:706:A:O4'	2.03	0.57
25:BA:1434:A:H61	25:BA:1558:A:H62	1.52	0.57
25:BA:2662:A:H2'	25:BA:2663:G:O4'	2.04	0.57
40:B0:2:ALA:O	40:B0:4:LYS:N	2.34	0.57
49:B8:51:ALA:N	49:B8:53:PRO:HD2	2.19	0.57
1:AA:59:A:H2'	1:AA:60:A:OP1	2.04	0.57
1:AA:149:A:HO2'	1:AA:150:C:H6	1.47	0.57
13:AS:47:HIS:O	13:AS:62:ILE:HG22	2.04	0.57
25:BA:2165:G:C2'	25:BA:2166:G:H5"	2.34	0.57
32:BS:15:ARG:O	32:BS:18:ILE:HG22	2.04	0.57
58:BL:100:UNK:O	58:BL:101:UNK:CB	2.52	0.57
1:AA:986:A:H2'	1:AA:987:G:O4'	2.04	0.57
1:AA:1054:C:C2'	1:AA:1055:A:H5"	2.34	0.57
9:AO:15:PHE:CZ	9:AO:85:LEU:HD13	2.39	0.57
15:AB:84:GLU:HB3	15:AB:219:VAL:HG21	1.86	0.57
25:BA:1058:G:H5"	25:BA:1058:G:C8	2.40	0.57
25:BA:1742:G:C8	25:BA:1743:C:C6	2.93	0.57
29:BP:97:PRO:HB3	29:BP:112:LEU:HB2	1.86	0.57
33:BT:27:THR:OG1	33:BT:28:VAL:N	2.36	0.57
35:BV:39:LEU:HA	35:BV:47:VAL:HG11	1.85	0.57
38:BY:55:TYR:O	38:BY:56:PRO:C	2.41	0.57
1:AA:838:G:N2	1:AA:849:C:C2	2.72	0.57
2:AV:43:C:O2	2:AV:43:C:O4'	2.21	0.57
6:AL:41:ARG:HB3	6:AL:41:ARG:HH11	1.68	0.57
25:BA:1982:C:H5"	25:BA:1983:C:OP2	2.04	0.57
26:BB:76:G:O3'	39:BZ:19:ARG:NH2	2.33	0.57
36:BW:6:ILE:HA	36:BW:103:ILE:O	2.04	0.57
53:BF:167:ALA:O	53:BF:169:ASN:N	2.38	0.57
57:BJ:14:ALA:O	57:BJ:18:ALA:HB3	2.05	0.57
1:AA:416:G:C5	1:AA:417:C:C4	2.93	0.57
17:AD:25:ARG:O	17:AD:27:TYR:N	2.37	0.57
25:BA:470:A:OP1	53:BF:59:TYR:HE2	1.87	0.57
25:BA:1062:G:P	25:BA:1070:A:H4'	2.45	0.57
25:BA:1496:A:C8	25:BA:1577:C:O2'	2.52	0.57
25:BA:1688:U:H1'	25:BA:1701:A:C6	2.39	0.57
25:BA:2208:A:H1'	25:BA:2219:G:C5	2.39	0.57
25:BA:2602:A:OP2	25:BA:2602:A:C4'	2.52	0.57
25:BA:2688:U:O2	25:BA:2688:U:O5'	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:343:U:O2'	1:AA:346:G:O6	2.13	0.57
1:AA:1181:G:O2'	1:AA:1182:G:H5'	2.03	0.57
11:AQ:45:HIS:HB2	11:AQ:65:ILE:HD13	1.86	0.57
25:BA:1918:A:O2'	25:BA:1919:A:H2	1.87	0.57
29:BP:58:THR:O	29:BP:61:ARG:NH2	2.37	0.57
35:BV:18:LEU:HD13	35:BV:19:LYS:N	2.19	0.57
49:B8:50:LEU:HA	49:B8:53:PRO:CD	2.35	0.57
56:BK:19:PRO:HB3	56:BK:34:ILE:HD12	1.87	0.57
15:AB:121:LEU:HB3	15:AB:127:ILE:HD11	1.86	0.57
27:BN:4:TYR:N	27:BN:4:TYR:CD1	2.71	0.57
33:BT:28:VAL:HG13	33:BT:46:GLU:HA	1.87	0.57
39:BZ:15:PRO:HA	39:BZ:18:LEU:HD13	1.87	0.57
43:BD:30:GLU:HG3	43:BD:63:ARG:CZ	2.34	0.57
1:AA:1452:C:C4'	1:AA:1456:G:N2	2.67	0.57
13:AS:79:THR:O	13:AS:80:TYR:O	2.22	0.57
60:AY:702:GCP:PG	61:AY:803:HOH:O	2.62	0.57
25:BA:523:C:H4'	25:BA:540:C:O2	2.04	0.57
25:BA:2320:A:N3	25:BA:2320:A:H2'	2.20	0.57
25:BA:2845:G:O2'	25:BA:2846:G:H5'	2.05	0.57
51:BC:53:ARG:O	51:BC:54:SER:C	2.43	0.57
55:BH:106:THR:HG22	55:BH:112:PRO:HG3	1.87	0.57
2:AV:74:C:O2'	2:AV:75:C:P	2.63	0.57
12:AR:31:LEU:HD22	19:AF:97:PHE:O	2.05	0.57
26:BB:80:U:H2'	26:BB:81:G:H21	1.68	0.57
27:BN:119:ARG:HH11	27:BN:119:ARG:HG3	1.69	0.57
38:BY:76:CYS:HB3	38:BY:96:ILE:HD11	1.87	0.57
11:AQ:27:PHE:CZ	11:AQ:36:ILE:HD11	2.40	0.56
14:AT:96:GLY:O	14:AT:97:ALA:HB3	2.05	0.56
16:AC:156:ARG:NE	16:AC:160:ALA:O	2.34	0.56
23:AY:680:PRO:HD2	23:AY:683:VAL:HG22	1.87	0.56
25:BA:8:A:H2'	25:BA:9:U:C5	2.39	0.56
43:BD:136:ILE:HG22	43:BD:140:THR:OG1	2.05	0.56
52:BE:60:ASN:N	52:BE:60:ASN:ND2	2.50	0.56
53:BF:23:ASP:N	53:BF:23:ASP:OD1	2.38	0.56
1:AA:250:A:C4'	1:AA:251:G:O5'	2.51	0.56
25:BA:102:G:C4'	25:BA:102:G:OP1	2.53	0.56
27:BN:32:THR:O	27:BN:35:ARG:O	2.23	0.56
29:BP:6:LEU:HD12	29:BP:8:PRO:HG2	1.86	0.56
34:BU:90:VAL:HG22	35:BV:39:LEU:CB	2.36	0.56
36:BW:92:ARG:O	36:BW:93:ALA:HB3	2.05	0.56
42:B2:47:ASN:O	42:B2:48:HIS:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:B5:34:PRO:O	46:B5:35:GLU:HG2	2.04	0.56
1:AA:432:A:N7	1:AA:433:C:C5	2.73	0.56
1:AA:664:G:H22	1:AA:741:G:H1	1.52	0.56
1:AA:975:A:C4'	1:AA:976:G:H5"	2.34	0.56
1:AA:1104:G:OP1	15:AB:111:ARG:NE	2.38	0.56
7:AM:79:LYS:O	7:AM:82:MET:SD	2.63	0.56
15:AB:239:VAL:O	15:AB:239:VAL:HG12	2.06	0.56
16:AC:165:THR:HG23	16:AC:165:THR:O	2.05	0.56
23:AY:418:LYS:O	23:AY:419:ALA:HB3	2.05	0.56
25:BA:272(J):C:C2'	25:BA:274:G:OP1	2.53	0.56
25:BA:1210:A:H8	25:BA:1210:A:C5'	2.17	0.56
25:BA:1494:A:N3	25:BA:1494:A:C3'	2.65	0.56
25:BA:1786:A:N1	25:BA:2606:C:H1'	2.20	0.56
28:BO:80:ASP:OD2	33:BT:64:ARG:NH2	2.37	0.56
33:BT:106:SER:HA	33:BT:110:ILE:HG13	1.86	0.56
38:BY:76:CYS:SG	38:BY:77:PRO:HD3	2.45	0.56
43:BD:182:LEU:O	43:BD:271:ILE:N	2.38	0.56
55:BH:167:GLU:HB3	55:BH:168:PRO:CD	2.35	0.56
1:AA:417:C:H2'	1:AA:418:C:H6	1.70	0.56
2:AV:46:G:H3'	2:AV:47:U:C5'	2.35	0.56
6:AL:27:LEU:C	6:AL:29:GLY:H	2.07	0.56
14:AT:53:LEU:HB2	14:AT:100:ILE:HG22	1.86	0.56
25:BA:252:G:P	29:BP:50:ARG:NH1	2.78	0.56
25:BA:1877:A:H5"	25:BA:1878:G:OP2	2.05	0.56
34:BU:108:GLU:OE2	34:BU:112:ARG:NH1	2.38	0.56
39:BZ:8:TYR:O	39:BZ:37:VAL:HB	2.05	0.56
1:AA:838:G:C2	1:AA:849:C:C2	2.94	0.56
15:AB:97:TRP:HH2	15:AB:176:GLU:CD	2.09	0.56
23:AY:70:THR:HA	23:AY:358:MET:O	2.06	0.56
25:BA:650:C:OP1	49:B8:48:PHE:CZ	2.58	0.56
25:BA:658:C:H2'	25:BA:659:C:C6	2.40	0.56
25:BA:1075:C:OP1	25:BA:1075:C:H4'	2.06	0.56
25:BA:2180:U:C6	25:BA:2180:U:H5'	2.39	0.56
25:BA:2238:G:H2'	25:BA:2238:G:N3	2.20	0.56
32:BS:89:ARG:HB3	32:BS:92:TYR:HB3	1.87	0.56
38:BY:17:SER:HB2	38:BY:71:LYS:HE2	1.87	0.56
49:B8:63:PRO:O	49:B8:64:TYR:C	2.43	0.56
51:BC:113:VAL:HG21	51:BC:131:LEU:HD11	1.88	0.56
1:AA:1014:A:H4'	13:AS:14:HIS:CE1	2.40	0.56
13:AS:63:THR:OG1	13:AS:65:ASN:OD1	2.23	0.56
17:AD:8:VAL:C	17:AD:10:ARG:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BP:16:ARG:NH1	29:BP:16:ARG:HB2	2.20	0.56
33:BT:24:PRO:HB3	33:BT:99:LEU:HD21	1.88	0.56
38:BY:90:LEU:HG	38:BY:91:GLU:HG3	1.87	0.56
15:AB:80:ILE:HD12	15:AB:80:ILE:N	2.20	0.56
23:AY:108:PHE:CE1	23:AY:114:VAL:HG22	2.41	0.56
25:BA:17:G:H4'	34:BU:25:TRP:CH2	2.41	0.56
53:BF:65:TRP:HB2	53:BF:66:PRO:HD2	1.87	0.56
54:BG:55:LYS:O	54:BG:59:GLU:HB2	2.06	0.56
56:BK:23:VAL:HG13	56:BK:27:LEU:HD22	1.87	0.56
23:AY:98:MET:HG3	23:AY:130:VAL:HG21	1.88	0.56
23:AY:215:LYS:HA	23:AY:218:GLU:HB3	1.88	0.56
25:BA:821:A:H2'	25:BA:946:G:H5"	1.88	0.56
25:BA:1022:G:N2	25:BA:1142(A):A:H2	1.97	0.56
29:BP:51:PHE:HB3	29:BP:52:GLU:HG2	1.87	0.56
33:BT:12:SER:O	33:BT:13:ARG:NE	2.38	0.56
33:BT:29:ARG:HD2	33:BT:30:VAL:HG13	1.87	0.56
23:AY:168:ILE:HD11	23:AY:178:ILE:CD1	2.35	0.56
23:AY:493:VAL:HG23	23:AY:512:ILE:HD11	1.87	0.56
25:BA:1448:G:H4'	25:BA:1542:A:OP1	2.06	0.56
25:BA:1584:C:O2	25:BA:1584:C:C2'	2.54	0.56
1:AA:149:A:O2'	1:AA:150:C:H6	1.89	0.56
1:AA:1133:G:C8	1:AA:1133:G:C3'	2.89	0.56
7:AM:82:MET:SD	7:AM:83:ASP:N	2.79	0.56
17:AD:17:VAL:O	17:AD:17:VAL:HG12	2.06	0.56
25:BA:528:A:C2	25:BA:2043:C:C5'	2.89	0.56
25:BA:810:U:O5'	25:BA:810:U:H6	1.89	0.56
25:BA:1504:C:HO2'	25:BA:1505:C:P	2.28	0.56
25:BA:1538:G:C5	25:BA:1539:G:N7	2.73	0.56
25:BA:2894:G:H2'	25:BA:2894:G:N3	2.21	0.56
43:BD:24:ILE:O	43:BD:25:THR:C	2.43	0.56
25:BA:762:U:H4'	25:BA:763:G:O5'	2.06	0.55
30:BQ:84:GLY:O	30:BQ:85:LYS:HB2	2.06	0.55
38:BY:65:ALA:HB1	38:BY:66:PRO:CD	2.35	0.55
42:B2:9:GLN:HE22	42:B2:56:GLN:HG2	1.72	0.55
51:BC:58:VAL:HG13	51:BC:199:HIS:HB3	1.87	0.55
56:BK:56:GLU:O	56:BK:67:PHE:HA	2.06	0.55
25:BA:102:G:OP1	25:BA:102:G:O4'	2.23	0.55
25:BA:528:A:O2'	25:BA:529:A:H5'	2.06	0.55
25:BA:1778:U:H2'	25:BA:1784:A:N6	2.20	0.55
25:BA:2444:G:OP2	53:BF:68:LYS:HE2	2.06	0.55
26:BB:42:C:O2'	26:BB:43:C:O5'	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BN:41:ASP:O	27:BN:42:TRP:C	2.43	0.55
31:BR:104:ARG:NH1	31:BR:107:ASP:OD1	2.39	0.55
38:BY:65:ALA:HB1	38:BY:66:PRO:HD3	1.88	0.55
1:AA:1392:G:H21	1:AA:1502:A:H8	1.52	0.55
5:AK:54:ARG:O	5:AK:57:THR:HG22	2.06	0.55
16:AC:7:PRO:O	16:AC:11:ARG:HG2	2.06	0.55
16:AC:180:ALA:O	16:AC:181:ASN:HB3	2.06	0.55
23:AY:404:VAL:HG22	23:AY:405:PRO:O	2.07	0.55
23:AY:556:ILE:HD11	23:AY:601:ILE:HD13	1.88	0.55
25:BA:456:C:O2'	37:BX:68:ARG:NH1	2.40	0.55
25:BA:1754:C:OP1	33:BT:96:ARG:NH1	2.40	0.55
25:BA:2262:U:H4'	25:BA:2328:A:H2	1.71	0.55
43:BD:209:ALA:O	43:BD:210:GLY:O	2.24	0.55
52:BE:77:ILE:HG22	52:BE:78:LEU:N	2.21	0.55
11:AQ:9:VAL:HG12	11:AQ:56:VAL:HG22	1.88	0.55
25:BA:1188:U:H4'	35:BV:79:VAL:HG22	1.88	0.55
25:BA:1315:C:C2	25:BA:1338:G:N2	2.74	0.55
25:BA:1996:C:OP1	28:BO:31:LYS:HE2	2.06	0.55
25:BA:2243:U:H2'	25:BA:2244:U:C6	2.41	0.55
28:BO:7:TYR:CZ	28:BO:44:LYS:HG3	2.42	0.55
38:BY:7:VAL:HB	38:BY:8:LYS:CD	2.36	0.55
38:BY:73:ARG:HH21	38:BY:81:LYS:HA	1.71	0.55
44:B3:50:VAL:HG23	44:B3:54:VAL:HG21	1.88	0.55
23:AY:58:GLU:HG2	23:AY:63:ILE:O	2.05	0.55
25:BA:1054:A:C5'	25:BA:1054:A:C8	2.89	0.55
27:BN:5:VAL:O	27:BN:5:VAL:HG13	2.06	0.55
35:BV:2:PHE:CB	35:BV:42:GLY:HA3	2.36	0.55
36:BW:18:ARG:NH1	36:BW:76:VAL:O	2.40	0.55
52:BE:68:ALA:C	52:BE:70:ALA:H	2.10	0.55
56:BK:6:ALA:O	56:BK:58:THR:HG23	2.07	0.55
1:AA:694:A:N1	1:AA:787:A:O2'	2.39	0.55
1:AA:1140:C:O2'	1:AA:1141:C:H5'	2.06	0.55
2:AV:34:G:C3'	2:AV:35:A:H5"	2.36	0.55
5:AK:111:ASP:HA	12:AR:84:LYS:HG3	1.87	0.55
11:AQ:12:SER:HB3	11:AQ:20:THR:HB	1.88	0.55
25:BA:2584:U:H2'	25:BA:2585:U:H2'	1.88	0.55
1:AA:1311:G:N2	1:AA:1327:C:C2	2.74	0.55
19:AF:37:VAL:HG12	19:AF:38:GLU:O	2.07	0.55
20:AG:137:LYS:O	20:AG:141:VAL:HG23	2.07	0.55
23:AY:519:ARG:NE	23:AY:519:ARG:HA	2.21	0.55
23:AY:652:MET:HG2	23:AY:671:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1054:A:H5"	25:BA:1054:A:H8	1.72	0.55
25:BA:2365:G:O6	49:B8:39:LYS:HE3	2.07	0.55
27:BN:24:GLY:HA2	27:BN:27:ALA:HB3	1.87	0.55
32:BS:96:GLY:O	32:BS:98:VAL:N	2.39	0.55
1:AA:1178:G:N7	22:AI:97:LYS:NZ	2.48	0.55
7:AM:39:ILE:HD12	7:AM:56:LEU:HD23	1.88	0.55
23:AY:488:THR:OG1	23:AY:598:ASP:O	2.24	0.55
25:BA:372:G:O2'	25:BA:373:U:P	2.65	0.55
25:BA:1272:A:H4'	25:BA:1272:A:OP1	2.05	0.55
25:BA:1300:U:O2'	25:BA:1635:G:OP1	2.22	0.55
25:BA:2095:C:H6	25:BA:2095:C:H5"	1.72	0.55
29:BP:10:PRO:O	53:BF:34:TRP:CD1	2.60	0.55
29:BP:99:LEU:HD23	29:BP:99:LEU:O	2.07	0.55
56:BK:109:LYS:O	56:BK:112:MET:HG2	2.06	0.55
1:AA:1014:A:H5"	13:AS:14:HIS:CG	2.42	0.55
1:AA:1292:U:H2'	1:AA:1293:G:H5"	1.88	0.55
1:AA:1399:C:C2	1:AA:1502:A:N6	2.74	0.55
7:AM:108:ARG:O	7:AM:111:LYS:O	2.25	0.55
23:AY:212:TYR:O	23:AY:215:LYS:N	2.40	0.55
25:BA:36:G:O2'	25:BA:450:G:H2'	2.07	0.55
25:BA:111:A:O3'	42:B2:69:ARG:NH2	2.39	0.55
25:BA:583:G:P	34:BU:10:ARG:HH11	2.29	0.55
25:BA:1332:G:N2	25:BA:1610:A:C8	2.75	0.55
26:BB:73:A:C4	26:BB:105:A:C2	2.94	0.55
29:BP:18:ARG:NH1	29:BP:18:ARG:O	2.40	0.55
31:BR:101:ALA:O	31:BR:102:GLU:HB2	2.07	0.55
33:BT:1:MET:O	33:BT:2:ASN:C	2.44	0.55
33:BT:89:VAL:C	33:BT:91:ARG:N	2.52	0.55
49:B8:32:LEU:HB2	49:B8:36:LYS:HE2	1.88	0.55
51:BC:53:ARG:O	51:BC:55:ASP:OD1	2.25	0.55
52:BE:89:ASP:O	52:BE:90:THR:O	2.24	0.55
54:BG:17:PRO:HA	54:BG:20:ILE:HD12	1.89	0.55
1:AA:408:A:H4'	17:AD:112:VAL:HG11	1.88	0.55
1:AA:630:G:C8	1:AA:630:G:H5"	2.42	0.55
2:AV:33:U:C5	2:AV:36:A:OP2	2.59	0.55
23:AY:71:THR:CG2	23:AY:80:ASN:OD1	2.48	0.55
25:BA:2097:C:C2'	25:BA:2098:U:H5'	2.36	0.55
34:BU:98:LEU:O	34:BU:101:ARG:O	2.24	0.55
38:BY:42:VAL:HG12	38:BY:65:ALA:HB3	1.88	0.55
51:BC:42:GLU:HG2	51:BC:215:THR:HG23	1.87	0.55
53:BF:9:ILE:O	53:BF:128:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1036:G:H3'	1:AA:1037:C:C6	2.42	0.54
23:AY:212:TYR:HA	23:AY:215:LYS:CB	2.35	0.54
25:BA:1713:U:O2'	25:BA:1714:G:H5'	2.07	0.54
25:BA:2031:A:C6	25:BA:2498:C:H1'	2.43	0.54
25:BA:2095:C:H6	25:BA:2095:C:C5'	2.20	0.54
28:BO:18:LYS:HB2	28:BO:45:GLU:HG3	1.89	0.54
29:BP:97:PRO:O	29:BP:98:GLU:CG	2.55	0.54
42:B2:38:GLN:O	42:B2:41:ILE:HG12	2.06	0.54
53:BF:53:THR:HG23	53:BF:55:GLY:H	1.71	0.54
1:AA:1003:G:H2'	1:AA:1004:A:H4'	1.89	0.54
5:AK:48:ILE:HG22	5:AK:49:GLY:N	2.23	0.54
23:AY:679:VAL:HB	23:AY:680:PRO:HD2	1.88	0.54
25:BA:1539:G:H2'	25:BA:1540:U:C5'	2.37	0.54
25:BA:2136:C:C2	25:BA:2137:C:C5	2.96	0.54
26:BB:91:C:OP2	30:BQ:16:ARG:NH1	2.39	0.54
29:BP:8:PRO:O	29:BP:10:PRO:HD3	2.06	0.54
52:BE:74:PRO:O	52:BE:75:VAL:O	2.26	0.54
52:BE:115:GLY:C	52:BE:116:VAL:O	2.42	0.54
54:BG:116:ASP:O	54:BG:117:PHE:CB	2.55	0.54
13:AS:70:LYS:N	13:AS:70:LYS:HE3	2.22	0.54
22:AI:118:LYS:O	22:AI:119:ALA:CB	2.55	0.54
25:BA:607:U:O2	25:BA:621:A:N1	2.40	0.54
25:BA:1639:U:O2'	25:BA:1640:C:H5'	2.08	0.54
25:BA:2492:U:H2'	25:BA:2493:U:C6	2.42	0.54
27:BN:46:VAL:O	27:BN:47:ALA:CB	2.55	0.54
31:BR:9:LYS:O	31:BR:10:LEU:HD23	2.06	0.54
33:BT:3:ARG:HG3	33:BT:6:LEU:HB3	1.89	0.54
33:BT:30:VAL:HG12	33:BT:44:ASP:OD1	2.08	0.54
35:BV:62:LEU:CD2	35:BV:95:LEU:HB2	2.37	0.54
43:BD:27:THR:HG23	43:BD:83:GLU:HB3	1.87	0.54
47:B6:20:ASN:O	47:B6:21:TYR:CD1	2.60	0.54
53:BF:81:PRO:CB	53:BF:89:VAL:HG23	2.37	0.54
53:BF:202:PHE:O	53:BF:206:ILE:HG12	2.08	0.54
56:BK:37:PHE:O	56:BK:41:PHE:HB3	2.07	0.54
16:AC:167:TRP:O	16:AC:168:ALA:HB2	2.08	0.54
25:BA:528:A:C2	25:BA:2043:C:C4'	2.88	0.54
25:BA:1721:G:C2	25:BA:1739:U:OP2	2.61	0.54
28:BO:1:MET:HG3	28:BO:67:LYS:HG2	1.90	0.54
47:B6:41:PRO:CD	47:B6:46:HIS:HA	2.37	0.54
51:BC:84:LYS:HA	51:BC:87:GLU:HG3	1.89	0.54
52:BE:65:GLY:O	52:BE:67:PHE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1080:A:C5'	18:AE:16:THR:HG21	2.37	0.54
25:BA:242:G:H5'	49:B8:62:LEU:HD13	1.88	0.54
25:BA:598:G:H2'	25:BA:599:G:O4'	2.07	0.54
25:BA:900:A:H3'	25:BA:901:A:C8	2.42	0.54
25:BA:1539:G:H2'	25:BA:1540:U:H5"	1.87	0.54
25:BA:2312:U:O2'	54:BG:71:THR:HG21	2.08	0.54
27:BN:3:THR:C	27:BN:5:VAL:N	2.61	0.54
1:AA:134:A:H1'	1:AA:325:A:C5	2.43	0.54
1:AA:1226:C:H4'	1:AA:1227:A:OP1	2.08	0.54
1:AA:1504:G:OP1	1:AA:1507:A:H4'	2.08	0.54
2:AV:33:U:O4'	2:AV:33:U:O2	2.23	0.54
25:BA:213:A:H2'	25:BA:214:G:O4'	2.07	0.54
25:BA:524:U:H4'	25:BA:555:U:H4'	1.88	0.54
25:BA:1539:G:C3'	25:BA:1540:U:C5'	2.86	0.54
25:BA:1689:A:N7	25:BA:1698:A:N1	2.55	0.54
29:BP:7:ARG:HA	29:BP:7:ARG:CZ	2.36	0.54
29:BP:23:PRO:HB2	29:BP:33:ARG:CD	2.38	0.54
39:BZ:6:LYS:HG2	39:BZ:8:TYR:OH	2.07	0.54
52:BE:4:ILE:HD13	52:BE:28:ALA:HB1	1.90	0.54
55:BH:117:PRO:HB3	55:BH:123:PHE:CE2	2.42	0.54
55:BH:174:GLY:C	55:BH:176:ALA:HB2	2.27	0.54
1:AA:1133:G:H2'	1:AA:1134:G:O4'	2.08	0.54
1:AA:1202:G:C2	8:AN:42:ILE:HG21	2.43	0.54
26:BB:66:A:O2'	26:BB:67:G:OP2	2.19	0.54
29:BP:135:LEU:HD21	29:BP:144:GLU:HG3	1.89	0.54
42:B2:53:LEU:O	42:B2:57:ILE:HG13	2.07	0.54
55:BH:136:ILE:HD12	55:BH:136:ILE:H	1.71	0.54
2:AV:73:A:H2'	2:AV:74:C:C5'	2.37	0.54
16:AC:60:ALA:O	16:AC:62:ASP:N	2.41	0.54
21:AH:96:GLY:N	21:AH:99:GLU:OE1	2.41	0.54
25:BA:219:G:H2'	25:BA:220:G:O4'	2.07	0.54
25:BA:1131:G:OP2	25:BA:2515:C:H4'	2.07	0.54
25:BA:2743:C:H2'	25:BA:2744:G:O5'	2.08	0.54
35:BV:49:THR:HB	35:BV:50:PRO:HD2	1.90	0.54
54:BG:7:LEU:HD22	54:BG:176:LEU:HD22	1.89	0.54
7:AM:10:PRO:HB2	7:AM:18:ALA:HB1	1.89	0.54
15:AB:77:ALA:HB2	15:AB:211:ILE:HD13	1.89	0.54
25:BA:918:A:H1'	26:BB:80:U:O2'	2.08	0.54
25:BA:2019:A:C2'	25:BA:2020:A:O5'	2.56	0.54
29:BP:7:ARG:CB	29:BP:8:PRO:CD	2.84	0.54
29:BP:48:PRO:O	29:BP:49:ARG:C	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BK:77:LEU:HD23	56:BK:77:LEU:H	1.72	0.54
1:AA:991:U:O2	1:AA:991:U:H2'	2.08	0.54
2:AV:57:G:H8	2:AV:57:G:H5"	1.73	0.54
4:AJ:49:VAL:O	4:AJ:60:ARG:HB2	2.09	0.54
23:AY:148:LEU:O	23:AY:152:THR:OG1	2.15	0.54
25:BA:684:G:OP1	48:B7:16:HIS:CD2	2.61	0.54
25:BA:2477:C:C5	50:B9:4:ARG:NH2	2.76	0.54
25:BA:2609:U:OP1	25:BA:2609:U:H4'	2.07	0.54
2:AV:18:G:O2'	2:AV:57:G:N2	2.31	0.53
15:AB:31:TYR:CE1	15:AB:200:ILE:HD12	2.42	0.53
25:BA:646:A:H2'	25:BA:647:G:O5'	2.08	0.53
25:BA:1100:C:C6	25:BA:1100:C:H5'	2.43	0.53
25:BA:1818:U:O4	43:BD:154:LYS:HE3	2.09	0.53
33:BT:56:GLY:C	33:BT:57:PHE:O	2.43	0.53
39:BZ:11:GLU:O	39:BZ:36:LYS:NZ	2.28	0.53
41:B1:57:GLU:O	41:B1:58:ILE:HG23	2.07	0.53
51:BC:53:ARG:O	51:BC:55:ASP:N	2.41	0.53
20:AG:144:MET:C	20:AG:145:ALA:O	2.43	0.53
21:AH:38:ILE:CD1	21:AH:118:VAL:HG12	2.37	0.53
23:AY:151:ARG:O	23:AY:154:GLN:HG2	2.08	0.53
25:BA:1478:G:O2'	25:BA:1558:A:C2	2.60	0.53
25:BA:1763:G:H4'	25:BA:1763:G:OP1	2.07	0.53
25:BA:2287:A:C2	25:BA:2346:A:N1	2.76	0.53
29:BP:62:LEU:HD11	49:B8:30:ARG:HG2	1.90	0.53
30:BQ:6:ARG:HA	39:BZ:195:GLU:O	2.07	0.53
30:BQ:21:THR:O	30:BQ:22:LYS:CB	2.55	0.53
32:BS:98:VAL:HG12	32:BS:100:ALA:N	2.23	0.53
35:BV:5:VAL:HG21	35:BV:35:LEU:HD23	1.90	0.53
42:B2:46:GLN:OE1	42:B2:46:GLN:HA	2.08	0.53
1:AA:1360:A:H8	1:AA:1360:A:OP1	1.90	0.53
6:AL:23:LYS:C	6:AL:24:VAL:HG23	2.28	0.53
23:AY:484:ARG:HB2	23:AY:602:LEU:HB2	1.89	0.53
25:BA:2032:G:H21	52:BE:146:THR:HG23	1.74	0.53
25:BA:2052:G:H4'	52:BE:143:ASN:O	2.07	0.53
25:BA:2134:A:C2	25:BA:2158:A:C5	2.95	0.53
56:BK:115:LEU:HD22	56:BK:126:MET:HE2	1.90	0.53
1:AA:671:G:C2'	1:AA:672:U:H5'	2.39	0.53
1:AA:978:A:C4	1:AA:1319:A:C2	2.97	0.53
14:AT:100:ILE:O	14:AT:100:ILE:HG23	2.07	0.53
34:BU:91:ASP:O	34:BU:95:LEU:HB2	2.08	0.53
43:BD:30:GLU:CG	43:BD:63:ARG:NH2	2.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BC:92:ASP:N	51:BC:92:ASP:OD1	2.41	0.53
52:BE:116:VAL:HB	52:BE:122:PHE:CD2	2.43	0.53
55:BH:155:SER:CB	55:BH:156:ALA:HA	2.39	0.53
56:BK:109:LYS:HA	56:BK:112:MET:HE2	1.91	0.53
1:AA:633:G:C5'	1:AA:633:G:C8	2.92	0.53
10:AP:3:LYS:O	10:AP:21:VAL:HA	2.08	0.53
25:BA:2165:G:H2'	25:BA:2166:G:H5"	1.90	0.53
56:BK:7:VAL:HG13	56:BK:7:VAL:O	2.08	0.53
57:BJ:55:ALA:O	57:BJ:56:ALA:C	2.46	0.53
1:AA:396:G:O2'	1:AA:398:C:OP1	2.19	0.53
1:AA:973:G:H2'	1:AA:974:A:OP1	2.08	0.53
1:AA:1068:G:OP2	1:AA:1068:G:H8	1.91	0.53
20:AG:6:ARG:O	20:AG:7:ALA:HB3	2.07	0.53
23:AY:117:GLN:HA	23:AY:120:THR:OG1	2.08	0.53
23:AY:157:LEU:N	23:AY:157:LEU:HD23	2.23	0.53
25:BA:661:C:H4'	29:BP:16:ARG:NH1	2.24	0.53
25:BA:1024:G:H3'	25:BA:1025:G:H5"	1.91	0.53
25:BA:1570:A:H5'	43:BD:38:LYS:HG3	1.90	0.53
25:BA:2206:G:N3	25:BA:2206:G:H5"	2.24	0.53
25:BA:2298:A:H62	25:BA:2318:G:H8	1.55	0.53
28:BO:104:ARG:HH21	33:BT:33:LYS:HE2	1.74	0.53
29:BP:16:ARG:CZ	29:BP:18:ARG:HG3	2.39	0.53
29:BP:85:LEU:HA	29:BP:88:LEU:HD22	1.90	0.53
37:BX:27:THR:HA	37:BX:79:ALA:O	2.09	0.53
38:BY:96:ILE:CD1	38:BY:99:CYS:SG	2.92	0.53
56:BK:79:ARG:HD2	56:BK:85:GLU:O	2.09	0.53
1:AA:353:A:H2'	1:AA:354:G:OP2	2.09	0.53
1:AA:518:C:H5	1:AA:530:G:O5'	1.92	0.53
1:AA:1533:C:H4'	1:AA:1533:C:OP1	2.09	0.53
20:AG:26:PHE:CE2	20:AG:30:ILE:HD11	2.43	0.53
23:AY:250:THR:N	23:AY:255:ILE:HG22	2.23	0.53
25:BA:686:G:H1	48:B7:16:HIS:CE1	2.27	0.53
25:BA:1204:A:N1	25:BA:1241:A:C2	2.76	0.53
25:BA:1538:G:C4	25:BA:1539:G:N7	2.76	0.53
25:BA:1720:U:O2	25:BA:1742:G:O6	2.26	0.53
25:BA:1920:C:O2	25:BA:1920:C:O4'	2.23	0.53
25:BA:2019:A:H2'	25:BA:2020:A:O5'	2.08	0.53
25:BA:2109:U:H1'	25:BA:2181:G:N2	2.24	0.53
25:BA:2875:C:O2'	33:BT:3:ARG:HB2	2.09	0.53
31:BR:4:LEU:O	31:BR:5:LYS:HG2	2.09	0.53
32:BS:52:SER:CB	32:BS:55:ALA:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BU:81:HIS:NE2	34:BU:117:GLN:HG3	2.23	0.53
51:BC:137:LEU:HD22	51:BC:138:PRO:HD2	1.89	0.53
1:AA:460:G:O6	1:AA:470:C:C5'	2.55	0.53
4:AJ:90:LEU:N	4:AJ:91:PRO:HD3	2.24	0.53
25:BA:8:A:H2'	25:BA:9:U:C6	2.44	0.53
25:BA:661:C:H4'	29:BP:16:ARG:HH12	1.74	0.53
25:BA:1364:G:N7	41:B1:3:LYS:HE2	2.24	0.53
25:BA:1833:U:O2	25:BA:1969:A:H2	1.90	0.53
29:BP:100:LEU:O	29:BP:105:LEU:O	2.26	0.53
31:BR:78:LYS:HE2	31:BR:83:ILE:HD11	1.90	0.53
50:B9:29:ASN:ND2	50:B9:32:HIS:CE1	2.66	0.53
54:BG:114:ILE:HG12	54:BG:140:ILE:HG21	1.90	0.53
57:BJ:106:ALA:O	57:BJ:107:ALA:CB	2.57	0.53
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.44	0.53
1:AA:1192:C:OP2	16:AC:4:LYS:NZ	2.40	0.53
25:BA:551:G:O2'	25:BA:1220:A:N3	2.31	0.53
25:BA:1742:G:H3'	25:BA:1742:G:C8	2.44	0.53
31:BR:2:ARG:CZ	52:BE:111:ARG:HG3	2.39	0.53
51:BC:76:ALA:HB3	51:BC:94:VAL:HG22	1.90	0.53
1:AA:602:A:H2'	1:AA:603:U:O4'	2.09	0.53
1:AA:1278:U:O2	1:AA:1278:U:O4'	2.26	0.53
15:AB:145:LEU:CD1	15:AB:149:LEU:HD12	2.39	0.53
17:AD:3:ARG:HG2	17:AD:118:ARG:CD	2.39	0.53
17:AD:11:LEU:HA	17:AD:13:ARG:O	2.09	0.53
25:BA:185:U:H4'	25:BA:218:A:H4'	1.91	0.53
25:BA:2138:C:O2	25:BA:2154:G:C2	2.62	0.53
31:BR:117:VAL:O	31:BR:117:VAL:HG12	2.09	0.53
43:BD:238:GLY:O	43:BD:239:ARG:O	2.26	0.53
46:B5:33:CYS:HB2	46:B5:40:LYS:CE	2.34	0.53
52:BE:1:MET:HB3	52:BE:200:GLU:CD	2.29	0.53
56:BK:109:LYS:HA	56:BK:112:MET:CE	2.39	0.53
1:AA:421:U:O2	1:AA:421:U:O4'	2.27	0.52
1:AA:552:U:O2'	6:AL:86:ARG:O	2.27	0.52
1:AA:633:G:H8	1:AA:633:G:C5'	2.19	0.52
17:AD:31:CYS:C	17:AD:33:MET:H	2.12	0.52
23:AY:201:ILE:H	23:AY:201:ILE:HD12	1.74	0.52
25:BA:613:G:H8	25:BA:613:G:C5'	2.20	0.52
25:BA:1243:G:H2'	25:BA:1244:G:O4'	2.09	0.52
25:BA:2063:C:O2	25:BA:2451:A:C2	2.62	0.52
29:BP:5:ASP:N	53:BF:116:ASP:OD2	2.42	0.52
29:BP:112:LEU:HD13	29:BP:114:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BS:66:ALA:HA	32:BS:69:VAL:HG12	1.91	0.52
2:AV:10:G:H2'	2:AV:11:C:C6	2.43	0.52
25:BA:657:U:H2'	25:BA:658:C:C6	2.45	0.52
25:BA:1858:G:H8	25:BA:1858:G:OP2	1.92	0.52
25:BA:2096:U:OP1	25:BA:2096:U:H4'	2.09	0.52
25:BA:2306:C:H5	25:BA:2307:G:H1'	1.71	0.52
38:BY:42:VAL:CG1	38:BY:65:ALA:HB3	2.39	0.52
52:BE:1:MET:HG3	52:BE:83:ASP:HB2	1.92	0.52
1:AA:104:G:N7	14:AT:14:LYS:NZ	2.57	0.52
1:AA:427:U:OP2	17:AD:36:ARG:NH2	2.42	0.52
1:AA:539:A:H2'	1:AA:540:G:C8	2.44	0.52
1:AA:706:A:H2'	5:AK:31:THR:HG21	1.91	0.52
1:AA:986:A:C2	1:AA:1220:G:C2	2.98	0.52
16:AC:134:ILE:CG2	16:AC:168:ALA:HB3	2.39	0.52
25:BA:612:C:H2'	25:BA:613:G:H5"	1.91	0.52
25:BA:715:G:H2'	25:BA:716:A:O4'	2.08	0.52
25:BA:2305:A:H5"	54:BG:134:GLY:HA3	1.89	0.52
25:BA:2556:C:H2'	25:BA:2557:G:O4'	2.09	0.52
33:BT:24:PRO:HA	33:BT:49:VAL:O	2.08	0.52
37:BX:40:LYS:HG3	37:BX:51:VAL:HB	1.91	0.52
43:BD:83:GLU:OE1	43:BD:104:TYR:OH	2.27	0.52
52:BE:24:THR:CG2	52:BE:187:ALA:H	2.22	0.52
52:BE:117:MET:O	52:BE:118:LYS:CB	2.56	0.52
17:AD:28:SER:O	17:AD:30:LYS:N	2.36	0.52
25:BA:247:G:H4'	25:BA:386:G:C6	2.45	0.52
25:BA:889:C:H1'	25:BA:890:A:O4'	2.10	0.52
25:BA:1332:G:H5'	25:BA:1332:G:C8	2.44	0.52
25:BA:2111:C:H42	25:BA:2147:G:H1	1.56	0.52
25:BA:2492:U:H2'	25:BA:2493:U:H6	1.75	0.52
27:BN:3:THR:C	27:BN:5:VAL:H	2.13	0.52
29:BP:13:ASN:OD1	53:BF:31:HIS:HB2	2.09	0.52
29:BP:59:LEU:HA	29:BP:61:ARG:CZ	2.39	0.52
30:BQ:21:THR:HG23	30:BQ:101:ARG:HB2	1.90	0.52
33:BT:82:LEU:N	33:BT:82:LEU:HD12	2.24	0.52
52:BE:47:VAL:HG13	52:BE:47:VAL:O	2.09	0.52
52:BE:55:ASN:O	52:BE:57:LYS:N	2.41	0.52
25:BA:652:C:C6	25:BA:652:C:OP2	2.62	0.52
25:BA:771:G:OP1	48:B7:10:ARG:NH1	2.42	0.52
25:BA:1506:C:O2	25:BA:1506:C:H2'	2.08	0.52
29:BP:51:PHE:HB3	29:BP:52:GLU:CG	2.39	0.52
43:BD:30:GLU:HB2	43:BD:35:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BG:5:VAL:HG12	54:BG:6:ALA:H	1.74	0.52
55:BH:6:ARG:CB	55:BH:65:HIS:NE2	2.73	0.52
56:BK:121:GLU:CD	56:BK:121:GLU:H	2.12	0.52
12:AR:25:THR:HG22	12:AR:26:LEU:HG	1.92	0.52
15:AB:80:ILE:HD11	15:AB:208:ILE:HG23	1.92	0.52
15:AB:146:GLN:O	15:AB:150:SER:OG	2.27	0.52
16:AC:73:PRO:HB3	16:AC:103:VAL:HG11	1.91	0.52
25:BA:528:A:H2	25:BA:2043:C:H5'	1.74	0.52
25:BA:1403:C:H5"	25:BA:1471:A:C1'	2.40	0.52
25:BA:2415:G:H4'	29:BP:67:MET:N	2.24	0.52
37:BX:35:THR:O	37:BX:39:ILE:HG13	2.10	0.52
49:B8:6:THR:HB	49:B8:63:PRO:HG3	1.91	0.52
52:BE:2:LYS:HA	52:BE:84:PHE:CD2	2.44	0.52
39:BZ:24:LEU:CD2	39:BZ:25:PRO:O	2.57	0.52
47:B6:18:ARG:HG3	47:B6:19:ARG:N	2.25	0.52
49:B8:50:LEU:O	49:B8:51:ALA:CB	2.58	0.52
50:B9:10:ILE:HB	50:B9:32:HIS:CD2	2.44	0.52
55:BH:85:LYS:HE3	55:BH:145:ALA:HB1	1.92	0.52
1:AA:187:C:O2'	14:AT:89:ARG:NH2	2.40	0.52
18:AE:12:LEU:HB3	18:AE:31:LEU:HB2	1.92	0.52
20:AG:23:VAL:HG13	20:AG:43:PHE:CE2	2.45	0.52
25:BA:1771:C:H1'	25:BA:1786:A:C8	2.44	0.52
25:BA:2141:G:H2'	25:BA:2142:C:C6	2.45	0.52
25:BA:2164:C:O2	25:BA:2164:C:O4'	2.25	0.52
25:BA:2611:U:H6	25:BA:2611:U:C5'	2.18	0.52
32:BS:42:ASP:O	32:BS:43:GLU:HB2	2.10	0.52
32:BS:88:ASP:OD2	32:BS:89:ARG:N	2.42	0.52
43:BD:24:ILE:O	43:BD:26:LYS:HB3	2.09	0.52
56:BK:41:PHE:CE1	56:BK:45:THR:HG21	2.45	0.52
1:AA:1074:G:O2'	1:AA:1101:A:N1	2.39	0.52
1:AA:1080:A:H5"	18:AE:16:THR:HG21	1.92	0.52
1:AA:1309:G:OP1	7:AM:88:ARG:NH1	2.42	0.52
15:AB:109:SER:C	15:AB:111:ARG:H	2.12	0.52
25:BA:301:G:C4	25:BA:302:C:C5	2.98	0.52
25:BA:613:G:C5'	25:BA:613:G:C8	2.93	0.52
25:BA:2063:C:O2	25:BA:2450:A:N1	2.43	0.52
25:BA:2619:C:OP1	52:BE:152:LYS:NZ	2.39	0.52
33:BT:93:ARG:HH11	33:BT:93:ARG:CG	2.23	0.52
39:BZ:108:PRO:HA	39:BZ:142:SER:HA	1.91	0.52
57:BJ:21:ALA:H	57:BJ:88:ALA:HB1	1.73	0.52
1:AA:1020:U:H2'	1:AA:1021:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:84:A:N1	25:BA:98:G:O2'	2.35	0.52
25:BA:195:A:H61	25:BA:198:C:H3'	1.75	0.52
25:BA:636:G:N7	29:BP:113:LYS:NZ	2.54	0.52
25:BA:807:U:OP2	29:BP:39:LYS:CG	2.51	0.52
25:BA:1170:G:N2	25:BA:1180:C:N3	2.58	0.52
25:BA:1963:U:H4'	25:BA:1964:G:OP1	2.10	0.52
25:BA:2262:U:H4'	25:BA:2328:A:C2	2.45	0.52
29:BP:130:PHE:CB	29:BP:135:LEU:HD23	2.39	0.52
31:BR:55:ALA:HB2	31:BR:79:LEU:HD13	1.91	0.52
39:BZ:153:SER:HA	39:BZ:155:LEU:HD23	1.91	0.52
49:B8:61:LEU:HD23	49:B8:61:LEU:H	1.75	0.52
18:AE:91:LEU:HG	18:AE:118:ILE:HD11	1.92	0.51
23:AY:493:VAL:HG23	23:AY:512:ILE:CD1	2.40	0.51
25:BA:1430:C:H2'	25:BA:1431:U:C6	2.45	0.51
25:BA:2518:A:H5'	25:BA:2518:A:C8	2.44	0.51
43:BD:166:GLN:HB2	43:BD:174:ILE:HG22	1.91	0.51
56:BK:58:THR:O	56:BK:66:THR:HG22	2.09	0.51
56:BK:99:ILE:HG23	56:BK:103:GLN:CB	2.39	0.51
1:AA:757:U:H2'	1:AA:758:G:O4'	2.10	0.51
1:AA:992:U:H4'	1:AA:993:G:O5'	2.09	0.51
1:AA:1531:A:O3'	1:AA:1532:U:H6	1.92	0.51
15:AB:97:TRP:CH2	15:AB:176:GLU:CD	2.83	0.51
17:AD:36:ARG:HG2	17:AD:36:ARG:HH11	1.75	0.51
25:BA:271(O):C:O2'	25:BA:271(P):C:P	2.68	0.51
25:BA:1296:G:OP1	25:BA:2709:G:O2'	2.23	0.51
25:BA:1299:G:H5'	25:BA:1301:A:O4'	2.10	0.51
25:BA:2261:C:O2'	25:BA:2262:U:H5'	2.10	0.51
32:BS:59:LYS:HB3	32:BS:65:VAL:HG22	1.92	0.51
33:BT:32:TYR:HD2	33:BT:81:PRO:O	1.92	0.51
43:BD:44:ASN:HB2	43:BD:49:ILE:HA	1.90	0.51
43:BD:77:ALA:HB2	43:BD:97:TYR:CE2	2.44	0.51
52:BE:75:VAL:O	52:BE:77:ILE:N	2.43	0.51
55:BH:19:VAL:HG11	55:BH:44:VAL:HA	1.93	0.51
1:AA:633:G:H5"	1:AA:633:G:C8	2.43	0.51
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.56	0.51
5:AK:82:VAL:O	5:AK:109:VAL:HG23	2.10	0.51
11:AQ:40:LYS:HD3	11:AQ:42:TYR:CZ	2.46	0.51
22:AI:16:ARG:HB2	22:AI:64:THR:HG22	1.92	0.51
23:AY:603:GLU:HG2	23:AY:679:VAL:HG13	1.92	0.51
25:BA:614:U:O2	25:BA:614:U:O4'	2.25	0.51
25:BA:1156:A:OP1	34:BU:55:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1385:G:H4'	25:BA:1386:C:OP1	2.10	0.51
25:BA:2179:C:HO2'	25:BA:2180:U:P	2.32	0.51
25:BA:2469:A:H2	25:BA:2481:G:H21	1.58	0.51
25:BA:2579:C:H2'	25:BA:2580:U:O4'	2.11	0.51
28:BO:64:ARG:HG2	28:BO:79:PHE:CG	2.45	0.51
33:BT:45:PHE:CE2	33:BT:63:VAL:HG12	2.45	0.51
1:AA:552:U:H4'	6:AL:86:ARG:HG2	1.93	0.51
1:AA:939:G:C6	1:AA:940:C:N4	2.78	0.51
1:AA:1140:C:C2	1:AA:1141:C:C5	2.98	0.51
15:AB:211:ILE:HG23	15:AB:215:LEU:HD23	1.92	0.51
23:AY:211:GLU:O	23:AY:215:LYS:HB2	2.10	0.51
25:BA:958:U:O2	26:BB:90:A:H4'	2.11	0.51
25:BA:1847:A:C5'	25:BA:1848:A:OP2	2.59	0.51
25:BA:2116:G:H3'	25:BA:2117:A:C8	2.45	0.51
25:BA:2391:G:OP1	49:B8:32:LEU:HD12	2.11	0.51
26:BB:78:A:C2	26:BB:100:A:C4	2.98	0.51
43:BD:43:ARG:HB2	43:BD:54:ARG:HB2	1.91	0.51
49:B8:50:LEU:O	49:B8:51:ALA:HB3	2.10	0.51
53:BF:64:ILE:HD12	53:BF:64:ILE:O	2.11	0.51
56:BK:112:MET:CE	56:BK:120:LEU:HD21	2.41	0.51
1:AA:680:C:O2'	43:BD:166:GLN:CG	2.59	0.51
1:AA:1371:G:C5	1:AA:1372:U:C5	2.99	0.51
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.46	0.51
2:AV:72:C:C6	2:AV:72:C:C3'	2.94	0.51
15:AB:166:ASP:HB3	15:AB:169:LYS:HB3	1.93	0.51
25:BA:285:C:O2'	25:BA:286:C:H5'	2.09	0.51
25:BA:479:A:H4'	25:BA:480:A:OP1	2.11	0.51
25:BA:1021:A:H3'	25:BA:1021:A:C8	2.45	0.51
25:BA:1447:G:HO2'	25:BA:1544:A:H8	0.69	0.51
25:BA:1478:G:O2'	25:BA:1558:A:N1	2.43	0.51
25:BA:1789:A:C2'	25:BA:1790:C:H5'	2.39	0.51
25:BA:2822:G:OP2	52:BE:110:GLY:O	2.28	0.51
26:BB:40:U:H3'	26:BB:41:U:C5'	2.41	0.51
26:BB:117:G:H5'	32:BS:55:ALA:HB1	1.92	0.51
42:B2:9:GLN:NE2	42:B2:56:GLN:HG2	2.26	0.51
53:BF:101:LEU:O	53:BF:106:ARG:NH1	2.36	0.51
56:BK:77:LEU:HD13	56:BK:110:GLN:OE1	2.11	0.51
1:AA:438:G:O2'	1:AA:494:U:O4	2.24	0.51
1:AA:685:G:O2'	1:AA:686:U:H5'	2.10	0.51
1:AA:1293:G:H8	1:AA:1293:G:C5'	2.22	0.51
25:BA:566:U:H2'	25:BA:567:A:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1039:G:C2'	25:BA:1040:C:H5'	2.41	0.51
25:BA:2136:C:N3	25:BA:2137:C:H5	2.07	0.51
25:BA:2199:A:H3'	25:BA:2200:C:H6	1.76	0.51
28:BO:64:ARG:HG2	28:BO:79:PHE:CD2	2.46	0.51
31:BR:113:LEU:HD23	31:BR:113:LEU:C	2.31	0.51
33:BT:28:VAL:O	33:BT:29:ARG:HB2	2.10	0.51
55:BH:148:ILE:O	55:BH:162:ILE:HD11	2.11	0.51
1:AA:1269:A:H5"	1:AA:1270:C:OP2	2.10	0.51
10:AP:20:VAL:HG21	10:AP:32:TYR:CE1	2.45	0.51
25:BA:221:A:H2'	25:BA:266:G:N7	2.26	0.51
25:BA:832:G:O2'	29:BP:52:GLU:HB3	2.11	0.51
25:BA:1281:G:C8	25:BA:1281:G:H5"	2.45	0.51
25:BA:2098:U:O2'	25:BA:2099:U:OP2	2.22	0.51
25:BA:2887:U:H2'	25:BA:2888:C:C6	2.46	0.51
28:BO:77:ILE:CD1	33:BT:74:ARG:HD3	2.41	0.51
38:BY:98:VAL:O	38:BY:98:VAL:CG1	2.58	0.51
39:BZ:124:ILE:HD13	39:BZ:155:LEU:HD11	1.91	0.51
39:BZ:151:HIS:HA	39:BZ:171:ILE:HG12	1.93	0.51
51:BC:66:HIS:CD2	51:BC:184:LYS:CG	2.94	0.51
5:AK:48:ILE:HD13	5:AK:48:ILE:N	2.26	0.51
6:AL:18:VAL:HG23	6:AL:19:ARG:N	2.26	0.51
7:AM:52:GLU:O	7:AM:56:LEU:HB2	2.11	0.51
9:AO:54:ARG:O	9:AO:58:MET:HG3	2.10	0.51
17:AD:61:LYS:HA	17:AD:203:VAL:HG22	1.92	0.51
25:BA:528:A:C2	25:BA:2043:C:H5'	2.46	0.51
25:BA:1046:A:C8	57:BJ:5:ALA:HB3	2.45	0.51
25:BA:1126:A:H8	25:BA:1126:A:OP1	1.93	0.51
25:BA:1281:G:H5"	25:BA:1281:G:H8	1.76	0.51
25:BA:1678:G:H22	25:BA:1989:G:H22	1.59	0.51
25:BA:2586:C:H6	25:BA:2586:C:O5'	1.93	0.51
28:BO:68:GLU:H	28:BO:68:GLU:CD	2.13	0.51
29:BP:57:THR:HB	29:BP:59:LEU:N	2.26	0.51
33:BT:28:VAL:HG22	33:BT:46:GLU:HA	1.93	0.51
33:BT:58:ASN:C	33:BT:58:ASN:HD22	2.14	0.51
41:B1:3:LYS:HB3	41:B1:61:ARG:NH2	2.26	0.51
47:B6:20:ASN:CG	47:B6:21:TYR:H	2.13	0.51
1:AA:1285:A:H4'	1:AA:1286:A:O5'	2.11	0.51
1:AA:1347:G:OP2	22:AI:107:ARG:HG2	2.10	0.51
5:AK:40:ILE:HG23	5:AK:75:TYR:CD2	2.46	0.51
15:AB:7:VAL:O	15:AB:11:LEU:HD12	2.10	0.51
15:AB:168:THR:CG2	15:AB:192:SER:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:319:C:H2'	25:BA:320:A:O5'	2.11	0.51
25:BA:806:C:OP1	29:BP:39:LYS:HB3	2.11	0.51
25:BA:1187:G:H8	25:BA:1187:G:O5'	1.92	0.51
25:BA:2312:U:H4'	54:BG:71:THR:CG2	2.40	0.51
25:BA:2387:U:OP1	40:B0:55:ARG:NH2	2.44	0.51
26:BB:75:G:H5"	26:BB:76:G:OP2	2.11	0.51
28:BO:115:VAL:HG13	28:BO:121:VAL:HG21	1.93	0.51
38:BY:39:VAL:O	38:BY:40:GLU:OE1	2.29	0.51
47:B6:19:ARG:CG	47:B6:20:ASN:N	2.70	0.51
1:AA:1532:U:H3'	1:AA:1533:C:H5"	1.92	0.51
9:AO:54:ARG:HG2	9:AO:58:MET:HE2	1.93	0.51
23:AY:204:GLU:C	23:AY:206:LEU:H	2.14	0.51
25:BA:537:C:H4'	27:BN:3:THR:HG21	1.92	0.51
25:BA:1210:A:C5'	25:BA:1210:A:C8	2.94	0.51
25:BA:1464:C:HO2'	25:BA:1528:A:H8	1.56	0.51
25:BA:2134:A:H8	25:BA:2159:G:HO2'	1.57	0.51
29:BP:18:ARG:HB3	29:BP:18:ARG:CZ	2.41	0.51
41:B1:82:LEU:O	41:B1:83:GLU:OE1	2.29	0.51
1:AA:148:G:O2'	1:AA:149:A:H5'	2.11	0.50
1:AA:1015:A:H2'	1:AA:1016:A:C8	2.46	0.50
1:AA:1135:U:O2	1:AA:1135:U:H2'	2.10	0.50
1:AA:1436:U:OP1	14:AT:23:ARG:NH2	2.43	0.50
4:AJ:85:LEU:C	4:AJ:87:THR:H	2.14	0.50
12:AR:32:ARG:HD2	12:AR:65:ILE:CG2	2.42	0.50
23:AY:180:VAL:O	23:AY:182:ARG:N	2.44	0.50
23:AY:342:TYR:CE1	23:AY:347:GLY:HA2	2.46	0.50
25:BA:857:C:N4	25:BA:858:U:O4	2.44	0.50
25:BA:2678:C:H2'	25:BA:2679:A:O4'	2.11	0.50
27:BN:56:ASN:O	27:BN:57:ALA:O	2.29	0.50
31:BR:83:ILE:O	31:BR:86:ARG:HB2	2.12	0.50
32:BS:34:HIS:HB3	32:BS:53:SER:HB3	1.93	0.50
33:BT:28:VAL:CG2	33:BT:46:GLU:HG3	2.41	0.50
38:BY:8:LYS:HE2	38:BY:72:VAL:O	2.10	0.50
56:BK:71:THR:HB	56:BK:72:PRO:HD2	1.92	0.50
1:AA:1293:G:C5'	1:AA:1293:G:C8	2.95	0.50
1:AA:1352:C:O2	1:AA:1371:G:C2	2.64	0.50
2:AV:27:G:N1	2:AV:43:C:H5	2.00	0.50
23:AY:377:VAL:CG2	23:AY:380:LEU:HD22	2.41	0.50
25:BA:285:C:H2'	25:BA:286:C:H6	1.75	0.50
25:BA:1025:G:C4	25:BA:1135:C:H1'	2.47	0.50
25:BA:1054:A:H4'	25:BA:1054:A:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1477:A:C2	25:BA:1515:G:C2	3.00	0.50
25:BA:2137:C:H5'	25:BA:2138:C:OP2	2.11	0.50
25:BA:2252:G:O6	40:B0:4:LYS:HB3	2.10	0.50
40:B0:43:THR:O	40:B0:43:THR:CG2	2.57	0.50
1:AA:310:G:H5"	10:AP:31:LYS:HB2	1.93	0.50
1:AA:706:A:C1'	5:AK:29:ILE:HD11	2.39	0.50
1:AA:1125:U:O2'	1:AA:1126:U:OP2	2.20	0.50
1:AA:1187:G:H5"	1:AA:1187:G:H8	1.76	0.50
1:AA:1212:U:C6	1:AA:1212:U:H5'	2.46	0.50
15:AB:15:VAL:H	15:AB:16:HIS:CD2	2.30	0.50
25:BA:628:G:H4'	25:BA:651:G:O2'	2.10	0.50
25:BA:686:G:C4	48:B7:11:LYS:HG2	2.47	0.50
25:BA:813:U:O2'	25:BA:1225:G:H1'	2.10	0.50
25:BA:1048:A:C4'	25:BA:1049:C:OP1	2.57	0.50
25:BA:1449:A:H5"	25:BA:1449:A:H8	1.75	0.50
25:BA:1709:U:H2'	25:BA:1710:C:C6	2.47	0.50
25:BA:2331:G:C4'	40:B0:42:GLY:HA3	2.42	0.50
26:BB:40:U:C2	26:BB:43:C:OP2	2.63	0.50
33:BT:91:ARG:O	33:BT:117:ASP:HB2	2.11	0.50
37:BX:27:THR:HB	37:BX:80:ILE:HB	1.94	0.50
47:B6:18:ARG:CG	47:B6:19:ARG:N	2.74	0.50
52:BE:67:PHE:O	52:BE:70:ALA:N	2.44	0.50
55:BH:64:LEU:O	55:BH:68:THR:OG1	2.18	0.50
55:BH:83:TYR:HB3	55:BH:134:SER:CA	2.41	0.50
2:AV:52:G:C2	2:AV:63:G:C2	2.99	0.50
25:BA:590:A:OP1	53:BF:95:ARG:NH1	2.44	0.50
25:BA:848:G:H2'	25:BA:849:A:C8	2.46	0.50
25:BA:1817:G:H2'	25:BA:1818:U:H5'	1.93	0.50
33:BT:3:ARG:HG3	33:BT:6:LEU:CB	2.40	0.50
48:B7:43:THR:O	48:B7:44:PRO:C	2.49	0.50
21:AH:114:THR:HG21	21:AH:119:LEU:HD12	1.94	0.50
22:AI:47:LEU:C	22:AI:49:PRO:HD2	2.32	0.50
25:BA:336:C:H5"	38:BY:7:VAL:HG21	1.94	0.50
25:BA:1504:C:O2'	25:BA:1505:C:O5'	2.30	0.50
25:BA:1858:G:HO2'	25:BA:1883:G:N2	2.08	0.50
25:BA:2121:G:H2'	25:BA:2122:U:C6	2.47	0.50
25:BA:2420:C:OP1	49:B8:34:TRP:HB2	2.11	0.50
29:BP:17:LYS:O	29:BP:19:VAL:HG22	2.12	0.50
33:BT:106:SER:O	33:BT:107:ASP:CG	2.50	0.50
35:BV:39:LEU:HB3	35:BV:47:VAL:HG21	1.93	0.50
53:BF:138:GLU:O	53:BF:141:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BG:81:LYS:O	54:BG:82:LEU:O	2.28	0.50
1:AA:979:C:H3'	1:AA:980:C:H5'	1.94	0.50
1:AA:1060:C:C5	16:AC:2:GLY:HA2	2.46	0.50
1:AA:1302:U:C5	7:AM:17:VAL:HG21	2.46	0.50
1:AA:1531:A:H2'	1:AA:1532:U:C5	2.46	0.50
17:AD:7:PRO:HB2	17:AD:10:ARG:HD2	1.93	0.50
25:BA:910:A:C6	25:BA:911:A:C6	2.99	0.50
25:BA:1260:G:H2'	25:BA:1261:C:O4'	2.12	0.50
25:BA:2355:C:H4'	40:B0:36:ILE:HD11	1.94	0.50
30:BQ:78:PRO:HG2	30:BQ:81:VAL:HG11	1.92	0.50
51:BC:77:ILE:HG22	51:BC:119:VAL:HG21	1.94	0.50
1:AA:63:C:C5'	1:AA:63:C:H6	2.24	0.50
1:AA:160:A:H2'	1:AA:161:A:O4'	2.12	0.50
1:AA:530:G:H3'	1:AA:531:U:C5'	2.41	0.50
1:AA:630:G:H5"	1:AA:630:G:H8	1.74	0.50
1:AA:738:C:OP1	19:AF:2:ARG:NH1	2.45	0.50
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.47	0.50
2:AV:4:C:O2'	25:BA:1850:G:H4'	2.12	0.50
13:AS:31:ILE:O	13:AS:31:ILE:HG23	2.11	0.50
23:AY:138:LYS:HE2	60:AY:702:GCP:C4	2.42	0.50
25:BA:1241:A:C2'	25:BA:1242:A:O5'	2.60	0.50
25:BA:1721:G:N1	25:BA:1739:U:OP2	2.45	0.50
25:BA:1901:A:OP2	25:BA:1901:A:H4'	2.12	0.50
25:BA:2206:G:N3	25:BA:2206:G:H3'	2.27	0.50
33:BT:55:ASN:O	33:BT:57:PHE:O	2.29	0.50
40:B0:11:ARG:O	40:B0:14:ARG:NH2	2.45	0.50
42:B2:39:ALA:HA	42:B2:45:SER:HB3	1.94	0.50
58:BL:113:UNK:HA	58:BL:117:UNK:O	2.12	0.50
1:AA:583:A:H2'	1:AA:584:G:O4'	2.12	0.50
1:AA:1138:G:OP1	1:AA:1140:C:C1'	2.60	0.50
1:AA:1269:A:C2	1:AA:1313:U:O4'	2.64	0.50
1:AA:1351:U:O4'	20:AG:33:ASP:HB3	2.11	0.50
6:AL:90:VAL:O	6:AL:92:ASP:N	2.41	0.50
16:AC:42:LEU:HD22	16:AC:94:LEU:HD23	1.93	0.50
25:BA:1658:C:OP1	52:BE:132:HIS:ND1	2.44	0.50
25:BA:2136:C:N3	25:BA:2137:C:C5	2.80	0.50
25:BA:2789:C:OP1	25:BA:2789:C:H4'	2.12	0.50
29:BP:130:PHE:CG	29:BP:135:LEU:HD23	2.46	0.50
30:BQ:14:ARG:HG2	30:BQ:41:TRP:HH2	1.77	0.50
38:BY:96:ILE:HG21	38:BY:99:CYS:SG	2.51	0.50
1:AA:961:U:OP2	1:AA:1223:C:H1'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1037:C:C4	1:AA:1038:C:N4	2.80	0.50
1:AA:1143:G:H8	1:AA:1143:G:O5'	1.94	0.50
8:AN:15:LYS:O	8:AN:16:PHE:O	2.30	0.50
14:AT:89:ARG:CZ	14:AT:104:LEU:HD21	2.42	0.50
25:BA:7:G:H2'	25:BA:8:A:O4'	2.11	0.50
25:BA:316:C:H2'	25:BA:317:G:O5'	2.11	0.50
25:BA:1058:G:H5"	25:BA:1058:G:H8	1.75	0.50
25:BA:1418:G:H8	25:BA:1418:G:O5'	1.95	0.50
25:BA:1615:C:C2	36:BW:87:PRO:HG2	2.47	0.50
25:BA:2824:C:H2'	25:BA:2825:C:O4'	2.12	0.50
26:BB:13:A:N1	26:BB:69:G:O2'	2.39	0.50
27:BN:131:GLN:HE22	27:BN:134:ARG:HH21	1.59	0.50
38:BY:13:VAL:HG13	38:BY:72:VAL:HB	1.94	0.50
51:BC:65:PRO:O	51:BC:188:ASN:OD1	2.30	0.50
51:BC:180:PHE:C	51:BC:181:PRO:O	2.50	0.50
53:BF:18:ARG:NH2	53:BF:20:LEU:HD12	2.27	0.50
56:BK:134:MET:HG3	56:BK:136:VAL:HG12	1.94	0.50
1:AA:1147:C:O2	22:AI:16:ARG:NH1	2.44	0.49
1:AA:1367:C:OP2	22:AI:112:LYS:NZ	2.45	0.49
25:BA:94:C:H5'	25:BA:94(A):G:OP2	2.11	0.49
25:BA:467:G:OP1	48:B7:33:ARG:NH1	2.44	0.49
25:BA:2821:A:OP2	52:BE:110:GLY:O	2.30	0.49
26:BB:12:C:O2'	40:B0:74:ARG:HG2	2.12	0.49
26:BB:77:U:P	39:BZ:19:ARG:NH2	2.85	0.49
35:BV:19:LYS:HG3	35:BV:20:LEU:C	2.32	0.49
35:BV:47:VAL:HB	35:BV:49:THR:O	2.12	0.49
49:B8:50:LEU:HA	49:B8:53:PRO:HD3	1.94	0.49
52:BE:132:HIS:CD2	52:BE:135:HIS:NE2	2.80	0.49
53:BF:53:THR:HB	53:BF:56:GLU:OE2	2.12	0.49
55:BH:89:ILE:HD13	55:BH:94:TYR:CB	2.42	0.49
55:BH:89:ILE:HD13	55:BH:94:TYR:HB3	1.93	0.49
1:AA:1263:C:C2	1:AA:1273:G:N2	2.81	0.49
23:AY:162:VAL:CG2	23:AY:255:ILE:HG12	2.41	0.49
25:BA:664:C:H4'	25:BA:941:A:OP1	2.11	0.49
25:BA:907:U:OP1	30:BQ:24:GLY:N	2.42	0.49
25:BA:2814:C:O2'	46:B5:29:THR:HG21	2.12	0.49
26:BB:81:G:O6	26:BB:96:U:C2	2.66	0.49
31:BR:2:ARG:NE	52:BE:111:ARG:HA	2.27	0.49
35:BV:69:LYS:HA	35:BV:87:HIS:O	2.12	0.49
42:B2:38:GLN:CD	42:B2:44:LEU:HD13	2.33	0.49
43:BD:32:SER:O	43:BD:36:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1293:G:H5"	1:AA:1293:G:C8	2.44	0.49
4:AJ:54:PHE:CZ	4:AJ:55:LYS:HE3	2.47	0.49
7:AM:40:ASN:HB3	7:AM:43:THR:HG23	1.93	0.49
7:AM:87:TYR:O	7:AM:91:ARG:HG2	2.12	0.49
15:AB:32:ILE:HD11	15:AB:40:HIS:CG	2.47	0.49
15:AB:167:PRO:HG3	15:AB:188:ALA:HB2	1.94	0.49
15:AB:211:ILE:CG2	15:AB:215:LEU:HD23	2.43	0.49
20:AG:116:ALA:O	20:AG:120:ILE:HD12	2.12	0.49
23:AY:98:MET:HA	23:AY:98:MET:CE	2.42	0.49
25:BA:1204:A:N1	25:BA:1241:A:N1	2.61	0.49
25:BA:2420:C:OP1	49:B8:34:TRP:CB	2.60	0.49
26:BB:4:C:H2'	26:BB:5:C:O4'	2.11	0.49
33:BT:83:ILE:HG13	33:BT:84:GLN:H	1.76	0.49
45:B4:62:CYS:C	45:B4:64:LYS:H	2.14	0.49
1:AA:1173:G:H2'	1:AA:1174:G:O4'	2.11	0.49
1:AA:1541:U:H2'	1:AA:1542:U:H4'	1.94	0.49
15:AB:17:PHE:CB	15:AB:44:LEU:HD21	2.42	0.49
15:AB:165:VAL:HG23	15:AB:166:ASP:N	2.27	0.49
18:AE:32:VAL:HB	18:AE:58:ALA:HB1	1.93	0.49
23:AY:546:ILE:HG12	23:AY:590:ILE:HG13	1.95	0.49
25:BA:1644:C:H2'	25:BA:1645:G:H5'	1.94	0.49
25:BA:2291:U:OP1	25:BA:2381:C:H5'	2.13	0.49
25:BA:2334:G:N3	32:BS:18:ILE:HD12	2.27	0.49
25:BA:2787:C:H1'	52:BE:61:ARG:HD3	1.94	0.49
26:BB:1:U:O2	26:BB:1:U:C2'	2.61	0.49
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.12	0.49
13:AS:19:VAL:O	13:AS:22:LEU:HB2	2.13	0.49
15:AB:33:TYR:HB2	15:AB:43:ASP:HB2	1.94	0.49
25:BA:582:G:H2'	25:BA:583:G:C8	2.48	0.49
25:BA:2165:G:H2'	25:BA:2166:G:C5'	2.42	0.49
25:BA:2285:C:OP2	47:B6:27:LYS:HB3	2.12	0.49
25:BA:2441:C:OP2	25:BA:2586:C:O2'	2.29	0.49
33:BT:28:VAL:O	33:BT:29:ARG:CG	2.60	0.49
38:BY:77:PRO:O	38:BY:78:ALA:CB	2.61	0.49
52:BE:46:ALA:HA	52:BE:82:ARG:O	2.13	0.49
53:BF:103:LYS:HA	53:BF:106:ARG:HG3	1.94	0.49
1:AA:706:A:C4'	5:AK:29:ILE:HD11	2.41	0.49
15:AB:165:VAL:O	15:AB:187:LEU:O	2.30	0.49
25:BA:1058:G:OP1	25:BA:1058:G:H4'	2.11	0.49
43:BD:24:ILE:HD13	43:BD:25:THR:N	2.27	0.49
54:BG:4:ASP:HB2	54:BG:8:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BJ:6:ALA:O	57:BJ:7:ALA:HB3	2.13	0.49
1:AA:33:A:N3	6:AL:32:PHE:HE2	2.10	0.49
1:AA:1066:C:O2'	1:AA:1067:A:H5'	2.13	0.49
1:AA:1152:A:H2'	1:AA:1153:C:C6	2.46	0.49
13:AS:9:VAL:O	13:AS:11:VAL:N	2.45	0.49
23:AY:413:ILE:HG21	23:AY:451:ILE:HD12	1.95	0.49
25:BA:90:U:C2'	25:BA:92:A:OP2	2.55	0.49
25:BA:1150:C:H2'	25:BA:1151:G:O4'	2.13	0.49
25:BA:1299:G:H5"	25:BA:1301:A:H5"	1.94	0.49
25:BA:2151:G:H5"	25:BA:2151:G:C8	2.48	0.49
26:BB:50:G:OP1	32:BS:62:LYS:HB2	2.12	0.49
27:BN:42:TRP:O	34:BU:64:ARG:NH1	2.38	0.49
28:BO:23:ARG:HG3	28:BO:24:VAL:N	2.27	0.49
29:BP:23:PRO:O	29:BP:33:ARG:NH1	2.46	0.49
29:BP:65:ARG:O	29:BP:66:GLY:C	2.51	0.49
29:BP:66:GLY:O	29:BP:67:MET:HB3	2.12	0.49
31:BR:2:ARG:C	31:BR:3:HIS:O	2.50	0.49
31:BR:45:ARG:HA	31:BR:95:THR:HG21	1.94	0.49
32:BS:89:ARG:HG2	32:BS:92:TYR:HA	1.93	0.49
42:B2:45:SER:O	42:B2:46:GLN:CD	2.51	0.49
46:B5:50:GLY:O	46:B5:51:TYR:CB	2.60	0.49
47:B6:15:GLU:HG2	47:B6:18:ARG:HE	1.78	0.49
56:BK:17:ALA:HB3	56:BK:38:VAL:HG13	1.93	0.49
57:BJ:124:ALA:HB3	57:BJ:127:ALA:HB3	1.93	0.49
1:AA:790:A:H2'	1:AA:791:G:C8	2.47	0.49
1:AA:1118:C:H1'	1:AA:1179:A:C5	2.48	0.49
1:AA:1297:C:N3	20:AG:115:ARG:NH2	2.61	0.49
16:AC:180:ALA:O	16:AC:181:ASN:CB	2.56	0.49
17:AD:30:LYS:C	17:AD:32:ALA:N	2.64	0.49
21:AH:112:LEU:N	21:AH:112:LEU:HD23	2.27	0.49
23:AY:210:ARG:C	23:AY:212:TYR:H	2.10	0.49
25:BA:263:C:O2'	25:BA:429:A:N3	2.40	0.49
25:BA:492:A:H2'	25:BA:493:G:O4'	2.13	0.49
25:BA:570:G:C6	25:BA:2030:A:C2	3.00	0.49
25:BA:638:G:C5	25:BA:651:G:C2	3.00	0.49
25:BA:748:G:C8	36:BW:89:ALA:HB1	2.48	0.49
25:BA:1076:C:O2'	25:BA:1076:C:O2	2.31	0.49
25:BA:1451:C:N3	25:BA:1459:G:O6	2.45	0.49
25:BA:2103:C:C3'	25:BA:2104:G:H5"	2.42	0.49
25:BA:2327:A:H2'	25:BA:2328:A:C8	2.48	0.49
39:BZ:23:LYS:N	39:BZ:23:LYS:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:B1:8:SER:HB3	41:B1:66:HIS:CD2	2.48	0.49
42:B2:45:SER:O	42:B2:45:SER:OG	2.30	0.49
49:B8:50:LEU:HD12	49:B8:51:ALA:H	1.78	0.49
51:BC:138:PRO:HA	51:BC:144:THR:OG1	2.13	0.49
6:AL:60:LEU:HB2	6:AL:64:TYR:O	2.12	0.49
23:AY:129:LYS:HB3	23:AY:253:LEU:HD11	1.95	0.49
25:BA:637:A:H4'	25:BA:638:G:O5'	2.13	0.49
25:BA:674:G:O2'	53:BF:74:ARG:HD3	2.13	0.49
25:BA:1241:A:H2'	25:BA:1242:A:O5'	2.13	0.49
29:BP:62:LEU:CD1	49:B8:30:ARG:HG2	2.42	0.49
35:BV:64:HIS:CE1	35:BV:92:THR:HG22	2.47	0.49
47:B6:19:ARG:NH1	47:B6:43:CYS:SG	2.81	0.49
56:BK:57:ILE:HD12	56:BK:57:ILE:N	2.28	0.49
1:AA:59:A:C2'	1:AA:60:A:OP1	2.61	0.49
1:AA:946:A:H2'	1:AA:947:G:C8	2.48	0.49
15:AB:109:SER:C	15:AB:111:ARG:N	2.66	0.49
17:AD:32:ALA:O	17:AD:36:ARG:N	2.46	0.49
28:BO:1:MET:HE2	28:BO:32:TYR:CE2	2.47	0.49
30:BQ:42:ILE:HD13	30:BQ:97:VAL:HB	1.95	0.49
36:BW:5:ALA:CB	36:BW:50:VAL:HG23	2.43	0.49
37:BX:57:LEU:HD22	37:BX:78:LYS:HG2	1.94	0.49
49:B8:51:ALA:O	49:B8:54:GLU:HB2	2.13	0.49
52:BE:14:ILE:HD11	52:BE:173:VAL:HG11	1.94	0.49
52:BE:16:ARG:O	52:BE:18:ASP:N	2.46	0.49
52:BE:201:THR:OG1	52:BE:202:LYS:N	2.46	0.49
53:BF:185:ASP:OD1	53:BF:188:ARG:NH1	2.41	0.49
1:AA:45:U:H2'	1:AA:46:G:C8	2.47	0.48
1:AA:1226:C:OP1	13:AS:81:ARG:HD2	2.13	0.48
2:AV:56:C:H2'	2:AV:57:G:H5"	1.94	0.48
15:AB:91:PRO:HG3	15:AB:155:LEU:HB2	1.94	0.48
25:BA:1356:G:N2	25:BA:1376:C:C2	2.81	0.48
25:BA:1632:A:C5	25:BA:1633:G:C6	3.01	0.48
25:BA:1914:C:O2'	25:BA:1915:U:O4'	2.30	0.48
25:BA:2836:U:C4	25:BA:2883:A:N6	2.81	0.48
29:BP:116:GLY:H	29:BP:134:ALA:HB2	1.78	0.48
32:BS:99:LYS:C	32:BS:101:LEU:H	2.16	0.48
34:BU:9:VAL:O	34:BU:13:LYS:HE3	2.12	0.48
46:B5:52:TYR:CD1	46:B5:52:TYR:C	2.86	0.48
52:BE:132:HIS:ND1	52:BE:132:HIS:O	2.46	0.48
1:AA:791:G:C6	1:AA:792:A:N7	2.81	0.48
2:AV:43:C:H4'	2:AV:44:G:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AC:164:ARG:O	16:AC:165:THR:HB	2.13	0.48
25:BA:1379:A:H4'	25:BA:1380:G:OP2	2.13	0.48
25:BA:1584:C:O2	25:BA:1584:C:O2'	2.28	0.48
25:BA:1952:A:OP1	28:BO:42:SER:OG	2.25	0.48
25:BA:2875:C:O2'	33:BT:5:ALA:HB3	2.12	0.48
26:BB:48:A:OP1	32:BS:92:TYR:O	2.31	0.48
46:B5:4:HIS:CB	46:B5:5:PRO:HD3	2.35	0.48
1:AA:192:U:O2'	14:AT:57:ARG:HG2	2.13	0.48
16:AC:124:ILE:HG12	16:AC:130:VAL:HG22	1.95	0.48
23:AY:517:LEU:HD11	23:AY:564:LYS:HB2	1.94	0.48
25:BA:272(J):C:H2'	25:BA:274:G:OP1	2.13	0.48
25:BA:500:G:N2	25:BA:502:A:H3'	2.28	0.48
25:BA:1002:G:H2'	25:BA:1003:G:O5'	2.13	0.48
25:BA:1021:A:H3'	25:BA:1021:A:H8	1.78	0.48
25:BA:2140:C:H5	25:BA:2151:G:H1	1.61	0.48
33:BT:106:SER:O	33:BT:107:ASP:CB	2.61	0.48
37:BX:12:VAL:HG12	37:BX:29:TRP:CE2	2.48	0.48
49:B8:50:LEU:HG	49:B8:51:ALA:N	2.28	0.48
53:BF:9:ILE:O	53:BF:9:ILE:HG22	2.13	0.48
53:BF:9:ILE:HG23	53:BF:13:SER:O	2.13	0.48
1:AA:29:G:O2'	1:AA:30:U:H5'	2.13	0.48
1:AA:376:G:P	10:AP:67:THR:HG21	2.53	0.48
1:AA:714:G:H2'	1:AA:715:A:C8	2.48	0.48
1:AA:760:G:O2'	11:AQ:98:LEU:HD23	2.12	0.48
1:AA:975:A:N6	1:AA:1367:C:O4'	2.47	0.48
1:AA:1346:A:C8	20:AG:10:ARG:NH2	2.81	0.48
8:AN:41:ARG:HG2	8:AN:41:ARG:HH11	1.79	0.48
16:AC:12:LEU:HD13	16:AC:18:TRP:CE2	2.48	0.48
23:AY:301:ILE:HG22	23:AY:332:SER:HB2	1.96	0.48
25:BA:118:A:C8	25:BA:119:A:C8	3.00	0.48
25:BA:244:A:C2	25:BA:255:A:C4	3.01	0.48
25:BA:330:A:H2	25:BA:1210:A:C2'	2.17	0.48
25:BA:1224:C:O2'	35:BV:85:LYS:HA	2.13	0.48
25:BA:2114:A:H2'	25:BA:2167:U:O2'	2.13	0.48
25:BA:2262:U:OP1	25:BA:2387:U:O2'	2.23	0.48
25:BA:2467:C:H4'	30:BQ:123:HIS:CD2	2.48	0.48
25:BA:2477:C:H1'	25:BA:2481:G:O6	2.14	0.48
25:BA:2801(A):A:H4'	25:BA:2802:G:H5'	1.95	0.48
25:BA:2849:U:P	33:BT:95:ARG:HH12	2.36	0.48
47:B6:33:LYS:HE2	47:B6:33:LYS:HA	1.94	0.48
1:AA:299:G:H2'	1:AA:300:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:738:C:H5”	19:AF:69:GLU:HB2	1.95	0.48
1:AA:1061:G:OP1	4:AJ:59:SER:OG	2.23	0.48
1:AA:1132:C:N3	1:AA:1142:G:N2	2.59	0.48
1:AA:1445:C:C4	1:AA:1446:U:C4	3.01	0.48
9:AO:16:ALA:HB1	9:AO:21:ASP:HB3	1.94	0.48
16:AC:24:ALA:HB1	16:AC:28:GLN:HB2	1.95	0.48
17:AD:25:ARG:C	17:AD:27:TYR:N	2.65	0.48
21:AH:83:ILE:HG13	21:AH:137:VAL:HG22	1.95	0.48
22:AI:95:LYS:NZ	22:AI:96:LEU:HD13	2.29	0.48
25:BA:620:G:H4’	25:BA:621:A:H5”	1.95	0.48
25:BA:1380:G:C2	25:BA:1381:G:C8	3.01	0.48
25:BA:2155:G:C6	25:BA:2156:G:C4	3.01	0.48
25:BA:2272:U:H5”	25:BA:2273:A:OP1	2.14	0.48
25:BA:2600:A:O2’	25:BA:2601:C:H5’	2.13	0.48
31:BR:33:ARG:HD2	46:B5:55:ARG:HG2	1.94	0.48
58:BL:61:UNK:O	58:BL:62:UNK:CB	2.61	0.48
1:AA:149:A:O2’	1:AA:150:C:P	2.71	0.48
1:AA:389:A:C6	1:AA:390:C:H1’	2.48	0.48
1:AA:986:A:H1’	13:AS:54:GLY:O	2.13	0.48
25:BA:848:G:C4	25:BA:933:A:H8	2.32	0.48
25:BA:1278:A:H4’	31:BR:34:ILE:HD12	1.96	0.48
25:BA:1329:U:H5”	25:BA:1330:C:H5	1.78	0.48
25:BA:1332:G:C2	25:BA:1609:A:O2’	2.54	0.48
25:BA:1977:A:H2’	25:BA:1978:A:O5’	2.13	0.48
25:BA:2023:G:H4’	25:BA:2617:C:O3’	2.14	0.48
25:BA:2123:G:H2’	25:BA:2124:G:O4’	2.13	0.48
1:AA:1004:A:C8	1:AA:1036:G:O6	2.67	0.48
14:AT:75:ASN:O	14:AT:79:ARG:HB2	2.14	0.48
17:AD:23:GLY:HA3	17:AD:112:VAL:HG22	1.96	0.48
23:AY:458:HIS:O	23:AY:461:ILE:HG13	2.13	0.48
25:BA:518:G:H4’	36:BW:18:ARG:NH1	2.29	0.48
25:BA:1199:U:H2’	25:BA:1200:C:O4’	2.14	0.48
25:BA:1449:A:H5”	25:BA:1449:A:C8	2.48	0.48
25:BA:1546:C:H5”	25:BA:1546:C:H6	1.78	0.48
26:BB:13:A:OP2	40:B0:74:ARG:NH2	2.45	0.48
30:BQ:39:PRO:HA	30:BQ:97:VAL:O	2.13	0.48
38:BY:7:VAL:HB	38:BY:8:LYS:HD2	1.96	0.48
43:BD:176:ARG:HA	43:BD:182:LEU:HD23	1.95	0.48
49:B8:62:LEU:N	49:B8:63:PRO:CD	2.76	0.48
53:BF:164:ARG:HG3	53:BF:175:THR:OG1	2.14	0.48
1:AA:155:C:H2’	1:AA:156:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:345:C:H4'	1:AA:346:G:O5'	2.14	0.48
1:AA:428:G:H4'	1:AA:429:U:O5'	2.13	0.48
1:AA:460:G:C6	1:AA:470:C:C5'	2.96	0.48
1:AA:520:A:N1	1:AA:536:C:H1'	2.29	0.48
1:AA:1456:G:O4'	1:AA:1456:G:OP1	2.31	0.48
21:AH:107:LEU:N	21:AH:107:LEU:HD23	2.29	0.48
25:BA:528:A:C2	25:BA:2042:A:H2'	2.48	0.48
25:BA:819:A:H2'	25:BA:820:A:H5'	1.95	0.48
25:BA:958:U:OP2	30:BQ:14:ARG:HD3	2.12	0.48
25:BA:1528:A:H2	25:BA:1542:A:H62	1.58	0.48
25:BA:1637:A:H5'	25:BA:1760:A:O2'	2.14	0.48
25:BA:2155:G:H2'	25:BA:2156:G:O5'	2.14	0.48
25:BA:2392:A:N1	25:BA:2424:C:N3	2.61	0.48
25:BA:2649:U:H2'	25:BA:2650:U:C6	2.48	0.48
27:BN:30:ILE:HG23	27:BN:52:VAL:HG11	1.96	0.48
27:BN:67:LEU:O	27:BN:68:GLU:HB2	2.13	0.48
27:BN:93:THR:OG1	27:BN:94:HIS:CD2	2.67	0.48
33:BT:28:VAL:CG1	33:BT:46:GLU:HB2	2.44	0.48
47:B6:15:GLU:OE2	47:B6:41:PRO:CB	2.62	0.48
49:B8:23:VAL:CG1	49:B8:46:ARG:HD3	2.44	0.48
52:BE:116:VAL:O	52:BE:117:MET:HB3	2.13	0.48
53:BF:107:LYS:HD2	53:BF:205:ARG:O	2.14	0.48
1:AA:62:U:H5"	1:AA:385:C:O2'	2.13	0.48
1:AA:441:A:OP2	1:AA:441:A:H8	1.96	0.48
16:AC:174:PRO:HD2	16:AC:182:ILE:HD11	1.95	0.48
25:BA:1364:G:OP2	41:B1:61:ARG:NH2	2.45	0.48
29:BP:35:HIS:C	29:BP:36:LYS:HG3	2.33	0.48
32:BS:106:ARG:HD2	32:BS:107:GLU:O	2.14	0.48
36:BW:20:VAL:HG22	36:BW:47:VAL:HG21	1.96	0.48
52:BE:55:ASN:O	52:BE:57:LYS:HD3	2.14	0.48
52:BE:55:ASN:C	52:BE:57:LYS:H	2.16	0.48
53:BF:65:TRP:HB2	53:BF:66:PRO:CD	2.43	0.48
56:BK:105:LEU:CD2	56:BK:120:LEU:HD13	2.44	0.48
1:AA:1013:G:H22	1:AA:1015:A:H3'	1.79	0.48
5:AK:105:VAL:O	5:AK:105:VAL:HG23	2.13	0.48
20:AG:5:ARG:HB2	20:AG:5:ARG:HH11	1.77	0.48
22:AI:48:GLU:N	22:AI:49:PRO:HD2	2.28	0.48
23:AY:242:LEU:O	23:AY:245:ALA:N	2.46	0.48
25:BA:784:A:C6	43:BD:229:VAL:HG11	2.49	0.48
25:BA:1488:G:C5	25:BA:1489:U:C5	3.02	0.48
25:BA:1494:A:C2'	25:BA:1495:A:H5"	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2517:C:C6	25:BA:2542:A:C2	3.01	0.48
27:BN:66:LYS:O	27:BN:70:LYS:HB3	2.14	0.48
29:BP:146:VAL:O	29:BP:148:LEU:HG	2.14	0.48
34:BU:65:ILE:HG12	34:BU:96:ALA:HB3	1.96	0.48
38:BY:13:VAL:O	38:BY:24:VAL:HA	2.14	0.48
43:BD:27:THR:CG2	43:BD:83:GLU:OE2	2.62	0.48
52:BE:76:ARG:HA	52:BE:77:ILE:HG12	1.95	0.48
55:BH:154:PRO:HB3	55:BH:163:TYR:CZ	2.49	0.48
1:AA:881:G:P	6:AL:12:ARG:HH22	2.37	0.47
1:AA:1202:G:H1'	8:AN:29:ARG:HD2	1.96	0.47
15:AB:142:LEU:HD21	15:AB:146:GLN:OE1	2.13	0.47
15:AB:155:LEU:HD12	15:AB:157:ARG:O	2.14	0.47
16:AC:40:ARG:O	16:AC:44:GLU:HB2	2.14	0.47
17:AD:11:LEU:O	17:AD:13:ARG:O	2.32	0.47
25:BA:364:C:OP2	25:BA:365:C:OP2	2.32	0.47
25:BA:652:C:O2	25:BA:652:C:O2'	2.28	0.47
25:BA:1301:A:C8	25:BA:1303:G:C8	3.02	0.47
25:BA:2870:C:H2'	25:BA:2871:C:O4'	2.14	0.47
27:BN:115:ARG:O	27:BN:119:ARG:HG2	2.14	0.47
29:BP:17:LYS:C	29:BP:19:VAL:H	2.14	0.47
56:BK:13:PRO:HA	56:BK:52:ILE:HA	1.94	0.47
1:AA:264:U:H2'	1:AA:265:G:O4'	2.14	0.47
1:AA:731:G:H5'	1:AA:766:A:H4'	1.96	0.47
1:AA:1059:C:O3'	8:AN:45:ARG:NH2	2.47	0.47
14:AT:49:ALA:HB2	14:AT:92:LEU:HD22	1.96	0.47
15:AB:165:VAL:HG23	15:AB:166:ASP:H	1.79	0.47
25:BA:470:A:H2'	25:BA:471:A:O4'	2.14	0.47
25:BA:882:G:H2'	25:BA:883:G:C8	2.48	0.47
25:BA:883:G:N2	25:BA:893:C:O2	2.47	0.47
25:BA:1905:C:H2'	25:BA:1930:G:C8	2.49	0.47
28:BO:114:ILE:H	28:BO:114:ILE:HD12	1.79	0.47
30:BQ:27:VAL:O	30:BQ:28:ALA:CB	2.62	0.47
30:BQ:116:GLU:OE1	30:BQ:116:GLU:HA	2.13	0.47
32:BS:24:LEU:O	32:BS:85:VAL:HB	2.14	0.47
35:BV:2:PHE:O	35:BV:3:ALA:O	2.31	0.47
39:BZ:22:GLY:C	39:BZ:23:LYS:HD2	2.35	0.47
53:BF:3:GLU:O	53:BF:19:GLU:HA	2.14	0.47
53:BF:152:GLU:OE1	53:BF:191:ARG:HD2	2.15	0.47
54:BG:4:ASP:CB	54:BG:8:LYS:HG2	2.43	0.47
55:BH:173:PRO:O	55:BH:174:GLY:C	2.52	0.47
1:AA:756:C:H2'	1:AA:757:U:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AV:35:A:C5'	2:AV:35:A:H8	2.27	0.47
7:AM:54:VAL:O	7:AM:55:ARG:C	2.53	0.47
15:AB:145:LEU:HD12	15:AB:149:LEU:HD12	1.96	0.47
17:AD:134:ASP:OD2	17:AD:135:LEU:HD13	2.13	0.47
23:AY:162:VAL:HG21	23:AY:255:ILE:CG1	2.42	0.47
23:AY:401:SER:OG	23:AY:402:ILE:N	2.47	0.47
25:BA:239:U:H2'	25:BA:240:G:O4'	2.14	0.47
25:BA:714:U:H2'	25:BA:716:A:OP2	2.15	0.47
25:BA:1078:U:H4'	25:BA:1078:U:OP1	2.15	0.47
25:BA:2023:G:H5'	25:BA:2617:C:H4'	1.95	0.47
25:BA:2316:C:O2'	54:BG:128:ARG:NH2	2.47	0.47
25:BA:2876:G:O5'	33:BT:3:ARG:HB3	2.14	0.47
30:BQ:27:VAL:HG12	30:BQ:28:ALA:N	2.29	0.47
32:BS:89:ARG:O	32:BS:92:TYR:HB3	2.14	0.47
32:BS:97:ARG:HH21	32:BS:98:VAL:HA	1.79	0.47
33:BT:30:VAL:HG23	33:BT:30:VAL:O	2.14	0.47
53:BF:5:ALA:O	53:BF:6:VAL:CG2	2.62	0.47
1:AA:659:U:O2'	1:AA:660:G:H5'	2.14	0.47
1:AA:750:G:N3	9:AO:23:GLY:HA3	2.28	0.47
1:AA:1203:C:OP1	8:AN:3:ARG:HD3	2.13	0.47
18:AE:6:PHE:CE1	18:AE:66:MET:HE1	2.49	0.47
18:AE:93:PRO:HG2	21:AH:105:ARG:NH2	2.29	0.47
25:BA:71:A:H5'	25:BA:71:A:H8	1.76	0.47
25:BA:271(L):U:H4'	25:BA:271(M):G:C5	2.50	0.47
25:BA:558:G:H1'	27:BN:45:ASN:HB3	1.95	0.47
25:BA:1539:G:N2	25:BA:1540:U:C2	2.82	0.47
25:BA:1899:G:O2'	25:BA:1900:A:OP2	2.27	0.47
27:BN:47:ALA:HB2	27:BN:112:LEU:HD11	1.96	0.47
38:BY:7:VAL:HG13	38:BY:83:THR:HG21	1.97	0.47
39:BZ:51:ALA:HB1	39:BZ:57:ILE:HD11	1.95	0.47
54:BG:59:GLU:HA	54:BG:62:LEU:HD22	1.95	0.47
55:BH:6:ARG:CB	55:BH:65:HIS:CD2	2.97	0.47
55:BH:17:VAL:O	55:BH:45:VAL:HG13	2.14	0.47
1:AA:571:U:O5'	1:AA:571:U:H6	1.97	0.47
22:AI:54:ASP:O	22:AI:56:LEU:N	2.45	0.47
25:BA:9:U:O2'	25:BA:10:G:P	2.73	0.47
25:BA:285:C:H2'	25:BA:286:C:C6	2.50	0.47
25:BA:478:A:N1	25:BA:500:G:H4'	2.29	0.47
25:BA:889:C:O4'	25:BA:889:C:O2	2.29	0.47
25:BA:1429:G:H2'	25:BA:1430:C:C6	2.50	0.47
25:BA:2308:G:N7	25:BA:2310:A:H5'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2492:U:O2'	25:BA:2493:U:H5'	2.13	0.47
29:BP:146:VAL:HG13	29:BP:147:LEU:H	1.78	0.47
31:BR:34:ILE:HD13	31:BR:34:ILE:HA	1.78	0.47
32:BS:56:LEU:HD23	32:BS:56:LEU:O	2.15	0.47
43:BD:32:SER:O	43:BD:36:PRO:CD	2.62	0.47
43:BD:147:LEU:HD12	43:BD:155:LEU:HD21	1.96	0.47
52:BE:111:ARG:HD2	52:BE:160:TYR:CE1	2.50	0.47
1:AA:673:G:OP1	19:AF:87:ARG:HD3	2.15	0.47
1:AA:779:C:H2'	1:AA:780:A:O4'	2.14	0.47
1:AA:1318:A:H1'	13:AS:37:ARG:HH21	1.79	0.47
1:AA:1333:A:H2'	1:AA:1334:G:O4'	2.13	0.47
1:AA:1465:C:H2'	1:AA:1466:C:O4'	2.15	0.47
4:AJ:35:SER:OG	4:AJ:73:ASP:HB2	2.15	0.47
23:AY:250:THR:HA	23:AY:255:ILE:HG22	1.97	0.47
23:AY:319:ASP:OD1	23:AY:322:VAL:HG22	2.15	0.47
23:AY:377:VAL:HG21	23:AY:380:LEU:HD22	1.96	0.47
25:BA:71:A:OP2	25:BA:71:A:H3'	2.14	0.47
25:BA:806:C:OP2	29:BP:39:LYS:HB3	2.15	0.47
25:BA:814:C:H2'	25:BA:815:C:H6	1.79	0.47
25:BA:1406:U:H2'	25:BA:1407:C:C6	2.49	0.47
25:BA:1407:C:H5'	25:BA:1408:C:OP2	2.14	0.47
25:BA:1538:G:O2'	25:BA:1539:G:O5'	2.24	0.47
25:BA:1786:A:H2	25:BA:2606:C:H1'	1.76	0.47
25:BA:2134:A:C8	25:BA:2159:G:O2'	2.63	0.47
25:BA:2591:C:OP2	43:BD:239:ARG:HB3	2.14	0.47
33:BT:28:VAL:HG21	33:BT:46:GLU:HG3	1.97	0.47
35:BV:2:PHE:HB3	35:BV:42:GLY:HA3	1.96	0.47
36:BW:9:TYR:H	36:BW:102:HIS:HD2	1.62	0.47
36:BW:69:LEU:HA	36:BW:108:GLY:O	2.15	0.47
38:BY:2:ARG:O	38:BY:4:LYS:HG3	2.14	0.47
41:B1:29:GLY:O	41:B1:30:VAL:HG13	2.14	0.47
54:BG:18:GLU:O	54:BG:22:ARG:N	2.47	0.47
55:BH:23:ARG:C	55:BH:24:VAL:HG12	2.35	0.47
56:BK:59:ILE:HG12	56:BK:60:TYR:H	1.78	0.47
57:BJ:46:ALA:O	57:BJ:47:ALA:HB2	2.14	0.47
1:AA:148:G:C2	1:AA:175:C:C2	3.03	0.47
1:AA:264:U:O2'	11:AQ:64:PRO:O	2.32	0.47
1:AA:298:A:H2'	1:AA:299:G:O4'	2.14	0.47
1:AA:456:C:H2'	1:AA:457:C:C6	2.49	0.47
1:AA:547:A:H4'	1:AA:548:G:O5'	2.14	0.47
1:AA:590:C:OP1	21:AH:30:ARG:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:938:A:N6	1:AA:939:G:C6	2.83	0.47
1:AA:1307:U:H2'	1:AA:1308:U:O4'	2.13	0.47
1:AA:1368:G:OP2	22:AI:112:LYS:CD	2.61	0.47
5:AK:97:ALA:O	5:AK:101:SER:HB3	2.13	0.47
17:AD:81:GLU:OE1	17:AD:139:ARG:NH2	2.46	0.47
18:AE:37:ARG:C	18:AE:38:GLN:HG2	2.34	0.47
18:AE:76:ILE:O	18:AE:93:PRO:HB3	2.15	0.47
18:AE:84:PHE:HB3	18:AE:134:ALA:HB2	1.95	0.47
21:AH:38:ILE:HD11	21:AH:118:VAL:HG12	1.96	0.47
23:AY:92:ILE:O	23:AY:96:ARG:HB2	2.15	0.47
23:AY:218:GLU:O	23:AY:221:ALA:HB3	2.15	0.47
23:AY:438:PHE:CZ	23:AY:451:ILE:HG12	2.49	0.47
25:BA:129:C:H6	25:BA:129:C:H5"	1.79	0.47
25:BA:295:G:H5"	25:BA:295:G:C8	2.50	0.47
25:BA:479:A:N3	25:BA:481:G:H5"	2.30	0.47
25:BA:647:G:O5'	25:BA:647:G:H8	1.97	0.47
25:BA:1283:G:N2	25:BA:1285:G:H3'	2.30	0.47
25:BA:1653:G:H4'	25:BA:1654:A:O5'	2.15	0.47
25:BA:1809:A:H2'	25:BA:1810:A:C8	2.50	0.47
25:BA:2181:G:H2'	25:BA:2182:G:O5'	2.15	0.47
25:BA:2370:G:H2'	25:BA:2371:G:O4'	2.14	0.47
25:BA:2688:U:C5	25:BA:2720:U:OP2	2.67	0.47
25:BA:2712:U:H2'	25:BA:2712:U:O2	2.14	0.47
30:BQ:137:TYR:OH	39:BZ:81:ARG:HD3	2.15	0.47
33:BT:121:ILE:O	33:BT:124:ASP:HB2	2.14	0.47
42:B2:44:LEU:O	42:B2:45:SER:CB	2.62	0.47
43:BD:26:LYS:HG2	43:BD:81:ALA:HA	1.97	0.47
43:BD:32:SER:HA	43:BD:35:LYS:NZ	2.30	0.47
45:B4:64:LYS:C	45:B4:65:CYS:SG	2.93	0.47
47:B6:16:CYS:O	47:B6:18:ARG:CZ	2.62	0.47
49:B8:23:VAL:HA	49:B8:47:LYS:O	2.15	0.47
53:BF:129:PHE:CD2	53:BF:163:VAL:HG21	2.50	0.47
54:BG:82:LEU:HD23	54:BG:83:ARG:H	1.79	0.47
1:AA:407:G:OP1	17:AD:3:ARG:NH1	2.48	0.47
1:AA:437:U:H5"	17:AD:155:LEU:HD21	1.97	0.47
1:AA:515:G:H2'	1:AA:516:U:O4'	2.15	0.47
1:AA:712:A:H2'	1:AA:713:G:O4'	2.14	0.47
1:AA:863:U:O2'	1:AA:865:A:N7	2.33	0.47
1:AA:1152:A:H5"	4:AJ:13:HIS:CD2	2.50	0.47
1:AA:1277:C:C2'	1:AA:1279:A:H8	2.27	0.47
15:AB:238:LEU:O	15:AB:240:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AD:187:ARG:NH2	17:AD:193:ASP:OD2	2.48	0.47
19:AF:60:PHE:C	19:AF:61:LEU:HD12	2.34	0.47
23:AY:461:ILE:C	23:AY:461:ILE:HD12	2.36	0.47
25:BA:669:G:C2'	25:BA:669:G:N3	2.77	0.47
25:BA:1053:C:H2'	25:BA:1054:A:C5'	2.45	0.47
25:BA:1540:U:H2'	25:BA:1541:G:O4'	2.15	0.47
25:BA:1932:A:H2'	25:BA:1933:G:O4'	2.14	0.47
26:BB:101:G:H2'	26:BB:102:A:O4'	2.15	0.47
29:BP:61:ARG:H	29:BP:61:ARG:HD2	1.80	0.47
34:BU:91:ASP:O	34:BU:92:ARG:HB3	2.13	0.47
37:BX:55:ASN:HD22	37:BX:55:ASN:N	2.12	0.47
38:BY:20:TYR:O	38:BY:23:ARG:HB2	2.15	0.47
38:BY:74:PRO:O	38:BY:80:GLY:CA	2.60	0.47
53:BF:132:VAL:HG22	53:BF:133:ASN:H	1.80	0.47
1:AA:538:G:H2'	1:AA:539:A:H8	1.80	0.47
1:AA:997:U:O5'	1:AA:997:U:H6	1.97	0.47
1:AA:1063:C:H3'	1:AA:1064:G:H2'	1.96	0.47
1:AA:1397:C:O4'	1:AA:1397:C:O2	2.33	0.47
8:AN:25:VAL:HB	8:AN:38:GLY:O	2.15	0.47
10:AP:8:ARG:HH11	10:AP:8:ARG:CG	2.26	0.47
19:AF:69:GLU:O	19:AF:72:VAL:HG12	2.15	0.47
20:AG:116:ALA:O	20:AG:120:ILE:CD1	2.63	0.47
23:AY:380:LEU:HD21	23:AY:389:LEU:HD21	1.97	0.47
25:BA:1407:C:H5"	25:BA:1407:C:H6	1.76	0.47
25:BA:1794:U:H2'	25:BA:1795:C:C6	2.50	0.47
25:BA:1906:G:N7	25:BA:1929:G:C8	2.82	0.47
26:BB:2:C:O2	26:BB:2:C:C2'	2.62	0.47
26:BB:32:C:C2	26:BB:51:G:N2	2.83	0.47
31:BR:28:LEU:HD12	31:BR:48:VAL:HG21	1.96	0.47
32:BS:53:SER:O	32:BS:55:ALA:N	2.47	0.47
6:AL:111:LYS:O	6:AL:112:ASP:HB2	2.16	0.47
7:AM:2:ALA:N	7:AM:9:ILE:HG23	2.30	0.47
23:AY:10:LYS:O	23:AY:10:LYS:HD3	2.15	0.47
23:AY:21:ILE:HD13	25:BA:2661:G:H5'	1.97	0.47
27:BN:17:ASP:OD2	27:BN:56:ASN:ND2	2.44	0.47
33:BT:28:VAL:HG13	33:BT:46:GLU:CA	2.45	0.47
34:BU:92:ARG:O	34:BU:93:LYS:C	2.54	0.47
38:BY:30:VAL:HG12	38:BY:31:LEU:N	2.29	0.47
41:B1:68:PRO:O	41:B1:69:LYS:C	2.52	0.47
56:BK:17:ALA:CB	56:BK:38:VAL:HG22	2.43	0.47
21:AH:44:PHE:CE2	21:AH:109:ILE:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:607:U:C2	25:BA:621:A:N1	2.83	0.46
25:BA:1386:C:OP2	25:BA:1396:U:H5	1.97	0.46
25:BA:1742:G:C8	25:BA:1742:G:C3'	2.98	0.46
25:BA:1790:C:H2'	25:BA:1791:A:C5	2.50	0.46
25:BA:1865:G:C5'	25:BA:1865:G:H8	2.29	0.46
31:BR:28:LEU:O	31:BR:28:LEU:HD22	2.15	0.46
32:BS:28:VAL:HB	32:BS:89:ARG:HB2	1.97	0.46
33:BT:28:VAL:HG13	33:BT:46:GLU:HB2	1.96	0.46
34:BU:92:ARG:NH1	34:BU:94:ASN:ND2	2.61	0.46
53:BF:84:VAL:O	53:BF:86:GLY:N	2.48	0.46
53:BF:117:ARG:HA	53:BF:117:ARG:HD3	1.57	0.46
1:AA:710:G:OP1	19:AF:54:LYS:CE	2.63	0.46
1:AA:977:A:O2'	1:AA:979:C:OP2	2.26	0.46
5:AK:99:GLN:HA	5:AK:105:VAL:HG13	1.97	0.46
13:AS:50:ALA:HB1	13:AS:57:HIS:HB3	1.98	0.46
17:AD:162:LEU:HD13	17:AD:181:MET:HG2	1.97	0.46
25:BA:391:G:H1'	25:BA:411:G:O4'	2.14	0.46
25:BA:806:C:OP2	29:BP:39:LYS:HD3	2.15	0.46
25:BA:1177:A:H4'	25:BA:1178:C:C6	2.50	0.46
29:BP:7:ARG:NH1	29:BP:7:ARG:CA	2.62	0.46
32:BS:16:ASN:O	32:BS:19:LYS:CB	2.64	0.46
53:BF:65:TRP:CB	53:BF:66:PRO:CD	2.94	0.46
1:AA:162:A:H3'	1:AA:163:C:O4'	2.16	0.46
1:AA:538:G:H2'	1:AA:539:A:C8	2.49	0.46
1:AA:722:A:H3'	1:AA:722:A:N3	2.30	0.46
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.80	0.46
7:AM:56:LEU:O	7:AM:59:TYR:N	2.49	0.46
23:AY:89:ASP:HA	23:AY:454:MET:HB3	1.96	0.46
25:BA:527:C:OP2	25:BA:2779:U:H5	1.98	0.46
25:BA:1959:G:H2'	25:BA:1960:A:O5'	2.15	0.46
25:BA:2086:U:H2'	25:BA:2087:G:C8	2.49	0.46
25:BA:2291:U:O2'	25:BA:2374:C:O2	2.28	0.46
25:BA:2341:G:H2'	25:BA:2342:C:C6	2.50	0.46
27:BN:133:GLN:HG2	27:BN:134:ARG:N	2.30	0.46
35:BV:15:GLU:O	35:BV:16:PRO:C	2.53	0.46
38:BY:7:VAL:HB	38:BY:8:LYS:HE3	1.96	0.46
43:BD:58:HIS:HD2	43:BD:59:LYS:O	1.99	0.46
47:B6:39:TYR:HB3	47:B6:49:HIS:CD2	2.49	0.46
53:BF:3:GLU:HA	53:BF:24:LEU:HB3	1.96	0.46
53:BF:101:LEU:HD12	53:BF:102:PRO:HD2	1.97	0.46
1:AA:263:A:P	14:AT:79:ARG:HH11	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:629:G:H2'	1:AA:630:G:O4'	2.15	0.46
1:AA:938:A:C6	1:AA:939:G:C5	3.04	0.46
1:AA:1446:U:H4'	1:AA:1447:A:C5	2.51	0.46
1:AA:1507:A:C2	1:AA:1508:G:C4	3.03	0.46
2:AV:15:G:H8	2:AV:15:G:OP2	1.98	0.46
23:AY:684:GLN:O	23:AY:688:ILE:N	2.41	0.46
25:BA:215:G:O3'	25:BA:216:A:H4'	2.15	0.46
25:BA:250:G:H2'	25:BA:251:A:C8	2.51	0.46
25:BA:476:G:H4'	25:BA:502:A:N1	2.30	0.46
25:BA:528:A:N1	25:BA:2043:C:O5'	2.48	0.46
27:BN:132:ALA:C	27:BN:133:GLN:O	2.54	0.46
33:BT:108:ARG:HB3	33:BT:111:ARG:NH1	2.31	0.46
43:BD:68:LYS:HB2	43:BD:70:TRP:CH2	2.51	0.46
51:BC:46:LYS:NZ	51:BC:168:THR:O	2.48	0.46
51:BC:222:VAL:O	51:BC:224:ILE:HG23	2.14	0.46
1:AA:328:C:O2	1:AA:328:C:C2'	2.58	0.46
1:AA:499:A:C6	1:AA:547:A:C8	3.03	0.46
1:AA:1226:C:H5"	13:AS:81:ARG:HB3	1.96	0.46
1:AA:1237:C:C2'	1:AA:1238:A:OP1	2.63	0.46
4:AJ:90:LEU:HG	4:AJ:90:LEU:O	2.15	0.46
15:AB:84:GLU:HG3	15:AB:215:LEU:HB3	1.96	0.46
16:AC:54:ARG:NH1	16:AC:56:ASP:OD1	2.35	0.46
23:AY:162:VAL:HG21	23:AY:255:ILE:CD1	2.45	0.46
25:BA:1115:G:H2'	25:BA:1116:C:C6	2.51	0.46
25:BA:1353:A:H4'	43:BD:38:LYS:HE3	1.96	0.46
25:BA:1865:G:H8	25:BA:1865:G:H5"	1.80	0.46
25:BA:2290:G:C2	25:BA:2343:C:O2	2.69	0.46
25:BA:2316:C:OP2	25:BA:2316:C:H6	1.99	0.46
25:BA:2477:C:O2	25:BA:2481:G:O6	2.33	0.46
25:BA:2533:A:H5"	25:BA:2665:A:O2'	2.16	0.46
25:BA:2612:C:H2'	25:BA:2613:U:H5'	1.98	0.46
26:BB:27:C:O3'	32:BS:36:TYR:OH	2.31	0.46
33:BT:106:SER:O	33:BT:107:ASP:OD1	2.34	0.46
38:BY:28:LYS:HE3	38:BY:30:VAL:HG22	1.98	0.46
43:BD:65:ILE:HD11	43:BD:67:PHE:CZ	2.51	0.46
53:BF:24:LEU:HB3	53:BF:25:PRO:CD	2.38	0.46
54:BG:82:LEU:HD22	54:BG:87:PRO:HB3	1.97	0.46
54:BG:135:LEU:HD22	54:BG:140:ILE:HD11	1.97	0.46
1:AA:807:A:H2'	1:AA:808:C:O4'	2.16	0.46
7:AM:83:ASP:OD1	7:AM:84:ILE:N	2.49	0.46
7:AM:120:LYS:HE3	7:AM:121:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AO:56:LEU:O	9:AO:60:VAL:HG23	2.16	0.46
18:AE:50:GLU:CD	18:AE:51:VAL:H	2.19	0.46
22:AI:50:LEU:HB3	22:AI:56:LEU:HA	1.96	0.46
23:AY:463:VAL:C	23:AY:465:ARG:H	2.19	0.46
25:BA:651:G:H4'	49:B8:18:ALA:HB3	1.98	0.46
25:BA:1021:A:OP2	27:BN:65:LYS:NZ	2.48	0.46
25:BA:1050:A:H2'	25:BA:1051:G:H8	1.79	0.46
25:BA:1086:A:H3'	25:BA:1086:A:N3	2.31	0.46
25:BA:1434:A:O2'	25:BA:1435:G:H5'	2.16	0.46
25:BA:1914:C:OP1	25:BA:1914:C:H2'	2.15	0.46
25:BA:2125:G:H5"	25:BA:2126:A:OP1	2.16	0.46
25:BA:2134:A:H8	25:BA:2159:G:O2'	1.98	0.46
25:BA:2503:A:N3	25:BA:2503:A:H5'	2.31	0.46
29:BP:47:ASP:HB3	29:BP:48:PRO:CA	2.46	0.46
31:BR:56:LYS:NZ	31:BR:90:ARG:O	2.48	0.46
39:BZ:73:GLN:HB3	39:BZ:87:ASP:HB2	1.96	0.46
40:B0:24:LYS:HG3	40:B0:36:ILE:HD11	1.98	0.46
52:BE:2:LYS:HD2	52:BE:95:ILE:HG23	1.96	0.46
52:BE:128:SER:O	52:BE:129:HIS:C	2.53	0.46
53:BF:157:VAL:HG23	53:BF:198:ALA:HB1	1.96	0.46
54:BG:48:GLU:O	54:BG:49:ASP:CB	2.63	0.46
1:AA:706:A:C2'	5:AK:31:THR:HG21	2.46	0.46
1:AA:973:G:C2'	1:AA:974:A:OP1	2.64	0.46
1:AA:1265:G:H2'	1:AA:1266:G:O4'	2.16	0.46
1:AA:1349:A:C2	1:AA:1374:A:C4	3.04	0.46
1:AA:1521:G:H2'	1:AA:1522:U:C6	2.50	0.46
23:AY:293:THR:HG22	23:AY:297:GLU:O	2.15	0.46
25:BA:197:A:H2'	25:BA:198:C:H5'	1.98	0.46
25:BA:586:A:H2	25:BA:809:G:N3	2.14	0.46
25:BA:1328:G:H8	25:BA:1328:G:O5'	1.98	0.46
25:BA:2340:G:O2'	25:BA:2341:G:H5'	2.16	0.46
29:BP:6:LEU:HD23	29:BP:6:LEU:H	1.81	0.46
36:BW:73:ALA:HB3	36:BW:106:ILE:CG1	2.44	0.46
37:BX:52:VAL:O	37:BX:52:VAL:HG12	2.16	0.46
39:BZ:166:SER:OG	39:BZ:167:PRO:HA	2.16	0.46
51:BC:82:LYS:O	51:BC:83:ILE:C	2.53	0.46
52:BE:5:LEU:HD12	52:BE:51:PHE:HB2	1.96	0.46
53:BF:113:ALA:HB1	53:BF:186:ILE:HG21	1.98	0.46
54:BG:39:ILE:HD11	54:BG:94:LEU:HD11	1.96	0.46
56:BK:14:ALA:HA	56:BK:41:PHE:CZ	2.50	0.46
1:AA:55:A:H1'	23:AY:321:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:120:A:O2'	1:AA:121:C:H5'	2.16	0.46
1:AA:673:G:H5"	19:AF:87:ARG:CZ	2.45	0.46
1:AA:1031:G:H2'	1:AA:1032:G:O4'	2.16	0.46
1:AA:1234:C:H1'	1:AA:1364:U:O2	2.15	0.46
1:AA:1452:C:O4'	1:AA:1456:G:N2	2.49	0.46
2:AV:47:U:H3'	2:AV:48:C:C5'	2.46	0.46
21:AH:86:ILE:HB	21:AH:133:LEU:O	2.16	0.46
25:BA:64:A:C2	37:BX:66:LEU:HD22	2.50	0.46
25:BA:89:G:OP2	25:BA:90:U:H2'	2.16	0.46
25:BA:991:C:H6	25:BA:991:C:H5'	1.80	0.46
25:BA:1741:A:N7	25:BA:1742:G:C2	2.84	0.46
25:BA:1789:A:H2'	25:BA:1790:C:H5'	1.96	0.46
25:BA:2144:U:O2	25:BA:2147:G:O6	2.34	0.46
25:BA:2298:A:N6	25:BA:2318:G:C8	2.82	0.46
28:BO:77:ILE:HD12	33:BT:74:ARG:HD3	1.97	0.46
33:BT:125:ARG:O	33:BT:128:GLU:HG3	2.14	0.46
34:BU:90:VAL:HG12	34:BU:91:ASP:N	2.31	0.46
39:BZ:166:SER:OG	39:BZ:167:PRO:CA	2.64	0.46
47:B6:11:LEU:HD21	47:B6:51:GLU:HB2	1.97	0.46
53:BF:81:PRO:HB3	53:BF:89:VAL:HG23	1.98	0.46
57:BJ:100:ALA:O	57:BJ:104:ALA:HB3	2.16	0.46
1:AA:1190:G:OP1	16:AC:4:LYS:HA	2.15	0.46
1:AA:1319:A:C8	1:AA:1323:G:C5	3.04	0.46
1:AA:1508:G:O2'	1:AA:1509:C:H5'	2.16	0.46
7:AM:45:VAL:HA	7:AM:48:LEU:HD22	1.98	0.46
14:AT:26:ASN:OD1	14:AT:71:THR:OG1	2.27	0.46
14:AT:94:ALA:O	14:AT:95:ALA:CB	2.64	0.46
15:AB:114:ARG:NH1	15:AB:118:LEU:HD21	2.31	0.46
15:AB:235:SER:OG	15:AB:236:TYR:CD1	2.69	0.46
18:AE:7:GLU:O	18:AE:8:GLU:HB3	2.16	0.46
25:BA:796:C:H2'	25:BA:797:C:C6	2.51	0.46
25:BA:889:C:O2'	25:BA:890:A:OP2	2.32	0.46
25:BA:1051:G:H2'	25:BA:1052:C:O4'	2.16	0.46
25:BA:1055:G:H5'	25:BA:1056:G:OP2	2.16	0.46
32:BS:97:ARG:NH2	32:BS:98:VAL:HA	2.30	0.46
43:BD:134:ARG:HG3	43:BD:135:PHE:CD1	2.51	0.46
45:B4:38:ALA:O	45:B4:49:GLU:HG2	2.16	0.46
51:BC:215:THR:OG1	51:BC:216:THR:N	2.48	0.46
1:AA:503:C:O2	1:AA:510:A:H2	1.98	0.46
1:AA:1128:C:C2'	1:AA:1129:C:H5'	2.45	0.46
1:AA:1158:C:O2	1:AA:1158:C:C2'	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AF:89:MET:HG2	19:AF:91:VAL:HG23	1.98	0.46
21:AH:113:SER:O	21:AH:131:GLY:HA3	2.16	0.46
25:BA:309:G:O3'	38:BY:18:GLY:HA2	2.16	0.46
25:BA:451:C:H4'	53:BF:52:LYS:HE2	1.97	0.46
25:BA:814:C:H2'	25:BA:815:C:C6	2.51	0.46
25:BA:1208:C:C4	25:BA:1209:G:N7	2.84	0.46
25:BA:2151:G:C6	25:BA:2152:G:C5	3.03	0.46
27:BN:119:ARG:HH11	27:BN:119:ARG:CG	2.29	0.46
34:BU:65:ILE:HG12	34:BU:96:ALA:CB	2.46	0.46
43:BD:13:ARG:HD2	43:BD:16:MET:CE	2.43	0.46
43:BD:169:GLU:OE1	43:BD:169:GLU:HA	2.16	0.46
55:BH:64:LEU:HD23	55:BH:67:LEU:HD23	1.98	0.46
1:AA:503:C:O5'	1:AA:503:C:H6	1.99	0.45
1:AA:979:C:C3'	1:AA:980:C:C5'	2.93	0.45
18:AE:28:PHE:O	18:AE:47:LYS:HA	2.17	0.45
25:BA:35:G:C2'	25:BA:36:G:O5'	2.64	0.45
25:BA:428:A:H5'	25:BA:429:A:OP2	2.16	0.45
25:BA:2512:C:H2'	25:BA:2513:G:O4'	2.15	0.45
26:BB:41:U:C6	54:BG:69:ALA:HB1	2.51	0.45
29:BP:23:PRO:HB2	29:BP:33:ARG:HD2	1.97	0.45
38:BY:42:VAL:HG23	38:BY:67:LEU:HD13	1.99	0.45
39:BZ:166:SER:OG	39:BZ:167:PRO:C	2.55	0.45
45:B4:64:LYS:C	45:B4:65:CYS:HG	2.19	0.45
53:BF:20:LEU:HD23	53:BF:21:ALA:N	2.31	0.45
1:AA:1134:G:C5	1:AA:1135:U:C6	3.04	0.45
1:AA:1149:C:P	22:AI:9:ARG:HH11	2.38	0.45
7:AM:58:GLU:O	7:AM:62:ASN:ND2	2.50	0.45
20:AG:152:ALA:O	20:AG:155:ARG:NE	2.49	0.45
23:AY:78:ARG:C	23:AY:79:ILE:HD12	2.36	0.45
23:AY:551:GLN:O	23:AY:559:PRO:HA	2.15	0.45
25:BA:299:A:C5	25:BA:322:A:C2	3.05	0.45
25:BA:401:A:H2'	25:BA:402:A:O4'	2.16	0.45
25:BA:613:G:H5"	25:BA:613:G:C8	2.43	0.45
25:BA:659:C:H4'	53:BF:100:THR:O	2.16	0.45
25:BA:995:C:O2	27:BN:4:TYR:OH	2.28	0.45
25:BA:1499:C:O2'	25:BA:1500:G:H5'	2.16	0.45
25:BA:1761:C:H2'	25:BA:1762:A:H5'	1.98	0.45
25:BA:2388:A:H5'	25:BA:2389:G:OP2	2.16	0.45
25:BA:2654:A:O4'	25:BA:2656:U:C6	2.69	0.45
29:BP:33:ARG:O	29:BP:34:GLY:C	2.54	0.45
33:BT:92:GLY:O	33:BT:115:ARG:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BU:66:ASN:O	34:BU:70:ARG:HB2	2.16	0.45
34:BU:81:HIS:CD2	34:BU:117:GLN:HG3	2.52	0.45
38:BY:76:CYS:O	38:BY:96:ILE:HD13	2.16	0.45
43:BD:226:MET:O	43:BD:234:GLY:HA2	2.16	0.45
53:BF:20:LEU:HD23	53:BF:21:ALA:H	1.81	0.45
54:BG:72:ARG:HB3	54:BG:87:PRO:HD3	1.97	0.45
54:BG:149:VAL:HG13	54:BG:149:VAL:O	2.17	0.45
55:BH:105:LEU:CD2	55:BH:113:VAL:HB	2.46	0.45
1:AA:288:A:H2'	1:AA:289:G:H4'	1.98	0.45
1:AA:1013:G:H5"	1:AA:1013:G:H8	1.78	0.45
2:AV:73:A:H3'	2:AV:74:C:H5'	1.97	0.45
15:AB:7:VAL:O	15:AB:11:LEU:HB2	2.16	0.45
15:AB:178:ARG:HG2	15:AB:178:ARG:NH1	2.13	0.45
23:AY:409:ILE:HD13	23:AY:409:ILE:HA	1.86	0.45
25:BA:306:U:H2'	25:BA:307:G:O4'	2.16	0.45
25:BA:308:G:C8	25:BA:501:A:O4'	2.69	0.45
25:BA:387:U:H4'	25:BA:388:G:O5'	2.16	0.45
25:BA:1394:U:C6	25:BA:1394:U:H3'	2.52	0.45
25:BA:1426:G:C6	25:BA:1427:A:C6	3.04	0.45
25:BA:1918:A:O2'	25:BA:1919:A:C2	2.64	0.45
25:BA:2137:C:N4	25:BA:2154:G:O6	2.49	0.45
25:BA:2506:U:H4'	25:BA:2507:C:OP1	2.14	0.45
27:BN:134:ARG:O	27:BN:134:ARG:CD	2.64	0.45
30:BQ:76:LYS:HB3	30:BQ:91:GLU:HG2	1.99	0.45
33:BT:23:ARG:C	33:BT:25:GLY:N	2.69	0.45
46:B5:51:TYR:CD2	46:B5:52:TYR:CE2	3.05	0.45
51:BC:131:LEU:HD12	51:BC:137:LEU:HA	1.98	0.45
1:AA:33:A:O2'	1:AA:363:A:H1'	2.16	0.45
1:AA:35:G:H2'	1:AA:36:C:C6	2.51	0.45
1:AA:141:A:H1'	1:AA:182:U:O2	2.17	0.45
1:AA:353:A:C2'	1:AA:354:G:OP2	2.65	0.45
1:AA:501:C:H1'	1:AA:549:C:H1'	1.98	0.45
1:AA:695:A:H2'	1:AA:696:A:C8	2.51	0.45
1:AA:981:U:O4	1:AA:1222:G:O6	2.33	0.45
1:AA:1003:G:C2'	1:AA:1004:A:H4'	2.45	0.45
4:AJ:30:SER:CB	4:AJ:81:THR:OG1	2.65	0.45
18:AE:41:VAL:HG23	18:AE:67:VAL:HG13	1.99	0.45
23:AY:72:CYS:SG	23:AY:81:ILE:HD11	2.56	0.45
23:AY:289:ILE:HD11	23:AY:331:TYR:CD2	2.51	0.45
25:BA:30:G:H2'	25:BA:31:C:C6	2.51	0.45
25:BA:94:C:O2	25:BA:94:C:H2'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:271(A):A:N1	25:BA:272(D):G:O2'	2.46	0.45
25:BA:2138:C:H6	25:BA:2138:C:H5"	1.82	0.45
25:BA:2461:C:H2'	25:BA:2462:U:C6	2.51	0.45
25:BA:2517:C:C2'	25:BA:2542:A:C2	2.99	0.45
25:BA:2746:U:H2'	25:BA:2747:G:H5'	1.99	0.45
25:BA:2757:A:N1	55:BH:67:LEU:HD22	2.31	0.45
29:BP:38:GLN:HG3	29:BP:39:LYS:H	1.81	0.45
31:BR:38:VAL:HB	31:BR:39:PRO:CD	2.45	0.45
38:BY:38:ILE:CG2	38:BY:39:VAL:N	2.78	0.45
39:BZ:188:ALA:O	39:BZ:189:ALA:C	2.55	0.45
41:B1:4:VAL:HG13	41:B1:4:VAL:O	2.15	0.45
51:BC:99:ILE:HD13	51:BC:99:ILE:H	1.81	0.45
1:AA:737:A:O2'	19:AF:72:VAL:CG1	2.65	0.45
16:AC:40:ARG:HG3	16:AC:40:ARG:NH1	2.30	0.45
23:AY:212:TYR:O	23:AY:216:LEU:N	2.40	0.45
25:BA:1421:G:C2	25:BA:1422:G:C8	3.05	0.45
25:BA:1562:A:H2'	25:BA:1563:G:O4'	2.17	0.45
25:BA:1910:G:N1	25:BA:1920:C:H5	1.98	0.45
25:BA:2302:G:C3'	25:BA:2303:G:H5'	2.47	0.45
25:BA:2302:G:H2'	25:BA:2303:G:H5'	1.99	0.45
25:BA:2371:G:C6	25:BA:2372:G:N7	2.85	0.45
25:BA:2506:U:H5'	25:BA:2506:U:H6	1.79	0.45
35:BV:40:LEU:HD23	35:BV:46:VAL:HG23	1.98	0.45
35:BV:79:VAL:O	35:BV:79:VAL:HG13	2.16	0.45
38:BY:17:SER:HB2	38:BY:71:LYS:HB3	1.97	0.45
38:BY:28:LYS:HB3	38:BY:37:VAL:HB	1.97	0.45
42:B2:38:GLN:HB3	42:B2:44:LEU:CB	2.45	0.45
48:B7:5:TRP:CD1	48:B7:7:PRO:HD3	2.51	0.45
49:B8:33:ASN:HA	49:B8:36:LYS:CG	2.47	0.45
51:BC:193:ILE:HD12	51:BC:193:ILE:H	1.80	0.45
53:BF:114:VAL:HG21	53:BF:202:PHE:CE1	2.51	0.45
1:AA:262:A:C6	1:AA:263:A:C6	3.04	0.45
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.98	0.45
1:AA:1230:C:O2'	1:AA:1231:G:H5'	2.17	0.45
1:AA:1349:A:H2'	1:AA:1350:A:O5'	2.16	0.45
2:AV:19:G:C5	25:BA:2169:A:H1'	2.52	0.45
17:AD:22:LYS:O	17:AD:24:GLU:N	2.49	0.45
19:AF:72:VAL:HG13	19:AF:73:ASN:N	2.31	0.45
21:AH:83:ILE:HG23	21:AH:83:ILE:O	2.17	0.45
25:BA:338:G:C5	25:BA:339:U:C5	3.05	0.45
25:BA:780:G:H2'	25:BA:782:A:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2142:C:H5”	25:BA:2143:C:OP2	2.16	0.45
25:BA:2164:C:C4	25:BA:2165:G:C8	3.05	0.45
31:BR:4:LEU:O	31:BR:5:LYS:HD3	2.17	0.45
38:BY:85:VAL:HG13	38:BY:92:ASN:OD1	2.16	0.45
43:BD:24:ILE:O	43:BD:26:LYS:CB	2.65	0.45
47:B6:15:GLU:OE2	47:B6:41:PRO:HB2	2.16	0.45
53:BF:88:VAL:HG11	53:BF:91:GLY:HA3	1.98	0.45
54:BG:96:ARG:O	54:BG:97:ASP:C	2.55	0.45
55:BH:85:LYS:O	55:BH:85:LYS:NZ	2.42	0.45
1:AA:1371:G:C6	1:AA:1372:U:C4	3.04	0.45
6:AL:27:LEU:HB2	6:AL:62:SER:HB2	1.98	0.45
22:AI:112:LYS:HG2	22:AI:118:LYS:HA	1.98	0.45
23:AY:20:HIS:CG	23:AY:21:ILE:N	2.85	0.45
23:AY:490:PRO:O	23:AY:491:VAL:HG23	2.17	0.45
23:AY:627:ARG:NH1	23:AY:651:GLU:O	2.50	0.45
25:BA:529:A:N3	25:BA:529:A:O4’	2.50	0.45
25:BA:833:U:H5”	29:BP:48:PRO:HB3	1.97	0.45
25:BA:2592:G:H2’	25:BA:2593:U:O4’	2.17	0.45
41:B1:44:PRO:HB2	41:B1:46:LEU:HD13	1.98	0.45
45:B4:37:PRO:HA	45:B4:51:TYR:CD2	2.52	0.45
52:BE:98:PRO:HD3	52:BE:175:VAL:CG1	2.47	0.45
58:BL:79:UNK:C	58:BL:81:UNK:N	2.78	0.45
9:AO:78:TYR:O	9:AO:82:ILE:HG22	2.17	0.45
14:AT:100:ILE:C	14:AT:102:GLY:N	2.70	0.45
15:AB:31:TYR:CZ	15:AB:200:ILE:HD12	2.52	0.45
16:AC:95:THR:C	16:AC:97:LYS:H	2.19	0.45
18:AE:51:VAL:O	18:AE:55:VAL:HG23	2.16	0.45
23:AY:114:VAL:HG11	23:AY:157:LEU:HD22	1.98	0.45
23:AY:286:ILE:O	23:AY:287:PRO:C	2.55	0.45
25:BA:26:G:C6	25:BA:27:G:N1	2.85	0.45
25:BA:27:G:O2’	25:BA:28:A:P	2.73	0.45
25:BA:363(E):U:H5’	25:BA:363(F):A:OP2	2.17	0.45
25:BA:864:G:N7	30:BQ:22:LYS:NZ	2.62	0.45
25:BA:1063:G:C6	25:BA:1075:C:N4	2.84	0.45
25:BA:1449:A:C4	25:BA:1528(A):A:C2	3.05	0.45
25:BA:1569:A:O2’	43:BD:38:LYS:HG2	2.17	0.45
25:BA:2575:C:H6	25:BA:2575:C:O5’	1.99	0.45
25:BA:2645:G:N2	25:BA:2767:C:OP2	2.49	0.45
34:BU:74:LEU:HD23	34:BU:78:THR:HG22	1.98	0.45
38:BY:55:TYR:O	38:BY:57:GLN:N	2.50	0.45
39:BZ:188:ALA:O	39:BZ:190:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BC:28:LEU:HD12	51:BC:28:LEU:O	2.17	0.45
1:AA:918:A:H2'	1:AA:919:A:C8	2.51	0.45
1:AA:1028:C:N4	1:AA:1033:G:O6	2.49	0.45
1:AA:1100:C:OP2	15:AB:96:ARG:NE	2.50	0.45
6:AL:41:ARG:HB3	6:AL:41:ARG:NH1	2.32	0.45
16:AC:91:LEU:HD11	16:AC:101:LEU:HD12	1.99	0.45
20:AG:44:TYR:O	20:AG:45:ASP:C	2.55	0.45
20:AG:113:GLU:HG2	20:AG:119:ARG:HG2	1.99	0.45
23:AY:470:PHE:O	23:AY:471:LYS:HG3	2.17	0.45
25:BA:270:A:N1	25:BA:366:C:O2'	2.43	0.45
25:BA:571:A:H5'	25:BA:2030:A:N7	2.32	0.45
25:BA:1057:A:C6	25:BA:1086:A:C2	3.05	0.45
25:BA:1078:U:O2	25:BA:1088:A:H5'	2.17	0.45
25:BA:1089:G:C4'	25:BA:1090:U:OP1	2.63	0.45
25:BA:1204:A:C2	25:BA:1241:A:N1	2.85	0.45
25:BA:1775:U:H2'	25:BA:1776:G:O5'	2.16	0.45
25:BA:1805:U:O2	43:BD:50:THR:HB	2.16	0.45
25:BA:2208:A:O2'	25:BA:2219:G:C8	2.70	0.45
25:BA:2447:G:N7	25:BA:2501:C:O4'	2.50	0.45
26:BB:82:G:H2'	26:BB:83:G:O5'	2.16	0.45
30:BQ:35:VAL:HG11	30:BQ:130:LYS:HE3	1.99	0.45
33:BT:32:TYR:O	33:BT:41:ARG:O	2.35	0.45
37:BX:21:PHE:O	37:BX:23:GLU:O	2.35	0.45
39:BZ:152:ALA:HB1	39:BZ:167:PRO:HB2	1.98	0.45
43:BD:125:ILE:HD11	43:BD:131:LEU:HD22	1.98	0.45
52:BE:67:PHE:O	52:BE:68:ALA:C	2.55	0.45
54:BG:60:LEU:HD13	54:BG:60:LEU:C	2.37	0.45
1:AA:62:U:C2'	1:AA:63:C:H5"	2.45	0.45
1:AA:927:G:OP2	1:AA:927:G:H4'	2.17	0.45
7:AM:13:LYS:O	7:AM:44:ARG:HA	2.16	0.45
15:AB:166:ASP:HB3	15:AB:169:LYS:CB	2.46	0.45
15:AB:178:ARG:CG	15:AB:178:ARG:NH1	2.65	0.45
18:AE:148:VAL:O	18:AE:152:ARG:HG3	2.17	0.45
23:AY:58:GLU:HG3	23:AY:65:ILE:HG22	1.98	0.45
23:AY:180:VAL:HG23	23:AY:181:LEU:N	2.31	0.45
23:AY:224:ASP:HB2	23:AY:227:ILE:HD12	1.98	0.45
23:AY:685:GLU:HA	23:AY:688:ILE:HG22	1.99	0.45
25:BA:251:A:H5"	29:BP:51:PHE:HZ	1.82	0.45
25:BA:301:G:H1'	25:BA:302:C:C6	2.52	0.45
25:BA:854:G:H5"	25:BA:855:G:OP2	2.17	0.45
25:BA:1076:C:O2'	25:BA:1077:A:O4'	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1914:C:C2’	25:BA:1915:U:O5’	2.59	0.45
25:BA:2637:U:C2’	25:BA:2638:G:H5’	2.46	0.45
27:BN:15:LEU:O	27:BN:136:GLU:HA	2.17	0.45
29:BP:57:THR:HB	29:BP:59:LEU:HB2	1.99	0.45
52:BE:68:ALA:O	52:BE:70:ALA:N	2.50	0.45
54:BG:28:VAL:O	54:BG:31:VAL:HG12	2.17	0.45
57:BJ:21:ALA:HB3	57:BJ:88:ALA:HA	1.98	0.45
1:AA:711:G:O2’	1:AA:712:A:H5’	2.17	0.44
1:AA:1138:G:O2’	1:AA:1139:G:P	2.75	0.44
2:AV:55:U:O2	2:AV:55:U:O4’	2.35	0.44
15:AB:223:ILE:O	15:AB:224:GLN:C	2.55	0.44
23:AY:343:ASN:C	23:AY:343:ASN:HD22	2.20	0.44
25:BA:316:C:C2’	25:BA:317:G:O5’	2.65	0.44
25:BA:861:A:H2’	25:BA:862:G:O4’	2.17	0.44
25:BA:1246:A:P	29:BP:16:ARG:NH2	2.90	0.44
25:BA:1367:A:H5”	25:BA:1368:G:OP2	2.17	0.44
25:BA:1458:C:C4’	25:BA:1459:G:O5’	2.64	0.44
25:BA:1462:C:H4’	25:BA:2703:C:H5’	1.98	0.44
25:BA:1527:G:H2’	25:BA:1544:A:C2	2.52	0.44
25:BA:1817:G:C6	25:BA:1818:U:C4	3.04	0.44
25:BA:1943:U:H4’	25:BA:1944:U:OP1	2.17	0.44
25:BA:2166:G:O2’	25:BA:2167:U:H5’	2.17	0.44
25:BA:2179:C:O2	25:BA:2179:C:O4’	2.35	0.44
29:BP:120:ALA:HB1	29:BP:138:LEU:HD12	1.99	0.44
31:BR:44:LEU:HD22	31:BR:48:VAL:HG23	1.98	0.44
33:BT:82:LEU:HD12	33:BT:82:LEU:H	1.80	0.44
37:BX:66:LEU:HD23	37:BX:66:LEU:O	2.16	0.44
41:B1:3:LYS:HG2	41:B1:4:VAL:H	1.82	0.44
42:B2:35:LEU:CD1	42:B2:53:LEU:HD12	2.46	0.44
51:BC:23:ASP:O	51:BC:24:GLU:C	2.56	0.44
51:BC:84:LYS:C	51:BC:86:ALA:H	2.20	0.44
1:AA:180:U:H2’	1:AA:181:G:H5’	1.99	0.44
1:AA:1037:C:H2’	1:AA:1038:C:C6	2.52	0.44
1:AA:1533:C:H3’	1:AA:1534:A:H5”	1.98	0.44
15:AB:215:LEU:HA	15:AB:215:LEU:HD13	1.76	0.44
17:AD:22:LYS:HE2	17:AD:25:ARG:HD2	1.98	0.44
23:AY:79:ILE:HD12	23:AY:79:ILE:N	2.32	0.44
25:BA:332:A:O2’	25:BA:334:C:OP2	2.29	0.44
25:BA:852:G:O2’	25:BA:853:G:H5’	2.17	0.44
25:BA:1903:G:OP1	43:BD:241:PRO:HB2	2.17	0.44
25:BA:2343:C:O2’	25:BA:2344:U:H5’	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2685:G:P	33:BT:51:ARG:HH12	2.40	0.44
28:BO:104:ARG:HH11	28:BO:107:ARG:HH12	1.63	0.44
31:BR:78:LYS:CE	31:BR:83:ILE:HD11	2.47	0.44
47:B6:41:PRO:O	47:B6:42:TRP:C	2.55	0.44
49:B8:54:GLU:O	49:B8:58:ILE:HG13	2.17	0.44
53:BF:22:ALA:HB1	53:BF:26:ALA:CB	2.47	0.44
54:BG:32:PRO:HB2	54:BG:172:LEU:HD13	1.99	0.44
1:AA:501:C:H2'	1:AA:502:G:C8	2.53	0.44
5:AK:38:ASN:HA	5:AK:39:PRO:HD3	1.91	0.44
7:AM:65:LYS:CG	7:AM:65:LYS:O	2.65	0.44
8:AN:47:LEU:O	8:AN:48:ALA:C	2.56	0.44
15:AB:19:HIS:HB2	15:AB:204:ASN:HD22	1.83	0.44
18:AE:7:GLU:OE1	18:AE:37:ARG:NE	2.49	0.44
23:AY:26:THR:HA	23:AY:83:ASP:OD2	2.16	0.44
23:AY:325:LEU:HD21	23:AY:358:MET:CE	2.47	0.44
23:AY:632:LEU:HD11	23:AY:646:PHE:CD2	2.52	0.44
25:BA:370:G:O5'	25:BA:370:G:C8	2.70	0.44
25:BA:1268:A:C2	25:BA:2013:A:C4	3.05	0.44
25:BA:1899:G:HO2'	25:BA:1900:A:P	2.38	0.44
25:BA:2469:A:H2'	25:BA:2470:G:O4'	2.18	0.44
26:BB:84:C:OP1	44:B3:15:TYR:OH	2.35	0.44
28:BO:9:GLU:O	28:BO:83:ALA:HA	2.18	0.44
34:BU:88:ILE:HD13	34:BU:109:LEU:CD2	2.44	0.44
38:BY:28:LYS:O	38:BY:29:GLU:C	2.56	0.44
38:BY:52:SER:O	38:BY:54:LYS:N	2.50	0.44
49:B8:32:LEU:CB	49:B8:36:LYS:NZ	2.80	0.44
49:B8:33:ASN:HA	49:B8:36:LYS:HG2	2.00	0.44
55:BH:23:ARG:O	55:BH:24:VAL:HG12	2.18	0.44
56:BK:3:LYS:HD3	56:BK:29:GLN:HG2	2.00	0.44
1:AA:684:A:C6	1:AA:685:G:C6	3.05	0.44
1:AA:702:A:H4'	1:AA:703:G:OP2	2.17	0.44
15:AB:51:LEU:O	15:AB:55:PHE:HB2	2.17	0.44
15:AB:92:TYR:O	15:AB:151:GLY:HA3	2.18	0.44
15:AB:126:GLU:O	15:AB:130:ARG:HG3	2.18	0.44
23:AY:86:GLY:O	23:AY:117:GLN:CG	2.66	0.44
23:AY:281:PRO:HB2	23:AY:286:ILE:HD11	2.00	0.44
23:AY:495:GLY:O	23:AY:510:VAL:N	2.51	0.44
25:BA:92:A:C2	25:BA:93:G:H1'	2.52	0.44
25:BA:358:U:O2	25:BA:358:U:H2'	2.18	0.44
25:BA:484:C:H2'	25:BA:485:C:C6	2.52	0.44
25:BA:1491:G:OP2	25:BA:1494:A:C6	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2287:A:N1	25:BA:2346:A:N1	2.65	0.44
25:BA:2743:C:C2'	25:BA:2744:G:O5'	2.65	0.44
27:BN:134:ARG:HD2	27:BN:134:ARG:N	2.32	0.44
28:BO:63:VAL:HG11	28:BO:85:VAL:HG23	1.99	0.44
29:BP:143:GLY:HA3	29:BP:145:PRO:HD3	1.99	0.44
32:BS:53:SER:OG	32:BS:54:LEU:N	2.50	0.44
33:BT:80:SER:HB3	33:BT:81:PRO:HD3	1.98	0.44
35:BV:19:LYS:CG	35:BV:20:LEU:O	2.65	0.44
39:BZ:151:HIS:HB3	39:BZ:170:THR:HA	1.99	0.44
41:B1:51:VAL:HG21	41:B1:74:VAL:HG21	2.00	0.44
53:BF:24:LEU:HD13	53:BF:118:ALA:HB1	1.98	0.44
54:BG:48:GLU:O	54:BG:49:ASP:HB3	2.17	0.44
1:AA:685:G:C2	1:AA:686:U:C4	3.05	0.44
7:AM:86:CYS:HA	13:AS:73:GLU:O	2.18	0.44
25:BA:510:C:OP1	25:BA:511:U:OP2	2.36	0.44
25:BA:603:A:O4'	25:BA:603:A:N3	2.50	0.44
25:BA:1692:U:O2'	25:BA:1693:U:H2'	2.18	0.44
25:BA:1835:G:H1'	25:BA:1931:U:C2	2.53	0.44
25:BA:2025:C:H2'	25:BA:2026:C:C6	2.52	0.44
25:BA:2151:G:C2	25:BA:2152:G:C4	3.05	0.44
25:BA:2392:A:OP1	49:B8:32:LEU:HD21	2.16	0.44
25:BA:2401:U:O2'	25:BA:2402:C:H5"	2.17	0.44
25:BA:2557:G:H2'	25:BA:2558:C:C6	2.52	0.44
27:BN:35:ARG:O	27:BN:37:LYS:N	2.50	0.44
32:BS:99:LYS:N	32:BS:99:LYS:HD3	2.27	0.44
33:BT:5:ALA:O	33:BT:6:LEU:C	2.55	0.44
33:BT:96:ARG:CZ	33:BT:96:ARG:HB3	2.47	0.44
41:B1:40:ARG:HD3	41:B1:40:ARG:C	2.38	0.44
55:BH:157:TYR:CE1	55:BH:173:PRO:HB3	2.53	0.44
56:BK:19:PRO:CB	56:BK:34:ILE:HD12	2.47	0.44
56:BK:77:LEU:HD23	56:BK:77:LEU:N	2.32	0.44
1:AA:96:U:O2'	1:AA:97:G:P	2.76	0.44
1:AA:909:A:H2'	1:AA:910:C:O4'	2.18	0.44
4:AJ:24:VAL:O	4:AJ:25:GLU:C	2.56	0.44
19:AF:72:VAL:CG2	19:AF:90:VAL:HG11	2.48	0.44
22:AI:10:ARG:CZ	22:AI:105:ASP:OD2	2.65	0.44
22:AI:48:GLU:N	22:AI:49:PRO:CD	2.80	0.44
23:AY:179:ASP:C	23:AY:180:VAL:O	2.56	0.44
23:AY:491:VAL:O	23:AY:513:LYS:HA	2.17	0.44
23:AY:512:ILE:CD1	23:AY:589:ALA:HB1	2.47	0.44
25:BA:104:U:C5	25:BA:105:C:C5	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:264:C:O2'	25:BA:265:A:H2'	2.18	0.44
25:BA:271(O):C:O2'	25:BA:271(P):C:OP2	2.31	0.44
25:BA:445:C:OP1	34:BU:2:PRO:HA	2.18	0.44
25:BA:614:U:O2	25:BA:614:U:O5'	2.35	0.44
25:BA:774:A:HO2'	25:BA:775:G:P	2.32	0.44
25:BA:2115:G:H2'	25:BA:2117:A:N7	2.33	0.44
25:BA:2165:G:C5	25:BA:2166:G:C6	3.05	0.44
25:BA:2266:A:H4'	25:BA:2267:A:O5'	2.18	0.44
25:BA:2667:C:H1'	55:BH:109:PHE:CD1	2.52	0.44
25:BA:2689:U:O2	25:BA:2713:A:O5'	2.36	0.44
28:BO:43:VAL:HG21	28:BO:52:VAL:CG1	2.47	0.44
29:BP:55:ARG:CG	29:BP:56:SER:H	2.30	0.44
29:BP:68:GLN:HE21	29:BP:68:GLN:HB2	1.61	0.44
33:BT:83:ILE:HG13	33:BT:84:GLN:N	2.33	0.44
35:BV:3:ALA:HA	35:BV:40:LEU:O	2.18	0.44
38:BY:23:ARG:O	38:BY:24:VAL:O	2.35	0.44
47:B6:14:THR:O	47:B6:49:HIS:HA	2.17	0.44
49:B8:61:LEU:H	49:B8:61:LEU:CD2	2.22	0.44
54:BG:16:ARG:NE	54:BG:31:VAL:HG11	2.33	0.44
54:BG:37:VAL:HG22	54:BG:159:VAL:HA	2.00	0.44
54:BG:130:ASN:OD1	54:BG:130:ASN:N	2.50	0.44
56:BK:21:PRO:HA	56:BK:23:VAL:N	2.33	0.44
1:AA:452:A:O2'	1:AA:453:A:H8	2.00	0.44
1:AA:804:U:H5"	1:AA:805:C:OP2	2.17	0.44
1:AA:926:G:H5"	1:AA:927:G:O5'	2.17	0.44
1:AA:1085:U:C2	1:AA:1094:G:O6	2.71	0.44
1:AA:1119:C:OP2	22:AI:9:ARG:NH2	2.50	0.44
2:AV:35:A:H5"	2:AV:35:A:H8	1.82	0.44
15:AB:15:VAL:O	15:AB:16:HIS:ND1	2.51	0.44
21:AH:31:PHE:O	21:AH:35:ILE:HG13	2.18	0.44
23:AY:321:TYR:CD1	23:AY:321:TYR:N	2.86	0.44
23:AY:627:ARG:O	23:AY:628:ARG:CB	2.66	0.44
25:BA:1375:C:H2'	25:BA:1376:C:H6	1.83	0.44
25:BA:1667:G:O2'	25:BA:1991:U:O4	2.26	0.44
25:BA:2097:C:H2'	25:BA:2098:U:H5'	1.99	0.44
25:BA:2648:C:H2'	25:BA:2649:U:C6	2.52	0.44
25:BA:2681:C:O2	25:BA:2681:C:H2'	2.17	0.44
25:BA:2712:U:O2'	25:BA:2712(A):A:OP2	2.29	0.44
25:BA:2769:C:H2'	25:BA:2770:G:O4'	2.17	0.44
31:BR:11:ASN:CG	31:BR:12:ARG:H	2.12	0.44
32:BS:35:ILE:HG23	32:BS:69:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BD:27:THR:CG2	43:BD:81:ALA:HB1	2.47	0.44
54:BG:64:THR:HG23	54:BG:66:GLN:H	1.83	0.44
54:BG:116:ASP:O	54:BG:117:PHE:HB3	2.18	0.44
1:AA:72:C:H2'	1:AA:73:G:C8	2.53	0.44
15:AB:191:ASP:OD1	15:AB:191:ASP:O	2.35	0.44
16:AC:91:LEU:CB	16:AC:99:VAL:HG21	2.48	0.44
18:AE:84:PHE:CB	18:AE:134:ALA:HB2	2.48	0.44
21:AH:44:PHE:HE2	21:AH:109:ILE:HG21	1.82	0.44
25:BA:485:C:C2	25:BA:496:G:N2	2.86	0.44
25:BA:508:G:N3	25:BA:508:G:H2'	2.32	0.44
25:BA:1599:C:OP1	37:BX:36:LYS:N	2.45	0.44
25:BA:2189:U:O5'	25:BA:2189:U:H6	2.00	0.44
25:BA:2302:G:C2'	25:BA:2303:G:H5'	2.47	0.44
25:BA:2451:A:H5'	40:B0:2:ALA:HB2	1.99	0.44
26:BB:40:U:H3'	26:BB:41:U:H5'	1.98	0.44
27:BN:58:ASP:O	27:BN:60:ILE:HG13	2.17	0.44
31:BR:94:TYR:O	31:BR:117:VAL:HB	2.18	0.44
34:BU:102:GLU:OE2	35:BV:13:ARG:NH2	2.51	0.44
1:AA:241:C:O2'	1:AA:242:C:H5'	2.18	0.44
1:AA:786:G:C2	1:AA:797:C:C2	3.06	0.44
1:AA:926:G:H2'	1:AA:1505:G:N3	2.33	0.44
1:AA:1499:A:H1'	1:AA:1520:G:H5'	2.00	0.44
4:AJ:51:ARG:HG3	4:AJ:60:ARG:HA	1.99	0.44
5:AK:114:VAL:HA	5:AK:115:PRO:HD2	1.88	0.44
11:AQ:66:SER:OG	11:AQ:69:LYS:HB2	2.17	0.44
17:AD:61:LYS:HD2	17:AD:207:TYR:OH	2.17	0.44
21:AH:9:MET:O	21:AH:13:ILE:HG12	2.18	0.44
25:BA:171:G:H2'	25:BA:172:C:O4'	2.18	0.44
25:BA:236:C:O2'	25:BA:431:U:H4'	2.17	0.44
25:BA:1676:A:H2'	25:BA:1677:A:O4'	2.18	0.44
25:BA:1859:A:C2	25:BA:1884:A:H1'	2.52	0.44
25:BA:1881:C:C6	25:BA:1881:C:H5"	2.53	0.44
25:BA:2193:G:C4	25:BA:2194:G:C8	3.06	0.44
25:BA:2762:G:H5"	25:BA:2762:G:H8	1.82	0.44
25:BA:2789:C:O2'	25:BA:2790:A:H1'	2.17	0.44
29:BP:143:GLY:CA	29:BP:145:PRO:HD3	2.48	0.44
35:BV:36:PRO:HA	35:BV:56:SER:CB	2.48	0.44
36:BW:88:ARG:HG3	36:BW:94:ASP:OD1	2.17	0.44
38:BY:3:VAL:O	38:BY:3:VAL:HG12	2.18	0.44
39:BZ:40:ASP:HB3	39:BZ:43:GLU:HB2	1.99	0.44
50:B9:29:ASN:HA	50:B9:30:PRO:HD3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BE:69:LYS:C	52:BE:71:GLY:H	2.20	0.44
53:BF:65:TRP:CH2	53:BF:73:ALA:O	2.70	0.44
1:AA:116:A:OP2	1:AA:116:A:H8	2.01	0.43
1:AA:243:A:C2	1:AA:246:A:C8	3.06	0.43
1:AA:325:A:H2'	1:AA:326:G:O4'	2.18	0.43
1:AA:693:G:C8	3:AX:15:A:H1'	2.52	0.43
1:AA:1317:C:C2	8:AN:16:PHE:CE1	3.06	0.43
1:AA:1423:G:H2'	1:AA:1424:C:O4'	2.19	0.43
1:AA:1442:G:C8	1:AA:1442(B):A:C2	3.06	0.43
1:AA:1531:A:O3'	1:AA:1532:U:C6	2.70	0.43
5:AK:33:THR:HG22	5:AK:39:PRO:HA	2.01	0.43
11:AQ:50:LYS:HG3	11:AQ:51:TYR:CE1	2.53	0.43
16:AC:10:PHE:CE2	16:AC:178:LEU:HD13	2.52	0.43
17:AD:176:LEU:HD12	17:AD:182:LYS:O	2.18	0.43
25:BA:105:C:H2'	25:BA:106:C:C6	2.53	0.43
25:BA:445:C:H2'	25:BA:446:G:O4'	2.18	0.43
25:BA:601:C:O2	25:BA:605:C:H4'	2.17	0.43
25:BA:1058:G:C8	25:BA:1058:G:C5'	3.01	0.43
25:BA:1168:G:H2'	25:BA:1169:G:O4'	2.17	0.43
25:BA:1344:G:H4'	25:BA:1384:A:C5	2.53	0.43
25:BA:2077:A:C2'	25:BA:2434:A:O2'	2.66	0.43
25:BA:2180:U:OP2	25:BA:2180:U:H3'	2.18	0.43
25:BA:2821:A:OP1	52:BE:110:GLY:N	2.47	0.43
29:BP:57:THR:CB	29:BP:59:LEU:HB2	2.47	0.43
33:BT:93:ARG:HD2	33:BT:93:ARG:HA	1.83	0.43
35:BV:47:VAL:O	35:BV:48:GLY:C	2.56	0.43
39:BZ:8:TYR:N	39:BZ:8:TYR:CD1	2.86	0.43
43:BD:2:ALA:O	43:BD:3:VAL:CB	2.54	0.43
47:B6:12:GLU:HB2	47:B6:52:VAL:HG13	1.99	0.43
53:BF:157:VAL:O	53:BF:157:VAL:CG2	2.65	0.43
54:BG:54:GLU:HA	54:BG:57:ALA:CB	2.44	0.43
1:AA:416:G:C6	1:AA:417:C:C4	3.06	0.43
1:AA:706:A:O2'	5:AK:31:THR:CG2	2.67	0.43
1:AA:985:C:C2	1:AA:1221:G:N2	2.86	0.43
1:AA:1069:C:C2'	1:AA:1070:U:O5'	2.66	0.43
1:AA:1158:C:O2	1:AA:1158:C:H2'	2.17	0.43
1:AA:1288:A:H2'	1:AA:1289:A:O4'	2.17	0.43
11:AQ:100:LYS:HD3	11:AQ:100:LYS:N	2.33	0.43
16:AC:155:GLY:O	16:AC:156:ARG:HB2	2.18	0.43
23:AY:190:ASN:ND2	23:AY:194:THR:OG1	2.44	0.43
25:BA:336:C:O3'	38:BY:7:VAL:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:998:C:H2'	25:BA:999:U:O5'	2.18	0.43
25:BA:1210:A:H5'	25:BA:1210:A:C8	2.50	0.43
25:BA:1569:A:O4'	43:BD:59:LYS:NZ	2.51	0.43
25:BA:1684:C:O2'	25:BA:1685:C:H5'	2.18	0.43
25:BA:2103:C:H3'	25:BA:2104:G:H5"	2.00	0.43
25:BA:2113:U:H5"	25:BA:2114:A:OP2	2.18	0.43
25:BA:2746:U:C2'	25:BA:2747:G:H5'	2.48	0.43
25:BA:2810:A:C2'	52:BE:61:ARG:NH2	2.79	0.43
25:BA:2876:G:H4'	33:BT:3:ARG:HE	1.83	0.43
33:BT:26:ASP:O	33:BT:26:ASP:OD2	2.35	0.43
33:BT:107:ASP:OD1	33:BT:107:ASP:N	2.51	0.43
39:BZ:7:ALA:C	39:BZ:8:TYR:CD1	2.91	0.43
42:B2:12:GLU:HA	42:B2:15:LYS:HE2	2.01	0.43
43:BD:108:PRO:HD2	43:BD:111:LEU:HD12	2.00	0.43
51:BC:131:LEU:CB	51:BC:137:LEU:HD23	2.46	0.43
1:AA:178:C:C2	1:AA:179:A:C8	3.06	0.43
1:AA:795:C:H5"	1:AA:796:C:OP2	2.18	0.43
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.53	0.43
1:AA:1053:G:H4'	1:AA:1054:C:H5'	2.00	0.43
1:AA:1206:G:H2'	1:AA:1207:G:O4'	2.17	0.43
1:AA:1245:A:H2'	1:AA:1246:C:O4'	2.18	0.43
1:AA:1328:C:H5"	7:AM:28:ALA:CB	2.48	0.43
1:AA:1534:A:H2'	1:AA:1535:C:C6	2.53	0.43
16:AC:141:VAL:HG11	16:AC:149:ALA:HB2	2.00	0.43
19:AF:16:GLN:HE21	19:AF:16:GLN:HB3	1.64	0.43
20:AG:15:ASP:O	20:AG:19:GLY:HA2	2.18	0.43
22:AI:49:PRO:HG2	22:AI:81:ILE:HG22	2.01	0.43
23:AY:485:GLU:O	23:AY:560:VAL:HA	2.18	0.43
25:BA:128:C:H3'	25:BA:128:C:C6	2.53	0.43
25:BA:2137:C:H3'	25:BA:2138:C:H5"	2.00	0.43
25:BA:2291:U:H2'	25:BA:2292:C:C6	2.53	0.43
25:BA:2419:U:O4	49:B8:30:ARG:NH1	2.48	0.43
25:BA:2577:A:H5"	25:BA:2578:G:H5'	1.99	0.43
26:BB:81:G:O6	26:BB:96:U:O2	2.36	0.43
29:BP:7:ARG:NH1	29:BP:7:ARG:O	2.52	0.43
33:BT:16:ARG:HG2	33:BT:79:HIS:HA	1.99	0.43
33:BT:31:SER:HB2	33:BT:32:TYR:CD2	2.54	0.43
36:BW:33:ARG:NH2	36:BW:52:GLU:OE1	2.42	0.43
39:BZ:71:VAL:HG11	39:BZ:74:VAL:HG23	2.00	0.43
47:B6:41:PRO:HG2	47:B6:44:ARG:O	2.18	0.43
57:BJ:118:ALA:O	57:BJ:119:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AV:35:A:C5'	2:AV:35:A:C8	3.01	0.43
23:AY:605:ILE:HD13	23:AY:677:GLN:HB3	1.99	0.43
25:BA:128:C:H4'	25:BA:129:C:OP1	2.19	0.43
25:BA:336:C:H4'	38:BY:7:VAL:HG21	2.00	0.43
25:BA:607:U:C5'	53:BF:103:LYS:HE2	2.48	0.43
25:BA:742:G:H4'	25:BA:1676:A:H5'	2.00	0.43
25:BA:1021:A:O2'	25:BA:1123:C:OP1	2.33	0.43
25:BA:1430:C:H2'	25:BA:1431:U:H6	1.83	0.43
25:BA:1644:C:C2'	25:BA:1645:G:H5'	2.48	0.43
25:BA:1762:A:H8	25:BA:1762:A:O5'	2.01	0.43
25:BA:1820:U:H4'	25:BA:1821:A:OP2	2.18	0.43
25:BA:2392:A:H2	25:BA:2424:C:N4	2.06	0.43
25:BA:2740:A:C6	25:BA:2741:A:C6	3.06	0.43
25:BA:2774:C:H2'	25:BA:2775:A:O4'	2.17	0.43
28:BO:43:VAL:HG12	28:BO:54:GLU:HA	2.01	0.43
29:BP:16:ARG:HD3	29:BP:17:LYS:N	2.33	0.43
33:BT:29:ARG:HE	33:BT:86:ILE:HG22	1.83	0.43
35:BV:28:GLU:HG3	35:BV:29:PRO:HD3	2.00	0.43
51:BC:84:LYS:O	51:BC:86:ALA:N	2.43	0.43
52:BE:61:ARG:HA	52:BE:63:LEU:HB2	1.99	0.43
1:AA:1378:C:OP1	20:AG:6:ARG:O	2.36	0.43
6:AL:18:VAL:CG2	6:AL:19:ARG:N	2.82	0.43
8:AN:57:ARG:NH2	16:AC:13:GLY:HA3	2.33	0.43
13:AS:78:ARG:HD2	13:AS:81:ARG:HH12	1.83	0.43
18:AE:11:ILE:HG22	18:AE:31:LEU:HB3	2.00	0.43
18:AE:36:ASP:O	18:AE:37:ARG:HB2	2.17	0.43
23:AY:169:GLY:HA3	23:AY:173:THR:O	2.18	0.43
25:BA:543:C:C5'	25:BA:543:C:H6	2.32	0.43
25:BA:623:G:H2'	25:BA:624:C:C6	2.53	0.43
25:BA:1881:C:H5"	25:BA:1881:C:H6	1.83	0.43
33:BT:65:LYS:HE3	33:BT:67:SER:HB2	2.01	0.43
41:B1:3:LYS:CG	41:B1:4:VAL:N	2.80	0.43
43:BD:43:ARG:CB	43:BD:54:ARG:HB2	2.47	0.43
51:BC:84:LYS:C	51:BC:86:ALA:N	2.72	0.43
1:AA:310:G:OP2	10:AP:27:LYS:HE2	2.18	0.43
1:AA:689:C:H2'	1:AA:690:G:O4'	2.18	0.43
1:AA:812:C:OP1	1:AA:903:G:H1'	2.19	0.43
1:AA:1157:A:H4'	1:AA:1158:C:O5'	2.19	0.43
7:AM:59:TYR:O	7:AM:63:THR:OG1	2.15	0.43
9:AO:82:ILE:HG13	9:AO:88:ARG:HB2	2.01	0.43
11:AQ:45:HIS:CB	11:AQ:65:ILE:HD13	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AQ:59:ILE:HA	11:AQ:59:ILE:HD13	1.75	0.43
15:AB:200:ILE:HB	15:AB:202:PRO:HD3	2.01	0.43
23:AY:181:LEU:HD23	23:AY:182:ARG:NH1	2.34	0.43
23:AY:205:TYR:HA	23:AY:208:GLN:HB3	2.00	0.43
23:AY:264:LEU:HD13	23:AY:265:LYS:HE3	2.01	0.43
23:AY:684:GLN:N	23:AY:687:LEU:HB2	2.33	0.43
25:BA:228:A:H3'	25:BA:229:A:C5'	2.48	0.43
25:BA:579:G:H2'	25:BA:580:C:C6	2.54	0.43
25:BA:876:C:H2'	25:BA:877:U:O4'	2.19	0.43
25:BA:1073:A:H2'	25:BA:1074:G:O4'	2.18	0.43
25:BA:1131:G:N2	27:BN:73:THR:HG23	2.33	0.43
25:BA:1674:G:H1'	25:BA:1676:A:N6	2.33	0.43
25:BA:2009:G:OP1	36:BW:41:LYS:HE2	2.19	0.43
25:BA:2352:A:C4	25:BA:2366:A:C2	3.06	0.43
26:BB:84:C:H2'	26:BB:85:G:O5'	2.18	0.43
27:BN:39:ARG:HD3	27:BN:41:ASP:OD1	2.18	0.43
27:BN:67:LEU:O	27:BN:68:GLU:CB	2.65	0.43
47:B6:51:GLU:HG3	47:B6:52:VAL:N	2.32	0.43
49:B8:62:LEU:O	49:B8:64:TYR:N	2.49	0.43
1:AA:1134:G:C4	1:AA:1135:U:C6	3.06	0.43
2:AV:1:G:C2	2:AV:73:A:C8	3.07	0.43
2:AV:36:A:C2	3:AX:19:U:C2	3.06	0.43
4:AJ:22:LYS:C	4:AJ:24:VAL:H	2.21	0.43
15:AB:23:ARG:HG3	15:AB:23:ARG:O	2.18	0.43
15:AB:62:ALA:C	15:AB:64:ARG:H	2.21	0.43
17:AD:28:SER:HB3	17:AD:30:LYS:HG3	2.01	0.43
18:AE:50:GLU:OE1	18:AE:50:GLU:HA	2.18	0.43
18:AE:107:ARG:O	18:AE:108:ALA:C	2.56	0.43
19:AF:3:ARG:CZ	19:AF:3:ARG:HB2	2.49	0.43
23:AY:86:GLY:O	23:AY:117:GLN:HG2	2.19	0.43
25:BA:385:C:O2	29:BP:71:VAL:HG21	2.18	0.43
25:BA:983:A:C6	25:BA:984:A:N1	2.87	0.43
25:BA:1181:C:C2'	25:BA:1182:A:H5'	2.48	0.43
25:BA:1538:G:C2'	25:BA:1539:G:O5'	2.66	0.43
25:BA:1722:A:C6	25:BA:1741:A:N1	2.87	0.43
25:BA:2056:G:N2	46:B5:5:PRO:HA	2.34	0.43
25:BA:2712:U:O2	25:BA:2712:U:H5'	2.19	0.43
25:BA:2815:C:O2'	46:B5:42:PRO:HG2	2.19	0.43
26:BB:42:C:C5'	54:BG:69:ALA:HB2	2.49	0.43
29:BP:13:ASN:OD1	53:BF:31:HIS:CB	2.67	0.43
30:BQ:16:ARG:O	30:BQ:17:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BZ:23:LYS:O	39:BZ:25:PRO:HD3	2.19	0.43
39:BZ:196:VAL:O	39:BZ:197:ILE:C	2.56	0.43
43:BD:10:THR:C	43:BD:11:PRO:O	2.55	0.43
54:BG:131:TYR:HB3	54:BG:159:VAL:CG1	2.49	0.43
55:BH:26:VAL:O	55:BH:32:GLU:HA	2.18	0.43
55:BH:37:VAL:HG13	55:BH:68:THR:HG21	2.00	0.43
56:BK:29:GLN:O	56:BK:59:ILE:HD12	2.19	0.43
1:AA:504:C:C2	1:AA:542:G:N2	2.87	0.43
21:AH:50:ARG:O	21:AH:51:VAL:CG1	2.67	0.43
23:AY:395:PRO:O	23:AY:397:VAL:N	2.51	0.43
25:BA:422:A:C6	25:BA:423:A:C6	3.06	0.43
25:BA:702:G:C2	25:BA:731:C:C2	3.06	0.43
25:BA:2035:G:H4'	25:BA:2036:C:OP2	2.18	0.43
25:BA:2298:A:H2'	25:BA:2299:G:O4'	2.17	0.43
25:BA:2305:A:C2	25:BA:2306:C:C1'	2.95	0.43
25:BA:2734:A:C5'	25:BA:2735:G:OP2	2.65	0.43
28:BO:66:LYS:HD2	28:BO:80:ASP:O	2.18	0.43
29:BP:136:GLU:O	29:BP:138:LEU:N	2.51	0.43
43:BD:224:ALA:N	43:BD:233:HIS:HB2	2.32	0.43
49:B8:26:LYS:HB2	49:B8:44:LYS:HG3	2.00	0.43
54:BG:37:VAL:HG22	54:BG:159:VAL:HG23	2.01	0.43
1:AA:1030:C:N4	1:AA:1032:G:C2	2.86	0.43
1:AA:1303:C:H2'	1:AA:1304:G:H5'	2.01	0.43
1:AA:1326:C:OP1	24:AU:12:LYS:NZ	2.25	0.43
15:AB:80:ILE:HD12	15:AB:80:ILE:H	1.84	0.43
23:AY:122:TRP:CZ2	23:AY:159:ALA:HB2	2.53	0.43
25:BA:27:G:HO2'	25:BA:28:A:P	2.41	0.43
25:BA:508:G:C5'	25:BA:509:C:OP1	2.67	0.43
25:BA:760:G:H4'	25:BA:1776:G:OP1	2.19	0.43
25:BA:1174:A:OP1	25:BA:1175:U:H5"	2.17	0.43
25:BA:1322:A:C5	25:BA:1323:U:C5	3.06	0.43
25:BA:1504:C:H1'	25:BA:1505:C:H5"	2.01	0.43
25:BA:1512:U:H2'	25:BA:1513:C:C6	2.53	0.43
25:BA:1975:G:H2'	25:BA:1976:U:O4'	2.19	0.43
25:BA:2151:G:H5"	25:BA:2151:G:H8	1.84	0.43
29:BP:144:GLU:N	29:BP:145:PRO:HD3	2.33	0.43
32:BS:89:ARG:HG2	32:BS:92:TYR:CA	2.49	0.43
33:BT:12:SER:O	33:BT:13:ARG:CZ	2.67	0.43
42:B2:63:VAL:O	42:B2:66:GLU:HG2	2.18	0.43
52:BE:59:VAL:C	52:BE:60:ASN:HD22	2.21	0.43
52:BE:61:ARG:H	52:BE:62:PRO:CD	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BE:144:ARG:HB3	52:BE:145:LYS:H	1.62	0.43
54:BG:56:ALA:CB	54:BG:153:ARG:NH1	2.82	0.43
1:AA:428:G:C4’	1:AA:429:U:O5’	2.66	0.43
1:AA:1237:C:H2’	1:AA:1238:A:OP1	2.18	0.43
2:AV:47:U:H3’	2:AV:48:C:H5”	2.01	0.43
4:AJ:24:VAL:HG22	4:AJ:34:VAL:HG11	2.00	0.43
7:AM:31:LYS:O	7:AM:35:GLU:HG2	2.18	0.43
25:BA:362:U:H6	25:BA:362:U:H5”	1.84	0.43
25:BA:459:U:H5”	48:B7:40:TRP:CD2	2.54	0.43
25:BA:464:U:O2’	48:B7:16:HIS:CE1	2.72	0.43
25:BA:1039:G:H1’	25:BA:1117:G:N2	2.34	0.43
25:BA:1786:A:N1	25:BA:2606:C:C1’	2.82	0.43
25:BA:1799:G:H5’	25:BA:1819:A:N6	2.34	0.43
25:BA:2623:G:H4’	25:BA:2825:C:O2	2.19	0.43
25:BA:2741:A:H2’	25:BA:2742:C:O4’	2.18	0.43
26:BB:46:A:C5	26:BB:47:C:C4	3.07	0.43
27:BN:89:LYS:O	27:BN:93:THR:HG22	2.18	0.43
29:BP:83:VAL:CG1	29:BP:112:LEU:HD21	2.49	0.43
33:BT:61:PHE:CE2	33:BT:76:PHE:HB2	2.54	0.43
36:BW:68:ARG:O	36:BW:110:LYS:HB3	2.19	0.43
43:BD:221:VAL:HG22	43:BD:226:MET:HE2	2.01	0.43
51:BC:185:LEU:O	51:BC:186:ALA:C	2.57	0.43
51:BC:215:THR:HB	51:BC:221:SER:HA	2.01	0.43
53:BF:114:VAL:HG21	53:BF:202:PHE:CZ	2.53	0.43
54:BG:72:ARG:HA	54:BG:87:PRO:HD2	2.00	0.43
56:BK:57:ILE:HD12	56:BK:57:ILE:H	1.84	0.43
1:AA:155:C:H2’	1:AA:156:G:O4’	2.19	0.42
1:AA:1013:G:H5’	1:AA:1014:A:OP2	2.19	0.42
5:AK:84:VAL:HG22	5:AK:110:ASP:HA	2.01	0.42
6:AL:60:LEU:HB3	6:AL:62:SER:H	1.84	0.42
16:AC:179:ARG:HG3	16:AC:207:VAL:H	1.84	0.42
21:AH:13:ILE:O	21:AH:17:THR:HG23	2.19	0.42
22:AI:4:TYR:CD2	22:AI:88:TYR:HB2	2.54	0.42
25:BA:387:U:O5’	25:BA:387:U:H6	2.01	0.42
25:BA:638:G:H2’	25:BA:639:U:O4’	2.19	0.42
25:BA:832:G:H21	29:BP:53:GLY:HA3	1.83	0.42
25:BA:973:A:O4’	25:BA:1188:U:C6	2.72	0.42
25:BA:1094:U:H6	25:BA:1094:U:C5’	2.32	0.42
25:BA:1445:A:N3	25:BA:1445:A:C2’	2.82	0.42
25:BA:1817:G:H5”	43:BD:88:ARG:NH2	2.34	0.42
25:BA:1876:A:H2’	25:BA:1877:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2134:A:C8	25:BA:2135:A:C8	3.06	0.42
25:BA:2139:C:O2'	25:BA:2140:C:O2	2.36	0.42
25:BA:2174:C:O2	51:BC:218:MET:SD	2.77	0.42
25:BA:2261:C:H3'	40:B0:16:SER:OG	2.19	0.42
25:BA:2864:G:H2'	25:BA:2865:U:O4'	2.19	0.42
26:BB:65:C:H2'	26:BB:66:A:H5'	2.01	0.42
33:BT:1:MET:O	33:BT:3:ARG:N	2.52	0.42
33:BT:125:ARG:C	33:BT:127:ALA:H	2.22	0.42
34:BU:64:ARG:O	34:BU:65:ILE:C	2.57	0.42
46:B5:33:CYS:SG	46:B5:34:PRO:O	2.76	0.42
46:B5:52:TYR:O	46:B5:52:TYR:CG	2.72	0.42
54:BG:6:ALA:HB3	54:BG:104:GLU:OE2	2.19	0.42
55:BH:41:MET:HE3	55:BH:43:VAL:N	2.34	0.42
57:BJ:94:ALA:O	57:BJ:97:ALA:HB3	2.19	0.42
1:AA:269:C:H2'	1:AA:270:A:H8	1.81	0.42
16:AC:12:LEU:O	16:AC:16:ARG:O	2.37	0.42
24:AU:12:LYS:O	24:AU:13:ILE:C	2.58	0.42
25:BA:370:G:O5'	25:BA:370:G:H8	2.02	0.42
25:BA:642:G:O3'	47:B6:42:TRP:CZ2	2.72	0.42
25:BA:1050:A:H2'	25:BA:1051:G:C8	2.54	0.42
25:BA:1313:U:O2	25:BA:1313:U:C2'	2.66	0.42
25:BA:1494:A:O2'	25:BA:1495:A:OP1	2.19	0.42
25:BA:1777:U:O2'	25:BA:1778:U:H5'	2.19	0.42
25:BA:1847:A:H5'	25:BA:1848:A:OP2	2.19	0.42
25:BA:2219:G:H8	25:BA:2219:G:O5'	2.02	0.42
25:BA:2273:A:H2'	25:BA:2274:A:C8	2.54	0.42
25:BA:2392:A:OP1	49:B8:32:LEU:HD22	2.19	0.42
27:BN:16:ILE:HD11	27:BN:26:LEU:CD1	2.34	0.42
27:BN:132:ALA:O	27:BN:133:GLN:O	2.37	0.42
29:BP:146:VAL:HG22	29:BP:147:LEU:H	1.83	0.42
30:BQ:98:LYS:HB3	30:BQ:99:PRO:HD2	2.00	0.42
35:BV:18:LEU:O	35:BV:19:LYS:O	2.37	0.42
36:BW:1:MET:HE3	36:BW:2:GLU:H	1.84	0.42
37:BX:10:ALA:HB1	37:BX:11:PRO:HD2	2.01	0.42
46:B5:34:PRO:O	46:B5:35:GLU:CB	2.67	0.42
1:AA:1051:C:O5'	1:AA:1051:C:H6	2.02	0.42
2:AV:30:G:H5"	2:AV:30:G:H8	1.84	0.42
4:AJ:61:GLU:OE2	8:AN:45:ARG:NH1	2.47	0.42
15:AB:59:GLU:HB2	15:AB:221:LEU:HD11	2.00	0.42
16:AC:87:LEU:O	16:AC:91:LEU:HG	2.18	0.42
16:AC:108:ASN:HA	16:AC:109:PRO:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AE:100:VAL:O	18:AE:107:ARG:NH2	2.50	0.42
22:AI:99:LEU:HD13	22:AI:99:LEU:N	2.33	0.42
23:AY:94:VAL:C	23:AY:96:ARG:N	2.72	0.42
23:AY:483:TYR:CE1	23:AY:603:GLU:HB3	2.54	0.42
25:BA:437:G:H8	25:BA:437:G:O5'	2.01	0.42
25:BA:1945:G:H2'	25:BA:1946:U:C6	2.55	0.42
25:BA:2001:A:H2'	25:BA:2002:G:C8	2.54	0.42
25:BA:2078:C:C4	25:BA:2079:U:C4	3.07	0.42
25:BA:2287:A:H62	25:BA:2344:U:H3	1.67	0.42
29:BP:108:LYS:C	29:BP:110:TYR:H	2.20	0.42
34:BU:92:ARG:HD2	35:BV:11:GLN:HB2	2.01	0.42
35:BV:47:VAL:C	35:BV:49:THR:O	2.58	0.42
38:BY:2:ARG:C	38:BY:4:LYS:H	2.11	0.42
53:BF:40:GLN:O	53:BF:44:ARG:HG2	2.19	0.42
53:BF:139:PHE:CZ	53:BF:156:LEU:HD22	2.54	0.42
1:AA:120:A:C6	1:AA:122:G:C2	3.07	0.42
1:AA:222:U:H2'	1:AA:223:U:C6	2.54	0.42
1:AA:417:C:H2'	1:AA:418:C:C6	2.51	0.42
1:AA:679:C:H2'	1:AA:680:C:C6	2.54	0.42
1:AA:1128:C:O2'	1:AA:1129:C:H5'	2.19	0.42
1:AA:1286:A:C8	1:AA:1287:A:H4'	2.55	0.42
7:AM:84:ILE:O	7:AM:84:ILE:HG22	2.20	0.42
18:AE:102:ALA:HB2	18:AE:120:THR:HG21	2.01	0.42
20:AG:138:LYS:O	20:AG:142:GLU:HG3	2.19	0.42
23:AY:181:LEU:HD23	23:AY:182:ARG:HG3	2.00	0.42
25:BA:185:U:C2	25:BA:212:G:N2	2.87	0.42
25:BA:300:A:H2'	25:BA:334:C:H1'	2.01	0.42
25:BA:954:G:N3	25:BA:2274:A:C2	2.88	0.42
25:BA:1532:C:O2	25:BA:1532:C:H2'	2.17	0.42
25:BA:1578:U:C2'	25:BA:1579:A:H5'	2.49	0.42
25:BA:1833:U:O2	25:BA:1969:A:C2	2.71	0.42
25:BA:1952:A:C4	28:BO:22:ILE:HG13	2.55	0.42
25:BA:1977:A:C2'	25:BA:1978:A:O5'	2.67	0.42
25:BA:2095:C:H2'	25:BA:2096:U:O4'	2.19	0.42
25:BA:2331:G:O4'	40:B0:42:GLY:HA3	2.19	0.42
26:BB:33:G:N3	26:BB:50:G:C2	2.88	0.42
27:BN:42:TRP:CD1	34:BU:63:VAL:HG11	2.55	0.42
33:BT:89:VAL:HG21	33:BT:91:ARG:CZ	2.49	0.42
35:BV:8:GLY:O	35:BV:10:LYS:HE3	2.19	0.42
42:B2:42:GLY:O	42:B2:44:LEU:O	2.37	0.42
1:AA:427:U:C4	1:AA:428:G:C6	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:990:C:C4	1:AA:991:U:C5	3.07	0.42
1:AA:1342:C:H2'	1:AA:1343:G:C8	2.54	0.42
15:AB:15:VAL:C	15:AB:16:HIS:CG	2.92	0.42
25:BA:300:A:H1'	25:BA:319:C:O4'	2.20	0.42
25:BA:562:U:C4	25:BA:2036:C:O4'	2.72	0.42
25:BA:586:A:C2	25:BA:809:G:N3	2.87	0.42
25:BA:588:U:H2'	25:BA:589:C:C6	2.54	0.42
25:BA:1006:C:O2'	27:BN:106:MET:HB3	2.20	0.42
25:BA:2754:U:H2'	25:BA:2756:U:OP1	2.18	0.42
25:BA:2820:A:C8	52:BE:109:LYS:HE2	2.54	0.42
30:BQ:76:LYS:HB3	30:BQ:91:GLU:CG	2.50	0.42
32:BS:16:ASN:OD1	32:BS:17:ARG:N	2.52	0.42
34:BU:112:ARG:NH2	35:BV:46:VAL:CG1	2.82	0.42
39:BZ:61:LEU:CD2	39:BZ:61:LEU:N	2.82	0.42
41:B1:44:PRO:HB2	41:B1:46:LEU:CD1	2.48	0.42
42:B2:21:LEU:HD23	42:B2:21:LEU:HA	1.83	0.42
43:BD:65:ILE:HD11	43:BD:67:PHE:CE1	2.55	0.42
43:BD:171:ASP:OD2	43:BD:171:ASP:N	2.53	0.42
43:BD:270:ILE:O	43:BD:270:ILE:HD12	2.20	0.42
44:B3:19:GLN:NE2	44:B3:52:HIS:NE2	2.67	0.42
47:B6:15:GLU:OE1	47:B6:18:ARG:HD2	2.19	0.42
52:BE:13:ARG:HD2	52:BE:20:ALA:HB1	2.01	0.42
56:BK:99:ILE:O	56:BK:139:VAL:N	2.52	0.42
1:AA:559:A:OP1	18:AE:126:ARG:NH2	2.48	0.42
1:AA:620:C:C2	17:AD:135:LEU:HG	2.55	0.42
1:AA:1078:U:H1'	18:AE:130:ASN:OD1	2.20	0.42
1:AA:1273:G:H8	1:AA:1273:G:H5"	1.83	0.42
5:AK:21:ILE:HG12	5:AK:30:VAL:CG1	2.50	0.42
11:AQ:45:HIS:HB2	11:AQ:65:ILE:CD1	2.49	0.42
14:AT:96:GLY:O	14:AT:97:ALA:CB	2.68	0.42
18:AE:131:ILE:HD13	18:AE:131:ILE:HA	1.93	0.42
23:AY:115:GLU:HB3	23:AY:116:PRO:CD	2.49	0.42
25:BA:304:G:H2'	25:BA:305:U:C6	2.55	0.42
25:BA:334:C:H2'	25:BA:335:C:OP1	2.19	0.42
25:BA:1394:U:H4'	25:BA:1603:A:H4'	2.00	0.42
26:BB:81:G:C6	26:BB:82:G:C5	3.07	0.42
27:BN:36:GLY:CA	27:BN:49:GLY:HA2	2.48	0.42
27:BN:93:THR:HG1	27:BN:94:HIS:CD2	2.38	0.42
27:BN:108:PRO:O	27:BN:113:GLY:HA3	2.19	0.42
29:BP:18:ARG:NH1	29:BP:18:ARG:HB3	2.35	0.42
31:BR:44:LEU:CD2	31:BR:48:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B0:50:ASN:HB3	40:B0:63:VAL:HG22	2.02	0.42
47:B6:42:TRP:CE3	47:B6:42:TRP:HA	2.55	0.42
49:B8:36:LYS:HD2	49:B8:41:ILE:HG22	2.02	0.42
55:BH:15:VAL:HG23	55:BH:15:VAL:O	2.18	0.42
55:BH:157:TYR:HD1	55:BH:173:PRO:HG3	1.84	0.42
1:AA:346:G:H5'	33:BT:41:ARG:CZ	2.50	0.42
1:AA:1092:A:C6	1:AA:1093:A:C6	3.08	0.42
1:AA:1118:C:C1'	1:AA:1179:A:C4	3.02	0.42
1:AA:1179:A:H2'	1:AA:1180:A:O4'	2.18	0.42
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.55	0.42
8:AN:9:LYS:O	8:AN:9:LYS:HG2	2.19	0.42
8:AN:23:ARG:NH1	8:AN:30:ALA:HB2	2.34	0.42
15:AB:8:LYS:HD3	15:AB:8:LYS:HA	1.92	0.42
15:AB:39:ILE:HG22	15:AB:41:ILE:CD1	2.50	0.42
15:AB:47:THR:HG22	15:AB:51:LEU:HD12	2.00	0.42
16:AC:167:TRP:O	16:AC:168:ALA:CB	2.68	0.42
17:AD:31:CYS:O	17:AD:33:MET:N	2.47	0.42
23:AY:335:LEU:HD11	23:AY:352:VAL:HG11	2.00	0.42
23:AY:587:SER:O	23:AY:591:LYS:HB2	2.20	0.42
25:BA:548:A:O2'	25:BA:549:G:P	2.77	0.42
25:BA:572:A:OP2	35:BV:78:LYS:HE2	2.19	0.42
25:BA:979:G:H3'	25:BA:980:A:H5"	2.02	0.42
25:BA:1090:U:H3	25:BA:1101:U:H3	1.67	0.42
25:BA:1329:U:H3'	25:BA:1330:C:H6	1.84	0.42
25:BA:1416:G:C4	25:BA:1417:C:C5	3.07	0.42
25:BA:1721:G:N2	25:BA:1739:U:OP2	2.53	0.42
25:BA:2151:G:N1	25:BA:2152:G:C5	2.88	0.42
25:BA:2811:G:H2'	25:BA:2812:G:O4'	2.20	0.42
29:BP:97:PRO:O	29:BP:98:GLU:CB	2.68	0.42
33:BT:32:TYR:CD2	33:BT:81:PRO:O	2.72	0.42
33:BT:62:THR:HA	33:BT:74:ARG:O	2.20	0.42
35:BV:64:HIS:HD1	35:BV:92:THR:HG22	1.78	0.42
43:BD:27:THR:HG22	43:BD:81:ALA:HB1	2.01	0.42
43:BD:45:ASN:ND2	43:BD:46:GLN:N	2.68	0.42
44:B3:50:VAL:CG2	44:B3:54:VAL:HG21	2.50	0.42
56:BK:105:LEU:HD21	56:BK:120:LEU:HD13	2.01	0.42
56:BK:136:VAL:O	56:BK:136:VAL:HG13	2.20	0.42
1:AA:73:G:H2'	1:AA:76:C:O4'	2.19	0.42
1:AA:339:C:OP2	28:BO:97:ARG:NH1	2.52	0.42
1:AA:355:C:H2'	1:AA:356:A:O4'	2.20	0.42
1:AA:920:U:H2'	1:AA:921:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AM:99:ARG:HB2	7:AM:101:GLN:HE21	1.84	0.42
15:AB:155:LEU:HD22	15:AB:155:LEU:HA	1.87	0.42
17:AD:71:SER:OG	17:AD:74:GLN:HB2	2.20	0.42
19:AF:23:LYS:O	19:AF:27:GLN:HG2	2.19	0.42
23:AY:209:ALA:O	23:AY:210:ARG:HB2	2.20	0.42
23:AY:344:THR:HG23	23:AY:390:VAL:HG22	2.02	0.42
25:BA:122:G:H2'	25:BA:123:G:O5'	2.20	0.42
25:BA:271(F):C:H2'	25:BA:271(G):C:C6	2.55	0.42
25:BA:309:G:N3	25:BA:329:G:O2'	2.48	0.42
25:BA:832:G:N3	29:BP:53:GLY:HA2	2.35	0.42
25:BA:962:G:H4'	25:BA:2496:C:O2'	2.19	0.42
25:BA:1005:C:H2'	25:BA:1006:C:C6	2.54	0.42
25:BA:1299:G:H8	25:BA:1299:G:O5'	2.02	0.42
25:BA:1816:G:H8	43:BD:62:TYR:OH	2.02	0.42
25:BA:1959:G:C2'	25:BA:1960:A:O5'	2.68	0.42
25:BA:2135:A:H2'	25:BA:2136:C:O4'	2.19	0.42
25:BA:2702:U:H4'	25:BA:2703:C:OP1	2.20	0.42
30:BQ:27:VAL:O	30:BQ:105:GLU:OE1	2.37	0.42
31:BR:10:LEU:HD22	31:BR:17:ARG:CD	2.50	0.42
34:BU:92:ARG:HD3	34:BU:94:ASN:HB3	2.02	0.42
35:BV:39:LEU:HD13	35:BV:39:LEU:N	2.34	0.42
41:B1:3:LYS:HG2	41:B1:4:VAL:N	2.34	0.42
46:B5:40:LYS:HE2	46:B5:40:LYS:HB3	1.70	0.42
1:AA:684:A:N6	1:AA:685:G:C6	2.88	0.42
1:AA:836:G:C6	1:AA:851:G:C6	3.08	0.42
7:AM:83:ASP:OD1	7:AM:85:GLY:N	2.48	0.42
22:AI:71:SER:HA	22:AI:74:ILE:HD12	2.02	0.42
23:AY:418:LYS:O	23:AY:419:ALA:CB	2.67	0.42
23:AY:689:LYS:HG3	23:AY:689:LYS:O	2.19	0.42
25:BA:26:G:OP1	36:BW:80:PRO:HB3	2.20	0.42
25:BA:97:C:H5"	42:B2:2:LYS:HB2	2.02	0.42
25:BA:453:C:O2	25:BA:457:A:O2'	2.35	0.42
25:BA:813:U:H2'	25:BA:814:C:C6	2.54	0.42
25:BA:996:A:OP2	34:BU:92:ARG:NH2	2.53	0.42
25:BA:1857:G:C6	25:BA:1858:G:N1	2.88	0.42
25:BA:2230:G:C6	25:BA:2231:C:C4	3.07	0.42
25:BA:2420:C:O5'	25:BA:2420:C:H6	2.01	0.42
25:BA:2690:C:OP2	31:BR:14:SER:CB	2.67	0.42
25:BA:2795:G:H2'	25:BA:2795:G:N3	2.35	0.42
27:BN:28:THR:HG22	27:BN:29:LYS:N	2.34	0.42
33:BT:29:ARG:HE	33:BT:86:ILE:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BV:23:GLU:O	35:BV:24:LYS:C	2.57	0.42
36:BW:17:VAL:O	36:BW:18:ARG:C	2.55	0.42
43:BD:129:ASN:O	43:BD:193:VAL:HG12	2.19	0.42
49:B8:52:LYS:N	49:B8:53:PRO:CD	2.82	0.42
51:BC:88:GLU:O	51:BC:89:ALA:CB	2.68	0.42
53:BF:184:TYR:O	53:BF:188:ARG:HG2	2.19	0.42
55:BH:171:LEU:O	55:BH:173:PRO:CD	2.67	0.42
56:BK:99:ILE:HD12	56:BK:103:GLN:CB	2.45	0.42
1:AA:302:G:O3'	6:AL:17:LYS:HE2	2.20	0.42
1:AA:346:G:OP1	33:BT:35:LYS:NZ	2.52	0.42
1:AA:1146:A:N3	1:AA:1146:A:H2'	2.33	0.42
5:AK:59:TYR:O	5:AK:62:GLN:HB3	2.19	0.42
12:AR:61:LYS:O	12:AR:65:ILE:HG12	2.20	0.42
15:AB:37:ASN:HD22	15:AB:37:ASN:HA	1.68	0.42
17:AD:3:ARG:NE	17:AD:5:ILE:HG13	2.35	0.42
20:AG:108:ALA:O	20:AG:119:ARG:HD2	2.19	0.42
23:AY:85:PRO:HG2	23:AY:90:PHE:HB2	2.02	0.42
25:BA:280:C:N4	25:BA:281:G:C6	2.88	0.42
25:BA:530:G:N3	25:BA:530:G:O4'	2.52	0.42
25:BA:785:G:O2'	25:BA:1779:U:H5'	2.19	0.42
25:BA:864:G:C6	25:BA:865:C:N4	2.88	0.42
25:BA:1364:G:P	41:B1:61:ARG:HH22	2.43	0.42
25:BA:1470:G:H5"	25:BA:1471:A:OP1	2.20	0.42
25:BA:2324:C:H5"	25:BA:2325:G:H5'	2.01	0.42
25:BA:2584:U:O2	25:BA:2584:U:O4'	2.37	0.42
25:BA:2801:A:H2'	25:BA:2895:U:H4'	2.01	0.42
29:BP:106:LEU:O	29:BP:107:LYS:O	2.38	0.42
32:BS:56:LEU:HD23	32:BS:58:LEU:HB2	2.01	0.42
33:BT:4:GLY:HA2	52:BE:9:VAL:HG23	2.02	0.42
34:BU:74:LEU:CD2	34:BU:78:THR:HG22	2.50	0.42
42:B2:65:ASN:HB3	42:B2:69:ARG:NH2	2.35	0.42
43:BD:26:LYS:CD	43:BD:113:VAL:HG21	2.50	0.42
43:BD:33:LEU:HD23	43:BD:34:VAL:HG13	2.02	0.42
50:B9:32:HIS:O	50:B9:34:GLN:HG3	2.20	0.42
1:AA:90:U:O2'	1:AA:91:C:H5	1.86	0.41
1:AA:126:G:H5'	1:AA:633:G:N2	2.35	0.41
1:AA:264:U:H4'	11:AQ:63:ARG:HD3	2.02	0.41
1:AA:640:A:N3	21:AH:115:SER:HB3	2.35	0.41
1:AA:950:U:H2'	1:AA:951:G:C8	2.55	0.41
1:AA:1226:C:H2'	7:AM:103:THR:OG1	2.20	0.41
1:AA:1319:A:OP2	13:AS:5:LEU:HD23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1325:C:P	24:AU:6:ARG:HH12	2.43	0.41
1:AA:1517:G:H1'	25:BA:1919:A:O3'	2.20	0.41
4:AJ:85:LEU:C	4:AJ:87:THR:N	2.74	0.41
16:AC:113:ALA:HB3	16:AC:114:PRO:HD3	2.01	0.41
17:AD:78:LEU:HB3	17:AD:93:PHE:HE2	1.85	0.41
17:AD:194:LEU:HD22	17:AD:194:LEU:N	2.35	0.41
20:AG:13:GLN:O	20:AG:24:THR:HG21	2.20	0.41
21:AH:17:THR:OG1	21:AH:18:ARG:NH1	2.53	0.41
22:AI:53:VAL:HG13	22:AI:95:LYS:NZ	2.35	0.41
23:AY:320:PRO:O	23:AY:320:PRO:CD	2.67	0.41
23:AY:343:ASN:O	23:AY:347:GLY:N	2.53	0.41
23:AY:349:LYS:H	23:AY:349:LYS:HD3	1.85	0.41
25:BA:435:C:C2'	25:BA:436:C:H5'	2.50	0.41
25:BA:881:G:C2	25:BA:882:G:H1'	2.55	0.41
25:BA:1019:U:C2'	25:BA:1021:A:C2	3.03	0.41
25:BA:1168:G:C2	25:BA:1182:A:C2	3.08	0.41
25:BA:1370:C:HO2'	25:BA:1811:G:HO2'	1.67	0.41
25:BA:1417:C:H2'	25:BA:1418:G:O4'	2.20	0.41
25:BA:1475:G:C8	25:BA:1475:G:H5"	2.54	0.41
25:BA:2287:A:C2	25:BA:2346:A:C2	3.08	0.41
27:BN:56:ASN:H	27:BN:125:GLY:HA3	1.85	0.41
29:BP:16:ARG:HB2	29:BP:16:ARG:CZ	2.50	0.41
29:BP:127:ALA:HB3	29:BP:130:PHE:CE2	2.55	0.41
33:BT:23:ARG:O	33:BT:24:PRO:C	2.58	0.41
33:BT:29:ARG:CB	33:BT:30:VAL:HG22	2.41	0.41
35:BV:18:LEU:HD13	35:BV:19:LYS:H	1.85	0.41
39:BZ:17:ALA:O	39:BZ:20:ARG:HB3	2.19	0.41
39:BZ:54:HIS:CE1	39:BZ:123:ASP:OD1	2.73	0.41
46:B5:4:HIS:CB	46:B5:5:PRO:CD	2.82	0.41
1:AA:232:G:H1'	1:AA:262:A:N1	2.34	0.41
1:AA:367:U:H4'	23:AY:351:ARG:NE	2.35	0.41
1:AA:782:A:C6	1:AA:801:U:C2	3.08	0.41
1:AA:1187:G:C5'	1:AA:1187:G:C8	3.03	0.41
10:AP:58:TYR:O	10:AP:62:VAL:HG22	2.20	0.41
17:AD:26:CYS:CB	17:AD:31:CYS:HB2	2.50	0.41
17:AD:31:CYS:C	17:AD:33:MET:N	2.73	0.41
22:AI:9:ARG:CG	22:AI:14:VAL:HG13	2.50	0.41
22:AI:110:GLU:OE2	22:AI:113:LYS:NZ	2.48	0.41
23:AY:120:THR:O	23:AY:124:GLN:HG3	2.20	0.41
25:BA:228:A:H2'	25:BA:230:U:O4'	2.21	0.41
25:BA:414:C:OP1	25:BA:1879:C:O2'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1156:A:C8	34:BU:51:LYS:HD2	2.54	0.41
25:BA:2286:A:H4'	25:BA:2287:A:O4'	2.20	0.41
25:BA:2430:A:H8	25:BA:2431:U:H5	1.68	0.41
25:BA:2468:G:HO2'	25:BA:2476:A:H8	1.63	0.41
26:BB:39:A:N3	26:BB:39:A:H2'	2.35	0.41
33:BT:56:GLY:O	33:BT:59:THR:HG23	2.19	0.41
33:BT:57:PHE:O	33:BT:58:ASN:C	2.59	0.41
49:B8:14:VAL:CG2	49:B8:22:VAL:HG13	2.50	0.41
55:BH:105:LEU:H	55:BH:105:LEU:HD22	1.84	0.41
1:AA:390:C:H2'	1:AA:391:G:C8	2.55	0.41
1:AA:665:A:N3	1:AA:732:C:H2'	2.35	0.41
1:AA:1260:C:OP1	1:AA:1284:C:H4'	2.20	0.41
2:AV:73:A:C2'	2:AV:74:C:C5'	2.98	0.41
8:AN:28:GLY:O	8:AN:29:ARG:C	2.58	0.41
14:AT:63:ILE:HG22	14:AT:77:ALA:HB1	2.02	0.41
16:AC:196:LEU:CD2	16:AC:196:LEU:N	2.84	0.41
19:AF:76:ALA:HB1	19:AF:80:ARG:NH2	2.35	0.41
25:BA:629:G:OP1	25:BA:650:C:O2'	2.36	0.41
25:BA:896:A:N7	39:BZ:146:ILE:HD13	2.36	0.41
25:BA:945:A:C4	25:BA:2448:A:C2	3.08	0.41
25:BA:1286:A:N1	25:BA:1329:U:O2'	2.46	0.41
25:BA:2016:U:O5'	25:BA:2016:U:H6	2.03	0.41
25:BA:2055:C:H5'	25:BA:2056:G:O5'	2.19	0.41
25:BA:2219:G:C2	25:BA:2220:G:C8	3.08	0.41
29:BP:28:GLY:HA3	29:BP:29:LYS:HD2	2.02	0.41
31:BR:2:ARG:HD2	52:BE:111:ARG:HG3	2.02	0.41
32:BS:12:PHE:O	32:BS:12:PHE:CD1	2.74	0.41
33:BT:11:GLU:N	33:BT:11:GLU:CD	2.74	0.41
33:BT:57:PHE:O	33:BT:59:THR:N	2.54	0.41
36:BW:51:LEU:HD23	36:BW:105:VAL:HG11	2.02	0.41
48:B7:34:ARG:HB3	48:B7:39:ARG:HG3	2.02	0.41
53:BF:123:LEU:HD12	53:BF:124:LEU:N	2.35	0.41
1:AA:1135:U:O2	1:AA:1135:U:C2'	2.67	0.41
13:AS:5:LEU:HG	13:AS:10:PHE:CD1	2.51	0.41
15:AB:169:LYS:O	15:AB:169:LYS:HD3	2.20	0.41
17:AD:191:ARG:NH1	17:AD:200:GLU:OE1	2.54	0.41
18:AE:80:ILE:CD1	18:AE:138:ALA:HB1	2.50	0.41
21:AH:75:ARG:HA	21:AH:76:PRO:HD2	1.88	0.41
21:AH:97:VAL:HG13	21:AH:98:LYS:N	2.35	0.41
25:BA:95:G:O2'	42:B2:48:HIS:ND1	2.40	0.41
25:BA:259:G:C2'	25:BA:621:A:O2'	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:319:C:C2'	25:BA:320:A:O5'	2.68	0.41
25:BA:535:C:O2'	25:BA:536:A:H5'	2.20	0.41
25:BA:923:C:H2'	25:BA:924:C:C6	2.56	0.41
25:BA:1151:G:H5'	34:BU:81:HIS:CE1	2.54	0.41
25:BA:1290:C:O2'	25:BA:1291:C:H5'	2.20	0.41
25:BA:1570:A:OP1	43:BD:36:PRO:HB2	2.20	0.41
25:BA:1839:G:H1'	25:BA:1927:A:O5'	2.20	0.41
31:BR:55:ALA:HA	31:BR:80:PHE:CZ	2.55	0.41
31:BR:58:GLY:HA2	31:BR:80:PHE:CE1	2.56	0.41
43:BD:26:LYS:HG2	43:BD:113:VAL:HG21	2.02	0.41
46:B5:20:ARG:HG2	46:B5:23:HIS:CD2	2.56	0.41
49:B8:2:PRO:O	49:B8:3:LYS:CB	2.68	0.41
49:B8:32:LEU:HB3	49:B8:36:LYS:HZ1	1.81	0.41
49:B8:32:LEU:HB2	49:B8:36:LYS:CE	2.48	0.41
51:BC:17:ASN:O	51:BC:18:LYS:C	2.59	0.41
56:BK:130:SER:HA	56:BK:133:SER:OG	2.21	0.41
57:BJ:25:ALA:O	57:BJ:85:ALA:N	2.53	0.41
1:AA:266:G:O3'	11:AQ:67:LYS:HB2	2.20	0.41
1:AA:859:A:H2	21:AH:19:VAL:HG11	1.83	0.41
1:AA:1213:A:C8	1:AA:1215:G:C5	3.08	0.41
1:AA:1228:C:P	7:AM:108:ARG:NH2	2.94	0.41
1:AA:1326:C:O2'	1:AA:1327:C:H5'	2.20	0.41
14:AT:89:ARG:NH1	14:AT:105:SER:O	2.49	0.41
15:AB:11:LEU:HD13	15:AB:217:ARG:NH2	2.36	0.41
15:AB:19:HIS:CD2	15:AB:189:ASP:OD2	2.73	0.41
15:AB:40:HIS:HB3	15:AB:190:THR:HG21	2.01	0.41
23:AY:156:ARG:HB3	23:AY:156:ARG:HH11	1.85	0.41
23:AY:250:THR:CA	23:AY:255:ILE:HG22	2.50	0.41
25:BA:30:G:H2'	25:BA:31:C:O4'	2.21	0.41
25:BA:103:A:H8	25:BA:103:A:O5'	2.03	0.41
25:BA:475:U:C4	25:BA:481:G:O6	2.73	0.41
25:BA:660:G:C6	25:BA:661:C:C4	3.08	0.41
25:BA:783:A:C8	25:BA:783:A:H3'	2.55	0.41
25:BA:1021:A:H62	25:BA:1141:U:H3	1.67	0.41
25:BA:1039:G:O6	25:BA:1116:C:N3	2.53	0.41
25:BA:1446:C:C2	25:BA:1466:G:N2	2.87	0.41
25:BA:1876:A:H2'	25:BA:1877:A:H8	1.85	0.41
25:BA:2141:G:N2	25:BA:2151:G:H1'	2.36	0.41
25:BA:2154:G:C5'	25:BA:2154:G:C8	3.04	0.41
25:BA:2419:U:O4	49:B8:30:ARG:NE	2.52	0.41
25:BA:2592:G:C5	25:BA:2593:U:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2695:C:H2'	25:BA:2696:U:C6	2.55	0.41
27:BN:119:ARG:HG3	27:BN:119:ARG:NH1	2.34	0.41
31:BR:96:ARG:NH1	31:BR:115:GLU:OE1	2.46	0.41
49:B8:39:LYS:O	49:B8:43:GLN:HB2	2.20	0.41
51:BC:64:LEU:HD23	51:BC:64:LEU:HA	1.95	0.41
54:BG:19:LEU:HA	54:BG:22:ARG:HB2	2.03	0.41
55:BH:72:ILE:O	55:BH:75:ALA:HB3	2.19	0.41
1:AA:130:A:N6	1:AA:234:C:O4'	2.53	0.41
1:AA:242:C:H2'	1:AA:243:A:H5'	2.03	0.41
1:AA:1048:G:OP1	8:AN:4:LYS:HB2	2.20	0.41
1:AA:1119:C:O2'	1:AA:1120:G:H5'	2.21	0.41
1:AA:1256:A:H4'	1:AA:1258:G:C4	2.56	0.41
1:AA:1347:G:C6	22:AI:107:ARG:NH2	2.89	0.41
2:AV:46:G:H3'	2:AV:47:U:H5"	2.02	0.41
10:AP:70:ALA:O	10:AP:74:LEU:HD12	2.21	0.41
14:AT:93:GLU:OE1	14:AT:93:GLU:C	2.59	0.41
20:AG:66:VAL:HG12	20:AG:70:LYS:HE3	2.03	0.41
20:AG:74:GLU:HG2	20:AG:91:VAL:HG22	2.01	0.41
20:AG:143:ARG:HG2	20:AG:143:ARG:O	2.21	0.41
23:AY:18:ALA:O	23:AY:106:VAL:HA	2.20	0.41
23:AY:79:ILE:N	23:AY:79:ILE:CD1	2.83	0.41
23:AY:435:ASP:OD1	23:AY:435:ASP:C	2.58	0.41
25:BA:83:G:H22	25:BA:102:G:H2'	1.84	0.41
25:BA:122:G:C2'	25:BA:123:G:O5'	2.69	0.41
25:BA:631:A:O2'	29:BP:67:MET:HB3	2.20	0.41
25:BA:1437:C:H6	25:BA:1437:C:H5"	1.86	0.41
25:BA:1655:A:H3'	25:BA:1656:C:H6	1.86	0.41
25:BA:2123:G:O6	25:BA:2175:C:N3	2.53	0.41
25:BA:2173:A:H5"	25:BA:2174:C:OP2	2.19	0.41
25:BA:2637:U:O2'	25:BA:2638:G:H5'	2.20	0.41
25:BA:2689:U:H5"	25:BA:2690:C:H5'	2.03	0.41
27:BN:47:ALA:HB2	27:BN:112:LEU:CD1	2.50	0.41
27:BN:93:THR:OG1	27:BN:94:HIS:NE2	2.53	0.41
32:BS:74:ALA:HB1	32:BS:103:GLU:CB	2.51	0.41
34:BU:65:ILE:CG1	34:BU:96:ALA:HB3	2.49	0.41
40:B0:14:ARG:HB2	40:B0:14:ARG:NH1	2.36	0.41
43:BD:124:PRO:HB2	43:BD:126:GLN:HG2	2.02	0.41
52:BE:101:ARG:NH1	52:BE:169:ASN:O	2.49	0.41
54:BG:7:LEU:O	54:BG:11:TYR:HB3	2.20	0.41
56:BK:115:LEU:HD13	56:BK:126:MET:SD	2.59	0.41
1:AA:401:C:H1'	1:AA:622:A:H1'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:600:C:C2	1:AA:639:G:C2	3.09	0.41
1:AA:620:C:H2'	1:AA:621:A:O4'	2.19	0.41
1:AA:781:A:H5'	1:AA:782:A:OP2	2.20	0.41
1:AA:789:U:O2'	1:AA:791:G:N7	2.46	0.41
1:AA:979:C:OP1	1:AA:981:U:O4	2.38	0.41
1:AA:1071:C:H2'	1:AA:1072:G:C8	2.55	0.41
1:AA:1134:G:C6	1:AA:1135:U:C5	3.09	0.41
1:AA:1144:G:C2'	1:AA:1145:C:H5'	2.50	0.41
1:AA:1411:C:O2'	1:AA:1412:C:H5'	2.20	0.41
2:AV:76:A:H2'	25:BA:2395:C:C2	2.56	0.41
5:AK:65:ALA:HB1	5:AK:98:LEU:CD2	2.50	0.41
14:AT:50:GLU:HG3	14:AT:100:ILE:HB	2.03	0.41
15:AB:62:ALA:O	15:AB:64:ARG:N	2.54	0.41
15:AB:172:ILE:HD12	15:AB:172:ILE:H	1.85	0.41
15:AB:239:VAL:O	15:AB:239:VAL:CG1	2.69	0.41
25:BA:685:A:C4'	25:BA:686:G:O5'	2.69	0.41
25:BA:957:A:N1	25:BA:2458:G:H4'	2.35	0.41
25:BA:1054:A:C8	25:BA:1054:A:H5'	2.56	0.41
25:BA:1190:G:H5"	29:BP:35:HIS:H	1.84	0.41
25:BA:1477:A:H2'	25:BA:1478:G:O4'	2.21	0.41
25:BA:1668:A:N3	25:BA:1670:C:C4	2.89	0.41
25:BA:1682:G:C5	25:BA:1683:C:C4	3.09	0.41
25:BA:2100:G:N3	25:BA:2100:G:H2'	2.35	0.41
25:BA:2176:A:N3	51:BC:44:HIS:HE1	2.18	0.41
26:BB:31:C:N4	32:BS:32:LEU:HD22	2.36	0.41
39:BZ:54:HIS:HB3	39:BZ:101:PRO:HD3	2.02	0.41
43:BD:158:ALA:O	43:BD:159:ALA:C	2.59	0.41
45:B4:36:VAL:HB	45:B4:37:PRO:HD2	2.03	0.41
55:BH:43:VAL:HG12	55:BH:46:GLU:OE2	2.20	0.41
56:BK:24:GLY:H	56:BK:25:PRO:HD2	1.86	0.41
57:BJ:37:ALA:C	57:BJ:39:ALA:H	2.23	0.41
1:AA:596:C:O2	1:AA:596:C:H2'	2.20	0.41
1:AA:693:G:H2'	1:AA:694:A:O4'	2.19	0.41
1:AA:801:U:H2'	1:AA:802:A:O5'	2.21	0.41
1:AA:859:A:H2'	1:AA:860:A:O4'	2.20	0.41
1:AA:1021:G:H2'	1:AA:1022:G:O4'	2.20	0.41
1:AA:1253:G:H1'	1:AA:1355:G:O2'	2.20	0.41
4:AJ:54:PHE:CE2	4:AJ:55:LYS:HE3	2.56	0.41
7:AM:36:LYS:O	7:AM:37:THR:HG23	2.21	0.41
15:AB:235:SER:OG	15:AB:236:TYR:N	2.54	0.41
24:AU:12:LYS:HG2	24:AU:22:ARG:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:729:G:H2'	25:BA:1775:U:H1'	2.02	0.41
25:BA:1069:A:N7	25:BA:1073:A:N6	2.68	0.41
25:BA:1396:U:O2	25:BA:1396:U:C2'	2.60	0.41
25:BA:1538:G:H8	25:BA:1538:G:H5'	1.85	0.41
25:BA:2061:G:H5"	25:BA:2503:A:C2	2.55	0.41
25:BA:2167:U:H2'	25:BA:2168:G:O4'	2.20	0.41
25:BA:2466:C:H5"	50:B9:6:SER:HB3	2.02	0.41
29:BP:64:LYS:O	29:BP:65:ARG:C	2.56	0.41
32:BS:83:LYS:HB3	32:BS:105:ALA:HB3	2.03	0.41
35:BV:64:HIS:CE1	35:BV:92:THR:CG2	3.04	0.41
38:BY:82:PRO:HD2	38:BY:97:ARG:HD3	2.03	0.41
41:B1:58:ILE:HD11	41:B1:60:PHE:CZ	2.56	0.41
42:B2:11:GLU:O	42:B2:15:LYS:HG3	2.21	0.41
55:BH:24:VAL:CG1	55:BH:37:VAL:HG21	2.51	0.41
55:BH:67:LEU:HD12	55:BH:71:LEU:HD13	2.03	0.41
1:AA:123:C:OP1	1:AA:312:C:H5'	2.21	0.41
1:AA:192:U:H4'	14:AT:57:ARG:HD2	2.03	0.41
1:AA:575:G:H4'	1:AA:575:G:OP1	2.21	0.41
1:AA:731:G:N2	1:AA:732:C:C2	2.89	0.41
1:AA:1003:G:N2	1:AA:1039:C:N4	2.69	0.41
1:AA:1140:C:H2'	1:AA:1141:C:H6	1.86	0.41
2:AV:55:U:H5	2:AV:58:A:OP2	2.04	0.41
5:AK:12:ARG:NH2	5:AK:34:ASP:OD1	2.53	0.41
7:AM:70:LEU:O	7:AM:71:ARG:C	2.59	0.41
7:AM:74:VAL:O	7:AM:77:ASN:HB2	2.20	0.41
9:AO:18:PHE:O	9:AO:19:PRO:C	2.58	0.41
9:AO:39:LEU:HD12	9:AO:56:LEU:HB2	2.01	0.41
15:AB:19:HIS:O	15:AB:39:ILE:HG23	2.21	0.41
16:AC:35:GLU:O	16:AC:36:ASP:C	2.59	0.41
20:AG:50:ILE:O	20:AG:54:THR:HG23	2.21	0.41
25:BA:57:C:H2'	25:BA:58:G:O4'	2.21	0.41
25:BA:408:G:O2'	25:BA:409:C:H5'	2.21	0.41
25:BA:536:A:H2'	25:BA:537:C:C6	2.55	0.41
25:BA:673:C:H5"	53:BF:81:PRO:HD2	2.03	0.41
25:BA:893:C:H2'	25:BA:894:C:C6	2.55	0.41
25:BA:901:A:H2'	25:BA:902:C:O4'	2.21	0.41
25:BA:991:C:O2'	25:BA:992:C:H5'	2.21	0.41
25:BA:1245:G:OP1	29:BP:16:ARG:HG2	2.20	0.41
25:BA:1299:G:H4'	25:BA:1300:U:H5"	2.02	0.41
25:BA:1405:U:H2'	25:BA:1406:U:C6	2.55	0.41
25:BA:1742:G:N7	25:BA:1743:C:C6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1848:A:H2'	25:BA:1849:G:O4'	2.21	0.41
25:BA:2135:A:H4'	25:BA:2160:G:H4'	2.03	0.41
25:BA:2155:G:C2'	25:BA:2156:G:O5'	2.69	0.41
25:BA:2164:C:C4	25:BA:2165:G:H8	2.39	0.41
25:BA:2346:A:H5'	25:BA:2383:G:O4'	2.21	0.41
25:BA:2505:G:HO2'	25:BA:2506:U:H6	1.67	0.41
25:BA:2680:C:O2'	25:BA:2681:C:H5'	2.21	0.41
25:BA:2766:G:N3	25:BA:2766:G:H2'	2.36	0.41
25:BA:2811:G:OP1	52:BE:60:ASN:CB	2.68	0.41
26:BB:104:U:C5'	30:BQ:141:GLN:HB3	2.50	0.41
26:BB:105:A:OP1	39:BZ:72:ARG:NH1	2.54	0.41
28:BO:10:VAL:O	28:BO:10:VAL:HG22	2.21	0.41
28:BO:35:VAL:CG2	28:BO:69:ILE:HD11	2.51	0.41
29:BP:85:LEU:H	29:BP:85:LEU:CD2	2.33	0.41
29:BP:144:GLU:N	29:BP:145:PRO:CD	2.84	0.41
30:BQ:21:THR:OG1	30:BQ:99:PRO:O	2.35	0.41
32:BS:58:LEU:O	32:BS:59:LYS:O	2.38	0.41
35:BV:55:ALA:HA	35:BV:100:ARG:O	2.20	0.41
38:BY:8:LYS:C	38:BY:28:LYS:HE2	2.41	0.41
38:BY:95:LYS:HD3	38:BY:99:CYS:O	2.21	0.41
41:B1:3:LYS:C	41:B1:46:LEU:HD21	2.41	0.41
43:BD:70:TRP:HZ3	43:BD:146:GLU:CD	2.24	0.41
43:BD:89:SER:HB2	43:BD:159:ALA:HB2	2.02	0.41
45:B4:36:VAL:HG22	45:B4:52:SER:O	2.21	0.41
51:BC:96:GLY:O	51:BC:97:GLU:HG3	2.20	0.41
51:BC:103:ILE:HG23	51:BC:105:ASP:OD2	2.21	0.41
53:BF:33:LEU:HD12	53:BF:33:LEU:HA	1.89	0.41
54:BG:83:ARG:O	54:BG:85:GLY:N	2.54	0.41
1:AA:500:G:H2'	1:AA:501:C:C6	2.56	0.41
1:AA:684:A:O3'	5:AK:12:ARG:NH1	2.54	0.41
1:AA:955:U:H2'	1:AA:956:U:O4'	2.21	0.41
1:AA:1053:G:N7	1:AA:1200:C:H5"	2.36	0.41
1:AA:1181:G:H8	1:AA:1181:G:H5"	1.86	0.41
5:AK:29:ILE:HG21	5:AK:29:ILE:HD13	1.75	0.41
6:AL:84:LEU:HD23	6:AL:84:LEU:HA	1.95	0.41
17:AD:16:GLY:C	17:AD:17:VAL:HG23	2.41	0.41
17:AD:28:SER:C	17:AD:30:LYS:N	2.75	0.41
25:BA:507:A:H5"	25:BA:508:G:H5'	2.02	0.41
25:BA:572:A:H3'	25:BA:573:G:O4'	2.21	0.41
25:BA:1451:C:H4'	25:BA:1452:A:C8	2.55	0.41
28:BO:87:ILE:HA	28:BO:87:ILE:HD13	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BP:23:PRO:O	29:BP:33:ARG:CZ	2.69	0.41
31:BR:4:LEU:O	31:BR:5:LYS:CG	2.68	0.41
34:BU:91:ASP:OD1	34:BU:96:ALA:HB2	2.20	0.41
40:B0:23:VAL:HG22	40:B0:38:VAL:CG2	2.44	0.41
44:B3:8:LEU:HD13	44:B3:31:LEU:HD23	2.03	0.41
47:B6:22:ALA:HB2	47:B6:39:TYR:CZ	2.56	0.41
51:BC:30:LYS:NZ	51:BC:30:LYS:HB3	2.36	0.41
53:BF:28:ILE:H	53:BF:28:ILE:CD1	2.31	0.41
55:BH:41:MET:HE3	55:BH:43:VAL:CG1	2.42	0.41
55:BH:86:GLU:HB3	55:BH:132:ARG:HB2	2.01	0.41
55:BH:137:ASP:HB3	55:BH:140:LYS:HB2	2.02	0.41
56:BK:121:GLU:O	56:BK:125:ARG:NE	2.53	0.41
1:AA:36:C:H2'	1:AA:37:U:O4'	2.21	0.40
1:AA:109:A:C6	1:AA:327:A:C6	3.09	0.40
1:AA:735:C:O2'	1:AA:736:C:H5'	2.21	0.40
1:AA:963:G:H21	4:AJ:55:LYS:HE3	1.86	0.40
12:AR:22:VAL:O	12:AR:23:LYS:C	2.58	0.40
16:AC:65:ALA:HA	16:AC:100:ALA:HB3	2.02	0.40
16:AC:85:ARG:HH12	16:AC:88:ARG:NH1	2.18	0.40
16:AC:91:LEU:HB2	16:AC:99:VAL:HG21	2.03	0.40
17:AD:2:GLY:C	17:AD:4:TYR:N	2.73	0.40
18:AE:11:ILE:HD12	18:AE:33:VAL:CG2	2.51	0.40
22:AI:8:GLY:O	22:AI:15:ALA:N	2.46	0.40
23:AY:61:ARG:NH1	25:BA:2663:G:OP1	2.54	0.40
23:AY:90:PHE:O	23:AY:91:THR:C	2.59	0.40
25:BA:41:C:H2'	25:BA:42:G:O4'	2.21	0.40
25:BA:52:A:O2'	25:BA:53:A:H5'	2.21	0.40
25:BA:1046:A:O5'	25:BA:1047:G:OP1	2.39	0.40
25:BA:1086:A:C5'	25:BA:1087:G:OP1	2.69	0.40
25:BA:1461:G:C6	25:BA:1462:C:C4	3.10	0.40
25:BA:1668:A:H4'	25:BA:1669:A:O5'	2.20	0.40
25:BA:1680:U:O2	25:BA:1763:G:H3'	2.21	0.40
25:BA:2313:C:H4'	54:BG:91:ARG:HG3	2.02	0.40
25:BA:2356:C:O3'	40:B0:20:ARG:HD3	2.21	0.40
25:BA:2472:G:H3'	25:BA:2475:C:H42	1.86	0.40
27:BN:5:VAL:O	27:BN:5:VAL:CG1	2.68	0.40
27:BN:30:ILE:HG22	27:BN:34:LEU:HD22	2.03	0.40
33:BT:91:ARG:HG2	33:BT:116:ALA:HA	2.03	0.40
38:BY:10:GLY:HA2	38:BY:27:VAL:HG13	2.03	0.40
38:BY:41:GLY:O	38:BY:42:VAL:C	2.59	0.40
38:BY:77:PRO:O	38:BY:78:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:B6:10:LEU:H	47:B6:10:LEU:CD2	2.34	0.40
51:BC:39:GLU:OE1	51:BC:216:THR:CB	2.69	0.40
53:BF:3:GLU:HA	53:BF:24:LEU:CB	2.51	0.40
53:BF:13:SER:HB2	53:BF:14:PRO:CD	2.50	0.40
53:BF:110:LEU:HA	53:BF:110:LEU:HD23	1.86	0.40
54:BG:54:GLU:O	54:BG:58:GLN:HG3	2.21	0.40
1:AA:375:U:O3'	10:AP:6:LEU:HB2	2.21	0.40
1:AA:488:C:O5'	1:AA:488:C:H6	2.04	0.40
1:AA:524:G:H2'	1:AA:525:C:C6	2.56	0.40
1:AA:1026:G:H2'	1:AA:1026:G:N3	2.36	0.40
7:AM:49:THR:O	7:AM:53:VAL:HG23	2.20	0.40
7:AM:121:LYS:O	7:AM:122:LYS:HG2	2.21	0.40
13:AS:22:LEU:HD13	13:AS:27:GLU:HB2	2.02	0.40
17:AD:15:GLU:OE1	17:AD:59:ARG:NE	2.43	0.40
18:AE:91:LEU:HD12	18:AE:91:LEU:HA	1.86	0.40
23:AY:128:TYR:OH	23:AY:402:ILE:O	2.36	0.40
23:AY:446:THR:O	23:AY:446:THR:HG23	2.21	0.40
24:AU:9:ARG:HH21	24:AU:22:ARG:HA	1.86	0.40
25:BA:565:C:H2'	25:BA:566:U:O4'	2.21	0.40
25:BA:570:G:C5	25:BA:2030:A:C2	3.09	0.40
25:BA:1285:G:C5	25:BA:1329:U:C4	3.09	0.40
25:BA:1338:G:N3	25:BA:1393:A:H2	2.19	0.40
25:BA:1491:G:C6	25:BA:1500:G:C2	3.09	0.40
25:BA:2519:U:C5	25:BA:2541:A:C6	3.09	0.40
34:BU:66:ASN:CG	34:BU:76:TYR:HB2	2.41	0.40
36:BW:46:PHE:O	36:BW:50:VAL:HG12	2.20	0.40
43:BD:39:LYS:HB2	43:BD:62:TYR:HB2	2.03	0.40
45:B4:51:TYR:O	54:BG:105:LYS:NZ	2.52	0.40
52:BE:134:ILE:C	52:BE:134:ILE:HD12	2.42	0.40
53:BF:136:THR:HA	53:BF:166:ALA:O	2.22	0.40
53:BF:167:ALA:CB	53:BF:173:VAL:HG11	2.43	0.40
54:BG:85:GLY:O	54:BG:86:MET:C	2.59	0.40
56:BK:58:THR:HB	56:BK:66:THR:CG2	2.52	0.40
1:AA:441:A:H3'	1:AA:442:C:H6	1.87	0.40
1:AA:1236:A:H4'	1:AA:1304:G:H4'	2.02	0.40
1:AA:1373:G:O5'	1:AA:1373:G:H8	2.04	0.40
4:AJ:26:ALA:O	4:AJ:27:ALA:HB2	2.22	0.40
7:AM:87:TYR:N	13:AS:73:GLU:O	2.54	0.40
21:AH:10:LEU:HD22	21:AH:83:ILE:HD11	2.03	0.40
25:BA:535:C:C2'	25:BA:536:A:H5'	2.52	0.40
25:BA:644:A:C2	25:BA:2369:A:H1'	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:687:C:O2'	25:BA:1780:A:N1	2.47	0.40
25:BA:1645:G:OP1	25:BA:1646:C:H5'	2.20	0.40
25:BA:1814:G:OP2	25:BA:1815:A:O2'	2.32	0.40
25:BA:2279:G:N7	40:B0:14:ARG:NH1	2.64	0.40
25:BA:2408:U:H2'	25:BA:2409:G:C8	2.56	0.40
25:BA:2468:G:H5'	30:BQ:120:ILE:HD12	2.03	0.40
25:BA:2810:A:H2'	52:BE:61:ARG:HH21	1.81	0.40
30:BQ:104:PHE:HE1	30:BQ:125:LEU:HD11	1.86	0.40
39:BZ:24:LEU:HD23	39:BZ:25:PRO:O	2.21	0.40
39:BZ:69:THR:HG22	39:BZ:90:VAL:HA	2.04	0.40
41:B1:58:ILE:HD11	41:B1:60:PHE:CE2	2.56	0.40
43:BD:26:LYS:HG2	43:BD:82:ILE:H	1.86	0.40
43:BD:32:SER:HA	43:BD:35:LYS:HZ2	1.85	0.40
51:BC:19:VAL:HG22	51:BC:223:ARG:HG3	2.02	0.40
53:BF:61:GLY:O	53:BF:62:ARG:C	2.59	0.40
58:BL:81:UNK:O	58:BL:85:UNK:C	2.69	0.40
1:AA:157:G:C6	1:AA:158:G:C5	3.10	0.40
1:AA:327:A:O3'	1:AA:328:C:H4'	2.21	0.40
1:AA:619:U:O2	17:AD:133:VAL:HA	2.21	0.40
11:AQ:26:GLN:HA	11:AQ:36:ILE:O	2.22	0.40
16:AC:19:GLU:O	16:AC:56:ASP:HA	2.22	0.40
17:AD:64:LEU:O	17:AD:67:ILE:HB	2.22	0.40
21:AH:111:ILE:C	21:AH:112:LEU:HD23	2.42	0.40
23:AY:329:ARG:HH21	23:AY:372:GLY:HA2	1.86	0.40
23:AY:486:THR:HG21	23:AY:519:ARG:HH12	1.86	0.40
25:BA:526:A:N3	25:BA:2044:C:H1'	2.36	0.40
25:BA:647:G:H2'	25:BA:648:G:O4'	2.21	0.40
25:BA:774:A:O2'	25:BA:775:G:P	2.78	0.40
25:BA:1263:U:O3'	46:B5:11:THR:OG1	2.39	0.40
25:BA:1684:C:H2'	25:BA:1685:C:C6	2.57	0.40
25:BA:1787:A:O4'	25:BA:2589:A:H4'	2.21	0.40
25:BA:2139:C:C2'	25:BA:2140:C:OP2	2.68	0.40
25:BA:2250:G:C8	25:BA:2496:C:H5"	2.57	0.40
25:BA:2392:A:OP1	49:B8:32:LEU:CD1	2.70	0.40
26:BB:24:G:N7	26:BB:56:G:H2'	2.37	0.40
28:BO:88:ASN:C	28:BO:88:ASN:ND2	2.73	0.40
31:BR:2:ARG:CD	52:BE:111:ARG:HG3	2.52	0.40
43:BD:131:LEU:HB2	43:BD:136:ILE:HD11	2.03	0.40
43:BD:245:PRO:HA	43:BD:246:PRO:HD3	1.87	0.40
52:BE:72:VAL:O	52:BE:74:PRO:N	2.53	0.40
53:BF:5:ALA:O	53:BF:6:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BK:104:VAL:CG2	56:BK:127:ILE:HB	2.51	0.40
58:BL:70:UNK:O	58:BL:74:UNK:N	2.54	0.40
1:AA:152:A:N6	1:AA:170:U:C2	2.89	0.40
1:AA:175:C:H2'	1:AA:176:C:C6	2.57	0.40
1:AA:1003:G:N2	1:AA:1038:C:C4	2.89	0.40
1:AA:1091:U:O2	1:AA:1093:A:C8	2.74	0.40
1:AA:1141:C:C2	1:AA:1142:G:C8	3.09	0.40
1:AA:1237:C:C4'	1:AA:1334:G:N2	2.84	0.40
1:AA:1299:A:O3'	1:AA:1300:G:H4'	2.21	0.40
9:AO:27:VAL:HG12	9:AO:31:LEU:HD22	2.04	0.40
10:AP:33:ILE:HD13	10:AP:33:ILE:N	2.36	0.40
15:AB:70:PHE:O	15:AB:92:TYR:HA	2.21	0.40
23:AY:168:ILE:HD11	23:AY:178:ILE:HD12	2.03	0.40
25:BA:435:C:H2'	25:BA:436:C:H5'	2.04	0.40
25:BA:732:C:H2'	25:BA:733:G:O4'	2.22	0.40
25:BA:1002:G:H2'	25:BA:1003:G:O4'	2.21	0.40
25:BA:1771:C:C1'	25:BA:1786:A:C8	3.05	0.40
25:BA:2092:U:C6	25:BA:2225:A:O2'	2.75	0.40
25:BA:2285:C:C5	47:B6:27:LYS:HE3	2.57	0.40
25:BA:2310:A:N3	25:BA:2310:A:H2'	2.36	0.40
25:BA:2550:G:C2'	25:BA:2551:C:H5'	2.51	0.40
25:BA:2731:G:OP1	52:BE:169:ASN:ND2	2.37	0.40
30:BQ:10:ARG:O	30:BQ:10:ARG:HG3	2.21	0.40
30:BQ:35:VAL:HG21	39:BZ:81:ARG:HH21	1.86	0.40
39:BZ:4:ARG:O	39:BZ:5:LEU:HB2	2.21	0.40
42:B2:12:GLU:O	42:B2:15:LYS:HE3	2.22	0.40
51:BC:53:ARG:HG3	51:BC:55:ASP:OD1	2.21	0.40
51:BC:162:GLU:HG2	51:BC:163:PHE:N	2.37	0.40
53:BF:123:LEU:HD12	53:BF:124:LEU:H	1.86	0.40
54:BG:77:ILE:O	54:BG:81:LYS:O	2.39	0.40
54:BG:103:LEU:HD22	54:BG:178:PHE:HZ	1.87	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 X-ray entries followed by that with respect to entries of similar resolution.

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
4	AJ	96/98 (98%)	80 (83%)	10 (10%)	6 (6%)	1 3
5	AK	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	5 17
6	AL	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	3 9
7	AM	122/124 (98%)	82 (67%)	32 (26%)	8 (7%)	1 3
8	AN	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3 12
9	AO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13 35
10	AP	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
11	AQ	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15 40
12	AR	68/70 (97%)	60 (88%)	5 (7%)	3 (4%)	2 8
13	AS	76/78 (97%)	60 (79%)	8 (10%)	8 (10%)	0 1
14	AT	97/99 (98%)	86 (89%)	5 (5%)	6 (6%)	1 3
15	AB	232/234 (99%)	191 (82%)	32 (14%)	9 (4%)	3 10
16	AC	204/206 (99%)	173 (85%)	22 (11%)	9 (4%)	2 8
17	AD	206/208 (99%)	171 (83%)	25 (12%)	10 (5%)	2 6
18	AE	148/150 (99%)	141 (95%)	5 (3%)	2 (1%)	11 31
19	AF	99/101 (98%)	91 (92%)	8 (8%)	0	100 100
20	AG	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	5 17
21	AH	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	6 21
22	AI	125/127 (98%)	99 (79%)	17 (14%)	9 (7%)	1 2
23	AY	612/680 (90%)	520 (85%)	72 (12%)	20 (3%)	4 13
24	AU	22/24 (92%)	17 (77%)	5 (23%)	0	100 100
27	BN	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	2 8
28	BO	120/122 (98%)	113 (94%)	3 (2%)	4 (3%)	4 13
29	BP	144/150 (96%)	90 (62%)	21 (15%)	33 (23%)	0 0
30	BQ	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3 11
31	BR	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	2 8
32	BS	96/112 (86%)	61 (64%)	20 (21%)	15 (16%)	0 0
33	BT	135/146 (92%)	96 (71%)	24 (18%)	15 (11%)	0 1
34	BU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3 12
35	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	BW	111/113 (98%)	101 (91%)	4 (4%)	6 (5%)	2 5
37	BX	90/96 (94%)	83 (92%)	7 (8%)	0	100 100
38	BY	98/110 (89%)	58 (59%)	18 (18%)	22 (22%)	0 0
39	BZ	194/206 (94%)	146 (75%)	32 (16%)	16 (8%)	1 1
40	B0	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	3 11
41	B1	91/98 (93%)	76 (84%)	12 (13%)	3 (3%)	4 13
42	B2	69/72 (96%)	58 (84%)	4 (6%)	7 (10%)	0 1
43	BD	269/276 (98%)	231 (86%)	24 (9%)	14 (5%)	2 5
44	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8 25
45	B4	28/71 (39%)	21 (75%)	4 (14%)	3 (11%)	0 1
46	B5	57/60 (95%)	47 (82%)	4 (7%)	6 (10%)	0 1
47	B6	42/54 (78%)	20 (48%)	15 (36%)	7 (17%)	0 0
48	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6 21
49	B8	61/65 (94%)	45 (74%)	11 (18%)	5 (8%)	1 1
50	B9	34/37 (92%)	32 (94%)	2 (6%)	0	100 100
51	BC	219/229 (96%)	166 (76%)	35 (16%)	18 (8%)	1 1
52	BE	202/206 (98%)	145 (72%)	30 (15%)	27 (13%)	0 0
53	BF	205/210 (98%)	165 (80%)	24 (12%)	16 (8%)	1 2
54	BG	179/182 (98%)	123 (69%)	44 (25%)	12 (7%)	1 2
55	BH	171/180 (95%)	128 (75%)	26 (15%)	17 (10%)	0 1
56	BK	121/147 (82%)	84 (69%)	30 (25%)	7 (6%)	1 4
57	BJ	128/130 (98%)	84 (66%)	31 (24%)	13 (10%)	0 1
All	All	6610/6949 (95%)	5383 (81%)	812 (12%)	415 (6%)	1 3

All (415) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AJ	23	ILE
4	AJ	59	SER
4	AJ	86	MET
5	AK	117	ASN
5	AK	128	ALA
6	AL	27	LEU
7	AM	46	LYS

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Mol	Chain	Res	Type
7	AM	83	ASP
7	AM	90	LEU
8	AN	16	PHE
11	AQ	49	GLU
12	AR	25	THR
13	AS	5	LEU
13	AS	10	PHE
13	AS	26	GLY
13	AS	28	LYS
13	AS	80	TYR
14	AT	95	ALA
15	AB	18	GLY
15	AB	237	ALA
16	AC	154	SER
16	AC	165	THR
16	AC	168	ALA
17	AD	3	ARG
17	AD	31	CYS
20	AG	155	ARG
22	AI	55	ALA
22	AI	89	ASN
22	AI	118	LYS
22	AI	119	ALA
23	AY	34	TYR
23	AY	95	GLU
23	AY	171	GLU
23	AY	180	VAL
23	AY	215	LYS
23	AY	683	VAL
23	AY	684	GLN
27	BN	4	TYR
27	BN	57	ALA
27	BN	59	LYS
27	BN	127	ASP
27	BN	133	GLN
29	BP	14	LYS
29	BP	18	ARG
29	BP	23	PRO
29	BP	25	SER
29	BP	47	ASP
29	BP	49	ARG
29	BP	52	GLU

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Mol	Chain	Res	Type
29	BP	57	THR
29	BP	65	ARG
29	BP	106	LEU
29	BP	107	LYS
30	BQ	18	LYS
30	BQ	22	LYS
31	BR	4	LEU
32	BS	59	LYS
32	BS	89	ARG
32	BS	97	ARG
32	BS	105	ALA
33	BT	24	PRO
33	BT	30	VAL
33	BT	80	SER
33	BT	91	ARG
33	BT	107	ASP
34	BU	91	ASP
34	BU	93	LYS
35	BV	3	ALA
35	BV	16	PRO
35	BV	19	LYS
35	BV	22	VAL
35	BV	24	LYS
35	BV	46	VAL
36	BW	63	ASP
38	BY	3	VAL
38	BY	10	GLY
38	BY	24	VAL
38	BY	27	VAL
38	BY	31	LEU
38	BY	42	VAL
38	BY	56	PRO
38	BY	62	GLU
38	BY	77	PRO
38	BY	78	ALA
38	BY	98	VAL
39	BZ	21	ALA
39	BZ	146	ILE
39	BZ	189	ALA
40	B0	3	HIS
41	B1	53	VAL
42	B2	43	GLN

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Mol	Chain	Res	Type
42	B2	44	LEU
42	B2	70	GLN
43	BD	3	VAL
43	BD	12	SER
43	BD	26	LYS
46	B5	4	HIS
46	B5	35	GLU
46	B5	49	CYS
46	B5	51	TYR
46	B5	52	TYR
46	B5	57	VAL
47	B6	19	ARG
47	B6	31	PRO
47	B6	46	HIS
49	B8	34	TRP
49	B8	61	LEU
51	BC	54	SER
51	BC	55	ASP
51	BC	80	GLY
51	BC	83	ILE
51	BC	109	ASP
51	BC	186	ALA
52	BE	60	ASN
52	BE	66	HIS
52	BE	69	LYS
52	BE	72	VAL
52	BE	75	VAL
52	BE	77	ILE
52	BE	82	ARG
52	BE	87	GLU
52	BE	88	GLY
52	BE	90	THR
52	BE	118	LYS
53	BF	21	ALA
53	BF	67	GLN
53	BF	168	ARG
53	BF	195	ASP
54	BG	82	LEU
54	BG	87	PRO
54	BG	97	ASP
55	BH	9	ILE
55	BH	10	PRO

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Mol	Chain	Res	Type
55	BH	13	LYS
55	BH	45	VAL
55	BH	83	TYR
55	BH	85	LYS
55	BH	92	ILE
55	BH	138	LYS
56	BK	115	LEU
57	BJ	47	ALA
57	BJ	50	ALA
57	BJ	56	ALA
57	BJ	61	ALA
57	BJ	73	ALA
57	BJ	107	ALA
57	BJ	128	ALA
4	AJ	27	ALA
6	AL	91	LYS
7	AM	66	LEU
8	AN	14	PRO
12	AR	28	GLU
14	AT	75	ASN
14	AT	101	GLY
15	AB	14	GLY
15	AB	110	GLN
16	AC	12	LEU
16	AC	61	ALA
16	AC	156	ARG
17	AD	9	CYS
17	AD	17	VAL
17	AD	23	GLY
17	AD	26	CYS
22	AI	105	ASP
23	AY	196	ILE
23	AY	211	GLU
23	AY	396	ARG
23	AY	551	GLN
28	BO	5	GLN
29	BP	11	GLY
29	BP	26	GLY
29	BP	33	ARG
29	BP	34	GLY
29	BP	66	GLY
29	BP	67	MET

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Mol	Chain	Res	Type
29	BP	98	GLU
29	BP	109	GLY
30	BQ	27	VAL
30	BQ	28	ALA
32	BS	14	VAL
32	BS	102	ALA
33	BT	2	ASN
33	BT	81	PRO
33	BT	126	ALA
33	BT	129	ARG
35	BV	37	VAL
35	BV	40	LEU
36	BW	65	LEU
38	BY	29	GLU
38	BY	39	VAL
39	BZ	142	SER
39	BZ	165	VAL
39	BZ	168	GLU
39	BZ	190	GLU
41	B1	58	ILE
42	B2	9	GLN
43	BD	11	PRO
43	BD	25	THR
43	BD	210	GLY
43	BD	224	ALA
43	BD	238	GLY
43	BD	239	ARG
45	B4	61	VAL
47	B6	23	THR
51	BC	85	GLU
51	BC	86	ALA
51	BC	89	ALA
51	BC	97	GLU
52	BE	45	THR
52	BE	63	LEU
52	BE	71	GLY
52	BE	74	PRO
52	BE	95	ILE
52	BE	130	GLY
53	BF	3	GLU
53	BF	5	ALA
53	BF	6	VAL

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Mol	Chain	Res	Type
53	BF	11	VAL
53	BF	25	PRO
53	BF	134	GLY
54	BG	61	ALA
54	BG	84	LYS
54	BG	117	PHE
55	BH	55	PRO
55	BH	84	SER
55	BH	172	LYS
56	BK	82	ALA
57	BJ	7	ALA
57	BJ	72	ALA
57	BJ	120	ALA
4	AJ	58	ASP
6	AL	28	LYS
7	AM	124	PRO
12	AR	87	ARG
13	AS	6	LYS
13	AS	76	PRO
14	AT	99	LEU
15	AB	153	ARG
15	AB	236	TYR
16	AC	4	LYS
16	AC	181	ASN
17	AD	18	LYS
18	AE	68	GLU
23	AY	96	ARG
23	AY	181	LEU
23	AY	403	GLU
23	AY	404	VAL
23	AY	581	ALA
27	BN	47	ALA
28	BO	29	ASN
29	BP	17	LYS
29	BP	35	HIS
29	BP	36	LYS
29	BP	39	LYS
29	BP	42	SER
29	BP	108	LYS
29	BP	136	GLU
29	BP	146	VAL
32	BS	19	LYS

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Mol	Chain	Res	Type
32	BS	53	SER
32	BS	88	ASP
32	BS	92	TYR
32	BS	103	GLU
33	BT	27	THR
33	BT	58	ASN
35	BV	2	PHE
35	BV	20	LEU
35	BV	23	GLU
35	BV	47	VAL
35	BV	48	GLY
38	BY	67	LEU
38	BY	82	PRO
38	BY	90	LEU
39	BZ	140	ASP
42	B2	45	SER
42	B2	48	HIS
43	BD	32	SER
43	BD	101	GLU
44	B3	51	ALA
45	B4	63	SER
47	B6	22	ALA
47	B6	28	ARG
49	B8	51	ALA
51	BC	141	LYS
52	BE	17	ASP
52	BE	61	ARG
52	BE	128	SER
53	BF	10	PRO
53	BF	141	ALA
54	BG	49	ASP
54	BG	64	THR
54	BG	142	PRO
55	BH	126	PRO
56	BK	51	ALA
57	BJ	84	ALA
6	AL	19	ARG
7	AM	67	GLU
14	AT	97	ALA
15	AB	15	VAL
15	AB	130	ARG
15	AB	131	PRO

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Mol	Chain	Res	Type
16	AC	36	ASP
17	AD	4	TYR
20	AG	81	GLY
21	AH	2	LEU
22	AI	92	TYR
28	BO	26	LYS
29	BP	43	GLY
29	BP	48	PRO
29	BP	122	PRO
29	BP	147	LEU
30	BQ	59	ARG
31	BR	3	HIS
31	BR	106	GLY
32	BS	54	LEU
33	BT	31	SER
33	BT	32	TYR
34	BU	33	ARG
36	BW	6	ILE
38	BY	32	PRO
38	BY	99	CYS
39	BZ	14	LYS
39	BZ	80	ARG
39	BZ	199	LYS
40	B0	6	GLY
40	B0	9	SER
41	B1	85	LEU
48	B7	47	ARG
49	B8	33	ASN
49	B8	53	PRO
51	BC	185	LEU
52	BE	18	ASP
52	BE	187	ALA
53	BF	131	GLY
54	BG	122	PRO
55	BH	168	PRO
56	BK	42	ASN
57	BJ	93	ALA
7	AM	7	VAL
7	AM	55	ARG
9	AO	24	SER
14	AT	100	ILE
17	AD	5	ILE

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Mol	Chain	Res	Type
18	AE	8	GLU
20	AG	54	THR
22	AI	54	ASP
22	AI	127	LYS
23	AY	136	ALA
29	BP	38	GLN
31	BR	86	ARG
31	BR	117	VAL
32	BS	13	ARG
33	BT	57	PHE
35	BV	44	LYS
39	BZ	156	LYS
47	B6	44	ARG
51	BC	140	PRO
51	BC	227	HIS
52	BE	44	TYR
53	BF	26	ALA
54	BG	43	LEU
55	BH	24	VAL
55	BH	137	ASP
55	BH	171	LEU
56	BK	62	ASP
57	BJ	38	ALA
4	AJ	90	LEU
13	AS	29	ARG
20	AG	7	ALA
21	AH	51	VAL
29	BP	9	ASN
32	BS	95	HIS
32	BS	107	GLU
35	BV	79	VAL
36	BW	11	ARG
36	BW	93	ALA
38	BY	81	LYS
39	BZ	78	LYS
39	BZ	147	GLY
42	B2	17	SER
43	BD	35	LYS
45	B4	54	LYS
51	BC	118	ASP
51	BC	181	PRO
52	BE	129	HIS

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Mol	Chain	Res	Type
54	BG	86	MET
55	BH	47	GLU
56	BK	10	LEU
22	AI	44	VAL
6	AL	121	GLY
17	AD	29	PRO
23	AY	243	VAL
23	AY	299	VAL
28	BO	48	PRO
34	BU	90	VAL
38	BY	53	PRO
38	BY	66	PRO
39	BZ	197	ILE
51	BC	96	GLY
52	BE	73	GLU
53	BF	84	VAL
5	AK	48	ILE
23	AY	516	PRO
43	BD	271	ILE
21	AH	73	ASP
33	BT	88	ILE
36	BW	112	GLY
38	BY	80	GLY
43	BD	28	GLU
51	BC	103	ILE
52	BE	116	VAL
53	BF	24	LEU
39	BZ	166	SER
52	BE	53	PRO
56	BK	4	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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
4	AJ	88/88 (100%)	70 (80%)	18 (20%)	1 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	AK	90/90 (100%)	68 (76%)	22 (24%)	0 1
6	AL	104/104 (100%)	85 (82%)	19 (18%)	1 4
7	AM	99/99 (100%)	83 (84%)	16 (16%)	2 6
8	AN	49/49 (100%)	38 (78%)	11 (22%)	1 2
9	AO	79/79 (100%)	67 (85%)	12 (15%)	3 7
10	AP	72/72 (100%)	61 (85%)	11 (15%)	2 7
11	AQ	94/94 (100%)	79 (84%)	15 (16%)	2 6
12	AR	61/61 (100%)	52 (85%)	9 (15%)	3 8
13	AS	69/69 (100%)	52 (75%)	17 (25%)	0 1
14	AT	76/76 (100%)	61 (80%)	15 (20%)	1 3
15	AB	202/202 (100%)	172 (85%)	30 (15%)	3 8
16	AC	160/160 (100%)	125 (78%)	35 (22%)	1 2
17	AD	180/180 (100%)	144 (80%)	36 (20%)	1 3
18	AE	115/115 (100%)	104 (90%)	11 (10%)	8 22
19	AF	90/90 (100%)	76 (84%)	14 (16%)	2 6
20	AG	126/126 (100%)	110 (87%)	16 (13%)	4 11
21	AH	119/119 (100%)	96 (81%)	23 (19%)	1 3
22	AI	98/98 (100%)	76 (78%)	22 (22%)	1 2
23	AY	528/573 (92%)	420 (80%)	108 (20%)	1 2
24	AU	19/19 (100%)	14 (74%)	5 (26%)	0 1
27	BN	117/119 (98%)	84 (72%)	33 (28%)	0 1
28	BO	100/100 (100%)	84 (84%)	16 (16%)	2 6
29	BP	112/116 (97%)	82 (73%)	30 (27%)	0 1
30	BQ	111/111 (100%)	96 (86%)	15 (14%)	4 9
31	BR	100/101 (99%)	80 (80%)	20 (20%)	1 3
32	BS	77/88 (88%)	62 (80%)	15 (20%)	1 3
33	BT	120/127 (94%)	91 (76%)	29 (24%)	0 1
34	BU	92/94 (98%)	76 (83%)	16 (17%)	2 5
35	BV	82/82 (100%)	56 (68%)	26 (32%)	0 0
36	BW	91/92 (99%)	75 (82%)	16 (18%)	2 4
37	BX	74/78 (95%)	59 (80%)	15 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	BY	84/91 (92%)	65 (77%)	19 (23%)	1 2
39	BZ	154/179 (86%)	127 (82%)	27 (18%)	2 4
40	B0	66/67 (98%)	56 (85%)	10 (15%)	3 7
41	B1	78/83 (94%)	63 (81%)	15 (19%)	1 3
42	B2	66/67 (98%)	51 (77%)	15 (23%)	1 2
43	BD	213/218 (98%)	170 (80%)	43 (20%)	1 3
44	B3	51/52 (98%)	41 (80%)	10 (20%)	1 3
45	B4	27/63 (43%)	23 (85%)	4 (15%)	3 8
46	B5	51/52 (98%)	42 (82%)	9 (18%)	2 4
47	B6	43/52 (83%)	31 (72%)	12 (28%)	0 1
48	B7	41/42 (98%)	35 (85%)	6 (15%)	3 8
49	B8	53/55 (96%)	33 (62%)	20 (38%)	0 0
50	B9	33/34 (97%)	23 (70%)	10 (30%)	0 0
51	BC	177/181 (98%)	159 (90%)	18 (10%)	7 20
52	BE	165/166 (99%)	131 (79%)	34 (21%)	1 2
53	BF	165/166 (99%)	134 (81%)	31 (19%)	1 3
54	BG	155/156 (99%)	128 (83%)	27 (17%)	2 5
55	BH	136/148 (92%)	107 (79%)	29 (21%)	1 2
56	BK	96/111 (86%)	85 (88%)	11 (12%)	5 15
All	All	5448/5654 (96%)	4402 (81%)	1046 (19%)	1 3

All (1046) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AJ	3	LYS
4	AJ	5	ARG
4	AJ	6	ILE
4	AJ	14	LYS
4	AJ	16	LEU
4	AJ	22	LYS
4	AJ	38	ILE
4	AJ	46	ARG
4	AJ	49	VAL
4	AJ	55	LYS
4	AJ	76	ASN

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Mol	Chain	Res	Type
4	AJ	78	ASN
4	AJ	79	ARG
4	AJ	80	LYS
4	AJ	81	THR
4	AJ	86	MET
4	AJ	96	ILE
4	AJ	99	LYS
5	AK	11	LYS
5	AK	14	VAL
5	AK	28	THR
5	AK	29	ILE
5	AK	30	VAL
5	AK	31	THR
5	AK	41	THR
5	AK	51	LYS
5	AK	53	SER
5	AK	87	THR
5	AK	92	GLU
5	AK	96	ARG
5	AK	103	LEU
5	AK	109	VAL
5	AK	112	THR
5	AK	114	VAL
5	AK	116	HIS
5	AK	117	ASN
5	AK	120	ARG
5	AK	122	LYS
5	AK	124	LYS
5	AK	126	ARG
6	AL	13	LYS
6	AL	20	LYS
6	AL	21	LYS
6	AL	27	LEU
6	AL	33	ARG
6	AL	41	ARG
6	AL	42	THR
6	AL	53	ARG
6	AL	60	LEU
6	AL	67	THR
6	AL	78	GLN
6	AL	83	VAL
6	AL	84	LEU

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Mol	Chain	Res	Type
6	AL	85	ILE
6	AL	89	ARG
6	AL	91	LYS
6	AL	92	ASP
6	AL	111	LYS
6	AL	126	LYS
7	AM	47	ASP
7	AM	48	LEU
7	AM	49	THR
7	AM	56	LEU
7	AM	64	TRP
7	AM	70	LEU
7	AM	79	LYS
7	AM	82	MET
7	AM	86	CYS
7	AM	90	LEU
7	AM	93	ARG
7	AM	94	ARG
7	AM	102	ARG
7	AM	108	ARG
7	AM	115	LYS
7	AM	120	LYS
8	AN	4	LYS
8	AN	7	ILE
8	AN	9	LYS
8	AN	18	VAL
8	AN	26	ARG
8	AN	27	CYS
8	AN	33	VAL
8	AN	35	ARG
8	AN	41	ARG
8	AN	44	LEU
8	AN	60	SER
9	AO	10	LYS
9	AO	17	ARG
9	AO	24	SER
9	AO	26	GLU
9	AO	31	LEU
9	AO	38	ARG
9	AO	39	LEU
9	AO	45	VAL
9	AO	65	ARG

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Mol	Chain	Res	Type
9	AO	66	LEU
9	AO	82	ILE
9	AO	83	GLU
10	AP	2	VAL
10	AP	4	ILE
10	AP	8	ARG
10	AP	20	VAL
10	AP	21	VAL
10	AP	25	ARG
10	AP	27	LYS
10	AP	28	ARG
10	AP	45	THR
10	AP	54	GLU
10	AP	81	ARG
11	AQ	7	THR
11	AQ	14	LYS
11	AQ	36	ILE
11	AQ	37	LYS
11	AQ	38	ARG
11	AQ	48	GLU
11	AQ	50	LYS
11	AQ	52	LYS
11	AQ	59	ILE
11	AQ	74	LEU
11	AQ	87	LYS
11	AQ	92	ARG
11	AQ	93	GLN
11	AQ	97	SER
11	AQ	100	LYS
12	AR	31	LEU
12	AR	32	ARG
12	AR	37	VAL
12	AR	45	SER
12	AR	47	THR
12	AR	54	ARG
12	AR	65	ILE
12	AR	76	LEU
12	AR	85	LEU
13	AS	5	LEU
13	AS	6	LYS
13	AS	7	LYS
13	AS	9	VAL

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Mol	Chain	Res	Type
13	AS	13	ASP
13	AS	15	LEU
13	AS	16	LEU
13	AS	18	LYS
13	AS	22	LEU
13	AS	30	LEU
13	AS	37	ARG
13	AS	44	MET
13	AS	60	VAL
13	AS	63	THR
13	AS	64	GLU
13	AS	70	LYS
13	AS	80	TYR
14	AT	23	ARG
14	AT	24	LEU
14	AT	27	LYS
14	AT	30	LYS
14	AT	35	THR
14	AT	38	LYS
14	AT	51	GLU
14	AT	58	LYS
14	AT	65	LYS
14	AT	75	ASN
14	AT	85	MET
14	AT	86	ARG
14	AT	89	ARG
14	AT	93	GLU
14	AT	104	LEU
15	AB	7	VAL
15	AB	15	VAL
15	AB	17	PHE
15	AB	24	TRP
15	AB	30	ARG
15	AB	32	ILE
15	AB	36	ARG
15	AB	37	ASN
15	AB	41	ILE
15	AB	42	ILE
15	AB	43	ASP
15	AB	52	GLU
15	AB	67	THR
15	AB	96	ARG

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Mol	Chain	Res	Type
15	AB	117	GLU
15	AB	119	GLU
15	AB	128	GLU
15	AB	133	LYS
15	AB	137	ARG
15	AB	140	HIS
15	AB	155	LEU
15	AB	156	LYS
15	AB	170	GLU
15	AB	178	ARG
15	AB	187	LEU
15	AB	196	LEU
15	AB	200	ILE
15	AB	212	GLN
15	AB	215	LEU
15	AB	223	ILE
16	AC	5	ILE
16	AC	12	LEU
16	AC	14	ILE
16	AC	16	ARG
16	AC	21	ARG
16	AC	22	TRP
16	AC	27	LYS
16	AC	34	LEU
16	AC	36	ASP
16	AC	38	ARG
16	AC	46	GLU
16	AC	47	LEU
16	AC	49	SER
16	AC	52	LEU
16	AC	54	ARG
16	AC	56	ASP
16	AC	62	ASP
16	AC	68	VAL
16	AC	72	LYS
16	AC	73	PRO
16	AC	82	GLU
16	AC	83	ARG
16	AC	85	ARG
16	AC	86	VAL
16	AC	94	LEU
16	AC	99	VAL

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Mol	Chain	Res	Type
16	AC	104	GLN
16	AC	131	ARG
16	AC	132	ARG
16	AC	136	GLN
16	AC	154	SER
16	AC	166	GLU
16	AC	167	TRP
16	AC	179	ARG
16	AC	196	LEU
17	AD	3	ARG
17	AD	5	ILE
17	AD	8	VAL
17	AD	9	CYS
17	AD	10	ARG
17	AD	11	LEU
17	AD	15	GLU
17	AD	18	LYS
17	AD	19	LEU
17	AD	22	LYS
17	AD	33	MET
17	AD	34	GLU
17	AD	36	ARG
17	AD	58	LEU
17	AD	73	ARG
17	AD	78	LEU
17	AD	85	LYS
17	AD	86	LYS
17	AD	91	SER
17	AD	96	LEU
17	AD	108	LEU
17	AD	115	ARG
17	AD	127	THR
17	AD	131	ARG
17	AD	132	ARG
17	AD	135	LEU
17	AD	139	ARG
17	AD	145	GLU
17	AD	150	GLU
17	AD	155	LEU
17	AD	162	LEU
17	AD	175	SER
17	AD	184	LYS

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Mol	Chain	Res	Type
17	AD	187	ARG
17	AD	194	LEU
17	AD	201	GLN
18	AE	11	ILE
18	AE	31	LEU
18	AE	34	VAL
18	AE	41	VAL
18	AE	47	LYS
18	AE	66	MET
18	AE	67	VAL
18	AE	76	ILE
18	AE	80	ILE
18	AE	100	VAL
18	AE	152	ARG
19	AF	3	ARG
19	AF	10	LEU
19	AF	16	GLN
19	AF	17	SER
19	AF	24	GLU
19	AF	25	ILE
19	AF	28	ARG
19	AF	43	LEU
19	AF	46	ARG
19	AF	54	LYS
19	AF	69	GLU
19	AF	78	GLU
19	AF	83	ASP
19	AF	92	LYS
20	AG	5	ARG
20	AG	8	GLU
20	AG	13	GLN
20	AG	22	LEU
20	AG	30	ILE
20	AG	32	ARG
20	AG	45	ASP
20	AG	54	THR
20	AG	61	VAL
20	AG	63	LYS
20	AG	67	GLU
20	AG	72	ARG
20	AG	84	ASN
20	AG	90	GLU

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Mol	Chain	Res	Type
20	AG	131	LYS
20	AG	137	LYS
21	AH	1	MET
21	AH	6	ILE
21	AH	18	ARG
21	AH	21	LYS
21	AH	24	THR
21	AH	30	ARG
21	AH	39	LEU
21	AH	41	ARG
21	AH	52	ASP
21	AH	56	LYS
21	AH	88	LYS
21	AH	91	ARG
21	AH	92	ARG
21	AH	99	GLU
21	AH	102	ARG
21	AH	104	ARG
21	AH	107	LEU
21	AH	109	ILE
21	AH	112	LEU
21	AH	115	SER
21	AH	125	ARG
21	AH	126	LYS
21	AH	127	LEU
22	AI	10	ARG
22	AI	14	VAL
22	AI	20	ARG
22	AI	42	ARG
22	AI	44	VAL
22	AI	47	LEU
22	AI	56	LEU
22	AI	64	THR
22	AI	65	VAL
22	AI	66	ARG
22	AI	70	LYS
22	AI	79	LEU
22	AI	86	VAL
22	AI	95	LYS
22	AI	97	LYS
22	AI	99	LEU
22	AI	111	ARG

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Mol	Chain	Res	Type
22	AI	112	LYS
22	AI	118	LYS
22	AI	121	ARG
22	AI	125	TYR
22	AI	128	ARG
23	AY	10	LYS
23	AY	12	LEU
23	AY	25	LYS
23	AY	30	GLU
23	AY	31	ARG
23	AY	33	LEU
23	AY	38	ARG
23	AY	39	ILE
23	AY	56	GLU
23	AY	61	ARG
23	AY	65	ILE
23	AY	69	VAL
23	AY	70	THR
23	AY	81	ILE
23	AY	91	THR
23	AY	96	ARG
23	AY	98	MET
23	AY	120	THR
23	AY	123	ARG
23	AY	146	LEU
23	AY	148	LEU
23	AY	152	THR
23	AY	156	ARG
23	AY	157	LEU
23	AY	165	GLN
23	AY	175	SER
23	AY	187	THR
23	AY	197	ARG
23	AY	201	ILE
23	AY	206	LEU
23	AY	224	ASP
23	AY	225	GLU
23	AY	230	LYS
23	AY	232	LEU
23	AY	254	LYS
23	AY	255	ILE
23	AY	260	LEU

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Mol	Chain	Res	Type
23	AY	264	LEU
23	AY	280	LEU
23	AY	284	LEU
23	AY	290	LYS
23	AY	295	GLU
23	AY	297	GLU
23	AY	298	VAL
23	AY	306	ASN
23	AY	312	LEU
23	AY	316	ILE
23	AY	319	ASP
23	AY	337	SER
23	AY	343	ASN
23	AY	346	LYS
23	AY	348	ARG
23	AY	349	LYS
23	AY	355	LEU
23	AY	356	LEU
23	AY	363	ARG
23	AY	369	LEU
23	AY	377	VAL
23	AY	378	VAL
23	AY	385	THR
23	AY	396	ARG
23	AY	399	LEU
23	AY	400	GLU
23	AY	402	ILE
23	AY	403	GLU
23	AY	409	ILE
23	AY	414	GLU
23	AY	422	GLU
23	AY	426	GLN
23	AY	431	LEU
23	AY	446	THR
23	AY	451	ILE
23	AY	452	SER
23	AY	459	LEU
23	AY	465	ARG
23	AY	471	LYS
23	AY	473	ASP
23	AY	476	VAL
23	AY	481	VAL

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Mol	Chain	Res	Type
23	AY	485	GLU
23	AY	488	THR
23	AY	492	ASP
23	AY	493	VAL
23	AY	512	ILE
23	AY	517	LEU
23	AY	544	LYS
23	AY	546	ILE
23	AY	548	GLU
23	AY	550	MET
23	AY	556	ILE
23	AY	566	THR
23	AY	584	ILE
23	AY	590	ILE
23	AY	591	LYS
23	AY	603	GLU
23	AY	610	VAL
23	AY	612	THR
23	AY	623	ASP
23	AY	628	ARG
23	AY	634	MET
23	AY	637	ARG
23	AY	647	VAL
23	AY	649	LEU
23	AY	679	VAL
23	AY	681	LYS
23	AY	684	GLN
23	AY	686	LYS
23	AY	687	LEU
24	AU	7	ARG
24	AU	9	ARG
24	AU	12	LYS
24	AU	15	ARG
24	AU	25	LYS
27	BN	1	MET
27	BN	3	THR
27	BN	4	TYR
27	BN	8	GLN
27	BN	9	VAL
27	BN	16	ILE
27	BN	19	GLU
27	BN	28	THR

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Mol	Chain	Res	Type
27	BN	33	LEU
27	BN	34	LEU
27	BN	39	ARG
27	BN	41	ASP
27	BN	43	THR
27	BN	48	MET
27	BN	55	VAL
27	BN	58	ASP
27	BN	60	ILE
27	BN	62	VAL
27	BN	63	THR
27	BN	65	LYS
27	BN	67	LEU
27	BN	68	GLU
27	BN	73	THR
27	BN	87	LEU
27	BN	93	THR
27	BN	99	LEU
27	BN	109	LYS
27	BN	119	ARG
27	BN	120	LEU
27	BN	121	LYS
27	BN	133	GLN
27	BN	134	ARG
27	BN	136	GLU
28	BO	3	GLN
28	BO	8	LEU
28	BO	10	VAL
28	BO	22	ILE
28	BO	23	ARG
28	BO	24	VAL
28	BO	47	ILE
28	BO	49	ARG
28	BO	66	LYS
28	BO	70	LYS
28	BO	88	ASN
28	BO	91	LEU
28	BO	94	ARG
28	BO	98	VAL
28	BO	104	ARG
28	BO	113	LYS
29	BP	6	LEU

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Mol	Chain	Res	Type
29	BP	13	ASN
29	BP	16	ARG
29	BP	27	HIS
29	BP	29	LYS
29	BP	39	LYS
29	BP	42	SER
29	BP	45	LEU
29	BP	55	ARG
29	BP	56	SER
29	BP	57	THR
29	BP	58	THR
29	BP	61	ARG
29	BP	62	LEU
29	BP	67	MET
29	BP	68	GLN
29	BP	76	LYS
29	BP	88	LEU
29	BP	91	PHE
29	BP	95	VAL
29	BP	98	GLU
29	BP	100	LEU
29	BP	105	LEU
29	BP	107	LYS
29	BP	110	TYR
29	BP	114	ILE
29	BP	115	LEU
29	BP	125	VAL
29	BP	135	LEU
29	BP	138	LEU
30	BQ	10	ARG
30	BQ	16	ARG
30	BQ	18	LYS
30	BQ	45	GLN
30	BQ	55	VAL
30	BQ	58	PHE
30	BQ	59	ARG
30	BQ	75	THR
30	BQ	76	LYS
30	BQ	96	VAL
30	BQ	115	MET
30	BQ	131	ILE
30	BQ	133	ARG

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Mol	Chain	Res	Type
30	BQ	134	ARG
30	BQ	138	ASP
31	BR	4	LEU
31	BR	8	ARG
31	BR	18	LEU
31	BR	28	LEU
31	BR	29	LEU
31	BR	33	ARG
31	BR	36	THR
31	BR	44	LEU
31	BR	51	LEU
31	BR	57	ARG
31	BR	63	ARG
31	BR	67	LEU
31	BR	74	LYS
31	BR	79	LEU
31	BR	88	ARG
31	BR	100	LEU
31	BR	105	ARG
31	BR	113	LEU
31	BR	116	LEU
31	BR	118	GLU
32	BS	15	ARG
32	BS	20	ARG
32	BS	27	SER
32	BS	30	ARG
32	BS	31	SER
32	BS	34	HIS
32	BS	49	VAL
32	BS	54	LEU
32	BS	73	LEU
32	BS	80	LEU
32	BS	89	ARG
32	BS	92	TYR
32	BS	97	ARG
32	BS	99	LYS
32	BS	107	GLU
33	BT	3	ARG
33	BT	6	LEU
33	BT	11	GLU
33	BT	15	VAL
33	BT	27	THR

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Mol	Chain	Res	Type
33	BT	29	ARG
33	BT	32	TYR
33	BT	43	GLN
33	BT	49	VAL
33	BT	50	ILE
33	BT	53	ARG
33	BT	58	ASN
33	BT	59	THR
33	BT	62	THR
33	BT	63	VAL
33	BT	64	ARG
33	BT	65	LYS
33	BT	78	LEU
33	BT	82	LEU
33	BT	86	ILE
33	BT	87	ASP
33	BT	90	GLN
33	BT	93	ARG
33	BT	96	ARG
33	BT	112	ARG
33	BT	118	ARG
33	BT	119	LYS
33	BT	123	GLN
33	BT	128	GLU
34	BU	8	VAL
34	BU	13	LYS
34	BU	15	LYS
34	BU	16	LYS
34	BU	19	LYS
34	BU	31	SER
34	BU	34	LYS
34	BU	60	LEU
34	BU	70	ARG
34	BU	74	LEU
34	BU	83	LEU
34	BU	88	ILE
34	BU	92	ARG
34	BU	108	GLU
34	BU	112	ARG
34	BU	114	LYS
35	BV	5	VAL
35	BV	6	LYS

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Mol	Chain	Res	Type
35	BV	13	ARG
35	BV	16	PRO
35	BV	18	LEU
35	BV	19	LYS
35	BV	20	LEU
35	BV	21	ARG
35	BV	28	GLU
35	BV	32	THR
35	BV	33	VAL
35	BV	35	LEU
35	BV	39	LEU
35	BV	40	LEU
35	BV	46	VAL
35	BV	47	VAL
35	BV	57	VAL
35	BV	61	VAL
35	BV	62	LEU
35	BV	66	ARG
35	BV	72	VAL
35	BV	73	SER
35	BV	79	VAL
35	BV	85	LYS
35	BV	95	LEU
35	BV	99	ILE
36	BW	11	ARG
36	BW	17	VAL
36	BW	20	VAL
36	BW	23	LEU
36	BW	41	LYS
36	BW	50	VAL
36	BW	51	LEU
36	BW	52	GLU
36	BW	60	ASN
36	BW	63	ASP
36	BW	76	VAL
36	BW	96	ILE
36	BW	100	THR
36	BW	106	ILE
36	BW	107	LEU
36	BW	110	LYS
37	BX	12	VAL
37	BX	27	THR

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Mol	Chain	Res	Type
37	BX	39	ILE
37	BX	48	LYS
37	BX	57	LEU
37	BX	60	ARG
37	BX	63	LYS
37	BX	64	LYS
37	BX	66	LEU
37	BX	68	ARG
37	BX	72	LYS
37	BX	73	ARG
37	BX	77	LYS
37	BX	78	LYS
37	BX	80	ILE
38	BY	4	LYS
38	BY	6	HIS
38	BY	8	LYS
38	BY	9	LYS
38	BY	31	LEU
38	BY	34	LYS
38	BY	38	ILE
38	BY	44	ILE
38	BY	45	VAL
38	BY	71	LYS
38	BY	75	ILE
38	BY	81	LYS
38	BY	83	THR
38	BY	85	VAL
38	BY	87	LYS
38	BY	88	LYS
38	BY	89	PHE
38	BY	97	ARG
38	BY	99	CYS
39	BZ	5	LEU
39	BZ	6	LYS
39	BZ	16	SER
39	BZ	23	LYS
39	BZ	31	ARG
39	BZ	34	ASN
39	BZ	42	VAL
39	BZ	46	LYS
39	BZ	61	LEU
39	BZ	63	ASP

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Mol	Chain	Res	Type
39	BZ	72	ARG
39	BZ	79	ARG
39	BZ	80	ARG
39	BZ	81	ARG
39	BZ	82	ARG
39	BZ	86	VAL
39	BZ	87	ASP
39	BZ	105	VAL
39	BZ	112	ARG
39	BZ	118	GLN
39	BZ	122	ARG
39	BZ	132	ASN
39	BZ	144	LEU
39	BZ	146	ILE
39	BZ	150	LEU
39	BZ	153	SER
39	BZ	156	LYS
40	B0	11	ARG
40	B0	19	LYS
40	B0	20	ARG
40	B0	30	VAL
40	B0	41	ARG
40	B0	43	THR
40	B0	49	LYS
40	B0	64	ASP
40	B0	68	GLU
40	B0	84	LEU
41	B1	7	ILE
41	B1	30	VAL
41	B1	38	SER
41	B1	39	LYS
41	B1	40	ARG
41	B1	46	LEU
41	B1	48	LYS
41	B1	52	ARG
41	B1	58	ILE
41	B1	59	THR
41	B1	61	ARG
41	B1	72	GLU
41	B1	75	GLU
41	B1	82	LEU
41	B1	83	GLU

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Mol	Chain	Res	Type
42	B2	2	LYS
42	B2	3	LEU
42	B2	8	LYS
42	B2	15	LYS
42	B2	16	LEU
42	B2	17	SER
42	B2	30	ARG
42	B2	32	LEU
42	B2	44	LEU
42	B2	47	ASN
42	B2	51	ARG
42	B2	52	ASP
42	B2	53	LEU
42	B2	64	LEU
42	B2	68	ARG
43	BD	3	VAL
43	BD	4	LYS
43	BD	13	ARG
43	BD	24	ILE
43	BD	26	LYS
43	BD	28	GLU
43	BD	33	LEU
43	BD	34	VAL
43	BD	35	LYS
43	BD	43	ARG
43	BD	44	ASN
43	BD	45	ASN
43	BD	49	ILE
43	BD	64	ILE
43	BD	65	ILE
43	BD	78	LYS
43	BD	88	ARG
43	BD	89	SER
43	BD	94	LEU
43	BD	103	ARG
43	BD	111	LEU
43	BD	117	VAL
43	BD	138	VAL
43	BD	140	THR
43	BD	155	LEU
43	BD	166	GLN
43	BD	169	GLU

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Mol	Chain	Res	Type
43	BD	171	ASP
43	BD	176	ARG
43	BD	192	THR
43	BD	193	VAL
43	BD	211	ARG
43	BD	218	ARG
43	BD	229	VAL
43	BD	232	PRO
43	BD	242	ARG
43	BD	244	ARG
43	BD	252	TRP
43	BD	257	LEU
43	BD	260	ARG
43	BD	262	ARG
43	BD	266	SER
43	BD	271	ILE
44	B3	3	ARG
44	B3	6	VAL
44	B3	8	LEU
44	B3	17	LYS
44	B3	18	ASP
44	B3	29	ARG
44	B3	31	LEU
44	B3	36	VAL
44	B3	37	LEU
44	B3	40	THR
45	B4	48	ILE
45	B4	49	GLU
45	B4	50	THR
45	B4	62	CYS
46	B5	4	HIS
46	B5	6	VAL
46	B5	11	THR
46	B5	23	HIS
46	B5	29	THR
46	B5	37	LYS
46	B5	48	GLU
46	B5	49	CYS
46	B5	56	LYS
47	B6	10	LEU
47	B6	11	LEU
47	B6	17	LYS

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Mol	Chain	Res	Type
47	B6	18	ARG
47	B6	26	ASN
47	B6	32	ASN
47	B6	33	LYS
47	B6	42	TRP
47	B6	44	ARG
47	B6	46	HIS
47	B6	50	ARG
47	B6	51	GLU
48	B7	11	LYS
48	B7	23	ARG
48	B7	24	THR
48	B7	41	ARG
48	B7	43	THR
48	B7	48	LYS
49	B8	6	THR
49	B8	8	LYS
49	B8	13	ARG
49	B8	14	VAL
49	B8	15	LYS
49	B8	23	VAL
49	B8	30	ARG
49	B8	31	HIS
49	B8	32	LEU
49	B8	33	ASN
49	B8	34	TRP
49	B8	35	GLN
49	B8	36	LYS
49	B8	44	LYS
49	B8	47	LYS
49	B8	49	VAL
49	B8	52	LYS
49	B8	56	GLU
49	B8	61	LEU
49	B8	64	TYR
50	B9	2	LYS
50	B9	4	ARG
50	B9	6	SER
50	B9	9	ARG
50	B9	14	CYS
50	B9	20	HIS
50	B9	22	ARG

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Mol	Chain	Res	Type
50	B9	26	ILE
50	B9	29	ASN
50	B9	32	HIS
51	BC	5	LYS
51	BC	23	ASP
51	BC	27	ARG
51	BC	30	LYS
51	BC	53	ARG
51	BC	63	SER
51	BC	68	LEU
51	BC	73	ARG
51	BC	81	GLU
51	BC	84	LYS
51	BC	92	ASP
51	BC	99	ILE
51	BC	104	LEU
51	BC	131	LEU
51	BC	141	LYS
51	BC	217	THR
51	BC	223	ARG
51	BC	227	HIS
52	BE	7	VAL
52	BE	9	VAL
52	BE	11	MET
52	BE	12	THR
52	BE	18	ASP
52	BE	24	THR
52	BE	33	VAL
52	BE	34	VAL
52	BE	40	GLU
52	BE	54	GLN
52	BE	55	ASN
52	BE	57	LYS
52	BE	60	ASN
52	BE	82	ARG
52	BE	87	GLU
52	BE	89	ASP
52	BE	92	THR
52	BE	93	VAL
52	BE	94	GLU
52	BE	111	ARG
52	BE	113	PHE

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Mol	Chain	Res	Type
52	BE	118	LYS
52	BE	144	ARG
52	BE	146	THR
52	BE	152	LYS
52	BE	154	LYS
52	BE	175	VAL
52	BE	181	LEU
52	BE	185	LYS
52	BE	188	VAL
52	BE	195	LEU
52	BE	197	ILE
52	BE	202	LYS
52	BE	203	LYS
53	BF	4	VAL
53	BF	8	GLN
53	BF	18	ARG
53	BF	19	GLU
53	BF	20	LEU
53	BF	23	ASP
53	BF	24	LEU
53	BF	27	GLU
53	BF	28	ILE
53	BF	43	LYS
53	BF	53	THR
53	BF	57	VAL
53	BF	65	TRP
53	BF	66	PRO
53	BF	68	LYS
53	BF	72	ARG
53	BF	74	ARG
53	BF	88	VAL
53	BF	102	PRO
53	BF	103	LYS
53	BF	106	ARG
53	BF	110	LEU
53	BF	117	ARG
53	BF	126	VAL
53	BF	157	VAL
53	BF	164	ARG
53	BF	170	LEU
53	BF	175	THR
53	BF	192	LEU

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Mol	Chain	Res	Type
53	BF	199	TRP
53	BF	200	GLU
54	BG	5	VAL
54	BG	8	LYS
54	BG	16	ARG
54	BG	21	ARG
54	BG	22	ARG
54	BG	33	ARG
54	BG	39	ILE
54	BG	43	LEU
54	BG	45	GLU
54	BG	47	LYS
54	BG	62	LEU
54	BG	71	THR
54	BG	80	PHE
54	BG	82	LEU
54	BG	86	MET
54	BG	98	ARG
54	BG	123	ASN
54	BG	126	ASP
54	BG	128	ARG
54	BG	130	ASN
54	BG	139	LEU
54	BG	143	GLU
54	BG	146	TYR
54	BG	148	MET
54	BG	152	LEU
54	BG	161	THR
54	BG	166	ASP
55	BH	23	ARG
55	BH	24	VAL
55	BH	25	LYS
55	BH	34	GLU
55	BH	36	PRO
55	BH	42	ARG
55	BH	43	VAL
55	BH	46	GLU
55	BH	53	GLU
55	BH	69	ARG
55	BH	71	LEU
55	BH	80	SER
55	BH	85	LYS

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Mol	Chain	Res	Type
55	BH	89	ILE
55	BH	97	ARG
55	BH	101	ARG
55	BH	105	LEU
55	BH	107	VAL
55	BH	119	GLU
55	BH	122	THR
55	BH	132	ARG
55	BH	139	GLN
55	BH	143	GLN
55	BH	153	LYS
55	BH	155	SER
55	BH	162	ILE
55	BH	168	PRO
55	BH	171	LEU
55	BH	173	PRO
56	BK	2	LYS
56	BK	3	LYS
56	BK	5	VAL
56	BK	29	GLN
56	BK	30	HIS
56	BK	38	VAL
56	BK	47	ASN
56	BK	65	PHE
56	BK	70	LYS
56	BK	77	LEU
56	BK	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
4	AJ	13	HIS
5	AK	93	GLN
5	AK	117	ASN
7	AM	62	ASN
7	AM	101	GLN
9	AO	9	GLN
13	AS	23	ASN
15	AB	37	ASN
15	AB	76	GLN
15	AB	95	GLN
15	AB	135	GLN

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Mol	Chain	Res	Type
17	AD	42	GLN
17	AD	62	GLN
19	AF	16	GLN
19	AF	64	GLN
20	AG	86	GLN
23	AY	124	GLN
23	AY	154	GLN
23	AY	343	ASN
23	AY	664	GLN
28	BO	3	GLN
28	BO	88	ASN
29	BP	38	GLN
29	BP	70	GLN
30	BQ	12	GLN
30	BQ	123	HIS
31	BR	13	HIS
31	BR	23	ASN
32	BS	95	HIS
33	BT	38	ASN
33	BT	90	GLN
34	BU	94	ASN
36	BW	61	ASN
36	BW	102	HIS
37	BX	55	ASN
39	BZ	34	ASN
40	B0	70	GLN
42	B2	70	GLN
43	BD	45	ASN
43	BD	58	HIS
43	BD	96	HIS
43	BD	227	ASN
44	B3	19	GLN
47	B6	26	ASN
47	B6	49	HIS
48	B7	16	HIS
49	B8	43	GLN
50	B9	29	ASN
50	B9	32	HIS
51	BC	66	HIS
51	BC	71	GLN
51	BC	188	ASN
52	BE	60	ASN

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Mol	Chain	Res	Type
52	BE	132	HIS
52	BE	180	ASN
53	BF	31	HIS
53	BF	169	ASN
55	BH	61	HIS
56	BK	29	GLN
56	BK	47	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1512/1516 (99%)	315 (20%)	65 (4%)
2	AV	73/76 (96%)	28 (38%)	9 (12%)
25	BA	2849/2915 (97%)	756 (26%)	130 (4%)
26	BB	119/122 (97%)	34 (28%)	4 (3%)
3	AX	5/25 (20%)	0	0
All	All	4558/4654 (97%)	1133 (24%)	208 (4%)

All (1133) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	U
1	AA	30	U
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	48	C
1	AA	49	U
1	AA	50	A
1	AA	51	A
1	AA	60	A
1	AA	61	G
1	AA	63	C
1	AA	76	C
1	AA	79	G
1	AA	80	G
1	AA	81	U
1	AA	88	A
1	AA	90	U
1	AA	91	C

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Mol	Chain	Res	Type
1	AA	92	C
1	AA	97	G
1	AA	101	A
1	AA	105	G
1	AA	108	G
1	AA	116	A
1	AA	121	C
1	AA	131	C
1	AA	144	G
1	AA	146	G
1	AA	147	G
1	AA	150	C
1	AA	160	A
1	AA	163	C
1	AA	179	A
1	AA	189(G)	G
1	AA	195	A
1	AA	197	A
1	AA	203	U
1	AA	204	U
1	AA	216	G
1	AA	217	C
1	AA	220	G
1	AA	221	C
1	AA	231	G
1	AA	244	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	301	G
1	AA	319	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	331	G
1	AA	332	G
1	AA	346	G
1	AA	347	G
1	AA	352	C
1	AA	353	A

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Mol	Chain	Res	Type
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	374	A
1	AA	381	C
1	AA	384	G
1	AA	398	C
1	AA	406	G
1	AA	409	G
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	422	C
1	AA	423	G
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	439	A
1	AA	441	A
1	AA	443	C
1	AA	452	A
1	AA	470	C
1	AA	485	G
1	AA	492	G
1	AA	495	A
1	AA	496	A
1	AA	498	U
1	AA	501	C
1	AA	505	G
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	518	C
1	AA	519	C
1	AA	522	C
1	AA	527	G
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	534	U
1	AA	539	A

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Mol	Chain	Res	Type
1	AA	545	C
1	AA	547	A
1	AA	559	A
1	AA	561	U
1	AA	562	C
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	577	G
1	AA	582	U
1	AA	592	G
1	AA	596	C
1	AA	617	G
1	AA	630	G
1	AA	631	G
1	AA	632	A
1	AA	633	G
1	AA	649	G
1	AA	653	A
1	AA	665	A
1	AA	671	G
1	AA	673	G
1	AA	688	G
1	AA	731	G
1	AA	734	G
1	AA	749	C
1	AA	755	G
1	AA	765	G
1	AA	773	G
1	AA	777	A
1	AA	785	G
1	AA	794	A
1	AA	801	U
1	AA	802	A
1	AA	816	A
1	AA	817	C
1	AA	827	U
1	AA	828	A
1	AA	838	G
1	AA	839	U
1	AA	840	C
1	AA	841	U

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Mol	Chain	Res	Type
1	AA	848	C
1	AA	851	G
1	AA	853	G
1	AA	859	A
1	AA	876	G
1	AA	890	G
1	AA	902	G
1	AA	913	A
1	AA	914	A
1	AA	919	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	947	G
1	AA	960	U
1	AA	961	U
1	AA	966	G
1	AA	968	A
1	AA	969	A
1	AA	973	G
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	980	C
1	AA	981	U
1	AA	984	C
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	994	A
1	AA	1001(A)	G
1	AA	1004	A
1	AA	1005	A
1	AA	1009	G
1	AA	1013	G
1	AA	1016	A
1	AA	1021	G
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G

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Mol	Chain	Res	Type
1	AA	1027	C
1	AA	1030	C
1	AA	1030(D)	A
1	AA	1031	G
1	AA	1044	A
1	AA	1046	A
1	AA	1050	G
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
1	AA	1065	U
1	AA	1067	A
1	AA	1068	G
1	AA	1081	G
1	AA	1086	U
1	AA	1087	G
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U
1	AA	1126	U
1	AA	1127	G
1	AA	1132	C
1	AA	1133	G
1	AA	1134	G
1	AA	1135	U
1	AA	1136	U
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1143	G
1	AA	1146	A
1	AA	1147	C
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1171	G
1	AA	1181	G
1	AA	1184	G

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Mol	Chain	Res	Type
1	AA	1187	G
1	AA	1192	C
1	AA	1196	U
1	AA	1197	G
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1218	C
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1259	C
1	AA	1260	C
1	AA	1269	A
1	AA	1273	G
1	AA	1281	U
1	AA	1285	A
1	AA	1286	A
1	AA	1287	A
1	AA	1288	A
1	AA	1290	G
1	AA	1293	G
1	AA	1299	A
1	AA	1300	G
1	AA	1301	U
1	AA	1302	U
1	AA	1305	G
1	AA	1310	G
1	AA	1317	C
1	AA	1319	A
1	AA	1320	C
1	AA	1322	C
1	AA	1323	G
1	AA	1328	C
1	AA	1332	A
1	AA	1336	C
1	AA	1337	G

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Mol	Chain	Res	Type
1	AA	1338	G
1	AA	1346	A
1	AA	1347	G
1	AA	1350	A
1	AA	1353	G
1	AA	1364	U
1	AA	1378	C
1	AA	1397	C
1	AA	1398	A
1	AA	1402	C
1	AA	1407	C
1	AA	1419	G
1	AA	1422	G
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1443	G
1	AA	1446	U
1	AA	1447	A
1	AA	1452	C
1	AA	1456	G
1	AA	1457	G
1	AA	1472	U
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1499	A
1	AA	1502	A
1	AA	1504	G
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1519	A
1	AA	1520	G
1	AA	1529	G
1	AA	1530	G
1	AA	1532	U
1	AA	1533	C
1	AA	1534	A
1	AA	1535	C
1	AA	1536	C
1	AA	1542	U

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Mol	Chain	Res	Type
1	AA	1543	C
2	AV	4	C
2	AV	13	C
2	AV	15	G
2	AV	19	G
2	AV	20	U
2	AV	21	A
2	AV	22	G
2	AV	23	A
2	AV	26	A
2	AV	27	G
2	AV	30	G
2	AV	34	G
2	AV	35	A
2	AV	38	A
2	AV	44	G
2	AV	46	G
2	AV	47	U
2	AV	48	C
2	AV	51	U
2	AV	52	G
2	AV	53	G
2	AV	57	G
2	AV	61	C
2	AV	72	C
2	AV	73	A
2	AV	74	C
2	AV	75	C
2	AV	76	A
25	BA	9	U
25	BA	10	G
25	BA	34	C
25	BA	35	G
25	BA	36	G
25	BA	41	C
25	BA	45	C
25	BA	49	A
25	BA	50	U
25	BA	55	G
25	BA	63	U
25	BA	71	A
25	BA	72	U

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Mol	Chain	Res	Type
25	BA	74	A
25	BA	75	G
25	BA	86	C
25	BA	88	G
25	BA	90	U
25	BA	92	A
25	BA	94	C
25	BA	95	G
25	BA	99	U
25	BA	100	G
25	BA	102	G
25	BA	103	A
25	BA	110	G
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	123	G
25	BA	128	C
25	BA	129	C
25	BA	131	G
25	BA	141	A
25	BA	154	G
25	BA	154(A)	C
25	BA	158	U
25	BA	171	G
25	BA	173	G
25	BA	174	C
25	BA	175	G
25	BA	181	A
25	BA	182	A
25	BA	196	A
25	BA	197	A
25	BA	199	A
25	BA	200	U
25	BA	204	A
25	BA	205	G
25	BA	214	G
25	BA	215	G
25	BA	216	A
25	BA	217	G
25	BA	221	A
25	BA	222	A

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Mol	Chain	Res	Type
25	BA	224	G
25	BA	228	A
25	BA	229	A
25	BA	233	A
25	BA	248	G
25	BA	250	G
25	BA	252	G
25	BA	259	G
25	BA	264	C
25	BA	265	A
25	BA	271(C)	C
25	BA	271(D)	G
25	BA	271(J)	C
25	BA	271(K)	U
25	BA	271(L)	U
25	BA	271(M)	G
25	BA	271(N)	U
25	BA	271(P)	C
25	BA	271(T)	C
25	BA	271(U)	G
25	BA	271(Y)	U
25	BA	271(Z)	C
25	BA	272	G
25	BA	272(G)	C
25	BA	272(H)	C
25	BA	272(I)	U
25	BA	272(J)	C
25	BA	274	G
25	BA	275	G
25	BA	280	C
25	BA	288	C
25	BA	289	A
25	BA	298	G
25	BA	310	A
25	BA	311	A
25	BA	320	A
25	BA	324	A
25	BA	327	G
25	BA	329	G
25	BA	330	A
25	BA	333	G
25	BA	334	C

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Mol	Chain	Res	Type
25	BA	335	C
25	BA	342	G
25	BA	345	A
25	BA	346	A
25	BA	349	G
25	BA	352	G
25	BA	353	G
25	BA	358	U
25	BA	360	G
25	BA	362	U
25	BA	363	G
25	BA	363(A)	A
25	BA	363(B)	G
25	BA	363(E)	U
25	BA	372	G
25	BA	374	A
25	BA	386	G
25	BA	387	U
25	BA	388	G
25	BA	389	G
25	BA	396	G
25	BA	405	U
25	BA	407	G
25	BA	411	G
25	BA	416	C
25	BA	428	A
25	BA	438	G
25	BA	441	U
25	BA	442	G
25	BA	443	A
25	BA	444	C
25	BA	448	U
25	BA	452	G
25	BA	454	A
25	BA	457	A
25	BA	470	A
25	BA	473	G
25	BA	479	A
25	BA	480	A
25	BA	481	G
25	BA	488	G
25	BA	494	G

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Mol	Chain	Res	Type
25	BA	504	U
25	BA	505	A
25	BA	508	G
25	BA	510	C
25	BA	513	A
25	BA	517	C
25	BA	528	A
25	BA	529	A
25	BA	530	G
25	BA	531	C
25	BA	532	A
25	BA	533	G
25	BA	543	C
25	BA	548	A
25	BA	549	G
25	BA	551	G
25	BA	563	G
25	BA	565	C
25	BA	571	A
25	BA	573	G
25	BA	574	C
25	BA	575	A
25	BA	584	C
25	BA	586	A
25	BA	587	C
25	BA	592	G
25	BA	593	G
25	BA	604	G
25	BA	606	U
25	BA	607	U
25	BA	609	A
25	BA	613	G
25	BA	614	U
25	BA	614(B)	G
25	BA	615	G
25	BA	620	G
25	BA	621	A
25	BA	622	G
25	BA	624	C
25	BA	627	A
25	BA	631	A
25	BA	637	A

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Mol	Chain	Res	Type
25	BA	645	C
25	BA	646	A
25	BA	647	G
25	BA	652	C
25	BA	669	G
25	BA	685	A
25	BA	686	G
25	BA	708	C
25	BA	715	G
25	BA	721	C
25	BA	722	A
25	BA	729	G
25	BA	730	C
25	BA	738	G
25	BA	764	A
25	BA	765	G
25	BA	775	G
25	BA	776	G
25	BA	782	A
25	BA	784	A
25	BA	785	G
25	BA	790	C
25	BA	791	C
25	BA	792	G
25	BA	805	G
25	BA	812	C
25	BA	819	A
25	BA	827	U
25	BA	828	U
25	BA	830	G
25	BA	836	G
25	BA	854	G
25	BA	858	U
25	BA	859	G
25	BA	878	A
25	BA	886	C
25	BA	888	C
25	BA	890	A
25	BA	896	A
25	BA	897	C
25	BA	900	A
25	BA	901	A

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Mol	Chain	Res	Type
25	BA	906	G
25	BA	907	U
25	BA	910	A
25	BA	917	A
25	BA	919	G
25	BA	932	G
25	BA	933	A
25	BA	934	G
25	BA	941	A
25	BA	945	A
25	BA	946	G
25	BA	958	U
25	BA	961	C
25	BA	973	A
25	BA	974	G
25	BA	983	A
25	BA	991	C
25	BA	996	A
25	BA	997	G
25	BA	999	U
25	BA	1012	U
25	BA	1013	C
25	BA	1022	G
25	BA	1023	U
25	BA	1025	G
25	BA	1026	U
25	BA	1027	A
25	BA	1033	U
25	BA	1038	C
25	BA	1039	G
25	BA	1040	C
25	BA	1042	G
25	BA	1045	A
25	BA	1046	A
25	BA	1047	G
25	BA	1048	A
25	BA	1049	C
25	BA	1050	A
25	BA	1053	C
25	BA	1054	A
25	BA	1055	G
25	BA	1057	A

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Mol	Chain	Res	Type
25	BA	1058	G
25	BA	1059	G
25	BA	1060	U
25	BA	1063	G
25	BA	1071	G
25	BA	1072	C
25	BA	1073	A
25	BA	1074	G
25	BA	1075	C
25	BA	1076	C
25	BA	1077	A
25	BA	1078	U
25	BA	1079	C
25	BA	1083	U
25	BA	1087	G
25	BA	1088	A
25	BA	1089	G
25	BA	1090	U
25	BA	1092	C
25	BA	1093	G
25	BA	1094	U
25	BA	1096	A
25	BA	1097	U
25	BA	1098	A
25	BA	1099	G
25	BA	1100	C
25	BA	1101	U
25	BA	1106	G
25	BA	1107	G
25	BA	1110	G
25	BA	1111	A
25	BA	1112	G
25	BA	1113	U
25	BA	1114	G
25	BA	1115	G
25	BA	1116	C
25	BA	1122	G
25	BA	1128	A
25	BA	1129	A
25	BA	1135	C
25	BA	1136	G
25	BA	1139	G

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Mol	Chain	Res	Type
25	BA	1142	U
25	BA	1143	A
25	BA	1148	A
25	BA	1151	G
25	BA	1155	A
25	BA	1168	G
25	BA	1171	G
25	BA	1173	G
25	BA	1174	A
25	BA	1175	U
25	BA	1176	G
25	BA	1177	A
25	BA	1179	C
25	BA	1180	C
25	BA	1187	G
25	BA	1193	G
25	BA	1194	A
25	BA	1195	G
25	BA	1210	A
25	BA	1211	U
25	BA	1218	C
25	BA	1220	A
25	BA	1235	G
25	BA	1237	A
25	BA	1242	A
25	BA	1244	G
25	BA	1246	A
25	BA	1247	A
25	BA	1249	U
25	BA	1253	A
25	BA	1256	G
25	BA	1263	U
25	BA	1271	G
25	BA	1272	A
25	BA	1273	U
25	BA	1281	G
25	BA	1284	A
25	BA	1288	U
25	BA	1289	C
25	BA	1300	U
25	BA	1301	A
25	BA	1302	A

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Mol	Chain	Res	Type
25	BA	1306	C
25	BA	1308	A
25	BA	1329	U
25	BA	1338	G
25	BA	1344	G
25	BA	1345	C
25	BA	1347	G
25	BA	1350	C
25	BA	1358	G
25	BA	1359	A
25	BA	1365	A
25	BA	1372	U
25	BA	1380	G
25	BA	1384	A
25	BA	1385	G
25	BA	1390	U
25	BA	1392	A
25	BA	1406	U
25	BA	1407	C
25	BA	1415	U
25	BA	1416	G
25	BA	1420	U
25	BA	1428	C
25	BA	1437	C
25	BA	1445	A
25	BA	1449	A
25	BA	1450	G
25	BA	1453	U
25	BA	1459	G
25	BA	1467	C
25	BA	1471	A
25	BA	1474	C
25	BA	1475	G
25	BA	1478	G
25	BA	1480	G
25	BA	1482	G
25	BA	1485	G
25	BA	1488	G
25	BA	1490	A
25	BA	1491	G
25	BA	1493	C
25	BA	1494	A

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Mol	Chain	Res	Type
25	BA	1495	A
25	BA	1496	A
25	BA	1497	U
25	BA	1502	C
25	BA	1503	U
25	BA	1505	C
25	BA	1506	C
25	BA	1508	A
25	BA	1509	C
25	BA	1509(A)	A
25	BA	1512	U
25	BA	1514	U
25	BA	1519	G
25	BA	1523	U
25	BA	1525	G
25	BA	1532	C
25	BA	1539	G
25	BA	1540	U
25	BA	1541	G
25	BA	1542	A
25	BA	1543	C
25	BA	1544	A
25	BA	1545	A
25	BA	1547	C
25	BA	1549	C
25	BA	1554	A
25	BA	1558	A
25	BA	1559	G
25	BA	1566	A
25	BA	1569	A
25	BA	1572	A
25	BA	1578	U
25	BA	1579	A
25	BA	1580	A
25	BA	1581	G
25	BA	1582	C
25	BA	1584	C
25	BA	1587	A
25	BA	1588	C
25	BA	1598	C
25	BA	1608	A
25	BA	1609	A

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Mol	Chain	Res	Type
25	BA	1610	A
25	BA	1616	A
25	BA	1617	C
25	BA	1618	A
25	BA	1622	G
25	BA	1624	G
25	BA	1647	G
25	BA	1648	C
25	BA	1652	A
25	BA	1653	G
25	BA	1654	A
25	BA	1655	A
25	BA	1672	C
25	BA	1674	G
25	BA	1678	G
25	BA	1681	G
25	BA	1686	C
25	BA	1695	G
25	BA	1696	G
25	BA	1701	A
25	BA	1722	A
25	BA	1739	U
25	BA	1740	G
25	BA	1741	A
25	BA	1742	G
25	BA	1744	C
25	BA	1745	C
25	BA	1745(A)	C
25	BA	1747	G
25	BA	1750	G
25	BA	1756	G
25	BA	1762	A
25	BA	1763	G
25	BA	1764	G
25	BA	1769	G
25	BA	1773	A
25	BA	1780	A
25	BA	1786	A
25	BA	1791	A
25	BA	1799	G
25	BA	1800	C
25	BA	1801	G

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Mol	Chain	Res	Type
25	BA	1802	A
25	BA	1810	A
25	BA	1816	G
25	BA	1820	U
25	BA	1829	A
25	BA	1834	U
25	BA	1835	G
25	BA	1838	C
25	BA	1839	G
25	BA	1843	C
25	BA	1847	A
25	BA	1848	A
25	BA	1858	G
25	BA	1859	A
25	BA	1864	U
25	BA	1865	G
25	BA	1876	A
25	BA	1877	A
25	BA	1878	G
25	BA	1880	C
25	BA	1881	C
25	BA	1882	C
25	BA	1885	A
25	BA	1888	G
25	BA	1889	A
25	BA	1900	A
25	BA	1907	G
25	BA	1913	A
25	BA	1914	C
25	BA	1915	U
25	BA	1919	A
25	BA	1924	C
25	BA	1925	C
25	BA	1930	G
25	BA	1936	A
25	BA	1938	A
25	BA	1944	U
25	BA	1947	C
25	BA	1955	U
25	BA	1963	U
25	BA	1964	G
25	BA	1965	C

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Mol	Chain	Res	Type
25	BA	1967	C
25	BA	1969	A
25	BA	1970	A
25	BA	1971	A
25	BA	1972	A
25	BA	1978	A
25	BA	1982	C
25	BA	1987	G
25	BA	1991	U
25	BA	1992	G
25	BA	1993	U
25	BA	1996	C
25	BA	1997	G
25	BA	2020	A
25	BA	2021	C
25	BA	2023	G
25	BA	2026	C
25	BA	2027	G
25	BA	2031	A
25	BA	2032	G
25	BA	2033	A
25	BA	2036	C
25	BA	2039	C
25	BA	2043	C
25	BA	2049	G
25	BA	2051	A
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2069	G
25	BA	2070	G
25	BA	2095	C
25	BA	2096	U
25	BA	2100	G
25	BA	2101	G
25	BA	2102	U
25	BA	2103	C
25	BA	2104	G
25	BA	2106	G
25	BA	2107	C

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Mol	Chain	Res	Type
25	BA	2108	C
25	BA	2113	U
25	BA	2115	G
25	BA	2116	G
25	BA	2122	U
25	BA	2123	G
25	BA	2126	A
25	BA	2127	G
25	BA	2131	G
25	BA	2137	C
25	BA	2138	C
25	BA	2140	C
25	BA	2141	G
25	BA	2142	C
25	BA	2145	C
25	BA	2146	C
25	BA	2147	G
25	BA	2148	G
25	BA	2151	G
25	BA	2152	G
25	BA	2153	G
25	BA	2154	G
25	BA	2156	G
25	BA	2158	A
25	BA	2159	G
25	BA	2163	C
25	BA	2172	U
25	BA	2173	A
25	BA	2178	C
25	BA	2179	C
25	BA	2180	U
25	BA	2182	G
25	BA	2183	C
25	BA	2186	G
25	BA	2187	G
25	BA	2191	G
25	BA	2192	G
25	BA	2193	G
25	BA	2194	G
25	BA	2198	A
25	BA	2199	A
25	BA	2201	C

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Mol	Chain	Res	Type
25	BA	2202	C
25	BA	2206	G
25	BA	2207	G
25	BA	2208	A
25	BA	2218	U
25	BA	2219	G
25	BA	2225	A
25	BA	2226	C
25	BA	2232	U
25	BA	2238	G
25	BA	2239	G
25	BA	2243	U
25	BA	2267	A
25	BA	2268	A
25	BA	2275	C
25	BA	2276	G
25	BA	2283	C
25	BA	2287	A
25	BA	2297	C
25	BA	2301	C
25	BA	2302	G
25	BA	2303	G
25	BA	2305	A
25	BA	2307	G
25	BA	2308	G
25	BA	2309	A
25	BA	2310	A
25	BA	2312	U
25	BA	2316	C
25	BA	2318	G
25	BA	2319	G
25	BA	2320	A
25	BA	2321	G
25	BA	2324	C
25	BA	2325	G
25	BA	2334	G
25	BA	2336	A
25	BA	2342	C
25	BA	2347	C
25	BA	2350	C
25	BA	2361	A
25	BA	2372	G

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Mol	Chain	Res	Type
25	BA	2383	G
25	BA	2385	C
25	BA	2386	C
25	BA	2393	A
25	BA	2394	C
25	BA	2402	C
25	BA	2406	U
25	BA	2410	G
25	BA	2418	A
25	BA	2423	U
25	BA	2424	C
25	BA	2425	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U
25	BA	2434	A
25	BA	2435	A
25	BA	2439	A
25	BA	2440	C
25	BA	2441	C
25	BA	2442	C
25	BA	2447	G
25	BA	2448	A
25	BA	2469	A
25	BA	2470	G
25	BA	2471	C
25	BA	2472	G
25	BA	2476	A
25	BA	2477	C
25	BA	2478	A
25	BA	2491	U
25	BA	2496	C
25	BA	2502	G
25	BA	2505	G
25	BA	2508	G
25	BA	2515	C
25	BA	2518	A
25	BA	2520	C
25	BA	2529	G
25	BA	2542	A
25	BA	2543	G
25	BA	2552	U

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Mol	Chain	Res	Type
25	BA	2554	U
25	BA	2556	C
25	BA	2564	A
25	BA	2566	A
25	BA	2567	G
25	BA	2572	A
25	BA	2573	C
25	BA	2576	G
25	BA	2581	G
25	BA	2582	G
25	BA	2585	U
25	BA	2586	C
25	BA	2602	A
25	BA	2603	G
25	BA	2604	U
25	BA	2609	U
25	BA	2611	U
25	BA	2612	C
25	BA	2615	U
25	BA	2630	G
25	BA	2634	G
25	BA	2655	G
25	BA	2656	U
25	BA	2669	G
25	BA	2670	A
25	BA	2673	G
25	BA	2690	C
25	BA	2691	C
25	BA	2712	U
25	BA	2712(A)	A
25	BA	2713	A
25	BA	2726	U
25	BA	2730	C
25	BA	2733	A
25	BA	2748	A
25	BA	2755	C
25	BA	2757	A
25	BA	2758	A
25	BA	2760	C
25	BA	2762	G
25	BA	2764	A
25	BA	2765	A

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Mol	Chain	Res	Type
25	BA	2766	G
25	BA	2778	A
25	BA	2779	U
25	BA	2780	G
25	BA	2789	C
25	BA	2790	A
25	BA	2791	C
25	BA	2793	G
25	BA	2794	C
25	BA	2795	G
25	BA	2801(A)	A
25	BA	2802	G
25	BA	2803	C
25	BA	2804	C
25	BA	2808	U
25	BA	2820	A
25	BA	2821	A
25	BA	2835	A
25	BA	2842	G
25	BA	2843	G
25	BA	2854	G
25	BA	2863	C
25	BA	2872	G
25	BA	2880	C
25	BA	2883	A
25	BA	2889	C
25	BA	2893	G
25	BA	2894	G
25	BA	2896	C
26	BB	2	C
26	BB	3	C
26	BB	5	C
26	BB	9	G
26	BB	12	C
26	BB	13	A
26	BB	15	A
26	BB	16	G
26	BB	17	C
26	BB	25	A
26	BB	26	A
26	BB	29	A
26	BB	32	C

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Mol	Chain	Res	Type
26	BB	34	U
26	BB	40	U
26	BB	41	U
26	BB	42	C
26	BB	43	C
26	BB	44	G
26	BB	47	C
26	BB	50	G
26	BB	53	A
26	BB	56	G
26	BB	67	G
26	BB	73	A
26	BB	75	G
26	BB	81	G
26	BB	99	G
26	BB	102	A
26	BB	106	G
26	BB	109	C
26	BB	110	G
26	BB	116	G
26	BB	118	G

All (208) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	30	U
1	AA	49	U
1	AA	60	A
1	AA	79	G
1	AA	108	G
1	AA	109	A
1	AA	115	G
1	AA	121	C
1	AA	149	A
1	AA	173	U
1	AA	243	A
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	305	G
1	AA	328	C

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Mol	Chain	Res	Type
1	AA	353	A
1	AA	428	G
1	AA	496	A
1	AA	509	A
1	AA	533	A
1	AA	560	U
1	AA	575	G
1	AA	576	G
1	AA	587	G
1	AA	687	A
1	AA	748	C
1	AA	766	A
1	AA	785	G
1	AA	793	U
1	AA	913	A
1	AA	931	C
1	AA	971	G
1	AA	973	G
1	AA	983	A
1	AA	992	U
1	AA	1049	U
1	AA	1067	A
1	AA	1086	U
1	AA	1124	G
1	AA	1133	G
1	AA	1135	U
1	AA	1136	U
1	AA	1138	G
1	AA	1139	G
1	AA	1145	C
1	AA	1181	G
1	AA	1212	U
1	AA	1225	A
1	AA	1257	U
1	AA	1280	A
1	AA	1285	A
1	AA	1300	G
1	AA	1319	A
1	AA	1332	A
1	AA	1337	G
1	AA	1397	C
1	AA	1442	G

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Mol	Chain	Res	Type
1	AA	1447	A
1	AA	1498	U
1	AA	1503	A
1	AA	1504	G
1	AA	1505	G
1	AA	1533	C
2	AV	7	A
2	AV	18	G
2	AV	19	G
2	AV	28	G
2	AV	34	G
2	AV	35	A
2	AV	43	C
2	AV	57	G
2	AV	72	C
25	BA	27	G
25	BA	49	A
25	BA	71	A
25	BA	74	A
25	BA	102	G
25	BA	119	A
25	BA	128	C
25	BA	196	A
25	BA	199	A
25	BA	221	A
25	BA	249	C
25	BA	271(U)	G
25	BA	271(Y)	U
25	BA	272(J)	C
25	BA	310	A
25	BA	311	A
25	BA	333	G
25	BA	370	G
25	BA	372	G
25	BA	387	U
25	BA	405	U
25	BA	479	A
25	BA	542	C
25	BA	549	G
25	BA	551	G
25	BA	603	A
25	BA	614(C)	A

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Mol	Chain	Res	Type
25	BA	615	G
25	BA	627	A
25	BA	685	A
25	BA	686	G
25	BA	746	A
25	BA	752	A
25	BA	764	A
25	BA	776	G
25	BA	790	C
25	BA	805	G
25	BA	827	U
25	BA	858	U
25	BA	889	C
25	BA	906	G
25	BA	933	A
25	BA	974	G
25	BA	989	G
25	BA	1022	G
25	BA	1026	U
25	BA	1033	U
25	BA	1048	A
25	BA	1053	C
25	BA	1054	A
25	BA	1057	A
25	BA	1058	G
25	BA	1076	C
25	BA	1087	G
25	BA	1089	G
25	BA	1100	C
25	BA	1128	A
25	BA	1142(A)	A
25	BA	1151	G
25	BA	1162	G
25	BA	1181	C
25	BA	1210	A
25	BA	1237	A
25	BA	1253	A
25	BA	1286	A
25	BA	1300	U
25	BA	1301	A
25	BA	1349	A
25	BA	1379	A

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Mol	Chain	Res	Type
25	BA	1396	U
25	BA	1403	C
25	BA	1494	A
25	BA	1497	U
25	BA	1540	U
25	BA	1543	C
25	BA	1558	A
25	BA	1559	G
25	BA	1608	A
25	BA	1609	A
25	BA	1610	A
25	BA	1617	C
25	BA	1653	G
25	BA	1740	G
25	BA	1763	G
25	BA	1780	A
25	BA	1784	A
25	BA	1786	A
25	BA	1799	G
25	BA	1819	A
25	BA	1847	A
25	BA	1858	G
25	BA	1888	G
25	BA	1913	A
25	BA	1914	C
25	BA	1943	U
25	BA	1962	C
25	BA	1963	U
25	BA	1970	A
25	BA	1992	G
25	BA	2019	A
25	BA	2031	A
25	BA	2141	G
25	BA	2146	C
25	BA	2179	C
25	BA	2180	U
25	BA	2191	G
25	BA	2207	G
25	BA	2225	A
25	BA	2275	C
25	BA	2282	G
25	BA	2296	U

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Mol	Chain	Res	Type
25	BA	2311	A
25	BA	2318	G
25	BA	2319	G
25	BA	2320	A
25	BA	2402	C
25	BA	2422	A
25	BA	2439	A
25	BA	2497	A
25	BA	2542	A
25	BA	2566	A
25	BA	2581	G
25	BA	2602	A
25	BA	2609	U
25	BA	2611	U
25	BA	2655	G
25	BA	2665	A
25	BA	2689	U
25	BA	2778	A
25	BA	2802	G
26	BB	1	U
26	BB	44	G
26	BB	66	A
26	BB	109	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 139 ligands modelled in this entry, 138 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	$\#\|Z\| > 2$
60	GCP	AY	702	59	27,34,34	2.37	10 (37%)	34,54,54	2.61	15 (44%)

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
60	GCP	AY	702	59	-	3/15/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AY	702	GCP	C6-N1	4.87	1.41	1.33
60	AY	702	GCP	C5-C6	-4.42	1.33	1.41
60	AY	702	GCP	PB-O2B	-4.23	1.46	1.56
60	AY	702	GCP	C2'-C3'	-3.97	1.42	1.53
60	AY	702	GCP	C2-N1	3.67	1.41	1.35
60	AY	702	GCP	PG-O2G	-3.56	1.46	1.54
60	AY	702	GCP	PG-O3G	-3.20	1.47	1.54
60	AY	702	GCP	PB-O3A	3.05	1.61	1.58
60	AY	702	GCP	C5-C4	-2.42	1.34	1.40
60	AY	702	GCP	PB-O1B	-2.03	1.46	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	AY	702	GCP	N3-C2-N1	-6.70	118.28	127.22
60	AY	702	GCP	O4'-C4'-C5'	-4.73	93.80	109.37
60	AY	702	GCP	C1'-N9-C4	-4.67	118.43	126.64
60	AY	702	GCP	C2-N3-C4	4.55	120.56	115.36
60	AY	702	GCP	C5-C6-N1	-4.05	117.89	123.43
60	AY	702	GCP	O1G-PG-C3B	-3.81	103.03	111.24
60	AY	702	GCP	N2-C2-N1	3.71	123.02	117.25
60	AY	702	GCP	C2'-C3'-C4'	-3.66	95.53	102.64
60	AY	702	GCP	O4'-C1'-C2'	-3.27	102.14	106.93
60	AY	702	GCP	O2B-PB-O1B	2.88	119.68	110.07
60	AY	702	GCP	O2'-C2'-C3'	-2.65	103.24	111.82
60	AY	702	GCP	C2-N1-C6	2.47	119.85	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	AY	702	GCP	O3'-C3'-C2'	-2.44	103.92	111.82
60	AY	702	GCP	O3G-PG-O2G	2.44	115.20	108.08
60	AY	702	GCP	PB-O3A-PA	-2.22	125.52	132.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AY	702	GCP	C5'-O5'-PA-O1A
60	AY	702	GCP	O4'-C4'-C5'-O5'
60	AY	702	GCP	C5'-O5'-PA-O3A

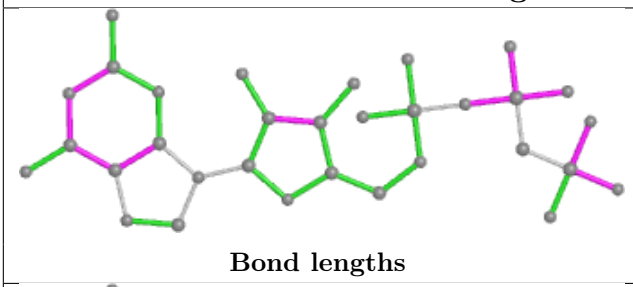
There are no ring outliers.

1 monomer is involved in 5 short contacts:

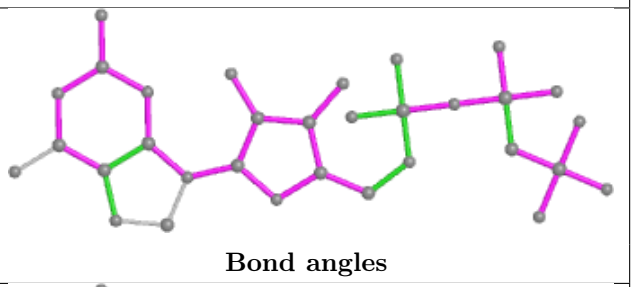
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AY	702	GCP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

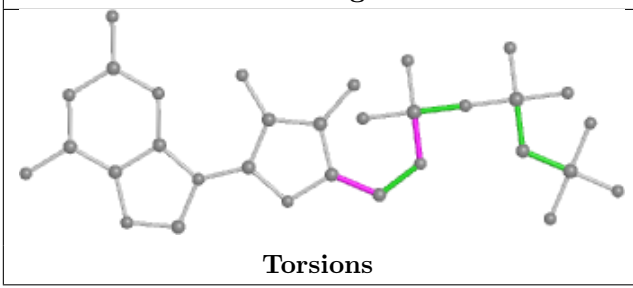
Ligand GCP AY 702



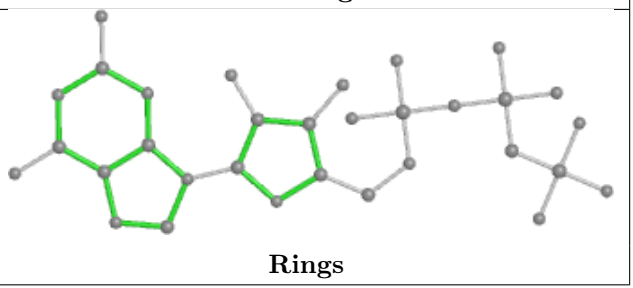
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2506:U	O3'	2507:C	P	1.76

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1514/1516 (99%)	-0.25	53 (3%) 44 38	9, 32, 113, 247	0
2	AV	74/76 (97%)	0.03	1 (1%) 75 74	23, 54, 91, 134	0
3	AX	6/25 (24%)	0.11	1 (16%) 1 1	18, 22, 53, 75	0
4	AJ	98/98 (100%)	0.20	3 (3%) 49 44	22, 49, 98, 108	0
5	AK	119/119 (100%)	-0.10	4 (3%) 45 39	18, 41, 65, 104	0
6	AL	124/124 (100%)	-0.19	3 (2%) 59 56	16, 32, 64, 107	0
7	AM	124/124 (100%)	0.74	12 (9%) 7 5	31, 69, 118, 161	0
8	AN	60/60 (100%)	-0.19	2 (3%) 46 41	21, 33, 69, 83	0
9	AO	88/88 (100%)	-0.25	0 100 100	24, 41, 67, 73	0
10	AP	83/83 (100%)	-0.28	1 (1%) 79 78	29, 40, 60, 112	0
11	AQ	99/99 (100%)	-0.46	0 100 100	20, 34, 53, 59	0
12	AR	70/70 (100%)	-0.26	0 100 100	23, 41, 75, 92	0
13	AS	78/78 (100%)	0.52	7 (8%) 9 6	39, 69, 107, 121	0
14	AT	99/99 (100%)	-0.16	4 (4%) 38 32	24, 39, 78, 90	0
15	AB	234/234 (100%)	0.04	14 (5%) 21 17	21, 55, 117, 134	0
16	AC	206/206 (100%)	-0.37	0 100 100	22, 41, 67, 103	0
17	AD	208/208 (100%)	-0.11	4 (1%) 66 64	26, 49, 75, 90	0
18	AE	150/150 (100%)	-0.41	1 (0%) 87 87	19, 30, 54, 81	0
19	AF	101/101 (100%)	-0.14	1 (0%) 82 81	28, 52, 75, 87	0
20	AG	155/155 (100%)	-0.02	9 (5%) 23 18	31, 53, 104, 148	0
21	AH	138/138 (100%)	-0.46	1 (0%) 87 87	19, 32, 55, 84	0
22	AI	127/127 (100%)	-0.09	3 (2%) 59 56	21, 51, 82, 108	0
23	AY	622/680 (91%)	-0.11	10 (1%) 72 70	30, 55, 97, 131	0
24	AU	24/24 (100%)	0.29	1 (4%) 36 31	33, 48, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	BA	2859/2915 (98%)	-0.30	67 (2%) 60 57	7, 27, 90, 267	0
26	BB	119/122 (97%)	-0.00	0 100 100	26, 63, 95, 134	0
27	BN	138/140 (98%)	-0.21	4 (2%) 51 47	18, 35, 66, 80	0
28	BO	122/122 (100%)	-0.56	0 100 100	18, 31, 49, 60	0
29	BP	146/150 (97%)	0.56	15 (10%) 6 4	18, 55, 94, 127	0
30	BQ	141/141 (100%)	-0.26	2 (1%) 75 74	23, 35, 64, 112	0
31	BR	117/118 (99%)	-0.27	5 (4%) 35 30	15, 33, 58, 75	0
32	BS	98/112 (87%)	0.72	8 (8%) 11 8	50, 80, 106, 125	0
33	BT	137/146 (93%)	0.43	15 (10%) 5 4	23, 50, 135, 151	0
34	BU	117/118 (99%)	-0.29	2 (1%) 70 68	16, 29, 58, 85	0
35	BV	101/101 (100%)	0.05	4 (3%) 38 32	15, 49, 77, 97	0
36	BW	113/113 (100%)	-0.21	3 (2%) 54 50	18, 29, 67, 122	0
37	BX	92/96 (95%)	-0.34	0 100 100	20, 34, 54, 61	0
38	BY	100/110 (90%)	0.92	16 (16%) 1 1	29, 56, 122, 168	0
39	BZ	198/206 (96%)	0.03	4 (2%) 65 62	33, 59, 92, 103	0
40	B0	84/85 (98%)	0.33	7 (8%) 11 8	26, 41, 96, 133	0
41	B1	93/98 (94%)	0.08	3 (3%) 47 42	18, 33, 72, 121	0
42	B2	71/72 (98%)	0.01	2 (2%) 53 48	30, 49, 82, 100	0
43	BD	271/276 (98%)	-0.41	5 (1%) 68 66	9, 20, 46, 89	0
44	B3	59/60 (98%)	0.06	2 (3%) 45 39	24, 40, 76, 137	0
45	B4	30/71 (42%)	1.63	10 (33%) 0 0	102, 130, 156, 174	0
46	B5	59/60 (98%)	0.37	7 (11%) 4 3	10, 35, 98, 134	0
47	B6	44/54 (81%)	1.08	9 (20%) 1 0	34, 59, 99, 109	0
48	B7	48/49 (97%)	-0.34	2 (4%) 36 31	10, 19, 59, 101	0
49	B8	63/65 (96%)	0.16	5 (7%) 12 9	22, 37, 61, 118	0
50	B9	36/37 (97%)	0.13	1 (2%) 53 48	26, 44, 69, 77	0
51	BC	225/229 (98%)	0.03	9 (4%) 38 32	36, 64, 111, 132	0
52	BE	204/206 (99%)	-0.16	8 (3%) 39 34	14, 32, 85, 109	0
53	BF	207/210 (98%)	0.02	13 (6%) 20 15	15, 37, 103, 187	0
54	BG	181/182 (99%)	1.01	30 (16%) 1 1	67, 101, 130, 147	0
55	BH	173/180 (96%)	0.33	11 (6%) 19 15	35, 60, 95, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	BK	127/147 (86%)	4.70	105 (82%) 0 0	127, 181, 237, 263	0
57	BJ	130/130 (100%)	1.18	26 (20%) 1 0	74, 106, 140, 195	0
58	BL	0/125	-	-	-	-
All	All	11304/11728 (96%)	-0.04	535 (4%) 31 27	7, 40, 108, 267	0

All (535) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	BH	44	VAL	18.6
7	AM	123	ALA	17.7
56	BK	136	VAL	14.8
56	BK	83	GLY	13.4
53	BF	11	VAL	12.9
38	BY	52	SER	11.6
56	BK	10	LEU	11.1
56	BK	105	LEU	11.1
56	BK	66	THR	11.0
38	BY	51	VAL	10.7
7	AM	122	LYS	10.3
56	BK	7	VAL	10.1
56	BK	76	TYR	9.7
55	BH	45	VAL	9.6
32	BS	54	LEU	9.4
56	BK	13	PRO	9.3
56	BK	64	SER	9.2
25	BA	2803	C	9.2
7	AM	124	PRO	9.1
38	BY	50	ARG	8.8
57	BJ	87	ALA	8.8
1	AA	89	C	8.8
56	BK	61	ALA	8.6
46	B5	58	LEU	8.5
56	BK	135	GLY	8.5
56	BK	12	LEU	8.5
25	BA	889	C	8.3
56	BK	52	ILE	8.3
56	BK	134	MET	8.3
57	BJ	88	ALA	8.2
56	BK	27	LEU	8.1
56	BK	63	ARG	8.0
56	BK	65	PHE	8.0

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Mol	Chain	Res	Type	RSRZ
7	AM	7	VAL	7.9
56	BK	53	VAL	7.9
53	BF	12	LEU	7.8
1	AA	82	U	7.8
56	BK	137	GLU	7.6
5	AK	129	SER	7.6
36	BW	112	GLY	7.5
56	BK	67	PHE	7.5
40	B0	3	HIS	7.4
25	BA	887	A	7.2
56	BK	84	LEU	7.2
25	BA	2801(A)	A	7.2
25	BA	2802	G	7.1
56	BK	132	ARG	7.1
56	BK	68	VAL	7.1
56	BK	140	GLY	7.1
36	BW	113	LYS	7.1
33	BT	36	GLU	7.1
25	BA	2801	A	7.0
38	BY	3	VAL	7.0
56	BK	51	ALA	7.0
35	BV	36	PRO	7.0
56	BK	77	LEU	7.0
56	BK	106	GLU	6.9
56	BK	56	GLU	6.7
56	BK	20	ALA	6.7
56	BK	29	GLN	6.7
40	B0	5	LYS	6.7
56	BK	26	ALA	6.7
56	BK	33	ASN	6.6
54	BG	2	PRO	6.6
40	B0	6	GLY	6.5
56	BK	3	LYS	6.5
56	BK	22	PRO	6.5
56	BK	28	GLY	6.5
33	BT	37	GLY	6.5
56	BK	17	ALA	6.4
46	B5	54	GLY	6.3
41	B1	85	LEU	6.2
57	BJ	49	ALA	6.2
33	BT	134	GLU	6.2
1	AA	81	U	6.1

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Mol	Chain	Res	Type	RSRZ
25	BA	1174	A	6.1
25	BA	1509	C	6.1
56	BK	16	LYS	5.9
56	BK	4	VAL	5.9
44	B3	1	MET	5.9
53	BF	24	LEU	5.9
56	BK	82	ALA	5.8
56	BK	110	GLN	5.8
7	AM	84	ILE	5.8
56	BK	21	PRO	5.8
1	AA	88	A	5.7
5	AK	128	ALA	5.7
46	B5	59	GLU	5.7
56	BK	8	VAL	5.7
53	BF	1	MET	5.6
56	BK	62	ASP	5.6
54	BG	126	ASP	5.5
7	AM	6	GLY	5.5
40	B0	7	LEU	5.5
56	BK	11	GLN	5.5
57	BJ	50	ALA	5.5
25	BA	2795	G	5.5
56	BK	50	ASP	5.5
47	B6	42	TRP	5.5
56	BK	74	ALA	5.4
56	BK	35	MET	5.4
54	BG	48	GLU	5.4
6	AL	128	ALA	5.3
56	BK	15	GLY	5.3
38	BY	58	GLY	5.3
33	BT	136	GLN	5.3
56	BK	31	GLY	5.3
57	BJ	7	ALA	5.2
33	BT	135	ALA	5.2
42	B2	72	ALA	5.1
33	BT	39	ARG	5.1
53	BF	133	ASN	5.0
56	BK	58	THR	5.0
56	BK	2	LYS	5.0
56	BK	80	LYS	4.9
52	BE	76	ARG	4.9
56	BK	36	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
56	BK	98	ARG	4.8
1	AA	1030(C)	G	4.8
56	BK	126	MET	4.8
56	BK	18	THR	4.8
25	BA	884	C	4.8
56	BK	47	ASN	4.7
56	BK	60	TYR	4.6
54	BG	84	LYS	4.6
46	B5	2	ALA	4.6
25	BA	886	C	4.6
33	BT	130	ALA	4.6
17	AD	9	CYS	4.6
54	BG	42	GLY	4.6
56	BK	9	LYS	4.5
1	AA	841	U	4.5
56	BK	19	PRO	4.5
57	BJ	4	ALA	4.5
1	AA	90	U	4.5
56	BK	133	SER	4.5
13	AS	43	GLU	4.5
1	AA	83	U	4.4
56	BK	14	ALA	4.4
56	BK	130	SER	4.4
57	BJ	132	ALA	4.3
45	B4	58	TYR	4.3
38	BY	28	LYS	4.3
29	BP	110	TYR	4.3
4	AJ	100	THR	4.3
55	BH	43	VAL	4.3
45	B4	61	VAL	4.3
34	BU	118	GLY	4.3
53	BF	21	ALA	4.2
54	BG	86	MET	4.2
1	AA	839	U	4.2
2	AV	20	U	4.2
54	BG	50	ALA	4.2
56	BK	5	VAL	4.2
1	AA	1001(A)	G	4.2
40	B0	4	LYS	4.2
56	BK	49	GLY	4.2
30	BQ	140	ALA	4.1
56	BK	101	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
25	BA	888	C	4.1
56	BK	81	ALA	4.1
38	BY	61	ILE	4.1
25	BA	880	G	4.1
25	BA	899	A	4.1
53	BF	7	TYR	4.1
43	BD	25	THR	4.1
56	BK	24	GLY	4.0
25	BA	2310	A	4.0
40	B0	2	ALA	4.0
1	AA	204	U	4.0
25	BA	2896	C	4.0
25	BA	1847	A	3.9
54	BG	47	LYS	3.9
56	BK	112	MET	3.9
1	AA	1541	U	3.9
54	BG	182	LYS	3.9
1	AA	1030(D)	A	3.8
25	BA	890	A	3.8
46	B5	53	ALA	3.8
56	BK	113	PRO	3.8
1	AA	1027	C	3.8
1	AA	1542	U	3.8
25	BA	2207	G	3.8
33	BT	137	LYS	3.8
56	BK	46	ALA	3.8
46	B5	60	VAL	3.8
56	BK	23	VAL	3.8
1	AA	1442(A)	G	3.8
25	BA	2892	A	3.7
30	BQ	141	GLN	3.7
56	BK	37	PHE	3.7
45	B4	54	LYS	3.7
54	BG	127	GLY	3.7
13	AS	10	PHE	3.7
56	BK	122	ALA	3.7
25	BA	2792	G	3.7
56	BK	43	ALA	3.7
54	BG	49	ASP	3.7
53	BF	25	PRO	3.7
29	BP	27	HIS	3.6
6	AL	28	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
45	B4	39	ARG	3.6
1	AA	1543	C	3.6
56	BK	138	VAL	3.6
22	AI	88	TYR	3.6
7	AM	121	LYS	3.6
25	BA	883	G	3.6
7	AM	119	GLY	3.6
25	BA	1173	G	3.5
25	BA	2793	G	3.5
25	BA	881	G	3.5
53	BF	10	PRO	3.5
1	AA	1492	A	3.5
1	AA	1493	A	3.5
8	AN	2	ALA	3.5
1	AA	1138	G	3.5
54	BG	3	LEU	3.4
49	B8	64	TYR	3.4
20	AG	81	GLY	3.4
25	BA	271(K)	U	3.4
15	AB	237	ALA	3.4
57	BJ	86	ALA	3.4
33	BT	2	ASN	3.4
56	BK	57	ILE	3.3
56	BK	128	ALA	3.3
54	BG	156	ASP	3.3
52	BE	204	ALA	3.3
25	BA	2794	C	3.3
25	BA	892	G	3.3
56	BK	75	SER	3.3
54	BG	139	LEU	3.3
56	BK	78	ILE	3.3
56	BK	48	MET	3.3
57	BJ	66	ALA	3.3
1	AA	78	G	3.3
25	BA	2833	G	3.3
31	BR	3	HIS	3.3
23	AY	582	PHE	3.3
57	BJ	8	ALA	3.3
13	AS	28	LYS	3.3
45	B4	53	THR	3.3
56	BK	120	LEU	3.3
7	AM	117	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
57	BJ	89	ALA	3.2
13	AS	30	LEU	3.2
39	BZ	6	LYS	3.2
8	AN	13	THR	3.2
56	BK	121	GLU	3.2
20	AG	82	GLY	3.2
25	BA	2894	G	3.2
27	BN	68	GLU	3.2
56	BK	102	GLU	3.2
35	BV	101	GLY	3.2
25	BA	2602	A	3.2
51	BC	95	GLY	3.2
52	BE	54	GLN	3.2
1	AA	470	C	3.2
38	BY	53	PRO	3.1
51	BC	202	GLU	3.1
1	AA	1533	C	3.1
17	AD	12	CYS	3.1
56	BK	73	PRO	3.1
15	AB	19	HIS	3.1
56	BK	117	THR	3.1
47	B6	44	ARG	3.1
23	AY	580	MET	3.1
51	BC	105	ASP	3.1
39	BZ	146	ILE	3.1
48	B7	48	LYS	3.1
15	AB	128	GLU	3.1
25	BA	2893	G	3.1
56	BK	40	ALA	3.0
54	BG	118	ARG	3.0
33	BT	32	TYR	3.0
44	B3	2	PRO	3.0
56	BK	38	VAL	3.0
56	BK	54	PRO	3.0
25	BA	882	G	3.0
25	BA	229	A	3.0
38	BY	2	ARG	3.0
54	BG	149	VAL	3.0
57	BJ	51	ALA	3.0
33	BT	105	LEU	3.0
25	BA	885	C	3.0
45	B4	41	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
47	B6	43	CYS	3.0
51	BC	71	GLN	3.0
25	BA	2897	U	2.9
17	AD	26	CYS	2.9
25	BA	352	G	2.9
38	BY	89	PHE	2.9
15	AB	122	PHE	2.9
25	BA	896	A	2.9
55	BH	42	ARG	2.9
36	BW	111	HIS	2.9
54	BG	52	ILE	2.9
54	BG	88	ILE	2.9
25	BA	508	G	2.9
53	BF	14	PRO	2.9
48	B7	47	ARG	2.9
21	AH	1	MET	2.9
27	BN	3	THR	2.9
54	BG	72	ARG	2.9
25	BA	2790	A	2.9
1	AA	77	G	2.9
1	AA	1002	G	2.9
1	AA	1026	G	2.9
57	BJ	31	ALA	2.9
5	AK	127	LYS	2.9
1	AA	1039	C	2.8
29	BP	65	ARG	2.8
33	BT	38	ASN	2.8
22	AI	3	GLN	2.8
32	BS	68	GLN	2.8
1	AA	91	C	2.8
54	BG	41	GLN	2.8
10	AP	83	GLU	2.8
15	AB	129	GLU	2.8
47	B6	17	LYS	2.8
45	B4	40	ILE	2.8
51	BC	124	GLY	2.8
1	AA	1456	G	2.8
43	BD	35	LYS	2.8
25	BA	1176	G	2.8
25	BA	2895	U	2.8
38	BY	60	PHE	2.8
4	AJ	83	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
56	BK	45	THR	2.8
1	AA	1030(B)	C	2.8
1	AA	1534	A	2.8
54	BG	78	SER	2.8
23	AY	567	LEU	2.8
25	BA	645	C	2.8
7	AM	115	LYS	2.7
56	BK	55	VAL	2.7
33	BT	1	MET	2.7
56	BK	114	ASP	2.7
1	AA	80	G	2.7
29	BP	118	GLY	2.7
29	BP	149	GLU	2.7
25	BA	271(N)	U	2.7
56	BK	109	LYS	2.7
1	AA	1031	G	2.7
56	BK	129	GLY	2.7
20	AG	156	TRP	2.7
57	BJ	6	ALA	2.7
55	BH	111	HIS	2.7
32	BS	107	GLU	2.7
23	AY	585	ALA	2.7
57	BJ	53	ALA	2.7
1	AA	161	A	2.6
31	BR	105	ARG	2.6
56	BK	79	ARG	2.6
45	B4	49	GLU	2.6
20	AG	79	ARG	2.6
32	BS	60	GLY	2.6
25	BA	2402	C	2.6
1	AA	1036	G	2.6
14	AT	9	ASN	2.6
42	B2	71	ASN	2.6
49	B8	34	TRP	2.6
57	BJ	52	ALA	2.6
57	BJ	98	ALA	2.6
15	AB	7	VAL	2.6
38	BY	91	GLU	2.6
1	AA	1447	A	2.5
20	AG	85	TYR	2.5
25	BA	275	G	2.5
29	BP	15	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
54	BG	115	ARG	2.5
56	BK	32	ALA	2.5
25	BA	897	C	2.5
54	BG	12	TYR	2.5
25	BA	11	G	2.5
29	BP	18	ARG	2.5
56	BK	99	ILE	2.5
20	AG	83	ALA	2.5
29	BP	33	ARG	2.5
49	B8	63	PRO	2.5
41	B1	81	LYS	2.5
43	BD	262	ARG	2.5
33	BT	91	ARG	2.5
1	AA	1034	G	2.5
56	BK	97	GLY	2.5
25	BA	893	C	2.5
53	BF	13	SER	2.5
57	BJ	83	ALA	2.5
57	BJ	131	ALA	2.5
15	AB	125	PRO	2.4
22	AI	53	VAL	2.4
27	BN	8	GLN	2.4
56	BK	41	PHE	2.4
1	AA	998	G	2.4
46	B5	37	LYS	2.4
1	AA	84	U	2.4
25	BA	879	G	2.4
43	BD	2	ALA	2.4
54	BG	164	GLU	2.4
47	B6	23	THR	2.4
55	BH	83	TYR	2.4
34	BU	91	ASP	2.4
1	AA	1538	C	2.4
25	BA	1076	C	2.4
15	AB	15	VAL	2.4
43	BD	36	PRO	2.4
57	BJ	116	ALA	2.4
15	AB	230	VAL	2.4
25	BA	614(A)	U	2.4
25	BA	1175	U	2.4
25	BA	547	A	2.4
52	BE	61	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
55	BH	170	ARG	2.4
15	AB	136	VAL	2.4
41	B1	79	GLY	2.4
25	BA	1742	G	2.4
57	BJ	54	ALA	2.4
18	AE	154	GLY	2.3
55	BH	110	SER	2.3
33	BT	133	GLU	2.3
29	BP	107	LYS	2.3
39	BZ	4	ARG	2.3
1	AA	1032	G	2.3
49	B8	48	PHE	2.3
1	AA	1000	U	2.3
25	BA	1091	G	2.3
47	B6	31	PRO	2.3
23	AY	203	GLU	2.3
38	BY	87	LYS	2.3
55	BH	85	LYS	2.3
3	AX	15	A	2.3
25	BA	1177	A	2.3
47	B6	36	LEU	2.3
56	BK	108	ALA	2.3
52	BE	56	PRO	2.3
56	BK	124	ALA	2.3
20	AG	84	ASN	2.3
52	BE	17	ASP	2.3
14	AT	106	ALA	2.3
25	BA	2179	C	2.3
57	BJ	19	ALA	2.3
1	AA	1030(A)	G	2.3
35	BV	48	GLY	2.3
7	AM	8	GLU	2.3
45	B4	47	VAL	2.2
38	BY	59	GLY	2.2
53	BF	128	ALA	2.2
1	AA	1003	G	2.2
29	BP	150	ALA	2.2
52	BE	132	HIS	2.2
51	BC	77	ILE	2.2
29	BP	92	GLU	2.2
25	BA	898	C	2.2
4	AJ	55	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
51	BC	205	LYS	2.2
7	AM	116	THR	2.2
1	AA	1532	U	2.2
25	BA	1740	G	2.2
51	BC	106	GLY	2.2
29	BP	94	GLU	2.2
32	BS	43	GLU	2.2
39	BZ	13	GLU	2.2
56	BK	25	PRO	2.2
57	BJ	75	ALA	2.2
20	AG	153	HIS	2.2
13	AS	81	ARG	2.2
23	AY	583	LYS	2.2
25	BA	878	A	2.2
56	BK	72	PRO	2.2
14	AT	75	ASN	2.2
35	BV	20	LEU	2.2
52	BE	1	MET	2.2
25	BA	2309	A	2.2
27	BN	4	TYR	2.2
38	BY	88	LYS	2.2
47	B6	39	TYR	2.2
40	B0	74	ARG	2.2
5	AK	117	ASN	2.2
25	BA	2805	G	2.2
32	BS	61	ASN	2.2
50	B9	12	ASP	2.1
54	BG	46	ALA	2.1
56	BK	116	ASN	2.1
15	AB	14	GLY	2.1
19	AF	101	ALA	2.1
57	BJ	30	ALA	2.1
57	BJ	97	ALA	2.1
1	AA	1038	C	2.1
47	B6	30	THR	2.1
6	AL	47	LYS	2.1
25	BA	1848	A	2.1
1	AA	1537	U	2.1
17	AD	150	GLU	2.1
14	AT	101	GLY	2.1
54	BG	74	LYS	2.1
54	BG	13	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	532	A	2.1
23	AY	596	LYS	2.1
55	BH	39	PRO	2.1
54	BG	147	ASP	2.1
1	AA	203	U	2.1
13	AS	68	GLY	2.1
24	AU	25	LYS	2.1
54	BG	116	ASP	2.1
1	AA	1025	U	2.1
1	AA	1540	U	2.1
32	BS	72	ALA	2.1
15	AB	231	GLU	2.1
31	BR	118	GLU	2.1
45	B4	56	GLU	2.1
29	BP	132	LYS	2.1
15	AB	23	ARG	2.1
53	BF	18	ARG	2.1
55	BH	167	GLU	2.1
38	BY	4	LYS	2.1
54	BG	141	PHE	2.1
1	AA	1030	C	2.0
13	AS	27	GLU	2.0
51	BC	12	GLU	2.0
31	BR	11	ASN	2.0
25	BA	2791	C	2.0
20	AG	154	TYR	2.0
25	BA	1060	U	2.0
23	AY	226	ASN	2.0
31	BR	2	ARG	2.0
49	B8	35	GLN	2.0
29	BP	87	ASP	2.0
1	AA	631	G	2.0
25	BA	157	U	2.0
57	BJ	15	ALA	2.0
56	BK	118	THR	2.0
23	AY	565	VAL	2.0
32	BS	30	ARG	2.0
23	AY	581	ALA	2.0
15	AB	33	TYR	2.0
29	BP	16	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3012	1/1	0.86	0.12	10,10,10,10	0
59	MG	BA	3004	1/1	0.87	0.15	46,46,46,46	0
59	MG	BA	3059	1/1	0.87	0.21	9,9,9,9	0
59	MG	BA	3013	1/1	0.88	0.20	26,26,26,26	0
59	MG	AA	1636	1/1	0.88	0.11	24,24,24,24	0
59	MG	AA	1629	1/1	0.89	0.14	38,38,38,38	0
59	MG	AA	1644	1/1	0.89	0.36	33,33,33,33	0
59	MG	AA	1635	1/1	0.89	0.22	24,24,24,24	0
59	MG	BA	3039	1/1	0.90	0.19	24,24,24,24	0
59	MG	BA	3065	1/1	0.90	0.30	24,24,24,24	0
59	MG	BA	3067	1/1	0.90	0.19	16,16,16,16	0
59	MG	BA	3072	1/1	0.90	0.25	19,19,19,19	0
59	MG	AA	1633	1/1	0.91	0.12	27,27,27,27	0
59	MG	BA	3027	1/1	0.91	0.34	30,30,30,30	0
59	MG	BA	3029	1/1	0.91	0.24	28,28,28,28	0
59	MG	BA	3070	1/1	0.91	0.29	24,24,24,24	0
59	MG	AA	1603	1/1	0.91	0.22	23,23,23,23	0
59	MG	BA	3073	1/1	0.91	0.26	14,14,14,14	0
59	MG	BA	3081	1/1	0.91	0.15	17,17,17,17	0
59	MG	AA	1615	1/1	0.92	0.17	24,24,24,24	0
59	MG	BA	3001	1/1	0.92	0.33	32,32,32,32	0
59	MG	BA	3071	1/1	0.92	0.32	29,29,29,29	0
59	MG	B8	101	1/1	0.92	0.12	15,15,15,15	0
59	MG	AA	1606	1/1	0.93	0.24	15,15,15,15	0
59	MG	AA	1621	1/1	0.93	0.17	14,14,14,14	0
59	MG	BA	3035	1/1	0.93	0.38	18,18,18,18	0
59	MG	AA	1637	1/1	0.93	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3047	1/1	0.93	0.35	27,27,27,27	0
59	MG	AA	1641	1/1	0.93	0.13	25,25,25,25	0
59	MG	AA	1643	1/1	0.93	0.14	31,31,31,31	0
59	MG	BA	3051	1/1	0.94	0.29	24,24,24,24	0
59	MG	AA	1602	1/1	0.94	0.31	16,16,16,16	0
59	MG	AA	1619	1/1	0.94	0.22	27,27,27,27	0
59	MG	BA	3080	1/1	0.94	0.23	16,16,16,16	0
59	MG	BA	3041	1/1	0.94	0.33	11,11,11,11	0
59	MG	BA	3083	1/1	0.94	0.11	37,37,37,37	0
59	MG	BA	3087	1/1	0.94	0.24	26,26,26,26	0
59	MG	AA	1639	1/1	0.94	0.17	20,20,20,20	0
59	MG	BF	301	1/1	0.94	0.16	27,27,27,27	0
59	MG	BA	3009	1/1	0.95	0.30	31,31,31,31	0
59	MG	BA	3010	1/1	0.95	0.30	14,14,14,14	0
59	MG	BA	3052	1/1	0.95	0.23	19,19,19,19	0
59	MG	AA	1623	1/1	0.95	0.23	15,15,15,15	0
59	MG	BA	3063	1/1	0.95	0.17	22,22,22,22	0
59	MG	BA	3064	1/1	0.95	0.17	22,22,22,22	0
59	MG	AA	1626	1/1	0.95	0.18	19,19,19,19	0
59	MG	BA	3066	1/1	0.95	0.27	15,15,15,15	0
59	MG	BA	3014	1/1	0.95	0.28	27,27,27,27	0
59	MG	BA	3018	1/1	0.95	0.23	12,12,12,12	0
59	MG	BA	3020	1/1	0.95	0.32	6,6,6,6	0
59	MG	BA	3025	1/1	0.95	0.21	16,16,16,16	0
59	MG	BA	3026	1/1	0.95	0.18	19,19,19,19	0
59	MG	BA	3074	1/1	0.95	0.15	16,16,16,16	0
59	MG	AA	1645	1/1	0.95	0.39	35,35,35,35	0
59	MG	AY	701	1/1	0.95	0.12	41,41,41,41	0
59	MG	AA	1604	1/1	0.95	0.09	3,3,3,3	0
59	MG	BA	3084	1/1	0.95	0.19	22,22,22,22	0
59	MG	BA	3002	1/1	0.95	0.17	17,17,17,17	0
59	MG	BA	3088	1/1	0.95	0.30	26,26,26,26	0
59	MG	AA	1642	1/1	0.95	0.23	30,30,30,30	0
59	MG	BE	301	1/1	0.95	0.27	16,16,16,16	0
59	MG	BA	3045	1/1	0.95	0.21	16,16,16,16	0
59	MG	BA	3021	1/1	0.96	0.20	25,25,25,25	0
59	MG	AA	1622	1/1	0.96	0.23	25,25,25,25	0
59	MG	AA	1613	1/1	0.96	0.17	6,6,6,6	0
59	MG	AA	1607	1/1	0.96	0.14	24,24,24,24	0
59	MG	BA	3076	1/1	0.96	0.23	8,8,8,8	0
59	MG	BA	3078	1/1	0.96	0.17	15,15,15,15	0
59	MG	AA	1609	1/1	0.96	0.24	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3060	1/1	0.96	0.30	22,22,22,22	0
59	MG	BA	3082	1/1	0.96	0.26	21,21,21,21	0
59	MG	BA	3030	1/1	0.96	0.32	12,12,12,12	0
59	MG	BA	3032	1/1	0.96	0.27	21,21,21,21	0
59	MG	BA	3085	1/1	0.96	0.27	18,18,18,18	0
59	MG	BA	3086	1/1	0.96	0.24	26,26,26,26	0
59	MG	AA	1640	1/1	0.96	0.16	21,21,21,21	0
59	MG	AA	1630	1/1	0.96	0.29	29,29,29,29	0
59	MG	AA	1611	1/1	0.96	0.24	7,7,7,7	0
59	MG	BA	3068	1/1	0.96	0.26	7,7,7,7	0
59	MG	BA	3043	1/1	0.96	0.30	7,7,7,7	0
59	MG	AA	1638	1/1	0.97	0.16	22,22,22,22	0
59	MG	AA	1616	1/1	0.97	0.18	5,5,5,5	0
59	MG	AA	1632	1/1	0.97	0.21	22,22,22,22	0
59	MG	BA	3033	1/1	0.97	0.26	12,12,12,12	0
59	MG	BA	3034	1/1	0.97	0.28	5,5,5,5	0
59	MG	BA	3015	1/1	0.97	0.22	10,10,10,10	0
59	MG	BA	3036	1/1	0.97	0.27	20,20,20,20	0
59	MG	BA	3038	1/1	0.97	0.36	19,19,19,19	0
59	MG	BA	3017	1/1	0.97	0.20	16,16,16,16	0
59	MG	BA	3040	1/1	0.97	0.25	10,10,10,10	0
59	MG	AA	1618	1/1	0.97	0.20	22,22,22,22	0
59	MG	BA	3075	1/1	0.97	0.19	12,12,12,12	0
59	MG	BA	3042	1/1	0.97	0.33	11,11,11,11	0
59	MG	BA	3077	1/1	0.97	0.14	17,17,17,17	0
59	MG	AA	1625	1/1	0.97	0.34	25,25,25,25	0
59	MG	BA	3008	1/1	0.97	0.27	13,13,13,13	0
59	MG	BA	3046	1/1	0.97	0.18	14,14,14,14	0
59	MG	BA	3023	1/1	0.97	0.25	9,9,9,9	0
59	MG	AA	1605	1/1	0.97	0.10	25,25,25,25	0
59	MG	AA	1612	1/1	0.97	0.15	14,14,14,14	0
59	MG	BA	3055	1/1	0.97	0.21	5,5,5,5	0
59	MG	BA	3056	1/1	0.97	0.15	18,18,18,18	0
59	MG	BA	3057	1/1	0.97	0.22	8,8,8,8	0
59	MG	BA	3058	1/1	0.97	0.17	3,3,3,3	0
59	MG	BA	3011	1/1	0.97	0.24	30,30,30,30	0
59	MG	BA	3028	1/1	0.97	0.20	23,23,23,23	0
59	MG	BA	3062	1/1	0.97	0.23	18,18,18,18	0
59	MG	AA	1614	1/1	0.98	0.24	11,11,11,11	0
59	MG	AA	1627	1/1	0.98	0.23	15,15,15,15	0
59	MG	BA	3048	1/1	0.98	0.25	9,9,9,9	0
59	MG	BA	3049	1/1	0.98	0.30	2,2,2,2	0

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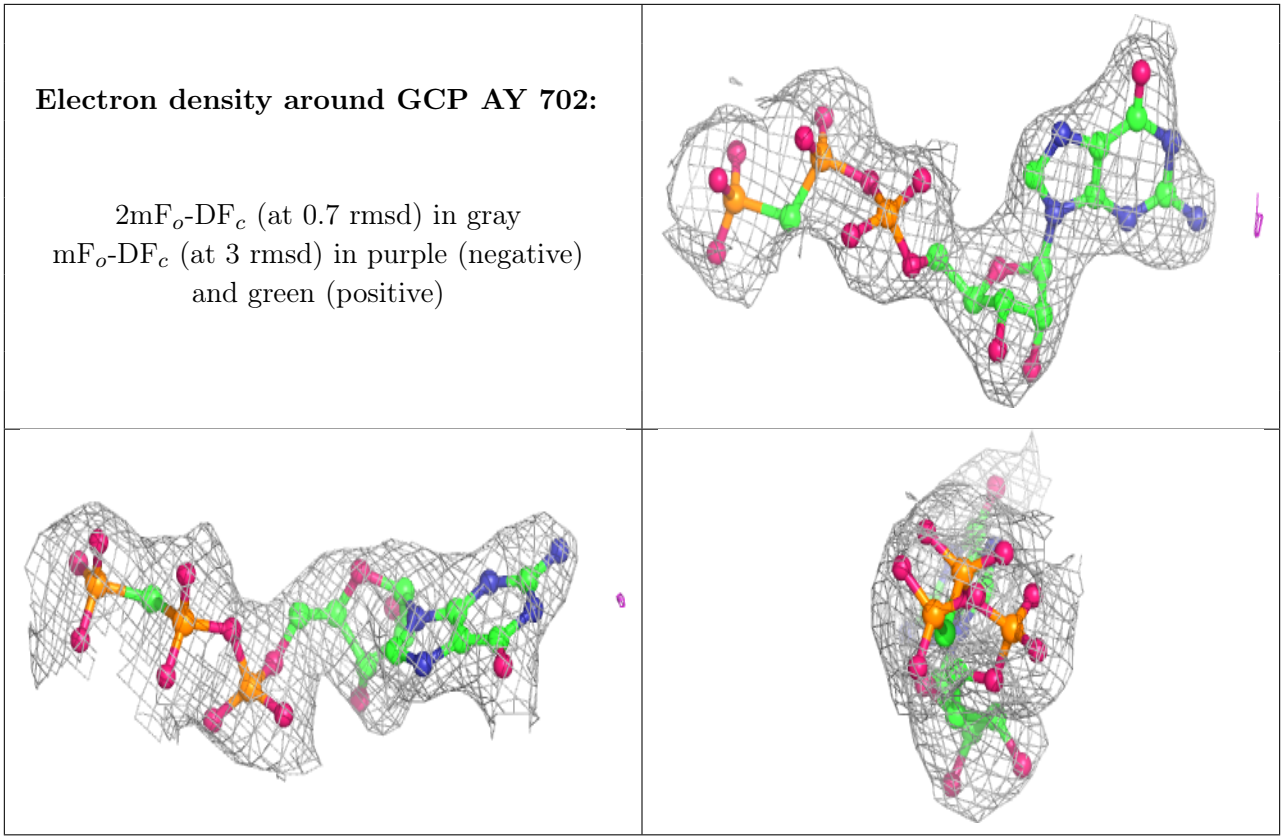
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1620	1/1	0.98	0.37	18,18,18,18	0
59	MG	BA	3031	1/1	0.98	0.29	16,16,16,16	0
59	MG	BA	3016	1/1	0.98	0.07	15,15,15,15	0
59	MG	AA	1608	1/1	0.98	0.42	23,23,23,23	0
59	MG	BA	3006	1/1	0.98	0.30	13,13,13,13	0
59	MG	BA	3079	1/1	0.98	0.23	14,14,14,14	0
59	MG	BA	3019	1/1	0.98	0.27	16,16,16,16	0
59	MG	BA	3007	1/1	0.98	0.30	4,4,4,4	0
59	MG	BA	3037	1/1	0.98	0.20	7,7,7,7	0
59	MG	BA	3061	1/1	0.98	0.30	8,8,8,8	0
59	MG	AA	1631	1/1	0.98	0.19	13,13,13,13	0
59	MG	BA	3022	1/1	0.98	0.33	13,13,13,13	0
59	MG	AA	1601	1/1	0.98	0.24	13,13,13,13	0
59	MG	BA	3024	1/1	0.98	0.28	2,2,2,2	0
59	MG	AA	1617	1/1	0.98	0.32	21,21,21,21	0
59	MG	BD	301	1/1	0.98	0.26	7,7,7,7	0
59	MG	AA	1624	1/1	0.98	0.19	14,14,14,14	0
59	MG	AA	1610	1/1	0.98	0.23	14,14,14,14	0
59	MG	BA	3069	1/1	0.98	0.34	14,14,14,14	0
60	GCP	AY	702	32/32	0.98	0.12	27,42,47,49	0
59	MG	BA	3005	1/1	0.99	0.32	12,12,12,12	0
59	MG	BA	3053	1/1	0.99	0.22	7,7,7,7	0
59	MG	BA	3054	1/1	0.99	0.27	9,9,9,9	0
59	MG	AA	1634	1/1	0.99	0.07	6,6,6,6	0
59	MG	BA	3003	1/1	0.99	0.36	2,2,2,2	0
59	MG	BA	3044	1/1	0.99	0.17	15,15,15,15	0
59	MG	AA	1628	1/1	0.99	0.07	18,18,18,18	0
59	MG	BA	3050	1/1	1.00	0.27	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GCP AY 702:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.