



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:15 PM UTC

PDB ID : 4W2E / pdb_00004w2e
Title : Crystal structure of Elongation Factor 4 (EF4/LepA) bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : 2014-06-04
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

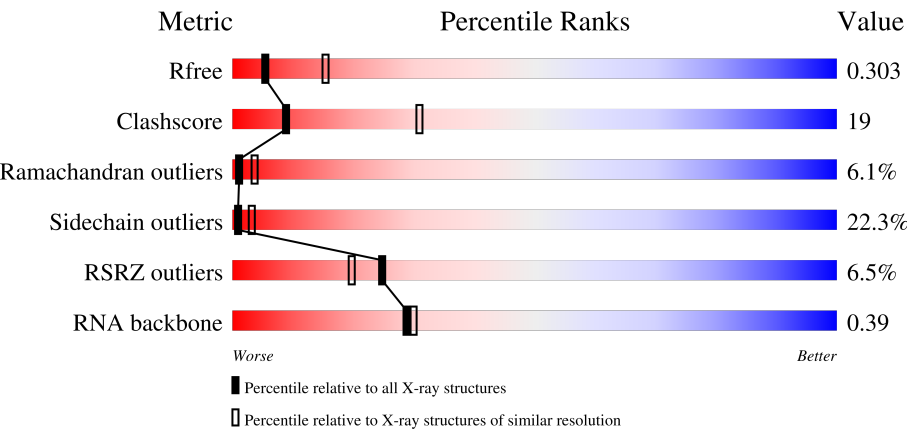
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$. 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	A	2915	
2	B	122	
3	D	276	
4	E	206	

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Mol	Chain	Length	Quality of chain
5	F	205	
6	G	182	
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	

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Mol	Chain	Length	Quality of chain
30	7	49	
31	8	65	
32	9	37	
33	w	76	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	

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Mol	Chain	Length	Quality of chain
54	u	27	
55	v	18	
56	y	679	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	SF4	d	501	-	-	X	-

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 152111 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2873	Total	C	N	O	P	0	0	0
			61879	27541	11577	19890	2871			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	130	Total	C	N	O	S	0	0	0
			641	381	130	130				

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	x	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		
33	w	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1496	Total	C	N	O	P		0	0
			32163	14314	5963	10390	1496			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	b	231	Total	C	N	O	S	0	0	0
			1850	1181	331	333	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	c	206	Total	C	N	O	S	0	0	0
			1550	974	302	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	g	155	Total	C	N	O	S	0	0	0
			1227	764	242	215	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	i	127	Total	C	N	O	0	0	0
			983	623	193	167			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	j	96	Total	C	N	O	0	0	0
			698	434	134	130			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	m	119	Total	C	N	O	S	0	0	0
			924	570	192	160	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	s	83	Total	C	N	O	S	0	0	0
			650	415	120	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	t	96	Total	C	N	O	S	0	0	0
			724	443	155	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	v	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			

- Molecule 56 is a protein called 50S ribosomal protein L9, Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	y	644	Total 4000	C 2438	N 760	O 799	S 3	0	0	0

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	A	635	Total 635	Mg 635	0	0
57	B	18	Total 18	Mg 18	0	0
57	D	5	Total 5	Mg 5	0	0
57	E	4	Total 4	Mg 4	0	0
57	F	5	Total 5	Mg 5	0	0
57	G	3	Total 3	Mg 3	0	0
57	N	1	Total 1	Mg 1	0	0
57	O	1	Total 1	Mg 1	0	0
57	P	2	Total 2	Mg 2	0	0
57	Q	5	Total 5	Mg 5	0	0
57	R	3	Total 3	Mg 3	0	0
57	U	4	Total 4	Mg 4	0	0
57	V	2	Total 2	Mg 2	0	0
57	W	1	Total 1	Mg 1	0	0
57	X	1	Total 1	Mg 1	0	0
57	Z	1	Total 1	Mg 1	0	0
57	0	3	Total 3	Mg 3	0	0
57	5	1	Total 1	Mg 1	0	0
57	6	1	Total 1	Mg 1	0	0

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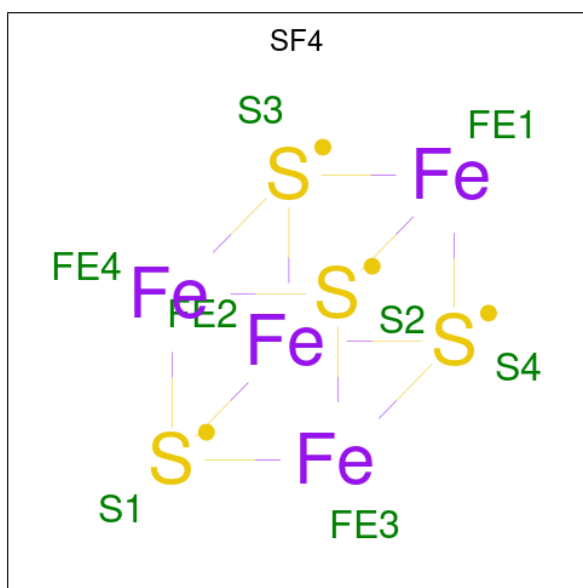
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7	3	Total 3	Mg 3	0	0
57	8	1	Total 1	Mg 1	0	0
57	9	1	Total 1	Mg 1	0	0
57	x	3	Total 3	Mg 3	0	0
57	a	187	Total 187	Mg 187	0	0
57	e	1	Total 1	Mg 1	0	0
57	f	1	Total 1	Mg 1	0	0
57	l	2	Total 2	Mg 2	0	0
57	m	1	Total 1	Mg 1	0	0
57	n	1	Total 1	Mg 1	0	0
57	w	6	Total 6	Mg 6	0	0
57	v	1	Total 1	Mg 1	0	0
57	y	2	Total 2	Mg 2	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

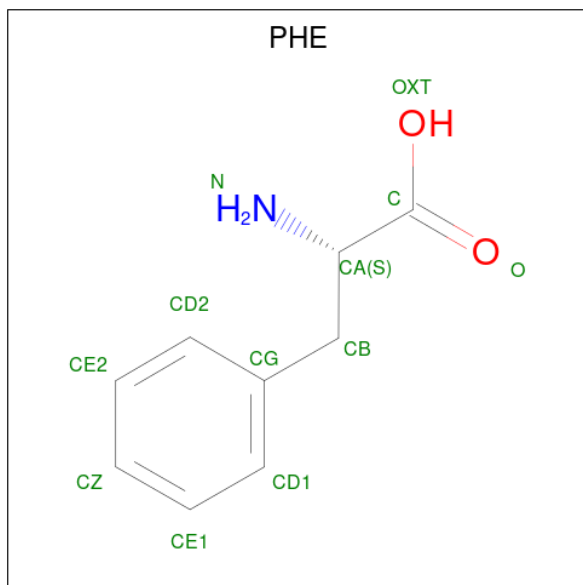
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y	1	Total 1	Zn 1	0	0
58	4	1	Total 1	Zn 1	0	0
58	5	1	Total 1	Zn 1	0	0
58	6	1	Total 1	Zn 1	0	0
58	9	1	Total 1	Zn 1	0	0
58	n	1	Total 1	Zn 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



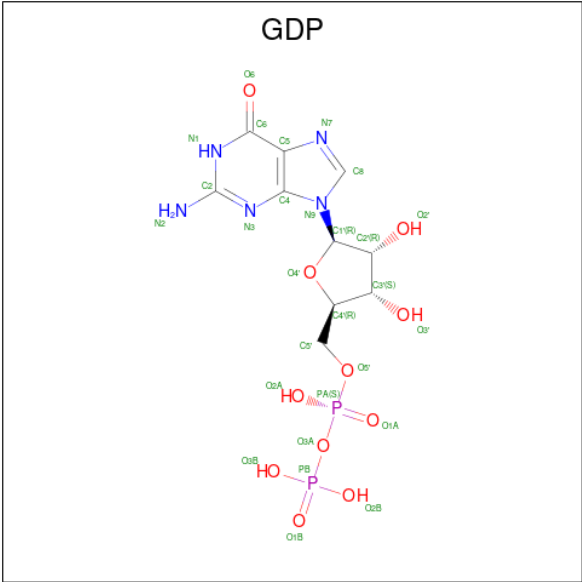
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula: $\text{C}_9\text{H}_{11}\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	w	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



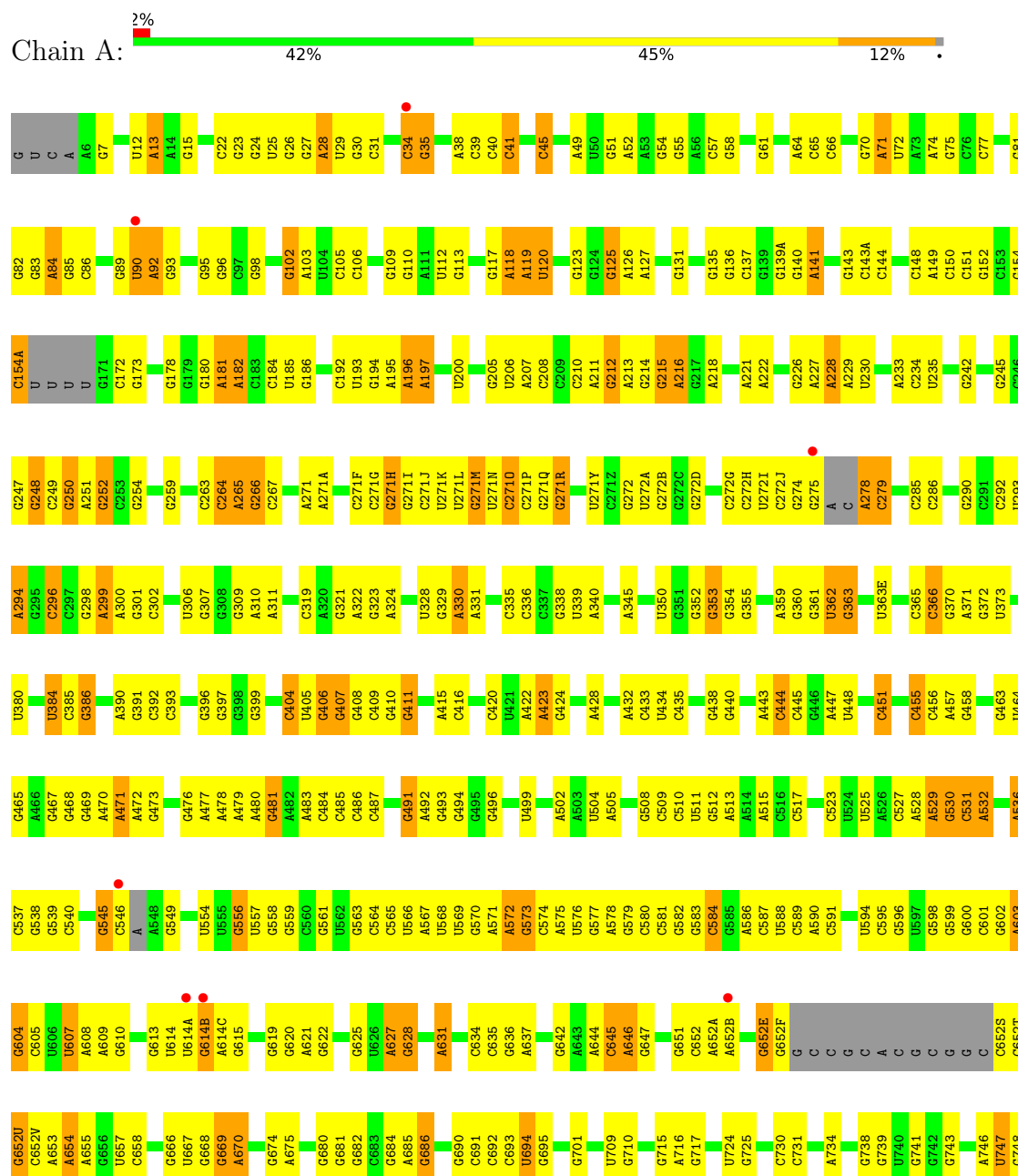
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	R	2	Total 2	O 2	0	0
62	T	1	Total 1	O 1	0	0
62	U	2	Total 2	O 2	0	0
62	V	1	Total 1	O 1	0	0
62	W	2	Total 2	O 2	0	0
62	Y	1	Total 1	O 1	0	0
62	0	4	Total 4	O 4	0	0
62	1	2	Total 2	O 2	0	0
62	3	1	Total 1	O 1	0	0
62	5	1	Total 1	O 1	0	0
62	7	2	Total 2	O 2	0	0
62	8	4	Total 4	O 4	0	0
62	9	1	Total 1	O 1	0	0
62	x	1	Total 1	O 1	0	0
62	a	167	Total 167	O 167	0	0
62	l	1	Total 1	O 1	0	0
62	v	3	Total 3	O 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: 23S Ribosomal RNA



U1779	U1680	C1588	A1509B	A1367	C1291	G1139	A1070	C998	G843	U1779
A1780	U1681	C1589	G1510	G1368	U1292	C1140	G1071	U999	C844	A1780
C1782	G1682	U1590	C1511	G1369	C1219	U1141	C1072	U922	C845	C1782
A1783	C1683	U1438	U1293	C1370	C1220	U1142	A1073	C923	G846	A1783
A1784	C1684	A1439	C1296	G1371	C1221	A1142A	C1006	C925	U847	A1784
A1785	C1685	G1440	C1297	G1372	C1222	A1143	C1007	A926	G848	A1785
A1786	U1688	G1441	C1297	G1373	G1223	G1144	C1008	G927	A849	A1786
A1787	A1689	G1442	U1300	C1375	C1224	G1145	A1009	G928	A764	A1787
A1788	U1689	G1443	A1301	C1376	G1227	G1149	U1012	U930	G855	A1788
A1789	G1696	G1444	A1302	G1377	G1228	G1150	C1013	G931	G768	A1789
A1790	G1697	G1445	G1303	A1378	G1229	G1151	U1014	G932	G769	A1790
G1792	A1603	G1450	A1308	A1379	C1230	G1152	A1084	A933	U773	G1792
C1793	C1604	C1451	G1309	G1380	G1231	G1153	U1015	A936	U774	C1793
U1794	C1607	C1452	U1234	G1381	U1235	G1154	A1085	A941	A775	U1794
A1795	A1608	A1453	G1236	C1382	A1155	A1156	G1087	G942	A776	A1795
C1796	A1609	G1455	G1237	U1312	A1157	G1157	A1088	A945	G775	C1796
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G1799	C1617	G1465	C1320	C1386	U1242	G1169	A1096	A953	A782	G1799
C1800	U1621	G1466	A1321	G1387	G1243	G1170	U1097	G954	A783	C1800
A1801	G1628	G1467	G1325	U1394	G1244	G1171	A1098	A955	G785	A1801
A1802	U1629	G1468	U1329	U1395	G1245	G1172	U1099	G956	A786	A1802
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C1914	C1504	C1504	C1504	C1504	G1282	G1194	U1099	A980	A900	C1914
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C1916	C1506	C1506	C1506	C1506	A1284	G1196	U1099	A982	A902	C1916
A1917	A1507	A1507	A1507	A1507	G1285	G1197	U1099	A983	A903	A1917
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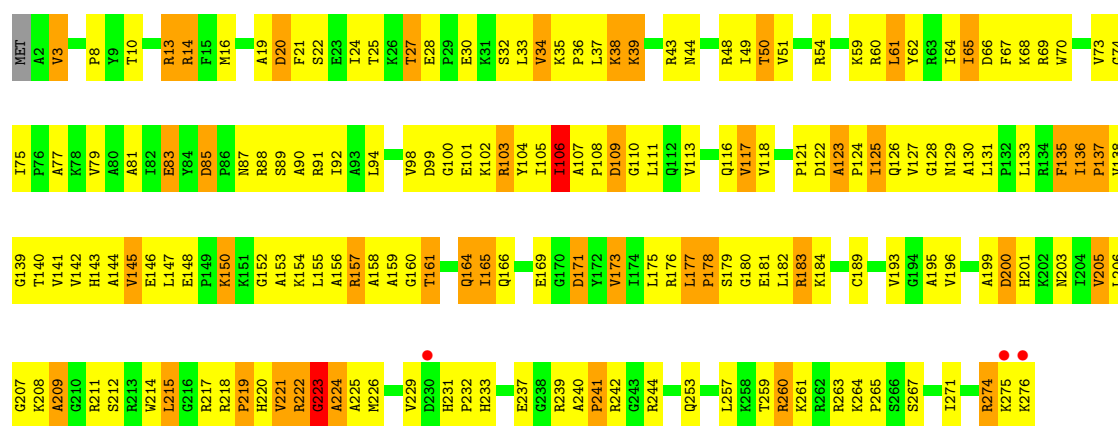
- Molecule 2: 5S Ribosomal RNA

Chain B: 



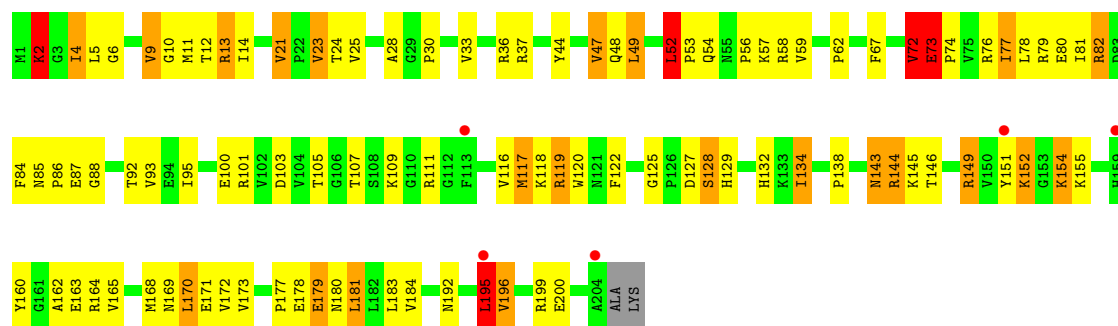
- Molecule 3: 50S ribosomal protein L2

Chain D: 



- Molecule 4: 50S ribosomal protein L3

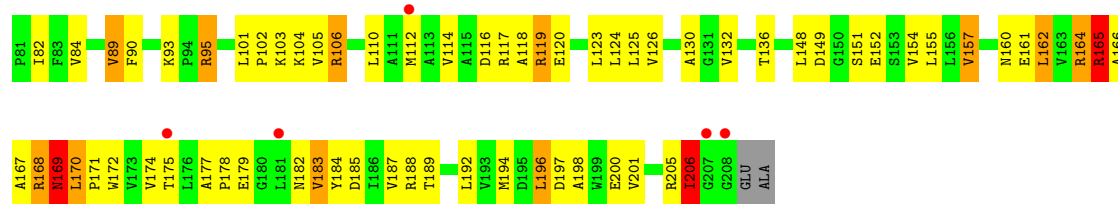
Chain E: 



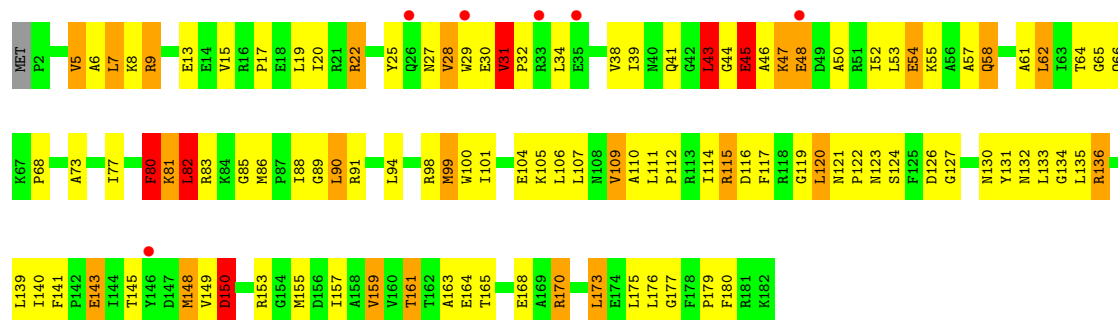
- Molecule 5: 50S ribosomal protein L4

Chain F: 

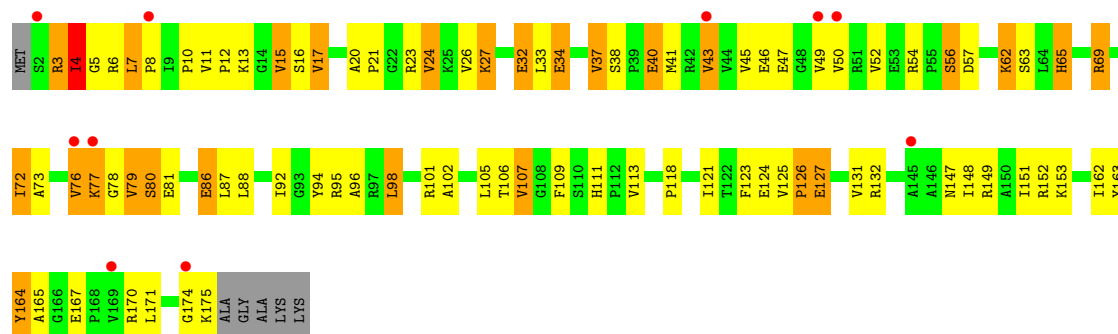




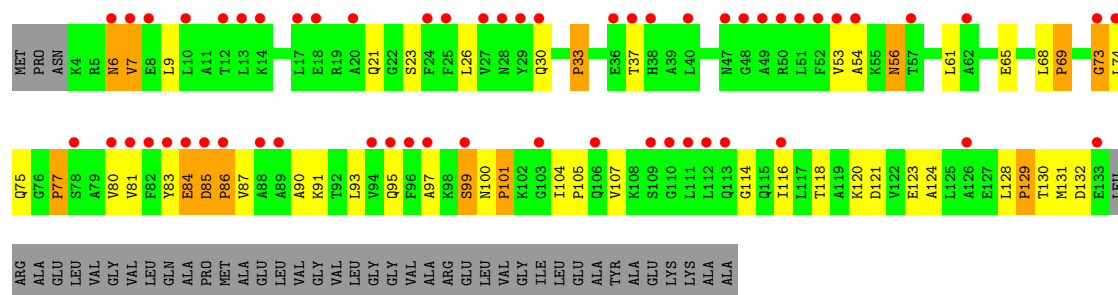
• Molecule 6: 50S ribosomal protein L5



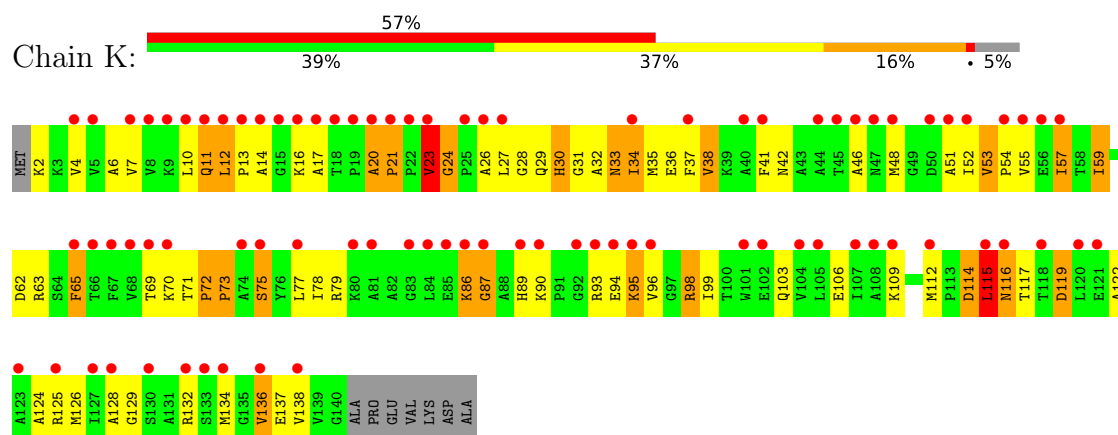
• Molecule 7: 50S ribosomal protein L6



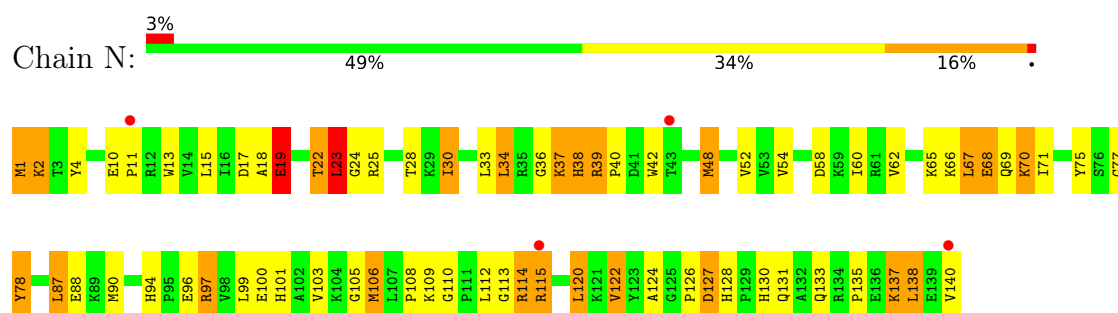
• Molecule 8: 50S ribosomal protein L10



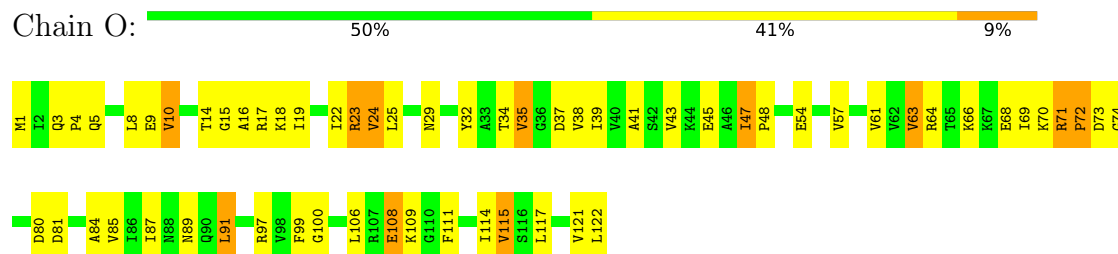
• Molecule 9: 50S ribosomal protein L11



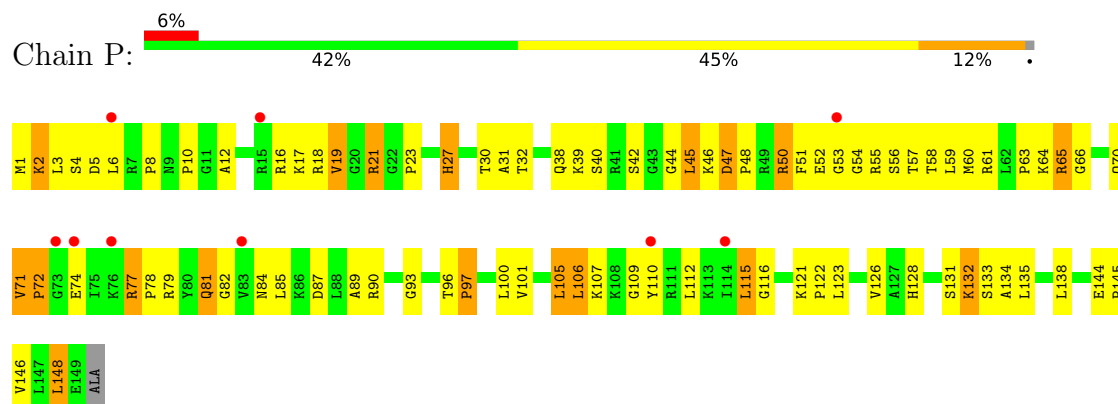
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14

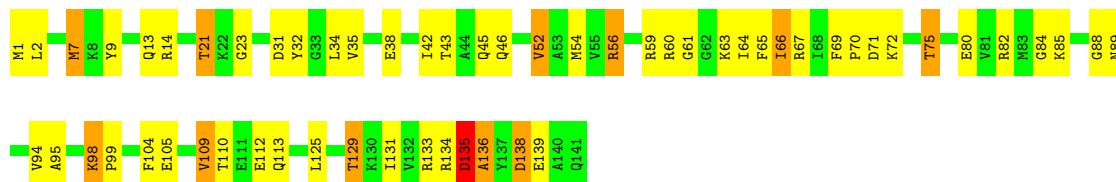


- Molecule 12: 50S ribosomal protein L15



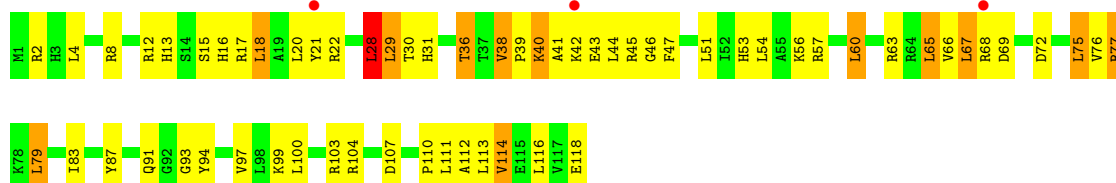
- Molecule 13: 50S ribosomal protein L16

Chain Q: 



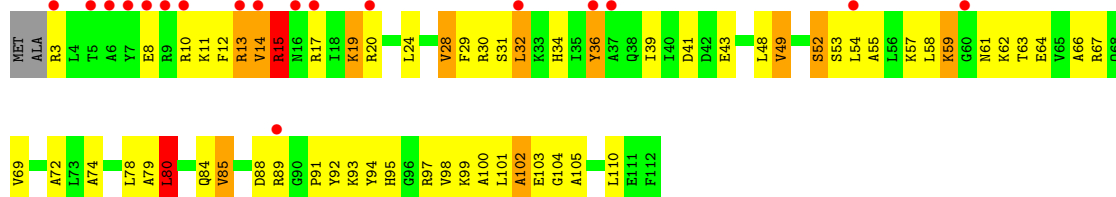
• Molecule 14: 50S ribosomal protein L17

Chain R: 



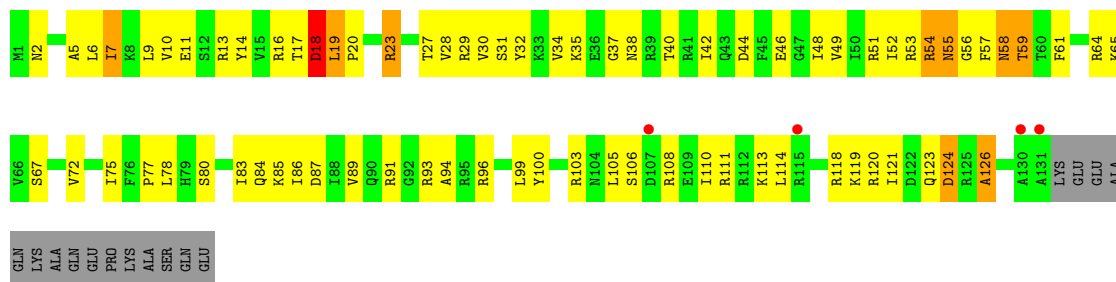
• Molecule 15: 50S ribosomal protein L18

Chain S: 



• Molecule 16: 50S ribosomal protein L19

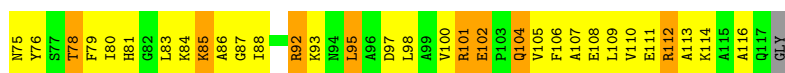
Chain T: 



• Molecule 17: 50S ribosomal protein L20

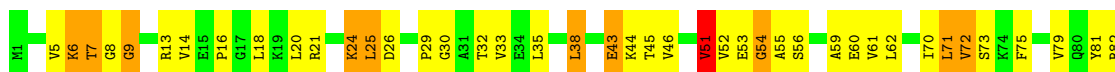
Chain U: 





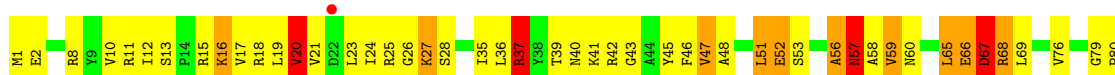
• Molecule 18: 50S ribosomal protein L21

Chain V: 47% 40% 13%



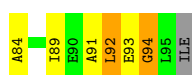
• Molecule 19: 50S ribosomal protein L22

Chain W: 46% 39% 10%



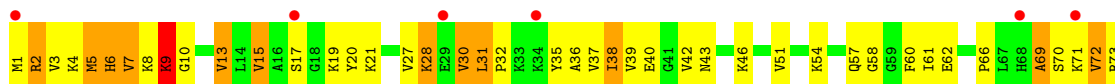
• Molecule 20: 50S ribosomal protein L23

Chain X: 6% 50% 36% 11%



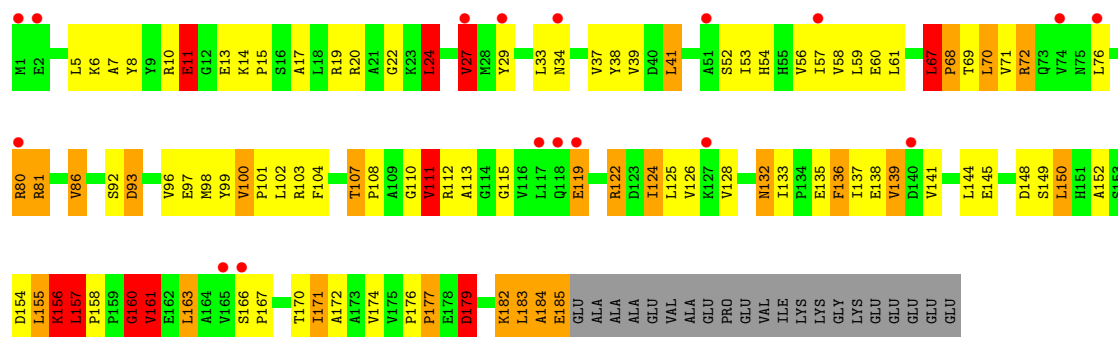
• Molecule 21: 50S ribosomal protein L24

Chain Y: 6% 39% 45% 13%

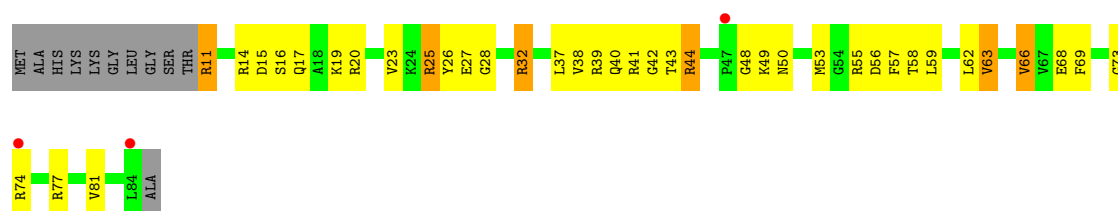
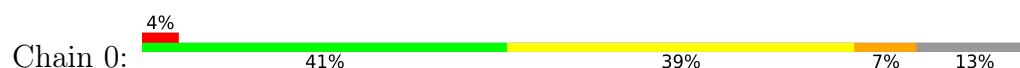


• Molecule 22: 50S ribosomal protein L25

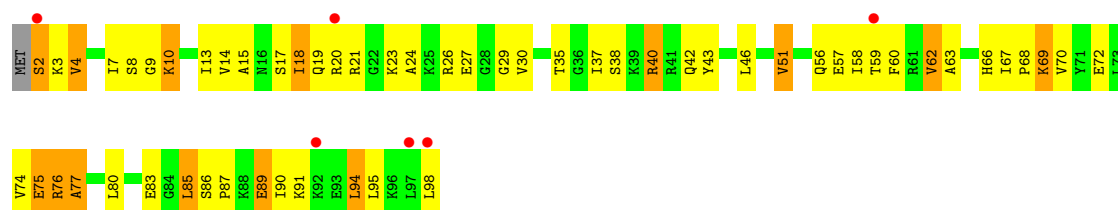
Chain Z: 8% 41% 32% 12% 5% 10%



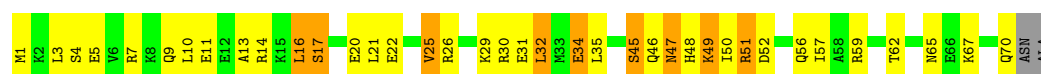
• Molecule 23: 50S ribosomal protein L27



• Molecule 24: 50S ribosomal protein L28

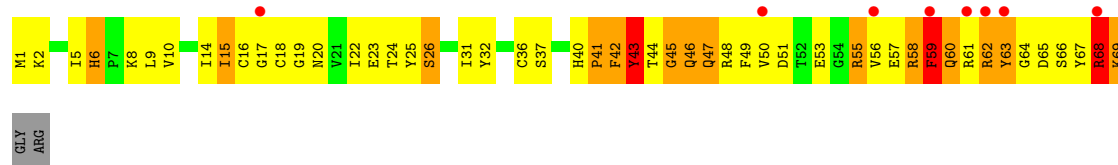


• Molecule 25: 50S ribosomal protein L29

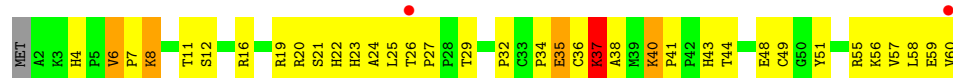


• Molecule 26: 50S ribosomal protein L30

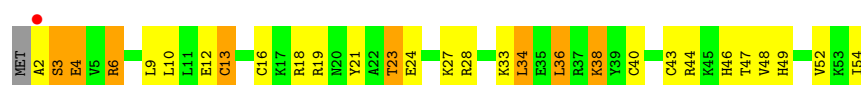




- Molecule 28: 50S ribosomal protein L32



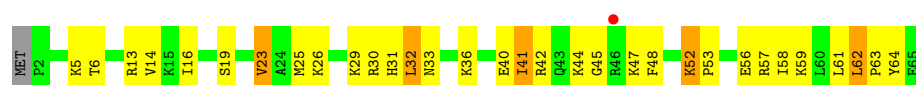
- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34



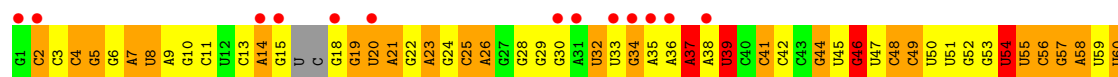
- Molecule 31: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L36

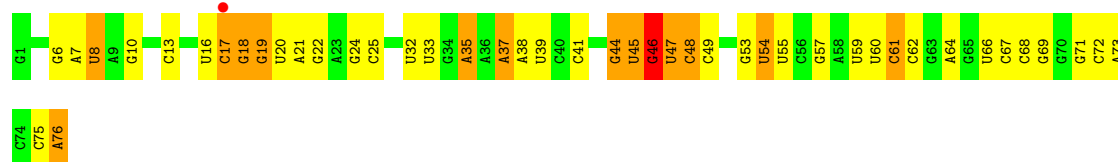


- Molecule 33: E-site tRNA

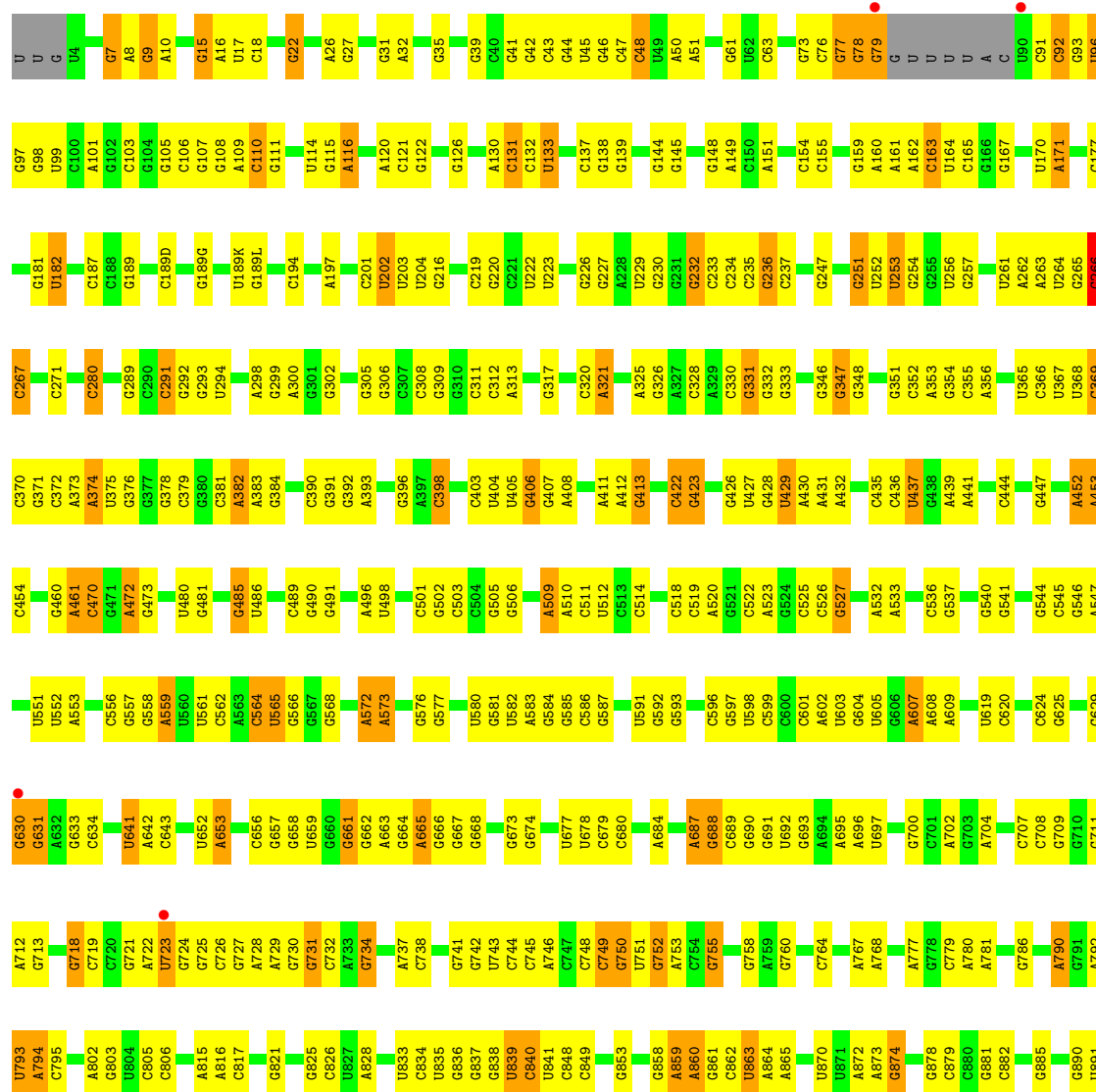


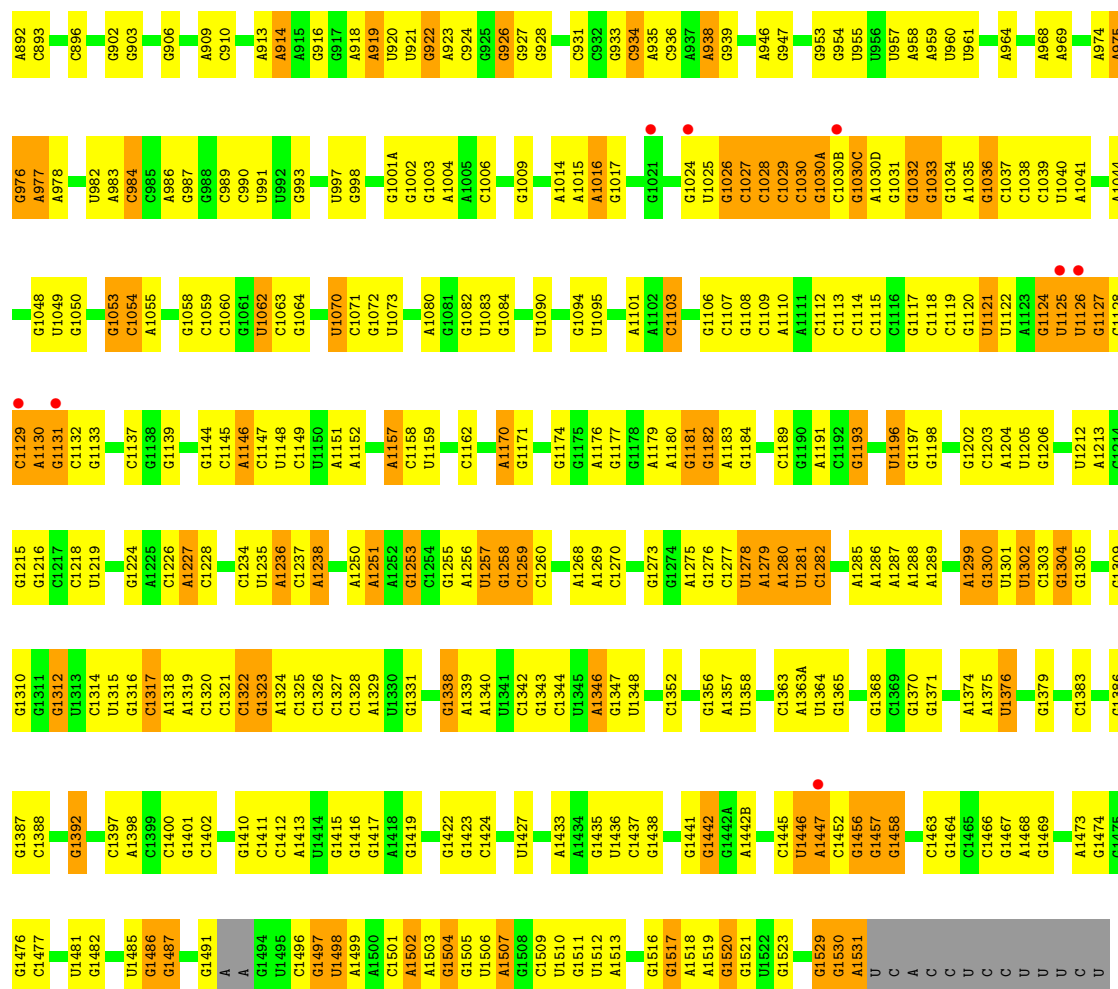


• Molecule 33: E-site tRNA

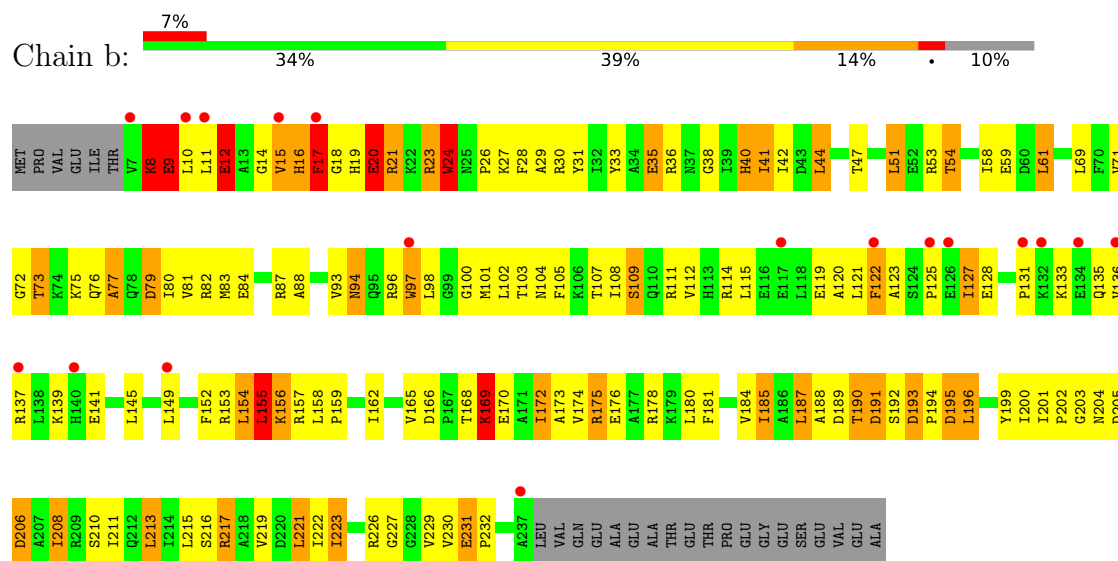


• Molecule 34: 16S Ribosomal RNA



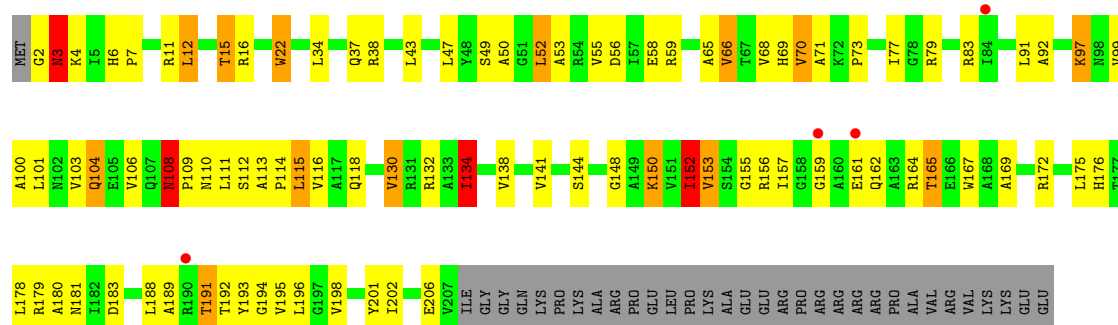


• Molecule 35: 30S ribosomal protein S2

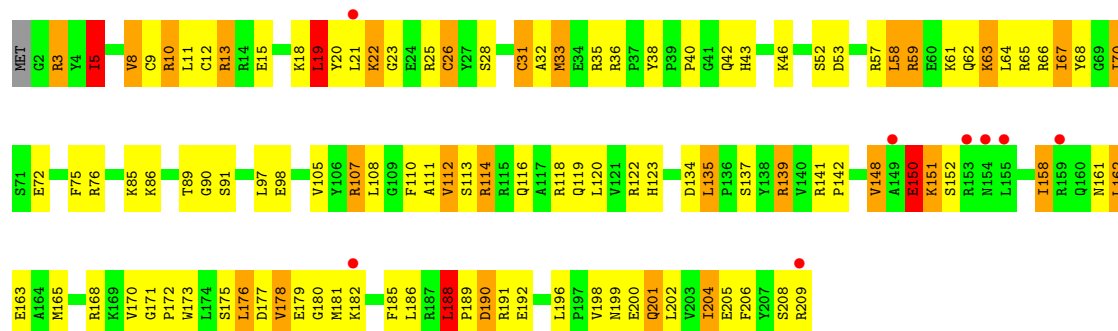


• Molecule 36: 30S ribosomal protein S3

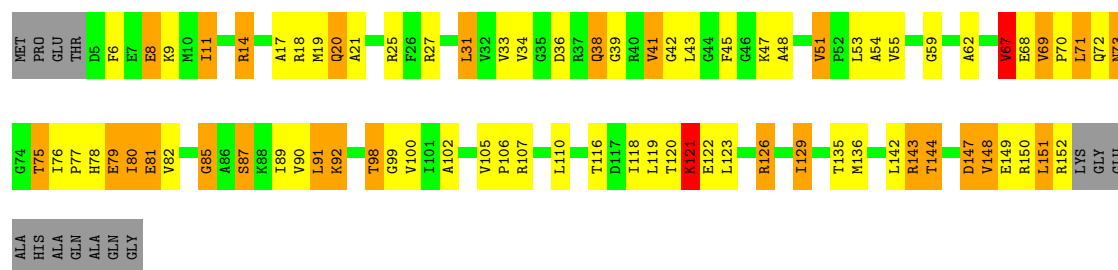




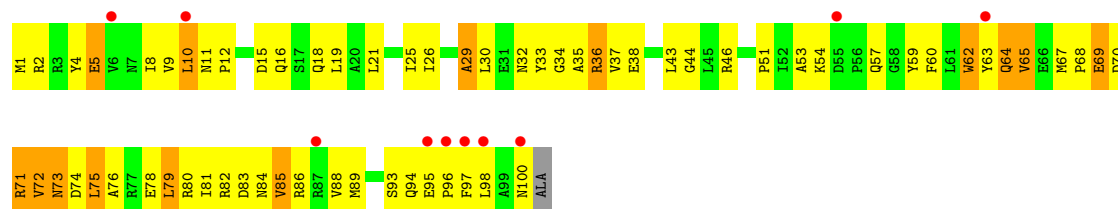
• Molecule 37: 30S ribosomal protein S4



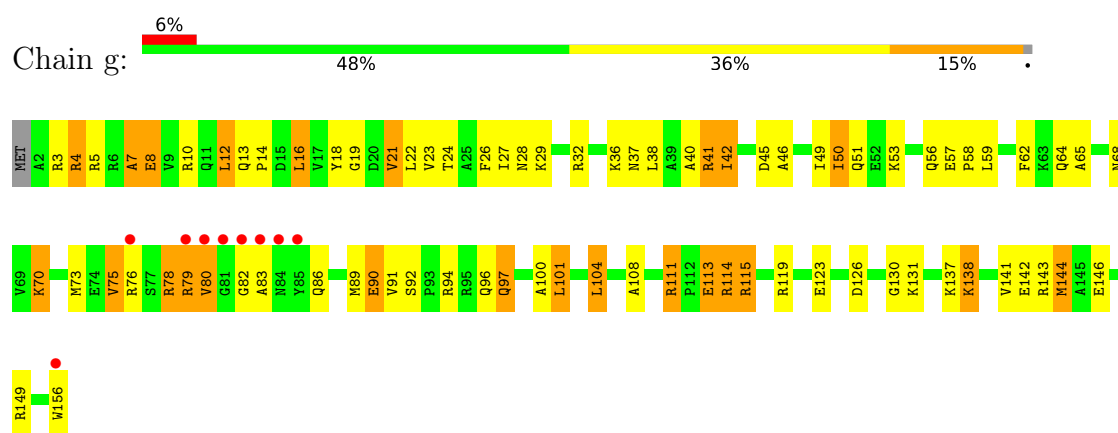
• Molecule 38: 30S ribosomal protein S5



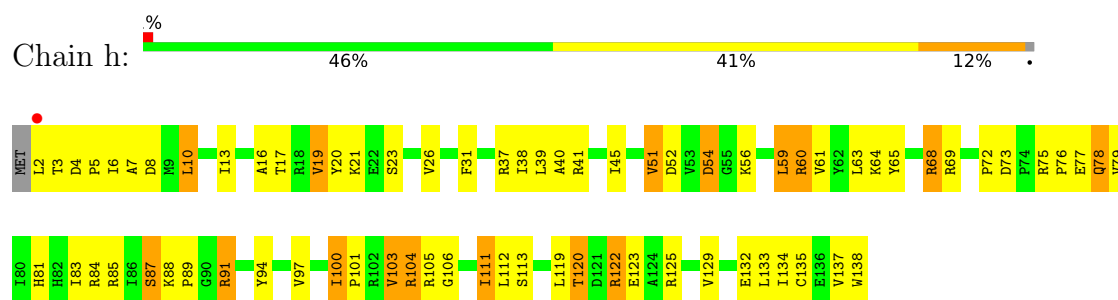
• Molecule 39: 30S ribosomal protein S6



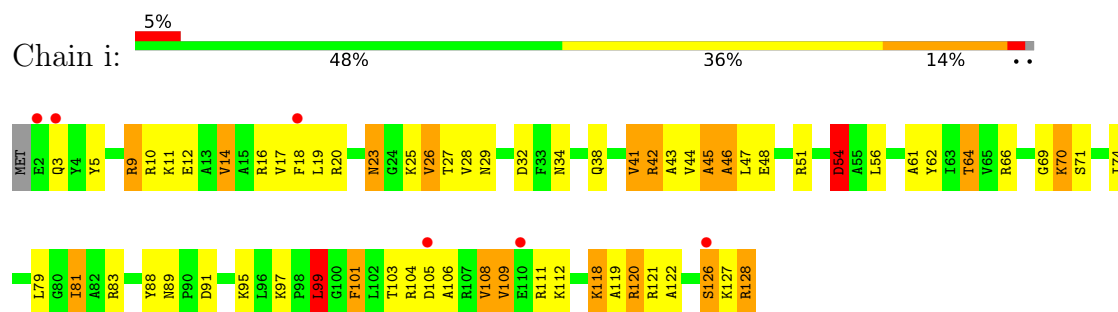
• Molecule 40: 30S ribosomal protein S7



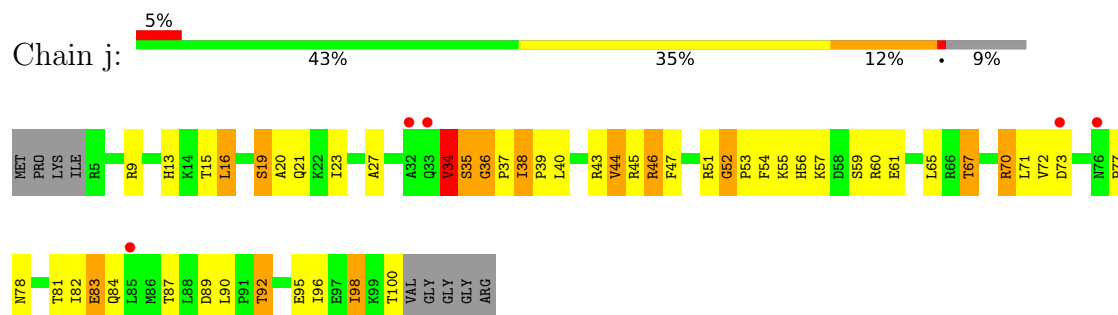
• Molecule 41: 30S ribosomal protein S8



• Molecule 42: 30S ribosomal protein S9

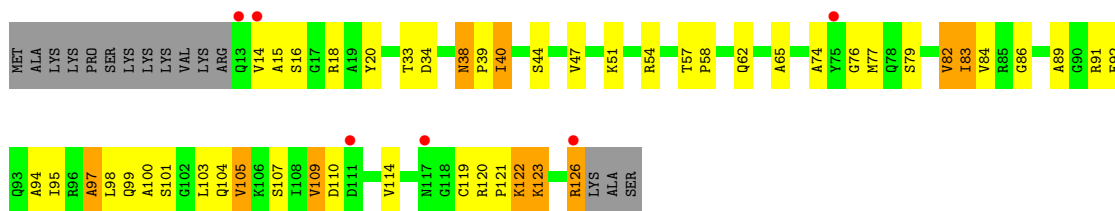


• Molecule 43: 30S ribosomal protein S10

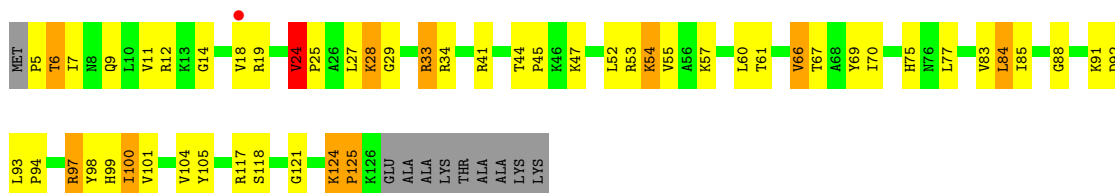


• Molecule 44: 30S ribosomal protein S11

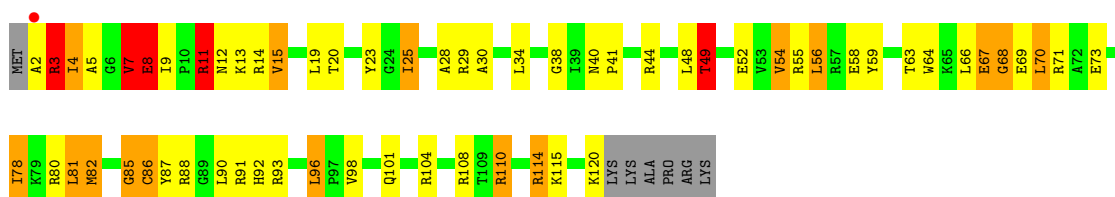
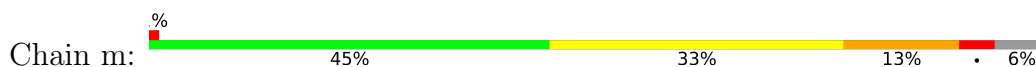




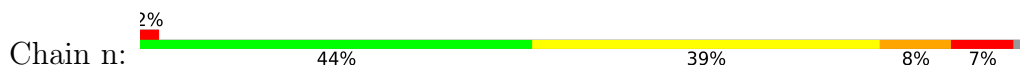
• Molecule 45: 30S ribosomal protein S12



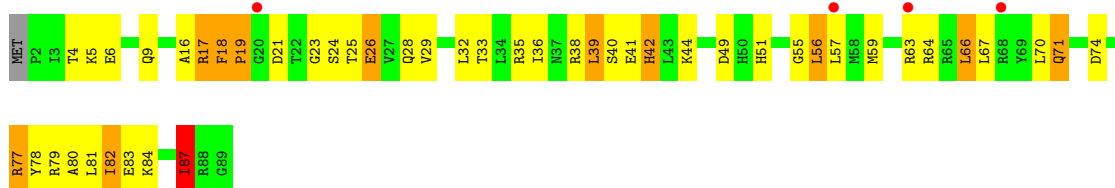
• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14 type Z

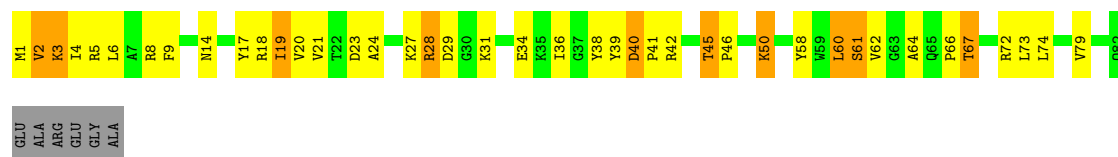


• Molecule 48: 30S ribosomal protein S15

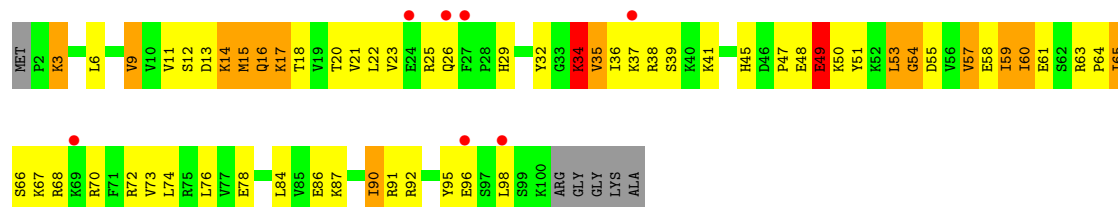
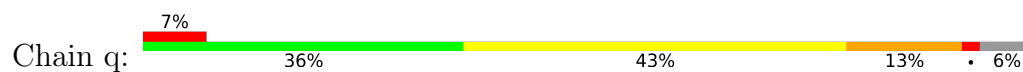


• Molecule 49: 30S ribosomal protein S16

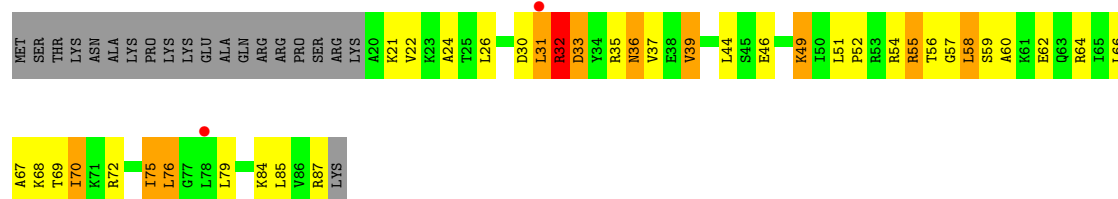




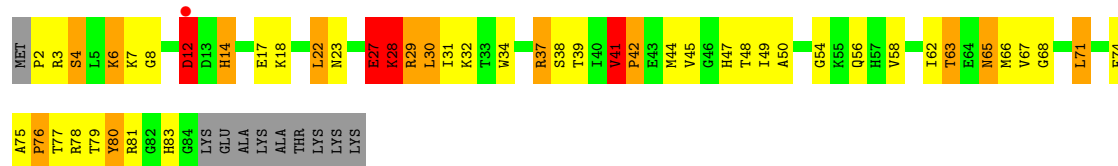
- Molecule 50: 30S ribosomal protein S17



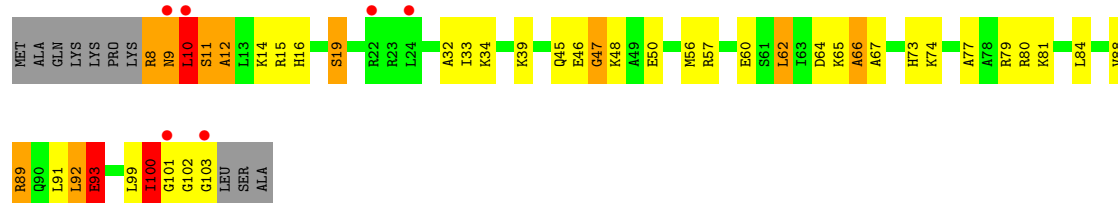
- Molecule 51: 30S ribosomal protein S18



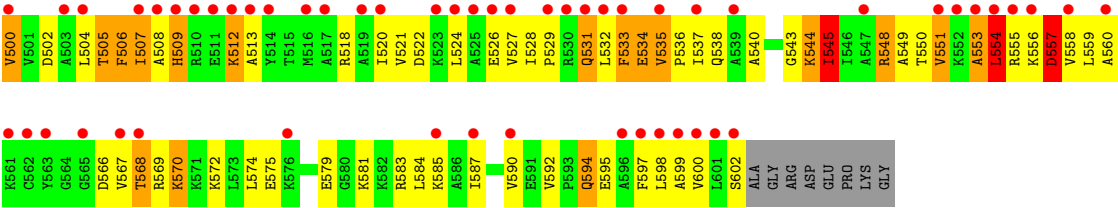
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	239.29Å 272.85Å 431.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.8 (49.76-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.238 , 0.304 0.239 , 0.303	Depositor DCC
R_{free} test set	29295 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, SF4, MIA, MG, 7MG, ZN, 4SU, GDP

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	A	0.46	0/69298	0.69	8/108168 (0.0%)
2	B	0.34	0/2878	0.54	0/4490
3	D	0.82	2/2186 (0.1%)	1.25	18/2944 (0.6%)
4	E	0.80	0/1592	1.28	10/2149 (0.5%)
5	F	0.73	0/1619	1.16	13/2193 (0.6%)
6	G	0.58	0/1450	1.12	14/1959 (0.7%)
7	H	0.59	0/1356	1.13	10/1834 (0.5%)
8	J	0.65	0/640	1.40	11/889 (1.2%)
9	K	0.46	0/1044	1.12	13/1416 (0.9%)
10	N	0.71	0/1144	1.09	8/1543 (0.5%)
11	O	0.91	0/943	1.35	7/1269 (0.6%)
12	P	0.62	0/1152	1.25	8/1533 (0.5%)
13	Q	0.75	0/1143	1.10	7/1527 (0.5%)
14	R	0.69	0/982	1.02	0/1312
15	S	0.55	0/887	1.02	2/1180 (0.2%)
16	T	0.72	0/1105	1.14	4/1477 (0.3%)
17	U	0.75	0/977	1.11	6/1301 (0.5%)
18	V	0.70	0/782	1.19	3/1049 (0.3%)
19	W	0.79	0/897	1.19	5/1205 (0.4%)
20	X	0.68	0/764	1.07	2/1025 (0.2%)
21	Y	0.70	0/819	1.11	3/1095 (0.3%)
22	Z	0.65	0/1483	1.16	14/2017 (0.7%)
23	0	0.63	0/599	0.99	1/798 (0.1%)
24	1	0.73	0/762	1.15	3/1014 (0.3%)
25	2	0.59	0/590	1.05	4/781 (0.5%)
26	3	0.74	0/474	1.28	4/635 (0.6%)
27	4	0.60	0/570	1.23	7/768 (0.9%)
28	5	0.69	0/473	1.15	2/639 (0.3%)
29	6	0.67	0/460	0.98	0/613
30	7	0.83	0/438	1.16	1/575 (0.2%)
31	8	0.74	0/519	1.06	2/684 (0.3%)
32	9	0.70	0/310	1.15	2/407 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	w	0.49	0/1651	0.74	2/2569 (0.1%)
33	x	0.34	1/1602 (0.1%)	0.59	0/2493
34	a	0.46	2/36002 (0.0%)	0.68	3/56188 (0.0%)
35	b	0.69	0/1885	1.22	15/2547 (0.6%)
36	c	0.74	0/1574	1.09	7/2127 (0.3%)
37	d	0.71	0/1685	1.14	8/2262 (0.4%)
38	e	0.86	0/1145	1.25	7/1543 (0.5%)
39	f	0.57	0/819	1.12	5/1111 (0.5%)
40	g	0.67	0/1246	1.12	8/1674 (0.5%)
41	h	0.76	0/1108	1.12	5/1494 (0.3%)
42	i	0.70	0/1002	1.18	6/1346 (0.4%)
43	j	0.73	0/711	1.26	6/968 (0.6%)
44	k	0.69	0/844	1.12	6/1145 (0.5%)
45	l	0.79	0/946	1.33	5/1274 (0.4%)
46	m	0.72	0/934	1.23	5/1256 (0.4%)
47	n	0.81	0/501	1.12	1/664 (0.2%)
48	o	0.67	0/739	1.08	5/985 (0.5%)
49	p	0.82	0/697	1.19	5/939 (0.5%)
50	q	0.77	0/836	1.15	4/1117 (0.4%)
51	r	0.61	0/560	0.97	1/746 (0.1%)
52	s	0.77	0/665	1.25	5/897 (0.6%)
53	t	0.71	0/726	1.13	4/961 (0.4%)
54	u	0.58	0/203	1.00	1/266 (0.4%)
55	v	0.46	0/165	0.61	0/254
56	y	1.14	30/4067 (0.7%)	1.86	169/5503 (3.1%)
All	All	0.57	35/162649 (0.0%)	0.88	475/242818 (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
3	D	0	1
8	J	0	1
42	i	0	1
46	m	0	2
52	s	0	1
53	t	0	1
56	y	0	23
All	All	0	30

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	y	191	ASP	C-N	8.27	1.40	1.33
56	y	460	LEU	C-O	7.74	1.32	1.24
56	y	188	PRO	C-N	-7.53	1.24	1.33
56	y	302	PHE	CA-C	-7.11	1.46	1.53
56	y	528	ILE	C-N	6.30	1.41	1.33
56	y	345	ARG	N-CA	6.20	1.54	1.46
56	y	189	LYS	C-N	6.04	1.42	1.33
56	y	194	ALA	C-N	5.96	1.41	1.33
3	D	136	ILE	CA-CB	-5.78	1.50	1.54
56	y	333	GLU	C-N	5.75	1.41	1.33
56	y	187	PRO	C-N	5.73	1.40	1.33
56	y	441	LEU	C-N	5.69	1.40	1.33
56	y	140	LEU	C-N	5.57	1.40	1.34
56	y	535	VAL	N-CA	5.57	1.50	1.46
56	y	141	PRO	N-CD	5.54	1.55	1.47
56	y	299	PRO	N-CD	5.52	1.55	1.47
56	y	246	THR	C-N	5.46	1.40	1.33
56	y	188	PRO	N-CD	5.45	1.55	1.47
56	y	195	PRO	N-CD	5.34	1.55	1.47
34	a	1125	U	O3'-P	5.33	1.69	1.61
56	y	397	PRO	N-CD	5.29	1.55	1.47
56	y	287	THR	C-N	5.27	1.41	1.34
34	a	1125	U	P-O5'	5.26	1.67	1.59
56	y	416	THR	CA-C	-5.26	1.46	1.52
56	y	529	PRO	N-CD	5.25	1.55	1.47
56	y	374	PRO	N-CD	5.24	1.55	1.47
56	y	288	PRO	N-CD	5.24	1.55	1.47
3	D	240	ALA	CA-CB	-5.21	1.46	1.54
56	y	334	PRO	N-CD	5.21	1.55	1.47
56	y	408	PRO	N-CD	5.16	1.54	1.47
56	y	412	LEU	CA-C	-5.16	1.46	1.52
56	y	467	LEU	CA-C	-5.09	1.45	1.52
56	y	292	PRO	N-CD	5.08	1.54	1.47
33	x	8	4SU	O3'-P	5.08	1.61	1.56
56	y	290	PRO	N-CD	5.06	1.54	1.47

All (475) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	463	PHE	N-CA-C	21.14	134.32	111.28
56	y	527	VAL	N-CA-C	12.72	123.57	110.72
56	y	388	VAL	N-CA-C	12.44	123.29	110.72
56	y	282	LEU	N-CA-C	-11.73	94.71	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	142	ASN	N-CA-C	-11.67	98.42	112.89
39	f	95	GLU	CA-C-N	11.57	134.30	119.84
39	f	95	GLU	C-N-CA	11.57	134.30	119.84
45	l	124	LYS	CA-C-N	11.27	133.93	119.84
45	l	124	LYS	C-N-CA	11.27	133.93	119.84
56	y	557	ASP	CA-C-N	11.18	136.29	120.53
56	y	557	ASP	C-N-CA	11.18	136.29	120.53
37	d	171	GLY	CA-C-N	11.03	133.62	119.84
37	d	171	GLY	C-N-CA	11.03	133.62	119.84
56	y	535	VAL	N-CA-C	10.83	118.87	108.15
56	y	136	ASN	N-CA-C	10.81	125.25	109.14
56	y	553	ALA	N-CA-C	10.74	126.55	113.12
12	P	44	GLY	N-CA-C	-10.68	99.04	111.85
45	l	18	VAL	N-CA-C	10.55	120.34	110.42
40	g	13	GLN	CA-C-N	10.38	130.49	119.90
40	g	13	GLN	C-N-CA	10.38	130.49	119.90
56	y	416	THR	N-CA-C	-10.37	98.84	108.07
11	O	100	GLY	CA-C-N	-10.19	110.43	120.52
11	O	100	GLY	C-N-CA	-10.19	110.43	120.52
56	y	159	PRO	CA-C-N	-10.08	106.77	120.28
56	y	159	PRO	C-N-CA	-10.08	106.77	120.28
43	j	52	GLY	CA-C-N	9.97	130.25	119.28
43	j	52	GLY	C-N-CA	9.97	130.25	119.28
56	y	209	GLN	N-CA-C	9.89	121.82	111.14
4	E	125	GLY	CA-C-N	9.76	131.04	120.11
4	E	125	GLY	C-N-CA	9.76	131.04	120.11
35	b	193	ASP	CA-C-N	9.69	131.96	119.84
35	b	193	ASP	C-N-CA	9.69	131.96	119.84
56	y	168	GLY	N-CA-C	9.62	124.27	112.73
35	b	231	GLU	CA-C-N	9.57	131.81	119.84
35	b	231	GLU	C-N-CA	9.57	131.81	119.84
56	y	528	ILE	N-CA-C	9.51	116.21	107.56
33	w	75	C	OP2-P-O3'	9.45	136.36	108.00
49	p	14	ASN	CA-C-N	-9.41	111.09	120.31
49	p	14	ASN	C-N-CA	-9.41	111.09	120.31
56	y	291	TYR	C-N-CD	9.26	140.98	120.60
56	y	252	ALA	N-CA-C	9.22	122.32	108.31
56	y	332	PHE	N-CA-C	9.15	123.65	108.73
56	y	251	VAL	N-CA-C	9.15	120.91	107.37
56	y	250	LEU	N-CA-C	9.11	123.91	108.23
6	G	15	VAL	N-CA-C	9.02	119.01	110.53
22	Z	157	LEU	CA-C-N	9.00	129.65	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Z	157	LEU	C-N-CA	9.00	129.65	120.38
56	y	343	GLY	O-C-N	-8.92	114.20	123.48
6	G	45	GLU	N-CA-C	-8.92	100.52	111.40
56	y	27	ASP	N-CA-C	-8.82	101.67	111.28
21	Y	9	LYS	N-CA-C	-8.66	97.46	110.28
56	y	155	VAL	CB-CA-C	-8.63	100.93	111.97
56	y	215	LEU	N-CA-C	-8.60	92.49	110.80
5	F	166	ALA	N-CA-C	-8.58	101.87	111.82
9	K	20	ALA	CA-C-N	8.56	129.20	120.38
9	K	20	ALA	C-N-CA	8.56	129.20	120.38
16	T	19	LEU	CA-C-N	8.51	128.55	119.78
16	T	19	LEU	C-N-CA	8.51	128.55	119.78
38	e	69	VAL	CA-C-N	8.51	129.02	119.92
38	e	69	VAL	C-N-CA	8.51	129.02	119.92
32	9	29	ASN	CA-C-N	8.48	128.99	119.32
32	9	29	ASN	C-N-CA	8.48	128.99	119.32
36	c	108	ASN	CA-C-N	8.45	129.28	119.47
36	c	108	ASN	C-N-CA	8.45	129.28	119.47
56	y	232	SER	N-CA-C	8.42	120.46	111.28
22	Z	111	VAL	N-CA-C	-8.36	98.01	109.55
56	y	130	VAL	CA-C-N	-8.36	111.92	122.37
56	y	130	VAL	C-N-CA	-8.36	111.92	122.37
56	y	95	ARG	N-CA-C	-8.33	102.16	111.07
56	y	373	ALA	C-N-CD	8.29	138.84	120.60
11	O	71	ARG	CA-C-N	8.19	130.07	119.84
11	O	71	ARG	C-N-CA	8.19	130.07	119.84
6	G	127	GLY	N-CA-C	-8.18	103.70	115.64
8	J	33	PRO	N-CA-CB	8.17	110.46	103.35
6	G	54	GLU	N-CA-C	-8.16	102.34	111.07
27	4	59	PHE	N-CA-C	8.14	123.37	112.30
36	c	134	ILE	N-CA-C	-8.13	103.89	111.45
26	3	9	VAL	N-CA-C	8.13	118.95	112.12
12	P	5	ASP	N-CA-C	-8.09	104.56	114.75
27	4	5	ILE	N-CA-C	8.06	118.86	110.72
36	c	92	ALA	N-CA-C	-7.96	104.73	114.75
1	A	1300	U	C2'-C3'-O3'	7.95	121.43	109.50
39	f	29	ALA	N-CA-C	-7.92	105.59	114.62
52	s	75	ALA	CA-C-N	7.91	129.73	119.84
52	s	75	ALA	C-N-CA	7.91	129.73	119.84
56	y	177	ILE	N-CA-C	7.87	118.65	110.62
56	y	202	ASP	N-CA-C	7.84	118.97	108.38
5	F	151	SER	N-CA-C	-7.77	103.82	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	U	93	LYS	N-CA-C	-7.75	102.77	111.07
1	A	2095	C	O3'-P-O5'	7.75	115.62	104.00
8	J	77	PRO	N-CA-CB	7.74	111.37	103.25
12	P	44	GLY	CA-C-O	-7.74	115.25	122.13
50	q	29	HIS	CA-C-N	7.70	129.46	119.84
50	q	29	HIS	C-N-CA	7.70	129.46	119.84
56	y	558	VAL	N-CA-C	7.65	119.34	110.62
56	y	268	ILE	CA-C-N	7.64	131.54	120.38
56	y	268	ILE	C-N-CA	7.64	131.54	120.38
33	w	75	C	OP1-P-O3'	-7.64	85.07	108.00
16	T	126	ALA	N-CA-C	-7.60	104.53	113.88
43	j	90	LEU	CA-C-N	7.58	129.32	119.84
43	j	90	LEU	C-N-CA	7.58	129.32	119.84
48	o	42	HIS	N-CA-C	-7.54	103.08	111.82
56	y	245	PHE	N-CA-C	7.52	119.98	109.15
42	i	46	ALA	N-CA-C	-7.51	100.56	111.30
56	y	441	LEU	CA-C-N	-7.50	113.01	120.21
56	y	441	LEU	C-N-CA	-7.50	113.01	120.21
56	y	297	ALA	N-CA-C	7.49	121.69	109.85
3	D	136	ILE	CA-C-N	7.49	129.20	119.84
3	D	136	ILE	C-N-CA	7.49	129.20	119.84
44	k	40	ILE	N-CA-C	-7.43	105.88	112.12
56	y	392	ASN	CA-C-O	7.42	124.11	119.29
1	A	1992	G	C2'-C3'-O3'	7.39	120.59	109.50
56	y	295	ARG	CA-C-N	7.38	127.83	120.52
56	y	295	ARG	C-N-CA	7.38	127.83	120.52
56	y	303	ALA	N-CA-C	-7.31	95.23	110.80
8	J	86	PRO	N-CA-CB	7.28	110.89	103.25
7	H	151	ILE	N-CA-C	-7.27	104.28	113.22
37	d	188	LEU	CA-C-N	7.26	128.91	119.84
37	d	188	LEU	C-N-CA	7.26	128.91	119.84
7	H	56	SER	N-CA-C	7.22	117.55	108.45
3	D	65	ILE	N-CA-C	7.22	118.54	107.78
3	D	218	ARG	CA-C-N	7.19	128.83	119.84
3	D	218	ARG	C-N-CA	7.19	128.83	119.84
44	k	97	ALA	N-CA-C	-7.17	105.06	114.31
56	y	535	VAL	CB-CA-C	-7.14	104.29	111.08
8	J	69	PRO	N-CA-CB	7.10	110.70	103.25
56	y	116	GLU	N-CA-C	-7.10	103.55	111.28
8	J	101	PRO	N-CA-CB	7.09	110.69	103.25
56	y	178	LEU	CA-C-N	7.09	129.78	120.28
56	y	178	LEU	C-N-CA	7.09	129.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	406	LEU	N-CA-C	7.08	120.31	108.13
19	W	68	ARG	N-CA-C	-7.08	104.27	114.12
56	y	344	PHE	CA-C-O	-7.08	113.11	121.11
4	E	117	MET	N-CA-C	-7.08	101.39	110.53
10	N	71	ILE	N-CA-C	7.08	118.31	108.12
44	k	38	ASN	CA-C-N	7.07	128.68	119.84
44	k	38	ASN	C-N-CA	7.07	128.68	119.84
56	y	187	PRO	CA-C-N	-7.06	113.43	120.21
56	y	187	PRO	C-N-CA	-7.06	113.43	120.21
46	m	96	LEU	CA-C-N	-7.05	113.05	120.03
46	m	96	LEU	C-N-CA	-7.05	113.05	120.03
56	y	543	GLY	N-CA-C	7.04	125.35	115.43
5	F	177	ALA	N-CA-C	-6.99	101.93	110.31
8	J	105	PRO	N-CA-CB	6.98	110.58	103.25
45	l	28	LYS	N-CA-C	6.98	121.01	111.17
10	N	39	ARG	CA-C-N	6.97	128.55	119.84
10	N	39	ARG	C-N-CA	6.97	128.55	119.84
7	H	153	LYS	CA-C-N	6.95	126.98	119.89
7	H	153	LYS	C-N-CA	6.95	126.98	119.89
6	G	80	PHE	N-CA-C	-6.92	99.42	109.59
21	Y	17	SER	N-CA-C	6.85	118.61	108.60
56	y	364	GLU	N-CA-C	6.84	118.39	111.07
12	P	77	ARG	CA-C-N	6.83	128.38	119.84
12	P	77	ARG	C-N-CA	6.83	128.38	119.84
5	F	27	GLU	N-CA-C	6.80	119.50	108.41
37	d	63	LYS	N-CA-C	-6.79	103.49	111.03
3	D	135	PHE	CA-C-N	-6.79	116.94	122.85
3	D	135	PHE	C-N-CA	-6.79	116.94	122.85
42	i	48	GLU	CA-C-N	-6.78	112.01	119.19
42	i	48	GLU	C-N-CA	-6.78	112.01	119.19
25	2	45	SER	N-CA-C	-6.77	101.80	110.53
56	y	242	VAL	N-CA-C	6.75	118.52	108.46
56	y	411	LYS	N-CA-C	-6.75	98.84	109.50
6	G	141	PHE	CA-C-N	6.72	126.68	119.28
6	G	141	PHE	C-N-CA	6.72	126.68	119.28
9	K	72	PRO	CA-C-N	6.72	128.24	119.84
9	K	72	PRO	C-N-CA	6.72	128.24	119.84
20	X	73	ARG	CA-C-N	-6.71	113.02	120.14
20	X	73	ARG	C-N-CA	-6.71	113.02	120.14
56	y	236	GLU	N-CA-C	6.71	119.07	108.67
3	D	116	GLN	N-CA-C	-6.70	99.30	109.95
56	y	344	PHE	CA-C-N	6.70	131.00	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	344	PHE	C-N-CA	6.70	131.00	121.42
56	y	479	TYR	N-CA-C	-6.70	97.61	108.52
13	Q	98	LYS	CA-C-N	6.68	128.19	119.84
13	Q	98	LYS	C-N-CA	6.68	128.19	119.84
7	H	113	VAL	N-CA-C	6.68	117.46	108.11
7	H	7	LEU	CA-C-N	6.67	127.06	119.93
7	H	7	LEU	C-N-CA	6.67	127.06	119.93
27	4	42	PHE	CA-C-N	6.66	133.68	121.70
27	4	42	PHE	C-N-CA	6.66	133.68	121.70
56	y	441	LEU	N-CA-C	-6.63	100.45	110.39
56	y	554	LEU	N-CA-C	-6.63	105.08	112.57
56	y	231	TYR	N-CA-C	6.62	118.50	111.28
11	O	47	ILE	CA-C-N	6.61	126.59	119.78
11	O	47	ILE	C-N-CA	6.61	126.59	119.78
5	F	169	ASN	N-CA-C	6.61	124.87	110.80
56	y	407	GLU	CA-C-N	-6.57	111.63	119.84
56	y	407	GLU	C-N-CA	-6.57	111.63	119.84
56	y	83	THR	CA-C-N	-6.56	112.91	119.93
56	y	83	THR	C-N-CA	-6.56	112.91	119.93
56	y	433	GLY	CA-C-N	-6.56	111.50	121.86
56	y	433	GLY	C-N-CA	-6.56	111.50	121.86
56	y	482	ALA	N-CA-C	6.56	119.45	109.62
35	b	158	LEU	CA-C-N	6.54	128.01	119.84
35	b	158	LEU	C-N-CA	6.54	128.01	119.84
56	y	114	GLU	N-CA-C	6.54	120.07	110.59
10	N	78	TYR	CA-C-N	-6.52	112.95	119.99
10	N	78	TYR	C-N-CA	-6.52	112.95	119.99
28	5	6	VAL	CA-C-N	6.52	126.55	119.90
28	5	6	VAL	C-N-CA	6.52	126.55	119.90
27	4	42	PHE	N-CA-C	6.50	121.58	112.93
4	E	47	VAL	CB-CA-C	-6.49	100.50	110.50
56	y	333	GLU	CA-C-N	-6.49	113.07	119.76
56	y	333	GLU	C-N-CA	-6.49	113.07	119.76
1	A	1653	G	C2'-C3'-O3'	6.49	119.23	109.50
15	S	80	LEU	N-CA-C	-6.49	105.94	114.31
56	y	304	GLY	CA-C-N	6.48	131.06	122.06
56	y	304	GLY	C-N-CA	6.48	131.06	122.06
8	J	129	PRO	N-CA-CB	6.47	110.04	103.25
13	Q	7	MET	N-CA-C	6.46	116.52	108.19
56	y	103	VAL	CB-CA-C	-6.46	101.00	110.81
3	D	215	LEU	N-CA-C	-6.46	104.72	112.59
12	P	12	ALA	N-CA-C	-6.40	103.48	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	123	LYS	N-CA-C	-6.40	104.67	113.18
56	y	348	PHE	N-CA-C	6.39	118.83	108.41
56	y	189	LYS	N-CA-C	6.39	118.87	108.26
56	y	372	THR	N-CA-C	-6.37	102.32	110.53
56	y	94	SER	CA-C-N	-6.36	112.17	120.44
56	y	94	SER	C-N-CA	-6.36	112.17	120.44
9	K	46	ALA	N-CA-C	-6.36	105.10	112.92
22	Z	171	ILE	CB-CA-C	-6.35	104.66	110.63
17	U	28	ARG	N-CA-C	-6.34	105.03	112.89
5	F	196	LEU	N-CA-C	6.33	119.48	111.69
37	d	176	LEU	N-CA-C	6.33	117.80	107.23
56	y	481	GLN	N-CA-C	6.33	119.02	108.20
1	A	2096	U	O5'-P-OP1	-6.32	89.04	108.00
56	y	294	PHE	CA-C-N	6.31	133.07	121.70
56	y	294	PHE	C-N-CA	6.31	133.07	121.70
27	4	6	HIS	N-CA-C	6.31	117.76	109.93
16	T	18	ASP	N-CA-C	-6.29	105.92	113.97
25	2	51	ARG	N-CA-C	-6.29	104.42	111.28
56	y	159	PRO	O-C-N	-6.29	114.16	122.64
56	y	149	ALA	N-CA-C	-6.28	104.44	111.28
56	y	191	ASP	CA-C-N	-6.27	113.46	121.04
56	y	191	ASP	C-N-CA	-6.27	113.46	121.04
9	K	12	LEU	CA-C-N	6.26	126.22	120.21
9	K	12	LEU	C-N-CA	6.26	126.22	120.21
8	J	95	GLN	N-CA-C	-6.26	105.64	113.28
56	y	424	LEU	CA-C-N	-6.26	112.30	120.44
56	y	424	LEU	C-N-CA	-6.26	112.30	120.44
35	b	188	ALA	N-CA-C	6.26	118.97	108.02
38	e	67	VAL	N-CA-C	6.25	116.06	108.06
43	j	36	GLY	CA-C-N	6.23	127.63	119.84
43	j	36	GLY	C-N-CA	6.23	127.63	119.84
56	y	464	HIS	N-CA-C	6.19	120.95	112.04
19	W	20	VAL	CB-CA-C	-6.18	103.96	112.24
38	e	80	ILE	N-CA-C	6.18	116.50	108.35
42	i	101	PHE	N-CA-C	6.15	117.98	111.28
56	y	230	ILE	CB-CA-C	-6.14	101.54	110.63
56	y	377	VAL	N-CA-C	6.14	117.43	108.53
49	p	45	THR	CA-C-N	6.13	127.50	119.84
49	p	45	THR	C-N-CA	6.13	127.50	119.84
36	c	83	ARG	N-CA-C	-6.12	103.94	112.45
9	K	98	ARG	N-CA-C	6.12	117.18	108.74
52	s	80	TYR	N-CA-C	6.12	118.57	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	194	ALA	CA-C-N	-6.09	113.49	119.76
56	y	194	ALA	C-N-CA	-6.09	113.49	119.76
56	y	184	ARG	N-CA-C	-6.08	103.97	111.75
26	3	20	LYS	N-CA-C	-6.06	104.80	111.82
34	a	266	G	P-O3'-C3'	6.04	129.26	120.20
3	D	177	LEU	CA-C-N	6.02	127.37	119.84
3	D	177	LEU	C-N-CA	6.02	127.37	119.84
56	y	346	CYS	CA-C-N	-6.02	117.13	122.73
56	y	346	CYS	C-N-CA	-6.02	117.13	122.73
6	G	82	LEU	N-CA-C	6.01	119.28	109.06
7	H	111	HIS	CA-C-N	-6.01	114.08	120.03
7	H	111	HIS	C-N-CA	-6.01	114.08	120.03
4	E	73	GLU	CA-C-N	6.00	125.94	119.76
4	E	73	GLU	C-N-CA	6.00	125.94	119.76
56	y	396	LEU	N-CA-C	5.99	117.25	109.64
37	d	19	LEU	N-CA-C	-5.98	98.78	108.41
56	y	28	ARG	N-CA-C	5.97	117.79	111.28
56	y	438	MET	N-CA-C	-5.97	98.07	110.80
12	P	21	ARG	N-CA-C	5.97	116.95	108.54
41	h	73	ASP	CA-C-N	5.97	127.30	119.84
41	h	73	ASP	C-N-CA	5.97	127.30	119.84
56	y	87	VAL	N-CA-C	5.97	116.15	110.42
35	b	169	LYS	N-CA-C	-5.95	104.71	111.07
56	y	524	LEU	N-CA-C	5.93	117.83	111.36
56	y	362	GLU	N-CA-C	5.92	117.40	111.07
47	n	18	VAL	CB-CA-C	-5.92	101.58	111.29
56	y	462	ASP	N-CA-C	-5.92	104.83	111.28
56	y	326	ASN	N-CA-C	5.88	117.69	111.28
56	y	246	THR	CA-C-N	-5.88	113.57	119.56
56	y	246	THR	C-N-CA	-5.88	113.57	119.56
56	y	508	ALA	N-CA-C	5.86	115.83	108.45
56	y	248	GLN	N-CA-C	-5.84	104.92	111.28
51	r	54	ARG	N-CA-C	-5.84	106.39	112.93
40	g	78	ARG	N-CA-C	5.83	118.16	108.13
12	P	54	GLY	N-CA-C	-5.82	106.63	115.00
42	i	5	TYR	N-CA-C	5.81	118.87	109.40
9	K	31	GLY	N-CA-C	-5.80	103.31	113.76
49	p	64	ALA	N-CA-C	-5.80	102.72	110.55
31	8	62	LEU	CA-C-N	5.79	125.16	118.85
31	8	62	LEU	C-N-CA	5.79	125.16	118.85
36	c	152	ILE	N-CA-C	5.78	116.32	107.77
5	F	80	ALA	CA-C-N	5.76	125.62	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	80	ALA	C-N-CA	5.76	125.62	119.28
56	y	213	PRO	CA-N-CD	-5.76	103.94	112.00
22	Z	160	GLY	CA-C-N	5.75	132.05	121.70
22	Z	160	GLY	C-N-CA	5.75	132.05	121.70
17	U	15	LYS	N-CA-C	-5.73	105.12	111.71
35	b	155	LEU	N-CA-C	-5.72	101.16	110.20
56	y	177	ILE	CB-CA-C	-5.72	104.41	112.14
46	m	5	ALA	CB-CA-C	-5.71	109.97	116.54
17	U	102	GLU	CA-C-N	5.70	126.97	119.84
17	U	102	GLU	C-N-CA	5.70	126.97	119.84
56	y	432	ARG	N-CA-C	-5.67	102.50	110.50
26	3	15	TYR	CA-C-N	5.67	125.68	119.90
26	3	15	TYR	C-N-CA	5.67	125.68	119.90
53	t	10	LEU	N-CA-C	5.67	122.87	110.80
5	F	95	ARG	N-CA-C	5.67	115.59	108.45
19	W	37	ARG	N-CA-C	-5.66	107.37	114.56
46	m	81	LEU	N-CA-C	-5.65	105.03	111.07
56	y	-2	ARG	N-CA-C	-5.64	105.28	111.82
56	y	287	THR	CA-C-N	-5.63	112.80	119.05
56	y	287	THR	C-N-CA	-5.63	112.80	119.05
22	Z	67	LEU	CA-C-N	5.60	126.84	119.84
22	Z	67	LEU	C-N-CA	5.60	126.84	119.84
3	D	10	THR	N-CA-C	-5.60	99.82	108.55
41	h	103	VAL	N-CA-C	5.59	116.29	109.30
45	l	124	LYS	N-CA-C	5.59	117.69	109.42
56	y	417	PRO	CA-N-CD	-5.59	104.18	112.00
17	U	40	PHE	N-CA-C	-5.58	105.34	111.82
56	y	208	TYR	N-CA-C	-5.58	105.20	111.28
40	g	79	ARG	CB-CA-C	-5.57	109.16	115.79
8	J	131	MET	N-CA-C	-5.57	106.34	113.02
6	G	159	VAL	N-CA-C	5.57	115.87	107.80
35	b	12	GLU	N-CA-C	-5.56	98.96	110.80
1	A	2428	G	P-O3'-C3'	5.55	128.52	120.20
22	Z	14	LYS	CA-C-N	5.55	126.78	119.84
22	Z	14	LYS	C-N-CA	5.55	126.78	119.84
38	e	11	ILE	N-CA-C	-5.55	108.09	113.53
35	b	54	THR	N-CA-C	-5.55	104.92	110.97
10	N	114	ARG	N-CA-C	-5.54	104.06	112.04
56	y	136	ASN	CA-C-N	5.54	132.13	121.54
56	y	136	ASN	C-N-CA	5.54	132.13	121.54
56	y	64	VAL	N-CA-C	5.53	117.86	109.12
56	y	343	GLY	CA-C-N	-5.53	114.12	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	y	343	GLY	C-N-CA	-5.53	114.12	122.81
6	G	38	VAL	N-CA-C	5.52	114.69	106.85
40	g	111	ARG	CA-C-N	-5.51	114.22	120.89
40	g	111	ARG	C-N-CA	-5.51	114.22	120.89
53	t	32	ALA	N-CA-C	-5.51	104.91	111.03
22	Z	24	LEU	CA-C-N	5.51	125.51	119.89
22	Z	24	LEU	C-N-CA	5.51	125.51	119.89
13	Q	38	GLU	CA-C-N	-5.50	112.96	119.84
13	Q	38	GLU	C-N-CA	-5.50	112.96	119.84
13	Q	125	LEU	N-CA-C	5.50	117.48	109.84
56	y	-47	LYS	CA-C-N	5.49	126.70	119.84
56	y	-47	LYS	C-N-CA	5.49	126.70	119.84
3	D	145	VAL	CB-CA-C	-5.48	103.63	111.31
19	W	60	ASN	N-CA-C	5.48	117.69	111.11
56	y	242	VAL	CA-C-N	5.48	127.00	121.35
56	y	242	VAL	C-N-CA	5.48	127.00	121.35
56	y	145	PRO	N-CA-C	5.48	123.76	112.47
48	o	18	PHE	CA-C-N	5.47	126.68	119.84
48	o	18	PHE	C-N-CA	5.47	126.68	119.84
56	y	374	PRO	CA-N-CD	-5.46	103.85	111.50
56	y	528	ILE	CA-C-N	-5.46	114.14	119.76
56	y	528	ILE	C-N-CA	-5.46	114.14	119.76
56	y	185	ILE	N-CA-C	5.45	112.95	107.55
56	y	243	GLY	N-CA-C	-5.45	102.84	110.96
22	Z	156	LYS	N-CA-C	5.44	116.89	111.07
24	l	35	THR	N-CA-C	-5.43	106.66	113.72
3	D	83	GLU	N-CA-C	5.43	117.93	109.52
3	D	209	ALA	N-CA-C	-5.42	106.71	113.38
6	G	31	VAL	CA-C-N	5.42	125.43	119.90
6	G	31	VAL	C-N-CA	5.42	125.43	119.90
36	c	198	VAL	N-CA-C	5.41	115.64	107.75
24	l	18	ILE	CB-CA-C	-5.40	102.77	110.12
56	y	0	LYS	N-CA-C	-5.39	106.76	113.55
18	V	51	VAL	CB-CA-C	-5.38	103.85	111.38
56	y	357	VAL	CA-C-N	-5.37	113.47	120.44
56	y	357	VAL	C-N-CA	-5.37	113.47	120.44
13	Q	139	GLU	N-CA-C	-5.36	106.87	113.41
48	o	29	VAL	CB-CA-C	-5.35	104.85	111.70
56	y	520	ILE	CB-CA-C	-5.35	105.01	112.02
53	t	93	GLU	N-CA-C	-5.34	105.12	111.69
56	y	488	ASP	CA-C-N	-5.34	115.67	122.77
56	y	488	ASP	C-N-CA	-5.34	115.67	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	f	11	ASN	CA-C-N	5.33	124.84	119.19
39	f	11	ASN	C-N-CA	5.33	124.84	119.19
56	y	405	ILE	N-CA-C	5.33	115.31	107.75
38	e	17	ALA	N-CA-C	5.32	118.11	108.69
42	i	9	ARG	N-CA-C	5.32	117.28	108.13
56	y	528	ILE	O-C-N	5.32	125.32	121.55
23	0	55	ARG	N-CA-C	5.31	117.98	111.82
40	g	114	ARG	N-CA-C	5.31	118.09	111.24
18	V	38	LEU	N-CA-C	-5.31	107.17	113.97
35	b	17	PHE	N-CA-C	5.31	122.11	110.80
56	y	597	PHE	N-CA-C	-5.31	106.06	112.54
3	D	123	ALA	N-CA-C	-5.31	102.43	110.50
56	y	140	LEU	CA-C-N	-5.30	113.07	118.85
56	y	140	LEU	C-N-CA	-5.30	113.07	118.85
6	G	119	GLY	N-CA-C	5.30	118.23	112.29
56	y	545	ILE	N-CA-C	5.30	115.48	107.80
11	O	4	PRO	CA-C-O	-5.29	115.31	121.34
4	E	143	ASN	N-CA-C	-5.29	104.44	108.78
56	y	180	ALA	N-CA-C	-5.29	105.59	111.36
4	E	52	LEU	CA-C-N	5.29	125.28	119.89
4	E	52	LEU	C-N-CA	5.29	125.28	119.89
24	l	30	VAL	N-CA-C	-5.28	107.68	112.96
56	y	437	ASN	N-CA-C	-5.27	99.58	110.80
7	H	147	ASN	N-CA-C	-5.27	104.45	111.24
15	S	32	LEU	N-CA-C	-5.27	106.70	113.23
56	y	416	THR	CA-C-N	-5.26	113.26	119.84
56	y	416	THR	C-N-CA	-5.26	113.26	119.84
56	y	335	GLU	N-CA-C	5.25	117.17	109.24
50	q	17	LYS	N-CA-C	5.24	121.97	110.80
37	d	204	ILE	CB-CA-C	-5.24	105.18	111.88
38	e	121	LYS	N-CA-C	-5.23	99.65	110.80
9	K	12	LEU	N-CA-C	5.23	116.66	110.07
56	y	294	PHE	O-C-N	-5.23	115.77	122.72
22	Z	11	GLU	N-CA-C	5.22	116.43	108.12
54	u	16	GLY	N-CA-C	-5.22	107.84	115.72
46	m	11	ARG	N-CA-C	-5.21	104.00	110.41
4	E	103	ASP	N-CA-C	-5.21	101.78	110.17
52	s	41	VAL	CA-C-N	5.20	126.33	119.84
52	s	41	VAL	C-N-CA	5.20	126.33	119.84
56	y	404	GLU	N-CA-C	5.19	117.70	109.50
56	y	292	PRO	CA-N-CD	-5.19	104.24	111.50
56	y	118	LEU	N-CA-C	5.19	117.01	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	48	GLU	N-CA-C	-5.18	105.63	111.28
56	y	4	GLU	N-CA-C	-5.18	106.91	113.18
35	b	191	ASP	N-CA-C	5.18	117.67	111.71
56	y	272	HIS	N-CA-C	5.18	117.01	111.36
56	y	378	TYR	N-CA-C	5.18	118.03	109.85
5	F	177	ALA	CA-C-N	-5.17	113.37	119.84
5	F	177	ALA	C-N-CA	-5.17	113.37	119.84
56	y	192	PRO	CA-N-CD	-5.17	104.76	112.00
8	J	65	GLU	N-CA-C	-5.17	106.66	113.17
1	A	2318	G	C2'-C3'-O3'	5.16	121.44	113.70
10	N	33	LEU	N-CA-C	-5.16	105.34	111.69
50	q	9	VAL	CB-CA-C	-5.16	103.64	111.33
56	y	291	TYR	CA-C-N	-5.16	114.63	127.00
56	y	291	TYR	C-N-CA	-5.16	114.63	127.00
3	D	237	GLU	CB-CA-C	5.15	117.98	110.26
53	t	12	ALA	N-CA-C	-5.15	105.85	111.82
34	a	266	G	C2'-C3'-O3'	5.15	117.22	109.50
1	A	2095	C	OP1-P-O3'	-5.14	92.57	108.00
56	y	216	ARG	N-CA-C	-5.13	100.67	109.24
56	y	78	PHE	N-CA-C	5.13	117.93	109.72
44	k	109	VAL	N-CA-C	5.13	115.30	108.27
56	y	195	PRO	CB-CA-C	-5.12	104.86	111.46
56	y	155	VAL	N-CA-C	5.11	115.33	110.42
3	D	60	ARG	N-CA-C	5.11	116.69	108.32
56	y	84	PRO	N-CA-C	-5.11	102.94	111.26
5	F	114	VAL	CB-CA-C	-5.09	105.45	111.97
18	V	5	VAL	N-CA-C	5.09	115.24	108.11
56	y	302	PHE	N-CA-C	-5.09	100.57	108.31
56	y	246	THR	N-CA-C	-5.09	102.63	110.01
19	W	100	THR	N-CA-C	5.07	116.95	108.99
9	K	114	ASP	O-C-N	5.06	124.58	120.83
10	N	19	GLU	N-CA-C	-5.06	100.02	110.80
40	g	76	ARG	N-CA-C	-5.06	100.82	108.46
9	K	53	VAL	CA-C-N	5.06	126.16	119.84
9	K	53	VAL	C-N-CA	5.06	126.16	119.84
8	J	7	VAL	N-CA-C	-5.04	98.85	109.34
34	a	687	A	P-O3'-C3'	5.04	127.76	120.20
56	y	152	VAL	N-CA-C	-5.04	105.47	110.62
25	2	17	SER	CA-C-N	5.03	126.13	119.84
25	2	17	SER	C-N-CA	5.03	126.13	119.84
30	7	27	GLY	N-CA-C	-5.03	108.08	114.16
41	h	106	GLY	N-CA-C	-5.03	107.76	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	o	87	ILE	N-CA-C	5.03	119.80	109.34
41	h	7	ALA	N-CA-C	-5.02	105.70	111.07
27	4	15	ILE	N-CA-C	5.01	115.07	107.75
5	F	157	VAL	N-CA-C	5.01	115.12	108.11
56	y	355	GLU	N-CA-C	5.01	117.63	111.82
21	Y	13	VAL	N-CA-C	5.01	115.91	108.65
35	b	155	LEU	CA-C-N	5.00	130.71	121.70
35	b	155	LEU	C-N-CA	5.00	130.71	121.70
56	y	400	THR	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	223	GLY	Peptide
8	J	6	ASN	Peptide
42	i	45	ALA	Peptide
46	m	7	VAL	Peptide
46	m	8	GLU	Peptide
52	s	28	LYS	Peptide
53	t	10	LEU	Peptide
56	y	127	HIS	Peptide
56	y	137	LYS	Peptide
56	y	152	VAL	Peptide
56	y	171	GLY	Peptide
56	y	174	VAL	Peptide
56	y	226	ASP	Peptide
56	y	230	ILE	Peptide
56	y	235	LYS	Peptide
56	y	250	LEU	Peptide
56	y	268	ILE	Peptide
56	y	292	PRO	Peptide
56	y	294	PHE	Mainchain
56	y	301	VAL	Peptide
56	y	331	THR	Peptide
56	y	389	GLU	Peptide
56	y	395	ASP	Peptide
56	y	419	GLU	Peptide
56	y	480	GLU	Peptide
56	y	553	ALA	Peptide
56	y	554	LEU	Peptide
56	y	557	ASP	Peptide

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Mol	Chain	Res	Type	Group
56	y	6	LEU	Peptide
56	y	86	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61879	0	31203	1296	0
2	B	2573	0	1306	33	0
3	D	2136	0	2217	147	0
4	E	1559	0	1618	77	0
5	F	1584	0	1625	73	0
6	G	1425	0	1443	68	0
7	H	1330	0	1407	59	0
8	J	641	0	309	13	0
9	K	1025	0	1066	58	0
10	N	1117	0	1184	59	0
11	O	933	0	996	40	0
12	P	1135	0	1212	73	0
13	Q	1122	0	1179	39	0
14	R	968	0	1033	40	0
15	S	877	0	938	40	0
16	T	1091	0	1151	54	0
17	U	959	0	1019	64	0
18	V	771	0	830	29	0
19	W	886	0	940	39	0
20	X	750	0	814	42	0
21	Y	806	0	881	37	0
22	Z	1451	0	1457	75	0
23	0	591	0	607	36	0
24	1	755	0	826	39	0
25	2	588	0	643	23	0
26	3	469	0	518	15	0
27	4	557	0	537	46	0
28	5	459	0	476	29	0
29	6	453	0	473	17	0
30	7	430	0	480	18	0
31	8	511	0	571	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	9	307	0	335	12	0
33	w	1632	0	838	26	0
33	x	1581	0	805	88	0
34	a	32163	0	16234	615	0
35	b	1850	0	1871	99	0
36	c	1550	0	1539	67	0
37	d	1655	0	1673	84	0
38	e	1129	0	1185	48	0
39	f	806	0	793	44	0
40	g	1227	0	1232	55	0
41	h	1088	0	1126	48	0
42	i	983	0	986	54	0
43	j	698	0	637	31	0
44	k	829	0	825	26	0
45	l	930	0	980	40	0
46	m	924	0	960	45	0
47	n	492	0	528	27	0
48	o	728	0	760	37	0
49	p	681	0	697	25	0
50	q	823	0	891	43	0
51	r	555	0	618	32	0
52	s	650	0	655	44	0
53	t	724	0	787	29	0
54	u	199	0	208	6	0
55	v	148	0	76	1	0
56	y	4000	0	3218	694	0
57	0	3	0	0	0	0
57	5	1	0	0	0	0
57	6	1	0	0	0	0
57	7	3	0	0	0	0
57	8	1	0	0	0	0
57	9	1	0	0	0	0
57	A	635	0	0	0	0
57	B	18	0	0	0	0
57	D	5	0	0	0	0
57	E	4	0	0	0	0
57	F	5	0	0	0	0
57	G	3	0	0	0	0
57	N	1	0	0	0	0
57	O	1	0	0	0	0
57	P	2	0	0	0	0
57	Q	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	R	3	0	0	0	0
57	U	4	0	0	0	0
57	V	2	0	0	0	0
57	W	1	0	0	0	0
57	X	1	0	0	0	0
57	Z	1	0	0	0	0
57	a	187	0	0	0	0
57	e	1	0	0	0	0
57	f	1	0	0	0	0
57	l	2	0	0	0	0
57	m	1	0	0	0	0
57	n	1	0	0	0	0
57	v	1	0	0	0	0
57	w	6	0	0	0	0
57	x	3	0	0	0	0
57	y	2	0	0	0	0
58	4	1	0	0	0	0
58	5	1	0	0	0	0
58	6	1	0	0	0	0
58	9	1	0	0	0	0
58	Y	1	0	0	0	0
58	n	1	0	0	0	0
59	d	8	0	0	2	0
60	w	11	0	8	0	0
61	y	28	0	12	8	0
62	0	4	0	0	0	0
62	1	2	0	0	0	0
62	3	1	0	0	0	0
62	5	1	0	0	0	0
62	7	2	0	0	0	0
62	8	4	0	0	0	0
62	9	1	0	0	0	0
62	A	710	0	0	109	0
62	B	34	0	0	2	0
62	D	4	0	0	2	0
62	E	7	0	0	1	0
62	F	5	0	0	0	0
62	G	1	0	0	0	0
62	H	1	0	0	0	0
62	N	1	0	0	0	0
62	O	3	0	0	0	0
62	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	Q	4	0	0	1	0
62	R	2	0	0	0	0
62	T	1	0	0	0	0
62	U	2	0	0	1	0
62	V	1	0	0	1	0
62	W	2	0	0	0	0
62	Y	1	0	0	0	0
62	a	167	0	0	17	0
62	l	1	0	0	0	0
62	v	3	0	0	0	0
62	x	1	0	0	0	0
All	All	152111	0	101436	4546	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 19.

All (4546) 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)
56:y:200:ILE:CA	56:y:215:LEU:HB3	1.30	1.57
56:y:245:PHE:CB	56:y:250:LEU:HA	1.37	1.50
56:y:306:TYR:HD2	56:y:343:GLY:CA	1.25	1.48
56:y:87:VAL:HG13	56:y:88:ASP:C	1.43	1.43
56:y:200:ILE:CA	56:y:215:LEU:CB	1.97	1.43
56:y:192:PRO:CB	56:y:258:ALA:HB3	1.46	1.42
56:y:306:TYR:CD2	56:y:343:GLY:HA3	1.53	1.42
56:y:369:LEU:HD22	56:y:370:ILE:N	1.05	1.38
56:y:369:LEU:CD2	56:y:370:ILE:H	1.43	1.31
56:y:11:ASN:O	56:y:101:GLU:N	1.63	1.31
56:y:223:ARG:HB3	56:y:255:ALA:CA	1.61	1.29
56:y:369:LEU:CD2	56:y:370:ILE:N	1.96	1.28
56:y:213:PRO:HD3	56:y:264:LEU:O	1.24	1.26
56:y:213:PRO:CD	56:y:264:LEU:O	1.84	1.25
56:y:417:PRO:CA	56:y:446:LYS:O	1.85	1.22
56:y:417:PRO:HA	56:y:446:LYS:O	1.10	1.22
56:y:306:TYR:CD2	56:y:343:GLY:CA	2.14	1.20
56:y:411:LYS:CA	56:y:452:TYR:O	1.90	1.20
56:y:192:PRO:CA	56:y:258:ALA:HB3	1.71	1.20
56:y:537:ILE:HB	56:y:549:ALA:CB	1.73	1.17
56:y:68:TYR:CZ	56:y:179:GLU:HB2	1.77	1.17
56:y:418:GLU:HB3	56:y:446:LYS:CG	1.76	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:109:ALA:N	56:y:136:ASN:O	1.76	1.15
56:y:369:LEU:HD21	56:y:370:ILE:O	1.45	1.15
56:y:417:PRO:HB2	56:y:446:LYS:HB3	1.28	1.15
56:y:192:PRO:HB3	56:y:258:ALA:CB	1.77	1.14
56:y:443:GLY:HA2	56:y:444:ALA:C	1.70	1.14
56:y:192:PRO:HA	56:y:258:ALA:HB2	1.28	1.14
56:y:192:PRO:HA	56:y:258:ALA:CB	1.76	1.14
56:y:192:PRO:CA	56:y:258:ALA:CB	2.26	1.12
56:y:166:ALA:O	56:y:167:SER:HB3	1.48	1.11
56:y:192:PRO:HB3	56:y:258:ALA:HB3	1.18	1.11
56:y:304:GLY:HA2	56:y:344:PHE:O	1.50	1.11
56:y:537:ILE:CB	56:y:549:ALA:HB3	1.80	1.11
56:y:200:ILE:CA	56:y:215:LEU:CA	2.28	1.10
56:y:306:TYR:HB3	56:y:340:LEU:HD21	1.19	1.10
56:y:418:GLU:HB3	56:y:446:LYS:HG2	1.20	1.10
56:y:12:PHE:HA	56:y:102:GLY:O	1.52	1.09
56:y:133:PRO:HG3	56:y:158:LEU:HD13	1.34	1.09
56:y:245:PHE:CB	56:y:250:LEU:CA	2.30	1.09
56:y:68:TYR:CE2	56:y:179:GLU:N	2.20	1.09
56:y:192:PRO:CB	56:y:258:ALA:CB	2.30	1.09
56:y:300:VAL:O	56:y:347:GLY:HA2	1.52	1.08
56:y:369:LEU:HD22	56:y:370:ILE:CA	1.84	1.08
56:y:200:ILE:CA	56:y:215:LEU:HA	1.84	1.07
33:x:49:C:N4	33:x:65:G:H1	1.51	1.07
56:y:306:TYR:O	56:y:369:LEU:CD2	2.03	1.06
56:y:15:ILE:HD11	56:y:103:VAL:HG11	1.36	1.06
56:y:87:VAL:CG1	56:y:88:ASP:C	2.28	1.06
56:y:228:ILE:HG13	56:y:237:PHE:O	1.55	1.06
56:y:25:LEU:O	56:y:28:ARG:HB3	1.55	1.06
56:y:166:ALA:CA	56:y:173:GLY:HA3	1.85	1.05
56:y:108:ASP:HB2	56:y:137:LYS:NZ	1.71	1.05
56:y:376:VAL:HG21	56:y:457:ALA:CB	1.85	1.05
56:y:497:HIS:N	56:y:536:PRO:O	1.89	1.05
56:y:537:ILE:HB	56:y:549:ALA:HB3	1.07	1.04
56:y:223:ARG:O	56:y:226:ASP:HB2	1.56	1.04
56:y:376:VAL:HG21	56:y:457:ALA:HB2	1.04	1.04
56:y:304:GLY:HA3	56:y:306:TYR:CZ	1.93	1.03
33:x:53:G:H1	33:x:61:C:N4	1.55	1.03
56:y:12:PHE:CA	56:y:102:GLY:O	2.07	1.03
56:y:188:PRO:HB2	56:y:216:ARG:NH2	1.71	1.03
56:y:108:ASP:CB	56:y:137:LYS:HZ2	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:418:GLU:CB	56:y:446:LYS:HG2	1.88	1.03
56:y:28:ARG:HH11	56:y:28:ARG:HB2	1.22	1.02
56:y:537:ILE:O	56:y:549:ALA:O	1.78	1.02
1:A:883:G:H1	1:A:893:C:N4	1.56	1.02
56:y:241:LYS:O	56:y:265:VAL:HG22	1.56	1.02
56:y:224:PRO:HD2	56:y:254:GLU:O	1.60	1.01
56:y:303:ALA:HB1	56:y:392:ASN:OD1	1.58	1.01
56:y:376:VAL:CG2	56:y:457:ALA:HB2	1.89	1.01
56:y:241:LYS:H	56:y:265:VAL:HG23	1.27	1.00
34:a:78:G:H1	34:a:91:C:H42	1.01	1.00
1:A:1019:U:HO2'	1:A:1021:A:H2	1.08	0.99
56:y:192:PRO:O	56:y:221:ARG:HD2	1.63	0.99
56:y:68:TYR:HE2	56:y:179:GLU:N	1.59	0.98
56:y:87:VAL:HG13	56:y:89:PHE:N	1.77	0.98
56:y:108:ASP:HB2	56:y:137:LYS:HZ2	0.85	0.97
56:y:250:LEU:H	56:y:250:LEU:HD22	1.28	0.97
56:y:121:PHE:CD1	56:y:156:LEU:HD12	2.00	0.96
1:A:2106:G:H1	1:A:2183:C:H42	0.98	0.96
56:y:223:ARG:CB	56:y:255:ALA:CA	2.43	0.96
56:y:24:THR:HG23	61:y:703:GDP:O2A	1.64	0.96
56:y:25:LEU:O	56:y:28:ARG:CB	2.13	0.96
56:y:243:GLY:O	56:y:263:TRP:N	1.97	0.96
12:P:100:LEU:HD12	12:P:112:LEU:HD11	1.48	0.96
56:y:241:LYS:H	56:y:265:VAL:CG2	1.78	0.95
56:y:369:LEU:CD2	56:y:370:ILE:O	2.13	0.95
1:A:143:G:H1'	20:X:37:THR:HG21	1.49	0.94
56:y:414:ILE:HG23	56:y:476:SER:O	1.65	0.94
56:y:159:PRO:HG2	56:y:162:GLU:CB	1.98	0.94
56:y:28:ARG:HA	56:y:31:GLU:CG	1.97	0.94
1:A:272(J):C:H42	1:A:363:G:H1	1.11	0.94
56:y:229:ARG:O	56:y:280:ILE:CA	2.16	0.94
8:J:26:LEU:HA	8:J:84:GLU:HA	1.50	0.93
56:y:17:HIS:O	56:y:20:HIS:HB2	1.68	0.93
56:y:306:TYR:HB3	56:y:340:LEU:CD2	1.99	0.93
56:y:443:GLY:CA	56:y:444:ALA:C	2.40	0.93
56:y:143:ALA:O	56:y:145:PRO:HD3	1.68	0.93
33:x:29:G:H1	33:x:41:C:N4	1.65	0.93
56:y:97:LEU:C	56:y:127:HIS:HE1	1.78	0.92
1:A:731:C:OP1	62:A:3701:HOH:O	1.86	0.92
56:y:108:ASP:OD2	56:y:137:LYS:NZ	2.02	0.92
56:y:537:ILE:HD11	56:y:551:VAL:CG2	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:445:GLN:C	56:y:447:ARG:H	1.77	0.91
56:y:335:GLU:OE2	56:y:336:SER:N	2.03	0.91
56:y:443:GLY:HA2	56:y:444:ALA:O	1.69	0.91
56:y:12:PHE:CB	56:y:102:GLY:O	2.19	0.91
56:y:68:TYR:HE2	56:y:179:GLU:H	1.02	0.90
56:y:418:GLU:H	56:y:446:LYS:CA	1.84	0.90
56:y:133:PRO:HG3	56:y:158:LEU:CD1	2.01	0.90
56:y:28:ARG:O	56:y:31:GLU:HG3	1.70	0.90
56:y:113:VAL:HG23	56:y:117:THR:HG21	1.52	0.90
56:y:411:LYS:CA	56:y:453:GLU:HA	2.02	0.90
1:A:2269:A:OP1	62:A:3702:HOH:O	1.88	0.89
1:A:1416:G:H1	1:A:1582:C:H42	1.21	0.89
56:y:137:LYS:O	56:y:139:ASP:N	2.06	0.89
34:a:406:G:H5'	37:d:5:ILE:HD12	1.55	0.89
56:y:245:PHE:HA	56:y:251:VAL:H	1.38	0.88
7:H:43:VAL:HA	7:H:52:VAL:HG12	1.54	0.88
33:x:49:C:N3	33:x:65:G:N2	2.21	0.88
35:b:155:LEU:HA	35:b:156:LYS:HD3	1.55	0.88
56:y:28:ARG:CZ	56:y:31:GLU:OE1	2.22	0.88
34:a:1491:G:O3'	45:l:47:LYS:NZ	2.05	0.88
56:y:15:ILE:HD11	56:y:103:VAL:CG1	2.03	0.88
56:y:223:ARG:HB2	56:y:224:PRO:CD	2.04	0.88
56:y:566:ASP:HB3	56:y:569:ARG:HG3	1.54	0.88
33:x:53:G:H1	33:x:61:C:H42	0.91	0.88
56:y:98:ALA:N	56:y:127:HIS:HE1	1.72	0.88
56:y:306:TYR:CD2	56:y:343:GLY:C	2.51	0.88
1:A:1143:A:OP1	10:N:25:ARG:NH2	2.07	0.87
1:A:818:G:OP2	62:A:3704:HOH:O	1.91	0.87
56:y:223:ARG:HB2	56:y:224:PRO:HD2	1.56	0.87
56:y:277:GLY:N	56:y:293:GLY:O	2.07	0.87
1:A:2121:G:H1	1:A:2177:C:H42	1.21	0.87
22:Z:138:GLU:H	22:Z:156:LYS:HZ1	1.23	0.87
56:y:306:TYR:HD2	56:y:343:GLY:HA2	1.39	0.87
56:y:301:VAL:CB	56:y:348:PHE:H	1.88	0.87
1:A:2106:G:H1	1:A:2183:C:N4	1.72	0.87
34:a:1030:C:N3	34:a:1031:G:N2	2.22	0.87
1:A:250:G:H2'	1:A:251:A:C8	2.10	0.86
34:a:1028:C:N3	34:a:1033:G:N2	2.21	0.86
46:m:87:TYR:HA	46:m:90:LEU:HD12	1.57	0.86
1:A:1603:A:OP1	62:A:3703:HOH:O	1.91	0.86
37:d:98:GLU:OE2	37:d:107:ARG:NH1	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:87:VAL:HG13	56:y:88:ASP:CA	2.05	0.86
56:y:192:PRO:HB3	56:y:258:ALA:CA	2.04	0.86
1:A:335:C:H4'	21:Y:73:ARG:HD3	1.54	0.86
56:y:306:TYR:O	56:y:369:LEU:HD21	1.75	0.86
56:y:544:LYS:C	56:y:545:ILE:HD13	2.01	0.86
1:A:1784:A:OP2	62:A:3705:HOH:O	1.92	0.86
1:A:2660:A:H61	56:y:465:ASP:HA	1.41	0.86
33:x:29:G:H1	33:x:41:C:H42	0.90	0.85
56:y:68:TYR:OH	56:y:179:GLU:HB2	1.74	0.85
56:y:373:ALA:HB1	56:y:374:PRO:HA	1.57	0.85
33:x:5:G:H1	33:x:68:C:H42	1.15	0.85
34:a:768:A:OP2	62:a:3501:HOH:O	1.94	0.85
56:y:89:PHE:O	56:y:90:THR:OG1	1.92	0.85
56:y:243:GLY:O	56:y:263:TRP:CA	2.25	0.85
56:y:304:GLY:HA3	56:y:306:TYR:CE1	2.11	0.85
56:y:378:TYR:HA	56:y:406:LEU:O	1.77	0.85
34:a:78:G:N2	34:a:91:C:N3	2.24	0.85
34:a:1028:C:N4	34:a:1033:G:H1	1.76	0.84
56:y:537:ILE:CD1	56:y:551:VAL:CG2	2.54	0.84
1:A:1170:G:H1	1:A:1179:C:H42	1.26	0.84
20:X:57:LEU:HD13	20:X:78:LYS:HB2	1.57	0.84
34:a:453:A:H4'	49:p:72:ARG:HG3	1.58	0.84
56:y:537:ILE:HD11	56:y:551:VAL:HG21	1.57	0.84
1:A:1036:G:H1	1:A:1119:C:H42	1.26	0.84
1:A:2705:A:OP2	62:A:3708:HOH:O	1.96	0.84
37:d:139:ARG:HG2	37:d:139:ARG:HH11	1.42	0.84
56:y:167:SER:OG	56:y:170:THR:OG1	1.93	0.84
1:A:370:G:OP2	62:A:3706:HOH:O	1.94	0.84
56:y:300:VAL:O	56:y:347:GLY:CA	2.25	0.84
34:a:78:G:N1	34:a:91:C:N4	2.25	0.84
34:a:1028:C:N4	34:a:1033:G:N1	2.26	0.84
56:y:449:GLU:HG2	56:y:450:LEU:N	1.91	0.84
1:A:1639:U:OP1	62:A:3709:HOH:O	1.96	0.83
27:4:59:PHE:HA	27:4:61:ARG:H	1.43	0.83
56:y:224:PRO:CD	56:y:254:GLU:O	2.27	0.83
1:A:817:C:OP2	62:A:3707:HOH:O	1.95	0.83
56:y:537:ILE:O	56:y:549:ALA:N	2.11	0.83
3:D:171:ASP:OD1	3:D:171:ASP:N	2.12	0.82
40:g:111:ARG:NH1	40:g:113:GLU:OE2	2.12	0.82
56:y:230:ILE:HG22	56:y:279:THR:C	2.04	0.82
56:y:28:ARG:HA	56:y:31:GLU:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:468:LYS:HB3	56:y:473:GLY:HA2	1.61	0.82
1:A:1364:G:OP1	24:1:2:SER:N	2.12	0.82
56:y:493:ASN:N	56:y:540:ALA:O	2.10	0.82
1:A:2006:C:OP1	62:A:3711:HOH:O	1.97	0.82
56:y:241:LYS:O	56:y:265:VAL:CG2	2.27	0.82
33:x:5:G:H1	33:x:68:C:N4	1.77	0.82
1:A:1604:C:OP2	62:A:3703:HOH:O	1.97	0.82
5:F:101:LEU:HD12	5:F:102:PRO:HD2	1.59	0.82
34:a:1030:C:N4	34:a:1031:G:N1	2.26	0.82
56:y:492:VAL:HB	56:y:506:PHE:CE2	2.14	0.82
56:y:418:GLU:HB3	56:y:446:LYS:CD	2.09	0.81
56:y:303:ALA:CB	56:y:392:ASN:OD1	2.26	0.81
56:y:418:GLU:H	56:y:446:LYS:HA	1.44	0.81
1:A:411:G:OP1	62:A:3712:HOH:O	1.98	0.81
1:A:999:U:OP2	62:A:3714:HOH:O	1.99	0.81
46:m:11:ARG:HG2	46:m:12:ASN:HD22	1.43	0.81
1:A:956:G:O6	62:A:3713:HOH:O	1.98	0.81
1:A:1268:A:OP1	62:A:3711:HOH:O	1.98	0.81
33:x:68:C:H2'	33:x:69:G:H5'	1.63	0.81
34:a:1321:C:H3'	34:a:1322:C:H5''	1.61	0.81
56:y:136:ASN:OD1	56:y:137:LYS:N	2.12	0.81
56:y:444:ALA:O	56:y:447:ARG:CB	2.29	0.81
5:F:168:ARG:O	5:F:170:LEU:N	2.14	0.81
56:y:166:ALA:CA	56:y:173:GLY:CA	2.59	0.81
56:y:182:VAL:O	56:y:185:ILE:O	1.98	0.81
56:y:242:VAL:O	56:y:252:ALA:O	1.98	0.81
12:P:39:LYS:HG3	12:P:45:LEU:HD12	1.63	0.81
31:8:33:ASN:HA	31:8:36:LYS:HD2	1.61	0.81
1:A:523:C:O2	1:A:554:U:O2'	2.00	0.81
56:y:246:THR:O	56:y:249:GLY:N	2.13	0.80
56:y:407:GLU:O	56:y:409:TYR:N	2.15	0.80
34:a:1014:A:H4'	52:s:14:HIS:CE1	2.16	0.80
36:c:179:ARG:NH1	36:c:206:GLU:OE1	2.14	0.80
56:y:68:TYR:CE1	56:y:70:ALA:HA	2.17	0.80
56:y:192:PRO:HB3	56:y:258:ALA:N	1.94	0.80
23:0:23:VAL:HG23	23:0:38:VAL:HG22	1.63	0.80
56:y:101:GLU:HA	56:y:129:HIS:CE1	2.16	0.80
56:y:433:GLY:CA	56:y:453:GLU:O	2.29	0.80
1:A:272(J):C:N4	1:A:363:G:H1	1.78	0.80
1:A:2292:C:OP1	15:S:17:ARG:NH2	2.15	0.80
33:x:8:4SU:H4'	33:x:48:C:H4'	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:U:O4	1:A:933:A:N6	2.15	0.80
34:a:934:C:OP1	62:a:3502:HOH:O	2.00	0.80
56:y:167:SER:HG	56:y:170:THR:HG1	1.22	0.80
1:A:993:G:OP1	17:U:50:ARG:NH2	2.15	0.80
1:A:1176:G:N2	1:A:1178:C:OP2	2.15	0.80
34:a:881:G:OP2	45:l:12:ARG:NH2	2.14	0.80
56:y:28:ARG:HH11	56:y:28:ARG:CB	1.95	0.80
56:y:87:VAL:CG1	56:y:88:ASP:CA	2.60	0.80
24:l:75:GLU:O	24:l:77:ALA:N	2.15	0.80
33:x:53:G:N2	33:x:61:C:N3	2.29	0.80
56:y:200:ILE:N	56:y:215:LEU:HB3	1.97	0.80
22:Z:52:SER:OG	22:Z:53:ILE:N	2.06	0.80
56:y:97:LEU:C	56:y:127:HIS:CE1	2.60	0.80
1:A:1067:A:H1'	56:y:429:GLN:OE1	1.82	0.79
4:E:12:THR:HG22	4:E:13:ARG:H	1.47	0.79
5:F:11:VAL:HB	5:F:18:ARG:HB3	1.65	0.79
56:y:277:GLY:CA	56:y:293:GLY:O	2.29	0.79
56:y:335:GLU:O	56:y:343:GLY:O	2.00	0.79
1:A:271(J):C:N3	1:A:271(M):G:O6	2.15	0.79
1:A:2125:G:H21	1:A:2173:A:H62	1.26	0.79
42:i:42:ARG:NH1	42:i:71:SER:OG	2.16	0.79
1:A:1059:G:N2	9:K:126:MET:O	2.16	0.79
56:y:159:PRO:CG	56:y:162:GLU:CB	2.61	0.79
22:Z:144:LEU:HD21	22:Z:150:LEU:HD21	1.64	0.79
56:y:302:PHE:CA	56:y:346:CYS:O	2.30	0.79
1:A:862:G:OP2	62:A:3715:HOH:O	1.99	0.79
33:x:5:G:N2	33:x:68:C:N3	2.31	0.79
56:y:193:GLU:HA	56:y:221:ARG:HD3	1.65	0.79
56:y:509:HIS:HB2	56:y:512:LYS:HE2	1.63	0.79
1:A:800:A:OP1	62:A:3716:HOH:O	2.01	0.79
2:B:81:G:OP2	62:B:301:HOH:O	2.00	0.79
56:y:418:GLU:H	56:y:446:LYS:C	1.90	0.79
2:B:17:C:H42	2:B:68:C:H42	1.31	0.79
7:H:109:PHE:HE2	7:H:152:ARG:HH21	1.31	0.79
31:8:6:THR:HG22	31:8:63:PRO:HD2	1.64	0.78
33:x:15:G:H22	33:x:48:C:H42	1.30	0.78
46:m:4:ILE:HD11	46:m:56:LEU:HB3	1.64	0.78
1:A:1095:A:H1'	56:y:426:GLN:NE2	1.97	0.78
1:A:759:G:O6	62:A:3710:HOH:O	1.97	0.78
7:H:3:ARG:HG3	7:H:3:ARG:HH11	1.48	0.78
1:A:1664:A:H2	11:O:1:MET:HE1	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2107:C:H42	1:A:2182:G:H1	1.31	0.78
56:y:531:GLN:HB2	56:y:533:PHE:CE1	2.19	0.78
1:A:883:G:N2	1:A:893:C:N3	2.31	0.78
1:A:943:U:OP2	62:A:3718:HOH:O	2.02	0.78
1:A:1009:A:OP2	10:N:37:LYS:NZ	2.16	0.78
44:k:79:SER:HA	44:k:104:GLN:HB2	1.65	0.78
56:y:306:TYR:O	56:y:369:LEU:CG	2.32	0.78
56:y:548:ARG:H	56:y:548:ARG:HD3	1.47	0.78
34:a:407:G:OP1	37:d:3:ARG:NH2	2.15	0.78
56:y:68:TYR:CE2	56:y:179:GLU:HB2	2.19	0.78
56:y:107:VAL:O	56:y:136:ASN:N	2.15	0.78
35:b:175:ARG:HG2	35:b:175:ARG:HH11	1.48	0.78
1:A:576:U:OP1	62:A:3717:HOH:O	2.01	0.78
1:A:1378:A:O2'	1:A:1380:G:N7	2.16	0.78
34:a:1310:G:N7	62:a:3510:HOH:O	2.15	0.78
56:y:192:PRO:CG	56:y:258:ALA:HB3	2.14	0.78
20:X:54:VAL:HG22	20:X:81:VAL:HG12	1.66	0.78
22:Z:29:TYR:HB3	22:Z:34:ASN:HD22	1.49	0.78
34:a:78:G:C2	34:a:91:C:N3	2.53	0.78
56:y:81:ILE:N	56:y:81:ILE:HD12	1.99	0.77
56:y:306:TYR:CB	56:y:340:LEU:HD21	2.09	0.77
56:y:306:TYR:O	56:y:369:LEU:HG	1.84	0.77
56:y:330:LEU:O	56:y:346:CYS:SG	2.43	0.77
56:y:12:PHE:HB2	56:y:102:GLY:O	1.82	0.77
1:A:693:C:H2'	1:A:694:U:H6	1.50	0.77
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.18	0.77
34:a:1303:C:OP1	62:a:3503:HOH:O	2.02	0.77
56:y:25:LEU:O	56:y:28:ARG:CA	2.33	0.77
1:A:862:G:OP2	62:A:3719:HOH:O	2.02	0.77
1:A:1766:U:H2'	1:A:1767:C:H6	1.49	0.77
5:F:51:THR:O	5:F:93:LYS:NZ	2.15	0.77
56:y:159:PRO:O	56:y:160:ALA:C	2.20	0.77
1:A:2600:A:N6	62:A:3779:HOH:O	2.18	0.77
34:a:308:C:H2'	34:a:309:G:H8	1.50	0.77
56:y:392:ASN:HD22	56:y:393:PRO:HD2	1.48	0.77
56:y:559:LEU:HD13	56:y:570:LYS:HG3	1.67	0.77
17:U:76:TYR:OH	17:U:92:ARG:NH1	2.18	0.76
22:Z:150:LEU:HB2	22:Z:172:ALA:HB3	1.67	0.76
56:y:172:GLU:C	56:y:174:VAL:H	1.91	0.76
56:y:291:TYR:CB	56:y:292:PRO:HA	2.16	0.76
34:a:509:A:N1	62:a:3511:HOH:O	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:U:H3	1:A:1142(A):A:H62	1.29	0.76
4:E:72:VAL:HA	4:E:73:GLU:HG2	1.68	0.76
56:y:28:ARG:HG3	56:y:31:GLU:OE1	1.85	0.76
1:A:1190:G:N7	62:A:3771:HOH:O	2.16	0.76
19:W:18:ARG:NH1	19:W:76:VAL:O	2.17	0.76
34:a:523:A:H2	45:l:91:LYS:HB3	1.48	0.76
1:A:1204:A:H2	1:A:1241:A:H62	1.33	0.76
1:A:2052:G:H4'	4:E:143:ASN:O	1.85	0.76
56:y:136:ASN:OD1	56:y:167:SER:HA	1.84	0.76
56:y:554:LEU:O	56:y:556:LYS:N	2.19	0.76
1:A:1999:C:O2	1:A:2687:U:O2'	2.04	0.76
34:a:918:A:H2'	34:a:919:A:C8	2.21	0.76
56:y:228:ILE:HA	56:y:281:THR:O	1.85	0.76
35:b:12:GLU:HA	35:b:15:VAL:HG23	1.66	0.76
35:b:223:ILE:HA	35:b:226:ARG:HG3	1.68	0.76
56:y:-63:LEU:HB2	56:y:-34:LEU:HB3	1.65	0.76
34:a:390:C:H2'	34:a:391:G:H8	1.50	0.76
1:A:2660:A:N6	56:y:465:ASP:HA	2.00	0.76
4:E:127:ASP:OD2	62:E:401:HOH:O	2.02	0.76
15:S:58:LEU:HB3	15:S:59:LYS:HB2	1.68	0.76
56:y:369:LEU:CD2	56:y:370:ILE:C	2.59	0.76
17:U:88:ILE:HD13	17:U:109:LEU:HD23	1.69	0.76
34:a:509:A:OP2	62:a:3505:HOH:O	2.04	0.76
33:x:67:C:H2'	33:x:68:C:C6	2.22	0.75
33:x:7:A:O2'	33:x:49:C:H5'	1.85	0.75
56:y:108:ASP:OD2	56:y:110:SER:OG	2.01	0.75
9:K:95:LYS:HG2	9:K:137:GLU:HB3	1.69	0.75
56:y:433:GLY:HA2	56:y:453:GLU:O	1.86	0.75
1:A:1315:C:OP2	62:A:3721:HOH:O	2.05	0.75
33:x:49:C:H42	33:x:65:G:H1	0.80	0.75
34:a:903:G:OP1	62:a:3504:HOH:O	2.02	0.75
40:g:70:LYS:HG2	40:g:96:GLN:HB3	1.67	0.75
46:m:12:ASN:O	46:m:44:ARG:NH1	2.19	0.75
1:A:883:G:H1	1:A:893:C:H42	0.81	0.75
34:a:1318:A:OP1	52:s:7:LYS:NZ	2.16	0.75
1:A:319:C:N4	1:A:323:G:O6	2.18	0.75
1:A:1639:U:OP2	62:A:3724:HOH:O	2.05	0.75
11:O:80:ASP:OD2	16:T:64:ARG:NH2	2.20	0.75
35:b:69:LEU:HB3	35:b:162:ILE:HG22	1.69	0.75
18:V:7:THR:O	62:V:301:HOH:O	2.05	0.75
23:0:39:ARG:HD3	23:0:58:THR:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:i:128:ARG:NH2	33:w:33:U:OP2	2.18	0.75
56:y:410:VAL:O	56:y:454:ALA:N	2.19	0.75
11:O:1:MET:HE3	11:O:32:TYR:CE2	2.21	0.75
20:X:18:TYR:O	20:X:20:GLY:N	2.20	0.74
22:Z:124:ILE:HG12	22:Z:125:LEU:H	1.51	0.74
42:i:46:ALA:HB2	42:i:74:ILE:HG23	1.69	0.74
43:j:35:SER:HB2	43:j:73:ASP:HB2	1.69	0.74
1:A:1566:A:OP1	3:D:211:ARG:NH1	2.21	0.74
1:A:2074:U:H2'	1:A:2075:U:C6	2.22	0.74
34:a:1323:G:H2'	34:a:1324:A:H8	1.52	0.74
29:6:3:SER:OG	29:6:4:GLU:N	2.18	0.74
46:m:78:ILE:HG22	46:m:82:MET:HE2	1.69	0.74
56:y:465:ASP:O	56:y:469:SER:HB2	1.87	0.74
1:A:2630:G:HO2'	1:A:2892:A:HO2'	1.36	0.74
34:a:781:A:OP2	62:a:3506:HOH:O	2.05	0.74
37:d:13:ARG:NH1	37:d:38:TYR:O	2.21	0.74
37:d:23:GLY:HA2	37:d:112:VAL:HG22	1.68	0.74
1:A:1058:G:N2	9:K:126:MET:SD	2.61	0.74
3:D:158:ALA:O	3:D:161:THR:OG1	2.03	0.74
10:N:120:LEU:HD22	10:N:122:VAL:HG22	1.68	0.74
56:y:418:GLU:HG3	56:y:419:GLU:N	2.03	0.74
3:D:141:VAL:HG12	3:D:164:GLN:HG3	1.70	0.74
7:H:3:ARG:NH1	7:H:4:ILE:H	1.86	0.74
34:a:15:G:H1'	38:e:19:MET:HE2	1.70	0.74
56:y:213:PRO:HD2	56:y:264:LEU:H	1.51	0.74
1:A:567:A:OP1	62:A:3720:HOH:O	2.04	0.74
22:Z:144:LEU:HD22	22:Z:148:ASP:HB3	1.69	0.74
36:c:58:GLU:HB3	43:j:92:THR:HG21	1.70	0.74
56:y:214:TYR:C	56:y:215:LEU:HD12	2.12	0.74
1:A:2581:G:OP2	62:A:3726:HOH:O	2.06	0.73
6:G:66:GLN:OE1	6:G:98:ARG:NE	2.16	0.73
27:4:16:CYS:HB2	27:4:36:CYS:HB3	1.70	0.73
45:l:84:LEU:HG	45:l:104:VAL:HG11	1.69	0.73
56:y:72:ASP:OD1	56:y:73:GLY:N	2.22	0.73
56:y:192:PRO:HB3	56:y:258:ALA:H	1.52	0.73
1:A:2150:U:H2'	1:A:2151:G:H8	1.52	0.73
38:e:43:LEU:H	38:e:136:MET:HE2	1.52	0.73
1:A:739:G:OP1	62:A:3727:HOH:O	2.06	0.73
34:a:222:U:H2'	34:a:223:U:H6	1.54	0.73
56:y:108:ASP:OD1	56:y:111:GLN:N	2.21	0.73
56:y:216:ARG:HG2	56:y:218:PHE:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:250:LEU:HD13	56:y:250:LEU:N	2.03	0.73
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.22	0.73
56:y:11:ASN:C	56:y:101:GLU:H	1.88	0.73
56:y:537:ILE:N	56:y:549:ALA:O	2.17	0.73
1:A:928:G:O6	62:A:3722:HOH:O	2.05	0.73
23:0:56:ASP:OD2	23:0:58:THR:OG1	2.07	0.73
1:A:120:U:OP2	62:A:3725:HOH:O	2.05	0.73
14:R:38:VAL:HG23	14:R:39:PRO:HD3	1.70	0.73
34:a:1323:G:H2'	34:a:1324:A:C8	2.24	0.73
9:K:13:PRO:HA	9:K:52:ILE:HA	1.69	0.73
1:A:1314:C:OP1	62:A:3721:HOH:O	2.06	0.73
50:q:16:GLN:O	50:q:18:THR:N	2.22	0.73
1:A:2349:G:OP1	62:A:3723:HOH:O	2.05	0.73
1:A:2683:C:OP1	16:T:55:ASN:ND2	2.21	0.73
33:x:56:C:H2'	33:x:57:G:O4'	1.88	0.73
34:a:333:G:H4'	53:t:16:HIS:CE1	2.23	0.73
34:a:390:C:H2'	34:a:391:G:C8	2.23	0.73
56:y:369:LEU:HD22	56:y:370:ILE:C	2.13	0.73
4:E:14:ILE:HG13	4:E:21:VAL:HG13	1.70	0.72
1:A:1108:U:O2'	1:A:1109:C:O5'	2.07	0.72
1:A:2592:G:OP1	62:A:3730:HOH:O	2.07	0.72
56:y:9:ILE:O	56:y:187:PRO:HG3	1.88	0.72
56:y:418:GLU:N	56:y:446:LYS:HA	2.02	0.72
17:U:69:CYS:HB3	17:U:74:LEU:HD13	1.71	0.72
46:m:11:ARG:HG2	46:m:12:ASN:ND2	2.04	0.72
34:a:964:A:OP1	62:a:3507:HOH:O	2.06	0.72
34:a:1441:G:H5''	34:a:1442:G:H5'	1.70	0.72
4:E:77:ILE:HG21	4:E:195:LEU:HD21	1.71	0.72
24:1:23:LYS:HB2	33:x:74:C:H4'	1.71	0.72
38:e:77:PRO:HD2	38:e:142:LEU:HD22	1.71	0.72
1:A:2591:C:H2'	1:A:2592:G:H8	1.54	0.72
45:l:53:ARG:NH1	45:l:92:ASP:OD2	2.20	0.72
56:y:445:GLN:C	56:y:447:ARG:N	2.41	0.72
21:Y:30:VAL:HG13	21:Y:37:VAL:HG12	1.71	0.72
34:a:1027:C:O2	34:a:1034:G:N1	2.23	0.72
9:K:51:ALA:HB1	9:K:73:PRO:HD2	1.72	0.72
34:a:429:U:OP2	37:d:36:ARG:NH2	2.23	0.72
1:A:944:G:OP2	62:A:3728:HOH:O	2.07	0.72
1:A:1095:A:H1'	56:y:426:GLN:HE21	1.55	0.72
1:A:2429:G:OP2	62:A:3732:HOH:O	2.08	0.72
13:Q:138:ASP:OD1	22:Z:81:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:300:VAL:C	56:y:347:GLY:HA2	2.15	0.72
1:A:2124:G:H1	1:A:2174:C:H42	1.36	0.72
5:F:20:LEU:HD22	5:F:21:ALA:H	1.54	0.72
21:Y:83:THR:OG1	21:Y:84:ARG:N	2.22	0.72
1:A:1153:C:OP2	62:A:3714:HOH:O	2.08	0.71
1:A:1434:A:H61	1:A:1558:A:H62	1.38	0.71
3:D:92:ILE:HG22	3:D:106:ILE:HA	1.72	0.71
12:P:81:GLN:HG2	12:P:106:LEU:HD22	1.72	0.71
34:a:931:C:H42	34:a:1386:G:H1	1.38	0.71
56:y:136:ASN:CG	56:y:137:LYS:H	1.98	0.71
56:y:250:LEU:HD22	56:y:250:LEU:N	2.03	0.71
56:y:306:TYR:HD2	56:y:343:GLY:C	1.91	0.71
1:A:444:C:H4'	5:F:49:ALA:HB2	1.72	0.71
1:A:1309:G:H4'	30:7:7:PRO:HG2	1.70	0.71
1:A:2793:G:H1	1:A:2803:C:H42	1.35	0.71
33:x:33:U:H3'	33:x:34:G:H5''	1.71	0.71
34:a:17:U:H2'	34:a:18:C:C6	2.25	0.71
1:A:1169:G:H1	1:A:1180:C:H42	1.38	0.71
16:T:65:LYS:HE3	16:T:67:SER:HB2	1.73	0.71
36:c:130:VAL:HG21	36:c:157:ILE:HG23	1.72	0.71
36:c:150:LYS:HG3	36:c:169:ALA:HB2	1.71	0.71
56:y:83:THR:O	56:y:84:PRO:C	2.30	0.71
56:y:435:LEU:HB2	56:y:452:TYR:CZ	2.26	0.71
12:P:89:ALA:HA	12:P:121:LYS:HD3	1.71	0.71
56:y:306:TYR:CE2	56:y:343:GLY:C	2.68	0.71
56:y:408:PRO:HG3	56:y:484:TYR:CZ	2.25	0.71
56:y:458:GLU:O	56:y:462:ASP:HB2	1.90	0.71
56:y:373:ALA:HB1	56:y:374:PRO:CA	2.21	0.71
1:A:1982:C:OP2	62:A:3731:HOH:O	2.08	0.71
34:a:502:G:OP1	45:l:118:SER:OG	2.08	0.71
40:g:80:VAL:HG12	40:g:82:GLY:H	1.55	0.71
38:e:71:LEU:O	38:e:73:ASN:N	2.24	0.71
1:A:372:G:OP2	24:l:69:LYS:NZ	2.21	0.71
9:K:59:ILE:HD11	9:K:63:ARG:HA	1.73	0.71
56:y:108:ASP:CG	56:y:110:SER:H	1.99	0.71
1:A:574:C:OP1	62:A:3733:HOH:O	2.08	0.71
1:A:2222:G:H2'	1:A:2223:G:H8	1.56	0.71
1:A:2357:U:OP1	23:0:20:ARG:NH1	2.24	0.71
34:a:975:A:H4'	34:a:976:G:H5''	1.73	0.71
56:y:-16:ALA:HB1	56:y:-12:ARG:HD3	1.73	0.71
9:K:99:ILE:HG23	9:K:103:GLN:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:9:LEU:HA	29:6:54:ILE:HB	1.73	0.70
33:x:22:G:N7	33:x:46:7MG:O6	2.25	0.70
34:a:1356:G:H2'	34:a:1357:A:C8	2.26	0.70
56:y:9:ILE:O	56:y:187:PRO:HB3	1.90	0.70
56:y:108:ASP:CG	56:y:111:GLN:H	1.99	0.70
35:b:84:GLU:HB3	35:b:219:VAL:HG21	1.72	0.70
56:y:531:GLN:OE1	56:y:590:VAL:HG23	1.91	0.70
1:A:2028:U:O4	62:A:3729:HOH:O	2.07	0.70
50:q:26:GLN:HG2	50:q:37:LYS:HG2	1.73	0.70
52:s:27:GLU:HB2	52:s:28:LYS:HD2	1.73	0.70
56:y:89:PHE:C	56:y:90:THR:HG23	2.16	0.70
56:y:154:GLU:OE2	56:y:155:VAL:HA	1.91	0.70
1:A:226:G:H21	1:A:228:A:H62	1.37	0.70
1:A:1021:A:C8	1:A:1021:A:H3'	2.26	0.70
1:A:1557:C:OP2	1:A:1558:A:O2'	2.10	0.70
1:A:2816:C:O3'	14:R:99:LYS:NZ	2.25	0.70
16:T:35:LYS:HZ1	16:T:38:ASN:HA	1.56	0.70
1:A:1187:G:H5''	18:V:81:TYR:CE2	2.27	0.70
1:A:2577:A:OP1	62:A:3734:HOH:O	2.08	0.70
56:y:28:ARG:NE	56:y:168:GLY:O	2.24	0.70
56:y:131:ILE:HD11	56:y:158:LEU:HD21	1.72	0.70
1:A:1375:C:OP1	62:A:3735:HOH:O	2.09	0.70
2:B:75:G:H1'	22:Z:27:VAL:HG11	1.74	0.70
13:Q:138:ASP:OD2	13:Q:138:ASP:N	2.21	0.70
19:W:13:SER:HB3	19:W:16:LYS:HG3	1.73	0.70
56:y:68:TYR:CD1	56:y:70:ALA:HA	2.26	0.70
56:y:277:GLY:HA3	56:y:293:GLY:O	1.91	0.70
40:g:78:ARG:HH21	40:g:156:TRP:HB3	1.57	0.70
56:y:85:GLY:C	56:y:86:HIS:ND1	2.49	0.70
5:F:17:ARG:HH12	5:F:19:GLU:HG3	1.57	0.70
11:O:87:ILE:HD12	11:O:91:LEU:HA	1.74	0.70
36:c:47:LEU:HD13	36:c:68:VAL:HG11	1.74	0.70
33:x:15:G:N1	33:x:48:C:N3	2.39	0.70
33:x:51:U:H2'	33:x:52:G:H8	1.56	0.70
36:c:189:ALA:HB3	36:c:196:LEU:HB2	1.73	0.70
56:y:113:VAL:HG23	56:y:117:THR:CG2	2.21	0.70
56:y:228:ILE:C	56:y:228:ILE:HD12	2.17	0.70
56:y:434:ARG:N	56:y:453:GLU:O	2.24	0.70
1:A:72:U:OP1	62:A:3736:HOH:O	2.09	0.70
1:A:2023:G:H5'	1:A:2617:C:H4'	1.73	0.70
1:A:2591:C:H2'	1:A:2592:G:C8	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:3:ARG:HH12	7:H:5:GLY:H	1.40	0.70
56:y:138:ILE:HG12	56:y:167:SER:HB2	1.74	0.70
56:y:418:GLU:N	56:y:446:LYS:CA	2.54	0.70
1:A:906:G:O2'	13:Q:67:ARG:NH2	2.21	0.69
1:A:1478:G:H2'	1:A:1479:G:H8	1.57	0.69
21:Y:13:VAL:HG12	21:Y:74:PRO:HA	1.73	0.69
27:4:44:THR:O	27:4:46:GLN:N	2.24	0.69
56:y:230:ILE:CD1	56:y:234:GLY:O	2.40	0.69
1:A:2478:A:OP2	32:9:2:LYS:NZ	2.20	0.69
1:A:588:U:OP2	62:A:3738:HOH:O	2.09	0.69
1:A:2822:G:H2'	1:A:2823:A:H5''	1.75	0.69
17:U:85:LYS:NZ	17:U:116:ALA:O	2.25	0.69
20:X:35:THR:HB	20:X:38:GLU:HG2	1.75	0.69
56:y:243:GLY:C	56:y:263:TRP:H	1.99	0.69
6:G:9:ARG:NH1	6:G:13:GLU:OE1	2.23	0.69
29:6:23:THR:OG1	29:6:24:GLU:N	2.17	0.69
44:k:91:ARG:HH12	51:r:87:ARG:HH12	1.41	0.69
56:y:241:LYS:N	56:y:265:VAL:CG2	2.55	0.69
43:j:52:GLY:O	47:n:41:ARG:NH2	2.25	0.69
56:y:492:VAL:HG13	56:y:540:ALA:C	2.18	0.69
1:A:801:G:OP2	62:A:3741:HOH:O	2.11	0.69
34:a:923:A:OP1	38:e:21:ALA:HB2	1.93	0.69
1:A:693:C:H2'	1:A:694:U:C6	2.27	0.69
1:A:1828:G:OP1	62:A:3739:HOH:O	2.10	0.69
27:4:45:GLY:C	27:4:47:GLN:H	2.01	0.69
34:a:926:G:H3'	34:a:1505:G:H21	1.58	0.69
1:A:690:G:O2'	1:A:780:G:OP1	2.10	0.69
1:A:1165:U:H2'	1:A:1166:C:C6	2.27	0.69
1:A:1936:A:H61	1:A:1963:U:H3	1.41	0.69
13:Q:54:MET:HE3	13:Q:64:ILE:HD13	1.73	0.69
13:Q:109:VAL:HG13	13:Q:113:GLN:HB3	1.75	0.69
56:y:15:ILE:CD1	56:y:103:VAL:HB	2.22	0.69
56:y:379:LYS:H	56:y:406:LEU:N	1.91	0.69
1:A:249:C:OP1	62:A:3743:HOH:O	2.11	0.69
1:A:833:U:O2	12:P:55:ARG:NH2	2.26	0.69
1:A:1395:A:OP1	62:A:3703:HOH:O	2.11	0.69
23:0:37:LEU:N	23:0:59:LEU:O	2.20	0.69
24:1:18:ILE:HG23	24:1:37:ILE:HG12	1.74	0.69
56:y:372:THR:O	56:y:373:ALA:HB2	1.91	0.69
56:y:131:ILE:CD1	56:y:158:LEU:HD21	2.23	0.69
56:y:531:GLN:HB2	56:y:533:PHE:HE1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:A:C8	1:A:119:A:C8	2.81	0.68
1:A:1345:C:OP2	62:A:3745:HOH:O	2.11	0.68
16:T:108:ARG:HA	16:T:111:ARG:HH11	1.57	0.68
34:a:642:A:N3	41:h:113:SER:OG	2.26	0.68
41:h:64:LYS:HB3	41:h:79:VAL:HG21	1.75	0.68
56:y:-3:GLU:HA	56:y:0:LYS:HB2	1.75	0.68
56:y:518:ARG:HH21	56:y:522:ASP:CA	2.05	0.68
1:A:1021:A:H3'	1:A:1021:A:H8	1.58	0.68
1:A:1968:G:OP1	62:A:3730:HOH:O	2.10	0.68
1:A:2417:C:OP1	12:P:65:ARG:NH2	2.26	0.68
56:y:412:LEU:N	56:y:452:TYR:O	2.26	0.68
16:T:100:TYR:HB3	16:T:103:ARG:NH1	2.07	0.68
31:8:31:HIS:O	31:8:36:LYS:NZ	2.26	0.68
56:y:495:LEU:HB2	56:y:538:GLN:HG3	1.76	0.68
1:A:1095:A:H4'	56:y:426:GLN:HE22	1.58	0.68
34:a:1149:C:P	42:i:9:ARG:HH21	2.16	0.68
33:x:69:G:H2'	33:x:70:G:O4'	1.94	0.68
34:a:1499:A:H1'	34:a:1520:G:H5'	1.75	0.68
56:y:9:ILE:O	56:y:187:PRO:CG	2.41	0.68
1:A:445:C:OP2	62:A:3740:HOH:O	2.10	0.68
1:A:2588:G:OP1	62:A:3749:HOH:O	2.11	0.68
6:G:115:ARG:O	6:G:117:PHE:N	2.27	0.68
20:X:92:LEU:C	20:X:94:GLY:H	2.02	0.68
34:a:954:G:H21	34:a:1227:A:H62	1.41	0.68
56:y:213:PRO:CG	56:y:264:LEU:O	2.41	0.68
4:E:13:ARG:HD3	16:T:58:ASN:HD21	1.59	0.68
27:4:56:VAL:HG23	27:4:57:GLU:HG3	1.76	0.68
34:a:222:U:H2'	34:a:223:U:C6	2.29	0.68
1:A:748:G:O6	19:W:90:ARG:NH1	2.27	0.68
1:A:1045:A:H5''	1:A:1047:G:H1'	1.76	0.68
1:A:1349:A:OP1	62:A:3748:HOH:O	2.11	0.68
36:c:6:HIS:HD2	36:c:7:PRO:HD2	1.56	0.68
50:q:53:LEU:O	50:q:55:ASP:N	2.25	0.68
1:A:1833:U:H2'	1:A:1834:U:H6	1.59	0.68
56:y:301:VAL:O	56:y:302:PHE:C	2.33	0.68
3:D:233:HIS:O	62:D:401:HOH:O	2.12	0.68
21:Y:99:CYS:HB2	21:Y:106:LEU:HD21	1.76	0.68
34:a:558:G:OP1	62:a:3508:HOH:O	2.11	0.68
40:g:78:ARG:HD3	40:g:79:ARG:HB2	1.74	0.68
4:E:54:GLN:HB2	4:E:76:ARG:HG2	1.75	0.67
34:a:1457:G:H2'	34:a:1458:G:H8	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:A:OP2	62:A:3747:HOH:O	2.11	0.67
1:A:2017:U:OP1	62:A:3750:HOH:O	2.12	0.67
56:y:24:THR:CG2	61:y:703:GDP:O2A	2.42	0.67
56:y:401:ARG:HG3	56:y:401:ARG:O	1.93	0.67
1:A:1269:A:OP2	62:A:3746:HOH:O	2.11	0.67
1:A:1332:G:OP2	62:A:3752:HOH:O	2.12	0.67
1:A:2035:G:OP1	62:A:3744:HOH:O	2.11	0.67
14:R:18:LEU:HD22	14:R:22:ARG:HG3	1.77	0.67
18:V:71:LEU:HD11	18:V:84:LYS:HE3	1.76	0.67
1:A:1792:G:H5''	3:D:205:VAL:HG22	1.75	0.67
1:A:2115:G:N1	1:A:2119:A:OP2	2.28	0.67
34:a:490:G:H2'	34:a:491:G:H8	1.59	0.67
56:y:68:TYR:CZ	56:y:179:GLU:CB	2.69	0.67
56:y:463:PHE:O	56:y:467:LEU:CA	2.42	0.67
1:A:574:C:OP2	62:A:3754:HOH:O	2.12	0.67
1:A:2405:G:OP2	62:A:3755:HOH:O	2.13	0.67
7:H:56:SER:OG	7:H:57:ASP:N	2.25	0.67
33:x:5:G:N1	33:x:68:C:N4	2.31	0.67
39:f:38:GLU:HB2	39:f:64:GLN:HG2	1.76	0.67
1:A:674:G:OP2	62:A:3756:HOH:O	2.13	0.67
20:X:31:HIS:CD2	20:X:33:LYS:H	2.13	0.67
26:3:35:ARG:HE	26:3:37:LEU:HD21	1.60	0.67
27:4:42:PHE:HB3	27:4:43:TYR:HB2	1.75	0.67
34:a:890:G:O2'	34:a:906:G:O6	2.09	0.67
1:A:794:G:OP2	62:A:3753:HOH:O	2.12	0.67
1:A:1175:U:OP1	1:A:1177:A:N6	2.27	0.67
1:A:1403:C:H5''	1:A:1471:A:H1'	1.77	0.67
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.77	0.67
56:y:192:PRO:O	56:y:221:ARG:CD	2.40	0.67
1:A:1060:U:H4'	1:A:1061:U:H5'	1.77	0.67
6:G:66:GLN:HA	27:4:6:HIS:ND1	2.10	0.67
17:U:53:ARG:HA	17:U:56:ASP:HB2	1.77	0.67
34:a:1003:G:C2	34:a:1004:A:H1'	2.29	0.67
34:a:1027:C:C2	34:a:1034:G:N1	2.62	0.67
34:a:1218:C:H2'	34:a:1219:U:C6	2.29	0.67
56:y:537:ILE:CD1	56:y:551:VAL:HG22	2.25	0.67
3:D:101:GLU:OE1	3:D:103:ARG:NH1	2.27	0.66
34:a:918:A:H2'	34:a:919:A:H8	1.61	0.66
46:m:15:VAL:HB	46:m:34:LEU:HD11	1.77	0.66
52:s:27:GLU:OE2	52:s:28:LYS:NZ	2.16	0.66
33:w:47:U:O2'	33:w:48:C:OP1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:245:PHE:HA	56:y:251:VAL:N	2.10	0.66
56:y:294:PHE:CB	56:y:295:ARG:CB	2.72	0.66
1:A:1219:G:OP2	17:U:19:LYS:NZ	2.20	0.66
34:a:1014:A:H4'	52:s:14:HIS:HE1	1.58	0.66
34:a:1456:G:O3'	53:t:39:LYS:NZ	2.29	0.66
34:a:1131:G:OP2	42:i:20:ARG:NH2	2.28	0.66
39:f:94:GLN:HB3	51:r:32:ARG:HH21	1.60	0.66
56:y:107:VAL:O	56:y:136:ASN:CB	2.44	0.66
56:y:109:ALA:HB1	56:y:145:PRO:HA	1.76	0.66
1:A:1021:A:H62	1:A:1141:U:H3	1.43	0.66
1:A:1590:U:H2'	1:A:1591:G:C8	2.30	0.66
3:D:123:ALA:HB3	3:D:131:LEU:HD11	1.77	0.66
19:W:35:ILE:O	19:W:37:ARG:N	2.27	0.66
22:Z:72:ARG:NH2	22:Z:97:GLU:O	2.28	0.66
26:3:31:LEU:HD13	26:3:32:GLN:HG2	1.78	0.66
35:b:17:PHE:HA	35:b:44:LEU:HD11	1.77	0.66
37:d:12:CYS:SG	37:d:19:LEU:HD12	2.36	0.66
56:y:227:ARG:CB	56:y:283:ALA:H	2.08	0.66
56:y:445:GLN:O	56:y:447:ARG:N	2.28	0.66
1:A:271(J):C:O2	1:A:271(M):G:N1	2.28	0.66
34:a:1003:G:H2'	34:a:1004:A:H4'	1.78	0.66
45:l:84:LEU:HD12	45:l:101:VAL:HB	1.78	0.66
46:m:11:ARG:H	46:m:11:ARG:NE	1.92	0.66
1:A:1395:A:OP1	62:A:3751:HOH:O	2.12	0.66
1:A:2101:G:H1	1:A:2188:C:H42	1.42	0.66
1:A:2589:A:OP1	62:A:3758:HOH:O	2.13	0.66
18:V:25:LEU:HD22	18:V:26:ASP:H	1.60	0.66
34:a:1181:G:O2'	34:a:1182:G:N7	2.26	0.66
36:c:103:VAL:HG12	36:c:104:GLN:H	1.60	0.66
1:A:192:C:OP2	62:A:3757:HOH:O	2.13	0.66
1:A:1405:U:H2'	1:A:1406:U:C6	2.30	0.66
56:y:228:ILE:CG1	56:y:237:PHE:O	2.39	0.66
9:K:10:LEU:HD11	9:K:27:LEU:HD11	1.77	0.66
34:a:181:G:H4'	34:a:182:U:H5'	1.78	0.66
38:e:79:GLU:HB3	38:e:92:LYS:HG2	1.78	0.66
50:q:13:ASP:CG	50:q:14:LYS:H	2.03	0.66
56:y:266:ALA:O	56:y:267:ALA:HB3	1.95	0.66
1:A:2111:C:OP2	1:A:2145:C:N4	2.29	0.66
42:i:45:ALA:HB2	42:i:51:ARG:HH21	1.61	0.66
1:A:40:C:H42	1:A:438:G:H1	1.42	0.66
5:F:17:ARG:NH1	5:F:18:ARG:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:59:ILE:HG22	50:q:73:VAL:HA	1.77	0.66
51:r:32:ARG:HA	51:r:69:THR:HG21	1.78	0.66
56:y:94:SER:O	56:y:95:ARG:C	2.37	0.66
1:A:2140:C:N3	1:A:2151:G:O6	2.29	0.65
5:F:178:PRO:HB2	5:F:201:VAL:HG21	1.75	0.65
34:a:1238:A:OP2	62:a:3509:HOH:O	2.14	0.65
41:h:10:LEU:HD13	41:h:83:ILE:HG12	1.76	0.65
56:y:28:ARG:CA	56:y:31:GLU:HG3	2.26	0.65
56:y:105:LEU:HD13	56:y:105:LEU:C	2.21	0.65
56:y:245:PHE:CA	56:y:250:LEU:HA	2.23	0.65
4:E:77:ILE:HD12	4:E:78:LEU:H	1.61	0.65
8:J:118:THR:N	8:J:121:ASP:O	2.29	0.65
27:4:58:ARG:HG2	52:s:67:VAL:HG12	1.78	0.65
34:a:1030:C:N3	34:a:1031:G:C2	2.64	0.65
1:A:322:A:H3'	5:F:169:ASN:HD21	1.61	0.65
1:A:2789:C:O2'	1:A:2790:A:O5'	2.13	0.65
3:D:133:LEU:HA	3:D:136:ILE:HD12	1.78	0.65
14:R:28:LEU:O	14:R:31:HIS:N	2.28	0.65
34:a:8:A:C6	37:d:209:ARG:HB3	2.32	0.65
34:a:429:U:H3'	37:d:9:CYS:SG	2.36	0.65
34:a:490:G:H2'	34:a:491:G:C8	2.31	0.65
34:a:523:A:C2	45:l:91:LYS:HB3	2.30	0.65
34:a:1124:G:C2	34:a:1127:G:N2	2.64	0.65
1:A:141:A:H8	1:A:1408:C:HO2'	1.41	0.65
34:a:233:C:H2'	34:a:234:C:H6	1.58	0.65
1:A:1783:A:H5'	1:A:2608:G:H4'	1.77	0.65
1:A:2106:G:N2	1:A:2183:C:N3	2.40	0.65
3:D:43:ARG:NH2	3:D:49:ILE:HD11	2.10	0.65
9:K:6:ALA:HB3	9:K:59:ILE:H	1.62	0.65
20:X:50:LYS:HB3	20:X:84:ALA:HB2	1.77	0.65
34:a:677:U:H3	34:a:713:G:H22	1.44	0.65
34:a:1521:G:N3	62:a:3521:HOH:O	2.28	0.65
33:w:53:G:H2'	33:w:54:5MU:H6	1.61	0.65
1:A:975:C:O2'	62:A:3764:HOH:O	2.15	0.65
22:Z:183:LEU:O	22:Z:185:GLU:N	2.29	0.65
34:a:187:C:O2'	53:t:89:ARG:NH2	2.29	0.65
35:b:79:ASP:OD2	35:b:79:ASP:N	2.26	0.65
56:y:166:ALA:O	56:y:167:SER:CB	2.34	0.65
56:y:340:LEU:O	56:y:340:LEU:HD13	1.97	0.65
1:A:1942:C:OP2	1:A:1943:U:O2'	2.12	0.65
12:P:63:PRO:HG2	31:8:25:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:138:ILE:HG12	56:y:167:SER:CB	2.27	0.65
1:A:180:G:N2	1:A:215:G:O6	2.30	0.65
1:A:2199:A:H5'	1:A:2200:C:OP2	1.96	0.65
3:D:274:ARG:HB2	3:D:275:LYS:HB2	1.79	0.65
14:R:104:ARG:HG3	14:R:111:LEU:HD11	1.76	0.65
30:7:9:ARG:HG3	30:7:46:VAL:HG23	1.79	0.65
31:8:29:LYS:HD3	31:8:44:LYS:HB2	1.79	0.65
52:s:14:HIS:HA	52:s:17:GLU:HB3	1.77	0.65
56:y:89:PHE:O	56:y:90:THR:CB	2.45	0.65
56:y:434:ARG:NH1	56:y:434:ARG:HG2	2.11	0.65
1:A:2036:C:OP1	62:A:3761:HOH:O	2.14	0.65
8:J:56:ASN:HA	8:J:83:TYR:HA	1.78	0.65
39:f:80:ARG:HG2	39:f:88:VAL:HG21	1.79	0.65
50:q:67:LYS:HA	50:q:70:ARG:HH12	1.62	0.65
1:A:83:G:O2'	1:A:102:G:N2	2.30	0.65
1:A:1254:A:OP2	62:A:3759:HOH:O	2.14	0.65
1:A:2025:C:H2'	1:A:2026:C:C6	2.32	0.65
24:1:7:ILE:HG22	24:1:8:SER:HB3	1.78	0.65
31:8:52:LYS:HG3	31:8:53:PRO:HD3	1.78	0.65
34:a:404:U:H2'	34:a:405:U:H6	1.61	0.65
35:b:33:TYR:HB3	35:b:41:ILE:HG22	1.78	0.65
40:g:41:ARG:O	40:g:45:ASP:HB2	1.96	0.65
56:y:9:ILE:O	56:y:187:PRO:CB	2.45	0.65
56:y:418:GLU:CA	56:y:446:LYS:HA	2.27	0.65
1:A:34:C:H2'	1:A:35:G:H5'	1.77	0.64
1:A:876:C:H2'	1:A:877:U:O4'	1.97	0.64
1:A:1250:G:N7	12:P:18:ARG:NH2	2.45	0.64
1:A:1790:C:O2'	3:D:209:ALA:HB2	1.96	0.64
1:A:2385:C:OP2	62:A:3762:HOH:O	2.14	0.64
37:d:199:ASN:O	37:d:201:GLN:N	2.30	0.64
1:A:467:G:OP1	30:7:33:ARG:NH1	2.29	0.64
1:A:979:G:N7	62:A:3804:HOH:O	2.29	0.64
33:x:6:G:O6	33:x:7:A:N6	2.29	0.64
1:A:1107:G:H4'	8:J:81:VAL:HA	1.79	0.64
1:A:2206:G:H5'	1:A:2207:G:C5	2.33	0.64
35:b:73:THR:OG1	35:b:170:GLU:OE1	2.08	0.64
37:d:43:HIS:HB3	37:d:46:LYS:HD2	1.79	0.64
44:k:15:ALA:HA	44:k:77:MET:HA	1.79	0.64
1:A:981:A:H8	1:A:982:C:C5	2.15	0.64
1:A:1451:C:H42	1:A:1459:G:H1	1.46	0.64
26:3:8:LEU:HB2	26:3:28:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:36:CYS:HB3	28:5:49:CYS:HB3	1.79	0.64
34:a:878:G:H5'	41:h:89:PRO:HG2	1.79	0.64
1:A:1071:G:O2'	1:A:1089:G:OP2	2.14	0.64
34:a:748:C:H4'	34:a:749:C:O5'	1.98	0.64
35:b:72:GLY:O	35:b:94:ASN:HA	1.97	0.64
49:p:74:LEU:HG	49:p:79:VAL:HG21	1.80	0.64
5:F:17:ARG:HG2	5:F:18:ARG:H	1.62	0.64
33:x:29:G:N2	33:x:41:C:N3	2.36	0.64
33:x:51:U:H2'	33:x:52:G:C8	2.32	0.64
37:d:178:VAL:O	37:d:180:GLY:N	2.28	0.64
40:g:78:ARG:HG2	40:g:79:ARG:HD3	1.78	0.64
56:y:308:VAL:HG13	56:y:369:LEU:HA	1.80	0.64
1:A:2109:U:O4	1:A:2179:C:N4	2.31	0.64
22:Z:7:ALA:HB2	22:Z:59:LEU:HD22	1.79	0.64
56:y:25:LEU:O	56:y:28:ARG:N	2.31	0.64
56:y:201:PHE:HD2	56:y:202:ASP:HB2	1.62	0.64
56:y:372:THR:HG22	56:y:373:ALA:N	2.11	0.64
1:A:747:U:H2'	19:W:88:ARG:HH21	1.62	0.64
1:A:1776:G:OP2	62:A:3763:HOH:O	2.15	0.64
1:A:2122:U:H2'	1:A:2123:G:H8	1.62	0.64
3:D:44:ASN:HB3	3:D:50:THR:HG21	1.79	0.64
5:F:161:GLU:O	5:F:165:ARG:HB2	1.98	0.64
6:G:115:ARG:H	6:G:136:ARG:HH21	1.46	0.64
1:A:1022:G:H22	1:A:1142(A):A:H2	1.46	0.64
1:A:1161:C:H4'	18:V:8:GLY:HA2	1.80	0.64
3:D:121:PRO:HB3	3:D:135:PHE:CE1	2.33	0.64
6:G:22:ARG:HH21	6:G:175:LEU:HD11	1.63	0.64
6:G:150:ASP:OD2	6:G:150:ASP:N	2.31	0.64
1:A:2121:G:H1	1:A:2177:C:N4	1.92	0.64
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.63	0.64
21:Y:51:VAL:HG13	21:Y:57:GLN:H	1.62	0.64
35:b:166:ASP:HB3	35:b:169:LYS:HB2	1.80	0.64
56:y:108:ASP:OD1	56:y:110:SER:N	2.28	0.64
56:y:215:LEU:HD12	56:y:215:LEU:N	2.13	0.64
1:A:1786:A:H1'	1:A:1938:A:N6	2.14	0.63
1:A:1951:U:O4	62:A:3742:HOH:O	2.11	0.63
1:A:2125:G:N2	1:A:2173:A:H62	1.93	0.63
1:A:2428:G:O2'	62:A:3760:HOH:O	2.14	0.63
27:4:58:ARG:NH1	52:s:68:GLY:H	1.96	0.63
1:A:120:U:OP2	62:A:3765:HOH:O	2.15	0.63
34:a:976:G:H5'	34:a:1358:U:O2'	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:162:LEU:HD13	37:d:181:MET:HG2	1.80	0.63
56:y:13:SER:O	56:y:103:VAL:HG12	1.99	0.63
22:Z:104:PHE:HA	22:Z:139:VAL:HG23	1.80	0.63
33:w:73:A:O2'	56:y:569:ARG:HG2	1.97	0.63
56:y:122:TYR:O	56:y:123:MET:C	2.38	0.63
1:A:1166:C:O2'	62:A:3768:HOH:O	2.16	0.63
12:P:27:HIS:HB3	12:P:32:THR:HG23	1.81	0.63
27:4:45:GLY:O	27:4:47:GLN:N	2.30	0.63
34:a:745:C:H2'	34:a:746:A:C8	2.33	0.63
56:y:140:LEU:HD23	56:y:142:ASN:H	1.62	0.63
56:y:230:ILE:HG22	56:y:279:THR:O	1.99	0.63
1:A:2319:G:H22	15:S:3:ARG:HA	1.64	0.63
8:J:6:ASN:HA	8:J:9:LEU:H	1.63	0.63
56:y:306:TYR:O	56:y:369:LEU:HD23	1.97	0.63
56:y:372:THR:O	56:y:373:ALA:CB	2.47	0.63
1:A:125:G:H5''	30:7:19:ARG:HD3	1.79	0.63
16:T:84:GLN:HG2	16:T:85:LYS:HG2	1.79	0.63
19:W:21:VAL:HG22	19:W:47:VAL:HG21	1.80	0.63
34:a:1145:C:O2'	34:a:1146:A:OP2	2.16	0.63
56:y:68:TYR:OH	56:y:179:GLU:CB	2.45	0.63
1:A:184:C:H2'	1:A:185:U:H6	1.64	0.63
1:A:2201:C:H2'	1:A:2202:C:H6	1.64	0.63
1:A:2419:U:OP2	31:8:33:ASN:ND2	2.31	0.63
2:B:51:G:N7	15:S:62:LYS:NZ	2.44	0.63
17:U:62:ILE:HG23	17:U:76:TYR:CE1	2.34	0.63
56:y:230:ILE:O	56:y:230:ILE:HG13	1.98	0.63
6:G:83:ARG:O	6:G:86:MET:HG3	1.99	0.63
33:x:25:C:O2'	33:x:26:A:H8	1.82	0.63
34:a:664:G:P	51:r:64:ARG:HH21	2.22	0.63
56:y:548:ARG:HD3	56:y:548:ARG:N	2.13	0.63
16:T:13:ARG:NH2	16:T:14:TYR:OH	2.31	0.63
34:a:41:G:H2'	34:a:42:G:C8	2.33	0.63
56:y:223:ARG:CB	56:y:224:PRO:CD	2.72	0.63
2:B:105:A:OP1	22:Z:72:ARG:NH1	2.31	0.62
4:E:56:PRO:HA	4:E:59:VAL:HG23	1.81	0.62
34:a:592:G:H2'	34:a:593:G:H8	1.64	0.62
34:a:1112:C:H5''	34:a:1113:C:OP2	1.99	0.62
49:p:6:LEU:HB3	49:p:17:TYR:CD1	2.33	0.62
56:y:496:VAL:O	56:y:496:VAL:HG13	1.97	0.62
1:A:1766:U:H2'	1:A:1767:C:C6	2.33	0.62
1:A:2305:A:H5''	6:G:134:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2369:A:H2'	1:A:2370:G:H8	1.64	0.62
3:D:155:LEU:HD23	3:D:177:LEU:HD22	1.81	0.62
22:Z:110:GLY:HA3	22:Z:174:VAL:HG11	1.80	0.62
56:y:28:ARG:C	56:y:31:GLU:HG3	2.24	0.62
1:A:1138:G:N2	10:N:106:MET:SD	2.67	0.62
1:A:2740:A:H2'	1:A:2741:A:C8	2.33	0.62
34:a:404:U:H2'	34:a:405:U:C6	2.34	0.62
37:d:150:GLU:O	37:d:152:SER:N	2.31	0.62
39:f:4:TYR:O	39:f:93:SER:OG	2.16	0.62
3:D:264:LYS:HG3	3:D:265:PRO:HD2	1.80	0.62
6:G:173:LEU:HA	6:G:176:LEU:HD12	1.81	0.62
7:H:54:ARG:NE	7:H:56:SER:O	2.17	0.62
22:Z:126:VAL:HG11	22:Z:161:VAL:HG22	1.79	0.62
34:a:1392:G:H21	34:a:1502:A:H8	1.47	0.62
36:c:155:GLY:HA3	36:c:196:LEU:HD13	1.81	0.62
1:A:1491:G:O4'	3:D:99:ASP:HB3	2.00	0.62
1:A:2051:A:H5'	1:A:2578:G:O4'	2.00	0.62
7:H:11:VAL:HG12	7:H:15:VAL:HG23	1.82	0.62
10:N:36:GLY:O	10:N:38:HIS:N	2.32	0.62
25:2:10:LEU:HD13	25:2:14:ARG:HH12	1.64	0.62
29:6:2:ALA:HA	29:6:6:ARG:HG2	1.82	0.62
56:y:392:ASN:HD22	56:y:393:PRO:CD	2.11	0.62
56:y:496:VAL:O	56:y:497:HIS:HB3	1.98	0.62
1:A:1048:A:OP2	1:A:1109:C:N4	2.33	0.62
34:a:673:G:H2'	34:a:674:G:C8	2.35	0.62
34:a:1027:C:H2'	34:a:1028:C:H5	1.65	0.62
56:y:113:VAL:HG13	56:y:113:VAL:O	1.99	0.62
56:y:308:VAL:O	56:y:311:GLY:HA3	1.99	0.62
1:A:2102:U:O2	1:A:2187:G:O6	2.18	0.62
1:A:2334:G:O6	23:0:74:ARG:NH2	2.33	0.62
21:Y:5:MET:HE3	21:Y:30:VAL:HG12	1.82	0.62
32:9:17:ILE:HG22	32:9:24:TYR:HB2	1.81	0.62
34:a:1027:C:N3	34:a:1034:G:O6	2.33	0.62
56:y:174:VAL:O	56:y:177:ILE:N	2.22	0.62
1:A:422:A:H2'	1:A:423:A:C8	2.35	0.62
1:A:1095:A:C1'	56:y:426:GLN:NE2	2.63	0.62
56:y:28:ARG:NH1	56:y:31:GLU:OE1	2.32	0.62
56:y:85:GLY:O	56:y:86:HIS:HB2	1.99	0.62
56:y:439:ASN:O	56:y:449:GLU:HB3	1.99	0.62
56:y:462:ASP:O	56:y:466:ARG:HD3	2.00	0.62
1:A:2482:G:H22	13:Q:52:VAL:HG11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:41:GLN:HE21	6:G:155:MET:HE2	1.64	0.62
6:G:161:THR:HG23	6:G:163:ALA:H	1.64	0.62
9:K:125:ARG:O	9:K:129:GLY:N	2.32	0.62
25:2:16:LEU:HD23	25:2:17:SER:H	1.64	0.62
29:6:47:THR:O	29:6:49:HIS:ND1	2.32	0.62
42:i:9:ARG:H	42:i:79:LEU:HD23	1.64	0.62
33:w:46:7MG:H3'	33:w:47:U:H5''	1.80	0.62
1:A:1412:A:H2'	1:A:1413:G:C8	2.34	0.62
3:D:8:PRO:HB3	3:D:14:ARG:HB2	1.82	0.62
10:N:96:GLU:OE2	10:N:96:GLU:N	2.23	0.62
11:O:115:VAL:HG12	11:O:121:VAL:HG21	1.81	0.62
1:A:610:G:N2	1:A:619:G:H1'	2.14	0.61
1:A:2784:C:H2'	1:A:2785:C:H6	1.65	0.61
6:G:27:ASN:O	6:G:29:TRP:N	2.31	0.61
53:t:57:ARG:HH12	53:t:100:ILE:HD12	1.65	0.61
56:y:108:ASP:CG	56:y:137:LYS:NZ	2.58	0.61
1:A:1187:G:H5''	18:V:81:TYR:HE2	1.64	0.61
1:A:1798:U:H5''	3:D:260:ARG:HB3	1.81	0.61
34:a:536:C:H2'	34:a:537:G:C8	2.34	0.61
43:j:46:ARG:HB3	43:j:46:ARG:HH11	1.65	0.61
1:A:2781:A:H5''	1:A:2782:G:H5'	1.82	0.61
35:b:208:ILE:HA	35:b:211:ILE:HD12	1.83	0.61
38:e:31:LEU:HD23	38:e:45:PHE:HB2	1.82	0.61
56:y:12:PHE:H	56:y:12:PHE:HD2	1.44	0.61
1:A:1394:U:OP1	62:A:3772:HOH:O	2.16	0.61
4:E:56:PRO:C	4:E:58:ARG:H	2.09	0.61
14:R:22:ARG:HE	14:R:69:ASP:HA	1.65	0.61
15:S:69:VAL:HA	15:S:72:ALA:HB3	1.83	0.61
25:2:47:ASN:ND2	25:2:47:ASN:H	1.96	0.61
29:6:13:CYS:SG	29:6:47:THR:HG21	2.40	0.61
34:a:1348:U:H4'	42:i:120:ARG:HD2	1.82	0.61
41:h:16:ALA:O	41:h:19:VAL:HG23	2.00	0.61
56:y:228:ILE:HD13	56:y:230:ILE:HG23	1.83	0.61
21:Y:102:CYS:SG	21:Y:103:GLY:N	2.74	0.61
27:4:55:ARG:O	27:4:60:GLN:NE2	2.33	0.61
34:a:308:C:H2'	34:a:309:G:C8	2.32	0.61
34:a:953:G:N7	46:m:104:ARG:NH2	2.47	0.61
56:y:575:GLU:O	56:y:579:GLU:HG2	2.00	0.61
1:A:910:A:H2'	1:A:911:A:C8	2.35	0.61
1:A:1819:A:H4'	1:A:1820:U:H5''	1.82	0.61
1:A:1940:U:H4'	1:A:1941:C:H5'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:81:GLU:HB3	38:e:90:VAL:HG22	1.83	0.61
53:t:45:GLN:HA	53:t:91:LEU:HD22	1.83	0.61
56:y:376:VAL:HG21	56:y:457:ALA:CA	2.30	0.61
1:A:1095:A:C4'	56:y:426:GLN:HE22	2.13	0.61
1:A:1135:C:H3'	1:A:1137:G:OP1	2.00	0.61
1:A:1165:U:H2'	1:A:1166:C:H6	1.66	0.61
9:K:28:GLY:C	9:K:30:HIS:H	2.07	0.61
34:a:1191:A:OP1	36:c:4:LYS:NZ	2.34	0.61
34:a:1251:A:H4'	42:i:12:GLU:OE1	2.01	0.61
46:m:81:LEU:HD13	46:m:88:ARG:HG2	1.81	0.61
49:p:5:ARG:NH2	49:p:24:ALA:O	2.33	0.61
56:y:68:TYR:CE2	56:y:179:GLU:CB	2.84	0.61
56:y:164:ILE:C	56:y:165:PHE:HD1	2.09	0.61
1:A:271(J):C:N3	1:A:271(M):G:C6	2.68	0.61
1:A:1259:G:H2'	1:A:1260:G:C8	2.35	0.61
1:A:2431:U:OP2	62:A:3770:HOH:O	2.16	0.61
18:V:62:LEU:HD11	18:V:95:LEU:HB2	1.83	0.61
26:3:8:LEU:HD12	26:3:31:LEU:HA	1.83	0.61
33:x:25:C:O2'	33:x:26:A:O5'	2.18	0.61
35:b:185:ILE:HG22	35:b:199:TYR:HB2	1.82	0.61
52:s:63:THR:HG23	52:s:66:MET:HE3	1.82	0.61
56:y:432:ARG:O	56:y:455:PRO:HD2	2.01	0.61
1:A:2222:G:H2'	1:A:2223:G:C8	2.35	0.61
17:U:78:THR:O	17:U:81:HIS:N	2.33	0.61
27:4:61:ARG:HH21	27:4:63:TYR:HB2	1.64	0.61
34:a:598:U:H4'	41:h:94:TYR:CG	2.36	0.61
34:a:1314:C:OP2	52:s:4:SER:OG	2.19	0.61
56:y:15:ILE:CD1	56:y:103:VAL:CB	2.78	0.61
56:y:113:VAL:CG2	56:y:117:THR:HG21	2.30	0.61
56:y:434:ARG:HG2	56:y:434:ARG:HH11	1.65	0.61
1:A:2793:G:N2	1:A:2803:C:N3	2.49	0.61
3:D:146:GLU:HB2	3:D:189:CYS:HB3	1.83	0.61
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.81	0.61
40:g:73:MET:HG3	40:g:89:MET:O	2.01	0.61
42:i:45:ALA:HB2	42:i:51:ARG:NH2	2.16	0.61
51:r:44:LEU:HD11	51:r:79:LEU:HD13	1.82	0.61
1:A:651:G:OP1	31:8:19:SER:OG	2.09	0.60
6:G:25:TYR:OH	6:G:168:GLU:OE1	2.18	0.60
7:H:20:ALA:HB1	7:H:21:PRO:HD2	1.83	0.60
34:a:489:C:H2'	34:a:490:G:C8	2.36	0.60
34:a:737:A:H1'	39:f:73:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2331:G:H4'	23:O:43:THR:H	1.66	0.60
1:A:2394:C:OP2	31:8:30:ARG:NH1	2.33	0.60
16:T:100:TYR:HB3	16:T:103:ARG:HH12	1.65	0.60
34:a:1502:A:H2	34:a:1505:G:H1	1.48	0.60
40:g:97:GLN:O	40:g:101:LEU:HD23	1.99	0.60
1:A:226:G:N2	1:A:228:A:H62	1.97	0.60
1:A:1651:G:H5'	14:R:39:PRO:HG2	1.83	0.60
1:A:2104:G:H1	1:A:2185:C:H42	1.49	0.60
1:A:2638:G:N2	1:A:2775:A:H2'	2.17	0.60
27:4:24:THR:OG1	27:4:25:TYR:N	2.32	0.60
36:c:43:LEU:HD22	36:c:47:LEU:HD11	1.82	0.60
1:A:944:G:H5''	1:A:945:A:O5'	2.01	0.60
1:A:1341:U:O4	20:X:16:LYS:NZ	2.35	0.60
1:A:2124:G:H1	1:A:2174:C:N4	1.99	0.60
1:A:2820:A:OP2	14:R:2:ARG:NH2	2.35	0.60
11:O:89:ASN:O	11:O:91:LEU:HD23	2.00	0.60
24:1:85:LEU:HD23	24:1:90:ILE:HG12	1.82	0.60
36:c:53:ALA:HB2	36:c:115:LEU:HD13	1.82	0.60
43:j:61:GLU:OE2	47:n:45:ARG:NE	2.34	0.60
56:y:250:LEU:H	56:y:250:LEU:CD2	2.00	0.60
1:A:2419:U:O4	62:A:3774:HOH:O	2.17	0.60
10:N:58:ASP:HB3	10:N:124:ALA:HB1	1.82	0.60
20:X:92:LEU:O	20:X:94:GLY:N	2.32	0.60
22:Z:110:GLY:N	22:Z:144:LEU:O	2.35	0.60
33:x:15:G:H22	33:x:48:C:N4	1.96	0.60
56:y:17:HIS:O	56:y:20:HIS:CB	2.47	0.60
56:y:214:TYR:C	56:y:215:LEU:HG	2.27	0.60
56:y:417:PRO:CB	56:y:446:LYS:O	2.49	0.60
4:E:154:LYS:HD3	4:E:155:LYS:H	1.67	0.60
22:Z:10:ARG:HD3	22:Z:38:TYR:HB3	1.83	0.60
33:x:62:C:H2'	33:x:63:G:H8	1.66	0.60
34:a:737:A:H1'	39:f:73:ASN:ND2	2.15	0.60
34:a:1476:G:H2'	34:a:1477:C:C6	2.36	0.60
35:b:156:LYS:HG2	35:b:157:ARG:N	2.17	0.60
50:q:22:LEU:HD11	50:q:39:SER:HB2	1.83	0.60
1:A:285:C:H2'	1:A:286:C:H6	1.67	0.60
19:W:1:MET:HG3	19:W:2:GLU:H	1.66	0.60
27:4:66:SER:OG	27:4:67:TYR:N	2.34	0.60
34:a:624:C:H2'	34:a:625:G:H8	1.67	0.60
34:a:641:U:O2'	34:a:642:A:OP2	2.20	0.60
34:a:725:G:H2'	34:a:726:C:H6	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:w:73:A:C2	56:y:572:LYS:HG3	2.36	0.60
56:y:109:ALA:O	56:y:143:ALA:HB1	2.02	0.60
12:P:84:ASN:HA	12:P:115:LEU:O	2.02	0.60
20:X:35:THR:HG22	20:X:37:THR:H	1.66	0.60
37:d:8:VAL:O	37:d:11:LEU:HB2	2.01	0.60
40:g:27:ILE:HD12	40:g:40:ALA:HA	1.84	0.60
56:y:122:TYR:O	56:y:126:GLU:N	2.33	0.60
56:y:245:PHE:CA	56:y:251:VAL:H	2.12	0.60
56:y:479:TYR:HD2	56:y:479:TYR:H	1.50	0.60
1:A:1709:U:C2	1:A:1750:G:N2	2.70	0.60
3:D:67:PHE:HD2	3:D:153:ALA:HB3	1.66	0.60
6:G:6:ALA:HA	6:G:9:ARG:HB2	1.84	0.60
34:a:1060:C:C5	36:c:2:GLY:HA3	2.37	0.60
56:y:68:TYR:O	56:y:70:ALA:N	2.35	0.60
56:y:192:PRO:CA	56:y:258:ALA:HB2	2.07	0.60
1:A:577:G:H2'	1:A:578:A:C8	2.37	0.60
4:E:23:VAL:HG21	4:E:183:LEU:HD23	1.84	0.60
34:a:1446:U:H4'	34:a:1447:A:N7	2.17	0.60
48:o:24:SER:OG	48:o:25:THR:N	2.35	0.60
56:y:220:GLY:O	56:y:258:ALA:HB2	2.02	0.60
56:y:411:LYS:CA	56:y:452:TYR:C	2.73	0.60
1:A:184:C:H2'	1:A:185:U:C6	2.37	0.59
1:A:576:U:H2'	1:A:577:G:C8	2.36	0.59
1:A:620:G:N3	1:A:620:G:H5'	2.17	0.59
1:A:1054:A:N6	1:A:1105:U:H3	2.01	0.59
1:A:1466:G:O2'	1:A:1546:C:O2'	2.19	0.59
34:a:1015:A:H2'	34:a:1016:A:C8	2.37	0.59
1:A:2793:G:H1	1:A:2803:C:N4	2.00	0.59
34:a:1030:C:N4	34:a:1031:G:C6	2.64	0.59
53:t:64:ASP:O	53:t:66:ALA:N	2.32	0.59
1:A:2025:C:H2'	1:A:2026:C:H6	1.66	0.59
1:A:2107:C:N4	1:A:2182:G:H1	2.00	0.59
34:a:750:G:N3	48:o:23:GLY:HA3	2.17	0.59
36:c:164:ARG:HG2	36:c:165:THR:H	1.68	0.59
47:n:2:ALA:O	47:n:3:ARG:HB2	2.03	0.59
51:r:35:ARG:O	51:r:37:VAL:N	2.33	0.59
1:A:264:C:O2'	1:A:428:A:N1	2.36	0.59
1:A:2577:A:H5''	1:A:2578:G:H5'	1.84	0.59
25:2:30:ARG:HH21	25:2:34:GLU:HG3	1.67	0.59
33:x:15:G:N2	33:x:48:C:H42	1.99	0.59
34:a:262:A:C6	34:a:263:A:C6	2.91	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:3:ARG:HD2	37:d:118:ARG:HD3	1.83	0.59
52:s:23:ASN:HA	52:s:27:GLU:HG2	1.85	0.59
56:y:107:VAL:HG12	56:y:108:ASP:O	2.01	0.59
56:y:221:ARG:HB2	56:y:256:LEU:O	2.03	0.59
56:y:306:TYR:CE2	56:y:343:GLY:HA3	2.30	0.59
1:A:31:C:OP1	62:A:3776:HOH:O	2.17	0.59
3:D:184:LYS:HG3	3:D:271:ILE:HD11	1.84	0.59
36:c:52:LEU:HD21	36:c:55:VAL:HG22	1.84	0.59
56:y:172:GLU:C	56:y:174:VAL:N	2.58	0.59
1:A:1246:A:OP1	5:F:38:ARG:NH1	2.36	0.59
1:A:1652:A:OP1	14:R:8:ARG:NH1	2.31	0.59
5:F:155:LEU:HB2	5:F:189:THR:HG21	1.85	0.59
7:H:80:SER:OG	7:H:81:GLU:N	2.35	0.59
19:W:56:ALA:O	19:W:58:ALA:N	2.35	0.59
22:Z:52:SER:HG	22:Z:53:ILE:H	1.47	0.59
27:4:58:ARG:HH12	52:s:68:GLY:H	1.51	0.59
34:a:662:G:H2'	34:a:663:A:C8	2.37	0.59
46:m:67:GLU:O	46:m:69:GLU:N	2.36	0.59
49:p:19:ILE:HD13	49:p:36:ILE:HG13	1.83	0.59
56:y:68:TYR:CE2	56:y:179:GLU:CA	2.84	0.59
56:y:411:LYS:C	56:y:452:TYR:O	2.45	0.59
1:A:1441:G:O2'	1:A:1628:G:OP1	2.21	0.59
1:A:2201:C:H2'	1:A:2202:C:C6	2.38	0.59
1:A:2287:A:O2'	1:A:2288:A:H5''	2.02	0.59
1:A:2287:A:H62	1:A:2344:U:H3	1.49	0.59
6:G:5:VAL:HG13	27:4:25:TYR:HE1	1.68	0.59
10:N:128:HIS:O	10:N:128:HIS:ND1	2.35	0.59
26:3:21:ALA:O	26:3:24:LYS:N	2.34	0.59
34:a:1126:U:O2'	34:a:1127:G:OP1	2.20	0.59
56:y:540:ALA:HB2	56:y:545:ILE:HG23	1.85	0.59
4:E:5:LEU:HD11	4:E:79:ARG:HB2	1.85	0.59
4:E:11:MET:HE2	4:E:24:THR:HB	1.85	0.59
18:V:82:ARG:O	18:V:83:ARG:NH1	2.28	0.59
34:a:78:G:H1	34:a:91:C:N4	1.86	0.59
34:a:1375:A:H2'	34:a:1376:U:O4'	2.03	0.59
35:b:12:GLU:C	35:b:14:GLY:H	2.10	0.59
56:y:103:VAL:HG23	56:y:103:VAL:O	2.03	0.59
9:K:124:ALA:O	9:K:128:ALA:N	2.34	0.59
34:a:413:G:N7	37:d:35:ARG:NH1	2.50	0.59
35:b:24:TRP:H	35:b:24:TRP:CD1	2.21	0.59
35:b:28:PHE:CD1	35:b:190:THR:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:65:ARG:HG3	37:d:70:ILE:HG22	1.85	0.59
37:d:150:GLU:HG3	37:d:151:LYS:H	1.68	0.59
56:y:98:ALA:N	56:y:127:HIS:CE1	2.63	0.59
56:y:537:ILE:CG2	56:y:549:ALA:HB3	2.31	0.59
1:A:2879:C:OP2	62:A:3773:HOH:O	2.16	0.58
16:T:91:ARG:HB2	16:T:121:ILE:HG13	1.84	0.58
27:4:40:HIS:O	27:4:43:TYR:HB3	2.03	0.58
34:a:396:G:O2'	34:a:398:C:OP1	2.20	0.58
44:k:84:VAL:HG21	44:k:95:ILE:HD11	1.84	0.58
56:y:434:ARG:HH11	56:y:434:ARG:CG	2.15	0.58
1:A:271:A:N3	1:A:365:C:O2'	2.33	0.58
7:H:170:ARG:O	7:H:171:LEU:HD23	2.03	0.58
11:O:63:VAL:HG21	11:O:85:VAL:HG23	1.85	0.58
16:T:55:ASN:H	16:T:59:THR:HG22	1.67	0.58
22:Z:128:VAL:HG22	22:Z:132:ASN:HD22	1.67	0.58
56:y:304:GLY:CA	56:y:344:PHE:O	2.41	0.58
1:A:2074:U:OP1	62:A:3777:HOH:O	2.17	0.58
1:A:2144:U:H1'	1:A:2148:G:H22	1.68	0.58
7:H:7:LEU:HB3	7:H:69:ARG:NH1	2.18	0.58
11:O:10:VAL:HG21	11:O:16:ALA:HB3	1.84	0.58
34:a:254:G:H1'	50:q:15:MET:HG2	1.85	0.58
34:a:1277:C:O2'	34:a:1279:A:H8	1.86	0.58
56:y:172:GLU:O	56:y:174:VAL:N	2.35	0.58
1:A:1124:C:OP1	62:A:3775:HOH:O	2.17	0.58
1:A:2640:G:OP1	10:N:97:ARG:NH2	2.36	0.58
2:B:63:G:H2'	2:B:64:C:C6	2.39	0.58
4:E:49:LEU:HD23	4:E:81:ILE:HG12	1.86	0.58
34:a:1203:C:H2'	34:a:1204:A:H8	1.68	0.58
56:y:357:VAL:O	56:y:361:LEU:HD23	2.04	0.58
1:A:855:G:H1	1:A:922:U:H3	1.51	0.58
1:A:1470:G:O6	62:A:3766:HOH:O	2.15	0.58
6:G:43:LEU:HB2	6:G:89:GLY:HA2	1.85	0.58
11:O:73:ASP:OD1	16:T:32:TYR:OH	2.22	0.58
33:x:30:G:H21	40:g:144:MET:HE1	1.68	0.58
34:a:1144:G:N2	34:a:1146:A:H62	2.02	0.58
56:y:410:VAL:O	56:y:453:GLU:HA	2.04	0.58
1:A:493:G:H2'	1:A:494:G:O4'	2.03	0.58
1:A:577:G:O2'	1:A:1254:A:OP1	2.22	0.58
1:A:1094:U:H2'	1:A:1095:A:H3'	1.85	0.58
1:A:1105:U:H2'	1:A:1106:G:C8	2.38	0.58
1:A:1174:A:H5''	1:A:1177:A:H61	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:126:VAL:HG12	12:P:148:LEU:HD22	1.85	0.58
33:x:60:U:H5'	33:x:61:C:H5	1.69	0.58
34:a:737:A:H2'	34:a:738:C:C6	2.39	0.58
34:a:781:A:OP1	34:a:1523:G:H5'	2.04	0.58
56:y:-7:LYS:O	56:y:-3:GLU:HB2	2.03	0.58
1:A:537:C:H2'	1:A:538:G:H8	1.68	0.58
5:F:117:ARG:NH2	5:F:189:THR:O	2.36	0.58
8:J:26:LEU:O	8:J:114:GLY:N	2.34	0.58
19:W:17:VAL:O	19:W:20:VAL:HG23	2.02	0.58
19:W:67:ASP:OD2	19:W:67:ASP:N	2.30	0.58
34:a:1289:A:OP1	54:u:10:ARG:NH2	2.36	0.58
36:c:58:GLU:HB2	36:c:65:ALA:HB3	1.86	0.58
40:g:111:ARG:HD2	40:g:123:GLU:HB2	1.86	0.58
56:y:363:ARG:NH2	56:y:363:ARG:HB3	2.18	0.58
1:A:557:U:H2'	1:A:558:G:H8	1.69	0.58
1:A:590:A:H2'	1:A:591:C:C6	2.38	0.58
1:A:857:C:H4'	23:0:23:VAL:HG11	1.85	0.58
10:N:30:ILE:HG23	10:N:52:VAL:HG11	1.86	0.58
21:Y:35:TYR:CE2	21:Y:69:ALA:HB3	2.39	0.58
34:a:582:U:OP1	48:o:64:ARG:NH1	2.37	0.58
34:a:975:A:H4'	34:a:976:G:C5'	2.33	0.58
34:a:1170:A:H2'	34:a:1171:G:O4'	2.04	0.58
53:t:88:VAL:O	53:t:92:LEU:HG	2.02	0.58
56:y:214:TYR:O	56:y:215:LEU:HG	2.03	0.58
56:y:292:PRO:HG2	56:y:294:PHE:H	1.69	0.58
1:A:1507:A:O2'	1:A:1508:A:O5'	2.22	0.58
1:A:1721:G:H5'	1:A:1722:A:OP2	2.04	0.58
1:A:1876:A:H2'	1:A:1877:A:C8	2.39	0.58
1:A:2249:U:O4	62:A:3767:HOH:O	2.15	0.58
3:D:19:ALA:HB3	3:D:21:PHE:CE2	2.39	0.58
34:a:1316:G:H4'	47:n:18:VAL:HG13	1.86	0.58
41:h:41:ARG:NH1	41:h:123:GLU:OE2	2.36	0.58
1:A:29:U:H2'	1:A:30:G:C8	2.39	0.58
1:A:272(J):C:N3	1:A:363:G:N2	2.47	0.58
1:A:2888:C:H2'	1:A:2889:C:H6	1.69	0.58
6:G:54:GLU:O	6:G:57:ALA:N	2.37	0.58
8:J:73:GLY:O	8:J:75:GLN:N	2.29	0.58
14:R:103:ARG:HH12	14:R:110:PRO:HD3	1.69	0.58
35:b:16:HIS:C	35:b:16:HIS:CD2	2.81	0.58
47:n:2:ALA:HB3	47:n:6:LEU:HD22	1.85	0.58
56:y:15:ILE:HD12	56:y:103:VAL:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:131:ILE:HD11	56:y:158:LEU:CD2	2.33	0.58
1:A:528:A:C8	1:A:528:A:H3'	2.38	0.57
19:W:66:GLU:O	19:W:68:ARG:N	2.35	0.57
28:5:20:ARG:C	28:5:22:HIS:H	2.12	0.57
34:a:976:G:N2	34:a:1363:C:OP2	2.34	0.57
53:t:10:LEU:HB3	53:t:12:ALA:H	1.69	0.57
56:y:16:ALA:CB	56:y:106:VAL:O	2.51	0.57
34:a:931:C:N4	34:a:1386:G:H1	2.02	0.57
42:i:16:ARG:HB2	42:i:64:THR:HB	1.87	0.57
56:y:11:ASN:O	56:y:100:VAL:C	2.41	0.57
56:y:192:PRO:O	56:y:220:GLY:C	2.47	0.57
56:y:223:ARG:HG2	56:y:223:ARG:NH1	2.19	0.57
56:y:537:ILE:HD12	56:y:551:VAL:HG22	1.84	0.57
1:A:299:A:N1	1:A:322:A:O2'	2.31	0.57
1:A:590:A:H2'	1:A:591:C:H6	1.69	0.57
3:D:211:ARG:HG3	3:D:214:TRP:CZ3	2.39	0.57
5:F:9:ILE:HG21	5:F:125:LEU:HD22	1.86	0.57
19:W:66:GLU:HA	19:W:69:LEU:HD12	1.86	0.57
20:X:50:LYS:O	20:X:84:ALA:N	2.34	0.57
41:h:5:PRO:HA	41:h:8:ASP:HB3	1.85	0.57
56:y:533:PHE:N	56:y:533:PHE:CD1	2.72	0.57
34:a:652:U:O4	34:a:752:G:O2'	2.15	0.57
34:a:1497:G:H2'	34:a:1498:U:H5'	1.86	0.57
56:y:-67:LYS:HB3	56:y:-30:ALA:HB3	1.86	0.57
56:y:88:ASP:O	56:y:89:PHE:CB	2.53	0.57
56:y:449:GLU:HG2	56:y:450:LEU:H	1.65	0.57
1:A:589:C:H2'	1:A:590:A:C8	2.39	0.57
1:A:1419:A:O2'	1:A:1421:G:N7	2.36	0.57
3:D:73:VAL:O	3:D:75:ILE:N	2.34	0.57
15:S:15:ARG:O	15:S:19:LYS:HG2	2.03	0.57
26:3:8:LEU:HD21	26:3:23:LEU:HD21	1.87	0.57
33:x:58:A:HO2'	33:x:60:U:H5	1.53	0.57
34:a:734:G:N2	51:r:75:ILE:HD11	2.19	0.57
34:a:1305:G:H5''	54:u:4:GLY:HA3	1.87	0.57
36:c:11:ARG:HD3	36:c:15:THR:HG21	1.85	0.57
56:y:250:LEU:H	56:y:250:LEU:HD13	1.68	0.57
1:A:1020:A:N6	1:A:1142:U:OP2	2.38	0.57
1:A:1431:U:H2'	1:A:1432:C:H6	1.70	0.57
1:A:2287:A:N6	1:A:2344:U:H3	2.03	0.57
1:A:2327:A:H2'	1:A:2328:A:C8	2.38	0.57
9:K:26:ALA:HA	9:K:29:GLN:CD	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:56:ALA:O	19:W:59:VAL:N	2.37	0.57
22:Z:6:LYS:HA	22:Z:60:GLU:HB2	1.86	0.57
56:y:418:GLU:N	56:y:446:LYS:O	2.37	0.57
1:A:796:C:H2'	1:A:797:C:C6	2.40	0.57
1:A:1221(A):C:H2'	1:A:1222:C:H6	1.69	0.57
1:A:1639:U:O2'	1:A:1640:C:H5'	2.05	0.57
1:A:1673:U:OP1	62:A:3778:HOH:O	2.18	0.57
1:A:2096:U:H6	1:A:2096:U:OP1	1.88	0.57
1:A:2330:G:H4'	23:O:44:ARG:HH12	1.69	0.57
1:A:2790:A:H2'	1:A:2790:A:N3	2.19	0.57
12:P:52:GLU:OE1	12:P:55:ARG:NH1	2.38	0.57
15:S:67:ARG:HG3	15:S:100:ALA:HB1	1.86	0.57
22:Z:126:VAL:HG22	22:Z:163:LEU:HA	1.87	0.57
34:a:1144:G:H21	34:a:1146:A:H62	1.52	0.57
37:d:13:ARG:HB2	37:d:40:PRO:HD3	1.86	0.57
56:y:28:ARG:HA	56:y:31:GLU:CD	2.29	0.57
56:y:108:ASP:CB	56:y:137:LYS:NZ	2.45	0.57
56:y:521:VAL:CB	56:y:549:ALA:HB2	2.35	0.57
56:y:537:ILE:O	56:y:549:ALA:C	2.46	0.57
1:A:1370:C:HO2'	1:A:1811:G:HO2'	1.53	0.57
1:A:1598:C:H5'	20:X:36:LYS:HB2	1.87	0.57
1:A:2319:G:N2	15:S:3:ARG:HA	2.20	0.57
5:F:33:LEU:O	5:F:37:VAL:HG23	2.05	0.57
6:G:120:LEU:HD22	6:G:131:TYR:OH	2.04	0.57
12:P:38:GLN:NE2	12:P:45:LEU:HD23	2.20	0.57
21:Y:38:ILE:HG23	21:Y:66:PRO:HA	1.87	0.57
34:a:920:U:H2'	34:a:921:U:C6	2.40	0.57
56:y:-68:MET:SD	56:y:-68:MET:N	2.71	0.57
56:y:114:GLU:O	56:y:117:THR:HG22	2.05	0.57
56:y:231:TYR:CB	56:y:290:PRO:HG3	2.34	0.57
1:A:38:A:H2'	1:A:39:C:C6	2.39	0.57
1:A:84:A:N1	1:A:98:G:O2'	2.33	0.57
34:a:1072:G:H2'	34:a:1073:U:C6	2.40	0.57
38:e:106:PRO:O	38:e:110:LEU:HG	2.05	0.57
1:A:2095:C:N4	1:A:2096:U:O4	2.38	0.57
5:F:37:VAL:O	5:F:41:LEU:HD12	2.03	0.57
27:4:48:ARG:HA	27:4:48:ARG:CZ	2.34	0.57
33:x:15:G:O6	33:x:48:C:O2	2.23	0.57
34:a:148:G:H2'	34:a:149:A:H8	1.70	0.57
34:a:657:G:H4'	48:o:28:GLN:HG2	1.87	0.57
43:j:20:ALA:HA	43:j:23:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:16:ALA:HB1	56:y:106:VAL:O	2.04	0.57
56:y:152:VAL:O	56:y:156:LEU:N	2.38	0.57
56:y:230:ILE:HA	56:y:280:ILE:N	2.20	0.57
56:y:375:SER:OG	56:y:393:PRO:HD3	2.05	0.57
56:y:534:GLU:O	56:y:585:LYS:NZ	2.37	0.57
1:A:330:A:HO2'	1:A:331:A:H8	1.53	0.56
1:A:528:A:H3'	1:A:528:A:H8	1.70	0.56
1:A:743:G:N7	62:A:3828:HOH:O	2.33	0.56
1:A:984:A:H5''	1:A:985:C:H5	1.70	0.56
1:A:1057:A:H62	1:A:1086:A:H2'	1.70	0.56
1:A:1810:A:H2'	1:A:1811:G:O4'	2.05	0.56
1:A:2749:A:OP2	1:A:2750:A:O2'	2.19	0.56
33:x:33:U:C3'	33:x:34:G:H5''	2.35	0.56
34:a:1510:U:H2'	34:a:1511:G:C8	2.40	0.56
56:y:79:HIS:CD2	56:y:261:VAL:CB	2.88	0.56
56:y:201:PHE:CD2	56:y:202:ASP:N	2.73	0.56
1:A:84:A:H5''	21:Y:8:LYS:HG2	1.87	0.56
1:A:479:A:N3	1:A:481:G:H5''	2.20	0.56
1:A:1800:C:OP1	3:D:260:ARG:NH2	2.38	0.56
1:A:2101:G:H1	1:A:2188:C:N4	2.03	0.56
48:o:70:LEU:HG	48:o:78:TYR:HB2	1.86	0.56
56:y:77:VAL:O	56:y:78:PHE:HD1	1.87	0.56
1:A:66:C:C2	1:A:89:G:N2	2.74	0.56
1:A:652:C:H2'	1:A:652(A):A:H5''	1.87	0.56
1:A:1809:A:H2'	1:A:1810:A:C8	2.41	0.56
1:A:2455:G:H2'	1:A:2456:C:C6	2.41	0.56
1:A:2857:G:N2	1:A:2860:A:OP2	2.37	0.56
10:N:4:TYR:CD2	17:U:100:VAL:HG11	2.41	0.56
12:P:71:VAL:HG22	12:P:72:PRO:HA	1.87	0.56
17:U:76:TYR:HH	17:U:92:ARG:NH1	2.04	0.56
19:W:35:ILE:C	19:W:37:ARG:H	2.13	0.56
19:W:45:TYR:HD2	19:W:46:PHE:CD1	2.23	0.56
31:8:26:LYS:HE3	31:8:48:PHE:CG	2.39	0.56
34:a:187:C:O2	53:t:103:GLY:HA2	2.06	0.56
34:a:564:C:H5'	50:q:32:TYR:CE1	2.40	0.56
34:a:663:A:O3'	51:r:64:ARG:NH2	2.38	0.56
34:a:1130:A:OP2	34:a:1131:G:C8	2.58	0.56
41:h:23:SER:HA	41:h:61:VAL:O	2.05	0.56
56:y:535:VAL:HB	56:y:551:VAL:HB	1.88	0.56
1:A:2469:A:H4'	13:Q:56:ARG:HG3	1.88	0.56
1:A:2794:C:N4	1:A:2802:G:H1	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:46:LYS:HD3	12:P:51:PHE:CE1	2.40	0.56
33:x:33:U:H2'	33:x:34:G:H3'	1.86	0.56
33:x:38:A:C2'	33:x:39:PSU:H5''	2.35	0.56
40:g:14:PRO:HB3	40:g:19:GLY:O	2.06	0.56
56:y:164:ILE:HG22	56:y:165:PHE:H	1.70	0.56
1:A:1339:G:H5''	20:X:16:LYS:HD2	1.87	0.56
1:A:1794:U:H2'	1:A:1795:C:C6	2.41	0.56
1:A:2360:A:H1'	12:P:61:ARG:HH12	1.71	0.56
1:A:2619:C:H2'	1:A:2620:C:H6	1.70	0.56
16:T:106:SER:O	16:T:110:ILE:HG13	2.04	0.56
34:a:447:G:H2'	34:a:485:G:N2	2.21	0.56
34:a:751:U:H4'	48:o:24:SER:HA	1.87	0.56
37:d:162:LEU:HA	37:d:165:MET:HB2	1.88	0.56
33:w:53:G:H2'	33:w:54:5MU:C6	2.41	0.56
56:y:295:ARG:CB	56:y:296:PRO:HD2	2.35	0.56
1:A:1312:U:OP2	20:X:63:LYS:NZ	2.30	0.56
1:A:2849:U:O4	16:T:23:ARG:NH2	2.39	0.56
3:D:161:THR:HG22	3:D:178:PRO:HG3	1.87	0.56
14:R:29:LEU:HD12	14:R:83:ILE:HD13	1.87	0.56
17:U:108:GLU:O	17:U:112:ARG:HG2	2.05	0.56
22:Z:124:ILE:HD12	22:Z:155:LEU:HD21	1.87	0.56
34:a:1415:G:H2'	34:a:1416:G:H8	1.71	0.56
35:b:27:LYS:HB3	35:b:194:PRO:HG2	1.88	0.56
56:y:-28:GLU:HA	56:y:-25:LEU:HB2	1.88	0.56
56:y:15:ILE:HD11	56:y:103:VAL:CB	2.35	0.56
56:y:158:LEU:HB3	56:y:159:PRO:HD2	1.86	0.56
56:y:492:VAL:HB	56:y:506:PHE:HE2	1.70	0.56
1:A:782:A:N1	3:D:226:MET:HE2	2.20	0.56
1:A:910:A:C6	1:A:911:A:C6	2.93	0.56
1:A:1933:G:N2	1:A:1968:G:H1'	2.21	0.56
1:A:2230:G:H2'	1:A:2231:C:C6	2.41	0.56
1:A:2428:G:H4'	1:A:2429:G:O5'	2.06	0.56
3:D:211:ARG:HG3	3:D:214:TRP:CE3	2.40	0.56
28:5:20:ARG:O	28:5:22:HIS:N	2.38	0.56
34:a:564:C:H5'	50:q:32:TYR:HE1	1.70	0.56
34:a:695:A:H2'	34:a:696:A:C8	2.41	0.56
37:d:58:LEU:HD23	37:d:206:PHE:CE2	2.41	0.56
37:d:139:ARG:HG2	37:d:139:ARG:NH1	2.15	0.56
56:y:11:ASN:H	56:y:101:GLU:HB2	1.68	0.56
1:A:2115:G:H2'	1:A:2116:G:H5''	1.88	0.56
1:A:2343:C:H2'	1:A:2344:U:H6	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:124:PRO:HB2	3:D:126:GLN:HB2	1.87	0.56
6:G:7:LEU:HD12	6:G:104:GLU:HA	1.87	0.56
13:Q:133:ARG:O	13:Q:135:ASP:N	2.38	0.56
21:Y:15:VAL:HG21	21:Y:42:VAL:HG11	1.87	0.56
34:a:232:G:H2'	34:a:233:C:C6	2.40	0.56
38:e:8:GLU:HA	38:e:33:VAL:O	2.06	0.56
50:q:3:LYS:HB3	50:q:61:GLU:HB3	1.88	0.56
1:A:139(A):G:N2	20:X:44:GLU:OE1	2.33	0.56
1:A:1843:C:H5'	3:D:253:GLN:NE2	2.20	0.56
1:A:2125:G:H21	1:A:2173:A:N6	1.99	0.56
1:A:2415:G:O3'	12:P:66:GLY:HA2	2.06	0.56
29:6:16:CYS:SG	29:6:18:ARG:NH1	2.78	0.56
34:a:77:G:O6	34:a:78:G:N2	2.38	0.56
34:a:333:G:H4'	53:t:16:HIS:HE1	1.70	0.56
34:a:501:C:H2'	34:a:502:G:C8	2.41	0.56
34:a:837:G:H1	34:a:849:C:H42	1.53	0.56
56:y:292:PRO:HG2	56:y:294:PHE:N	2.21	0.56
56:y:545:ILE:HD13	56:y:545:ILE:N	2.20	0.56
1:A:292:C:H2'	1:A:293:U:C6	2.40	0.56
1:A:2024:G:H2'	1:A:2025:C:H6	1.71	0.56
3:D:182:LEU:O	3:D:271:ILE:N	2.36	0.56
34:a:976:G:OP2	34:a:1358:U:O2'	2.23	0.56
34:a:986:A:H1'	52:s:54:GLY:O	2.06	0.56
37:d:19:LEU:HB3	37:d:67:ILE:HG13	1.87	0.56
38:e:98:THR:HG22	38:e:99:GLY:O	2.06	0.56
43:j:53:PRO:HA	47:n:42:ILE:HD11	1.88	0.56
56:y:331:THR:H	56:y:346:CYS:CB	2.19	0.56
56:y:449:GLU:CG	56:y:450:LEU:N	2.65	0.56
56:y:502:ASP:O	56:y:505:THR:OG1	2.22	0.56
1:A:2056:G:N2	28:5:4:HIS:O	2.37	0.55
1:A:2502:G:H5''	1:A:2503:A:C5'	2.36	0.55
6:G:62:LEU:HD23	6:G:143:GLU:HB2	1.87	0.55
7:H:96:ALA:HB2	7:H:105:LEU:HD13	1.86	0.55
43:j:43:ARG:HB2	43:j:67:THR:HG23	1.88	0.55
56:y:-64:LEU:HD12	56:y:-64:LEU:H	1.71	0.55
56:y:304:GLY:HA2	56:y:344:PHE:C	2.25	0.55
1:A:1061:U:O2'	1:A:1063:G:OP2	2.24	0.55
1:A:2512:C:H4'	4:E:122:PHE:CE2	2.42	0.55
35:b:19:HIS:CE1	35:b:206:ASP:HB2	2.41	0.55
1:A:192:C:H2'	1:A:193:U:H5'	1.87	0.55
1:A:263:C:H2'	1:A:264:C:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:A:O2'	1:A:331:A:H8	1.88	0.55
1:A:539:G:H2'	1:A:540:C:C6	2.41	0.55
1:A:2248:C:H2'	1:A:2249:U:H5'	1.87	0.55
15:S:31:SER:OG	15:S:32:LEU:N	2.40	0.55
15:S:52:SER:O	15:S:55:ALA:N	2.39	0.55
34:a:7:G:H21	38:e:121:LYS:HG3	1.72	0.55
34:a:48:C:H5''	34:a:365:U:O4	2.06	0.55
34:a:1127:G:H4'	34:a:1148:U:O2	2.06	0.55
47:n:27:CYS:SG	47:n:29:ARG:HB2	2.47	0.55
1:A:480:A:H2	1:A:499:U:O2	1.88	0.55
1:A:2199:A:H5''	1:A:2200:C:H5	1.71	0.55
4:E:105:THR:O	4:E:196:VAL:HG23	2.06	0.55
16:T:35:LYS:NZ	16:T:37:GLY:HA2	2.21	0.55
33:x:19:G:H4'	33:x:20:U:OP2	2.06	0.55
34:a:509:A:C8	34:a:509:A:H3'	2.40	0.55
40:g:28:ASN:HD21	40:g:36:LYS:NZ	2.03	0.55
50:q:45:HIS:NE2	50:q:47:PRO:HG3	2.21	0.55
56:y:108:ASP:OD2	56:y:137:LYS:HG3	2.07	0.55
56:y:358:GLN:O	56:y:359:GLU:C	2.49	0.55
1:A:604:G:H2'	1:A:605:C:H6	1.71	0.55
1:A:2257:U:O2'	1:A:2258:C:H5'	2.07	0.55
7:H:7:LEU:HB3	7:H:69:ARG:HH11	1.71	0.55
34:a:1124:G:N3	34:a:1127:G:N2	2.52	0.55
41:h:81:HIS:ND1	41:h:138:TRP:OXT	2.38	0.55
48:o:16:ALA:HB1	48:o:21:ASP:HB3	1.88	0.55
56:y:108:ASP:C	56:y:136:ASN:O	2.47	0.55
1:A:1062:G:H1	1:A:1076:C:H42	1.55	0.55
1:A:2286:A:H4'	1:A:2287:A:O5'	2.05	0.55
3:D:38:LYS:HE3	3:D:39:LYS:O	2.06	0.55
3:D:67:PHE:CD2	3:D:153:ALA:HB3	2.42	0.55
14:R:79:LEU:HD23	14:R:83:ILE:HB	1.88	0.55
22:Z:182:LYS:O	22:Z:184:ALA:N	2.40	0.55
28:5:40:LYS:NZ	28:5:41:PRO:O	2.28	0.55
34:a:261:U:OP2	53:t:79:ARG:NH2	2.40	0.55
34:a:1387:G:C6	34:a:1388:C:N4	2.75	0.55
39:f:69:GLU:O	39:f:71:ARG:N	2.38	0.55
56:y:369:LEU:CG	56:y:370:ILE:N	2.62	0.55
56:y:373:ALA:CB	56:y:374:PRO:HA	2.25	0.55
1:A:1268:A:C2	1:A:2013:A:C4	2.95	0.55
1:A:2788:C:O2'	1:A:2809:A:O2'	2.24	0.55
18:V:30:GLY:H	18:V:61:VAL:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:376:G:H4'	49:p:5:ARG:HD3	1.89	0.55
42:i:45:ALA:HB1	42:i:47:LEU:H	1.72	0.55
44:k:58:PRO:HG3	44:k:89:ALA:O	2.07	0.55
50:q:48:GLU:O	50:q:50:LYS:N	2.40	0.55
56:y:143:ALA:O	56:y:145:PRO:CD	2.48	0.55
56:y:214:TYR:C	56:y:215:LEU:CG	2.79	0.55
56:y:418:GLU:HA	56:y:446:LYS:HA	1.88	0.55
1:A:372:G:H3'	24:l:66:HIS:CE1	2.41	0.55
1:A:2144:U:H1'	1:A:2148:G:N2	2.21	0.55
1:A:2224:G:H4'	1:A:2226:C:C2	2.42	0.55
1:A:2537:U:H2'	1:A:2538:C:H6	1.71	0.55
3:D:43:ARG:CZ	3:D:49:ILE:HD11	2.36	0.55
4:E:101:ARG:NH1	4:E:169:ASN:O	2.39	0.55
11:O:19:ILE:HG22	11:O:43:VAL:HA	1.88	0.55
27:4:61:ARG:NH2	27:4:63:TYR:HB2	2.22	0.55
34:a:803:G:OP1	62:a:3513:HOH:O	2.18	0.55
34:a:1338:G:H2'	34:a:1339:A:C8	2.42	0.55
1:A:2270:G:H2'	1:A:2271:G:C8	2.42	0.55
4:E:37:ARG:HD2	4:E:44:TYR:OH	2.06	0.55
27:4:41:PRO:HA	27:4:44:THR:OG1	2.07	0.55
34:a:501:C:H2'	34:a:502:G:H8	1.72	0.55
34:a:663:A:H61	34:a:742:G:H1	1.52	0.55
34:a:946:A:H2'	34:a:947:G:C8	2.41	0.55
36:c:156:ARG:HH21	36:c:161:GLU:HA	1.72	0.55
36:c:191:THR:HG21	36:c:196:LEU:HD23	1.88	0.55
45:l:70:ILE:HG12	45:l:77:LEU:HD12	1.89	0.55
53:t:33:ILE:HG13	53:t:62:LEU:HB3	1.89	0.55
56:y:164:ILE:HG22	56:y:165:PHE:N	2.22	0.55
56:y:497:HIS:CA	56:y:536:PRO:O	2.55	0.55
1:A:680:G:H2'	1:A:681:G:C8	2.42	0.55
1:A:2751:G:H4'	7:H:4:ILE:HD11	1.89	0.55
11:O:25:LEU:HD12	11:O:38:VAL:HG12	1.87	0.55
53:t:9:ASN:O	53:t:10:LEU:HB2	2.07	0.55
56:y:68:TYR:CD1	56:y:68:TYR:C	2.85	0.55
56:y:89:PHE:O	56:y:90:THR:HG23	2.07	0.55
1:A:2025:C:C2	1:A:2026:C:C5	2.95	0.54
1:A:2419:U:P	31:8:33:ASN:HD22	2.30	0.54
5:F:33:LEU:HB3	12:P:6:LEU:HD21	1.89	0.54
34:a:16:A:C6	34:a:17:U:C5	2.95	0.54
34:a:833:U:H2'	34:a:834:C:C6	2.43	0.54
48:o:17:ARG:HB3	48:o:17:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:213:PRO:HD2	56:y:264:LEU:N	2.21	0.54
1:A:139(A):G:H2'	1:A:140:G:C8	2.41	0.54
1:A:2203:U:O2'	1:A:2205:C:H5'	2.07	0.54
1:A:2279:G:OP2	23:0:11:ARG:NH1	2.41	0.54
3:D:27:THR:OG1	3:D:28:GLU:N	2.41	0.54
5:F:172:TRP:CD1	5:F:172:TRP:H	2.22	0.54
11:O:108:GLU:H	11:O:108:GLU:CD	2.15	0.54
16:T:35:LYS:HD3	16:T:37:GLY:H	1.71	0.54
17:U:102:GLU:HB3	17:U:105:VAL:HB	1.89	0.54
30:7:43:THR:HG23	30:7:44:PRO:HD2	1.89	0.54
33:x:63:G:H2'	33:x:64:A:O4'	2.08	0.54
34:a:201:C:H2'	34:a:202:U:H5''	1.89	0.54
34:a:256:U:H2'	34:a:257:G:C8	2.43	0.54
34:a:1257:U:O2	34:a:1257:U:H2'	2.06	0.54
40:g:18:TYR:CD2	40:g:59:LEU:HD12	2.43	0.54
42:i:17:VAL:HG11	42:i:81:ILE:HG13	1.89	0.54
45:l:88:GLY:O	45:l:99:HIS:HD2	1.88	0.54
46:m:3:ARG:HB3	46:m:8:GLU:H	1.72	0.54
56:y:424:LEU:O	56:y:425:MET:C	2.48	0.54
1:A:2134:A:OP2	1:A:2156:G:N1	2.40	0.54
5:F:63:LYS:HA	5:F:76:GLY:O	2.08	0.54
6:G:32:PRO:HB3	6:G:163:ALA:HB2	1.89	0.54
11:O:63:VAL:HG13	11:O:106:LEU:HD11	1.90	0.54
23:0:23:VAL:HG13	23:0:26:TYR:HE2	1.72	0.54
24:1:24:ALA:O	24:1:27:GLU:N	2.41	0.54
26:3:32:GLN:HA	26:3:32:GLN:HE21	1.71	0.54
34:a:1080:A:H5'	38:e:14:ARG:HH21	1.73	0.54
35:b:54:THR:O	35:b:58:ILE:HG13	2.06	0.54
37:d:173:TRP:CD2	37:d:189:PRO:HG3	2.42	0.54
1:A:477:A:H2'	1:A:478:A:C8	2.42	0.54
1:A:1021:A:C8	1:A:1021:A:C3'	2.89	0.54
1:A:1063:G:O2'	9:K:87:GLY:HA3	2.06	0.54
1:A:1413:G:H2'	1:A:1414:G:H8	1.71	0.54
1:A:2100:G:N3	1:A:2190:G:N2	2.56	0.54
1:A:2554:U:H2'	1:A:2555:U:C6	2.42	0.54
1:A:2721:A:N7	62:A:3830:HOH:O	2.33	0.54
3:D:34:VAL:HG12	3:D:62:TYR:O	2.07	0.54
15:S:39:ILE:HB	15:S:49:VAL:HG13	1.89	0.54
17:U:44:ASN:HD21	18:V:75:PHE:H	1.55	0.54
31:8:31:HIS:CD2	31:8:32:LEU:HD22	2.43	0.54
34:a:407:G:H2'	34:a:408:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:140:LEU:HB2	61:y:703:GDP:N2	2.22	0.54
1:A:692:C:O2'	3:D:38:LYS:HE2	2.07	0.54
1:A:2867:G:OP2	16:T:119:LYS:NZ	2.40	0.54
3:D:30:GLU:HB3	3:D:33:LEU:HD12	1.90	0.54
5:F:41:LEU:HA	5:F:44:ARG:HG2	1.89	0.54
19:W:40:ASN:O	19:W:41:LYS:HD3	2.08	0.54
33:x:60:U:H5''	33:x:61:C:C5	2.43	0.54
39:f:8:ILE:HD11	39:f:79:LEU:HD13	1.90	0.54
47:n:25:VAL:HG22	47:n:38:GLY:O	2.07	0.54
56:y:291:TYR:CB	56:y:292:PRO:CA	2.85	0.54
56:y:331:THR:H	56:y:346:CYS:HB3	1.72	0.54
1:A:353:G:H2'	1:A:354:G:H8	1.73	0.54
1:A:1028:A:N6	1:A:1125:G:H2'	2.22	0.54
1:A:1266:G:O5'	19:W:15:ARG:NH2	2.40	0.54
1:A:1291:C:H2'	1:A:1292:U:C6	2.42	0.54
1:A:2312:U:H5'	6:G:88:ILE:HD11	1.88	0.54
1:A:2749:A:H1'	7:H:63:SER:OG	2.07	0.54
12:P:85:LEU:HG	12:P:116:GLY:HA2	1.88	0.54
20:X:89:ILE:HG22	20:X:92:LEU:H	1.73	0.54
35:b:82:ARG:HD2	35:b:83:MET:HE2	1.90	0.54
35:b:219:VAL:O	35:b:222:ILE:HB	2.08	0.54
41:h:38:ILE:HD12	41:h:111:ILE:HG23	1.90	0.54
43:j:15:THR:O	43:j:19:SER:HB2	2.08	0.54
48:o:78:TYR:C	48:o:80:ALA:H	2.15	0.54
56:y:221:ARG:CB	56:y:257:GLU:HA	2.38	0.54
1:A:254:G:O6	31:8:5:LYS:HD3	2.08	0.54
1:A:264:C:O2	62:A:3769:HOH:O	2.16	0.54
1:A:510:C:H2'	1:A:511:U:O4'	2.07	0.54
1:A:2385:C:H2'	1:A:2386:C:H6	1.73	0.54
1:A:2749:A:H4'	7:H:62:LYS:HG2	1.90	0.54
2:B:18:G:H2'	2:B:19:G:H8	1.72	0.54
3:D:121:PRO:HB3	3:D:135:PHE:HE1	1.73	0.54
15:S:28:VAL:HG21	15:S:98:VAL:HG13	1.89	0.54
18:V:56:SER:H	18:V:100:ARG:HB2	1.72	0.54
27:4:68:ARG:NH2	27:4:69:LYS:O	2.41	0.54
34:a:266:G:O3'	50:q:67:LYS:HB2	2.07	0.54
34:a:667:G:H4'	48:o:51:HIS:ND1	2.22	0.54
34:a:1277:C:H1'	34:a:1282:C:O2	2.07	0.54
35:b:17:PHE:HD1	35:b:18:GLY:N	2.06	0.54
39:f:44:GLY:HA2	39:f:59:TYR:CZ	2.42	0.54
45:l:54:LYS:HD3	45:l:54:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:85:GLY:O	56:y:86:HIS:CB	2.53	0.54
56:y:164:ILE:C	56:y:165:PHE:CD1	2.85	0.54
1:A:321:G:O2'	1:A:340:A:N3	2.41	0.54
1:A:715:G:H2'	1:A:716:A:O4'	2.07	0.54
1:A:998:C:OP2	17:U:92:ARG:NH2	2.41	0.54
1:A:2716:U:O2'	1:A:2717:G:H5'	2.07	0.54
5:F:13:SER:C	5:F:15:SER:H	2.16	0.54
16:T:16:ARG:NH2	16:T:83:ILE:O	2.30	0.54
20:X:67:GLY:C	20:X:69:TYR:H	2.16	0.54
22:Z:67:LEU:HD23	22:Z:68:PRO:HD2	1.90	0.54
34:a:1189:C:O2	62:a:3512:HOH:O	2.18	0.54
44:k:120:ARG:HH22	44:k:126:ARG:NH1	2.06	0.54
45:l:60:LEU:HD23	45:l:66:VAL:HG13	1.90	0.54
56:y:183:GLN:O	56:y:184:ARG:C	2.50	0.54
1:A:1553:A:O2'	1:A:1554:A:H8	1.90	0.54
1:A:2096:U:H2'	1:A:2097:C:H6	1.73	0.54
1:A:2141:G:H2'	1:A:2142:C:O4'	2.08	0.54
36:c:6:HIS:CD2	36:c:7:PRO:HD2	2.42	0.54
37:d:176:LEU:HD12	37:d:182:LYS:O	2.08	0.54
56:y:11:ASN:O	56:y:100:VAL:CA	2.56	0.54
56:y:230:ILE:HG13	56:y:234:GLY:O	2.06	0.54
1:A:52:A:N1	1:A:178:G:O2'	2.38	0.54
1:A:1079:C:H4'	9:K:132:ARG:HH22	1.73	0.54
3:D:77:ALA:HB3	3:D:117:VAL:HG23	1.88	0.54
3:D:125:ILE:HG13	3:D:137:PRO:HG2	1.90	0.54
6:G:126:ASP:OD2	6:G:130:ASN:HB2	2.06	0.54
9:K:14:ALA:HA	9:K:41:PHE:HE2	1.72	0.54
24:1:60:PHE:HE1	24:1:91:LYS:HG3	1.73	0.54
1:A:484:C:H42	1:A:496:G:H1	1.55	0.53
1:A:531:C:OP1	1:A:561:G:N1	2.41	0.53
1:A:1507:A:O2'	1:A:1508:A:O4'	2.27	0.53
1:A:2103:C:N3	1:A:2186:G:O6	2.41	0.53
4:E:152:LYS:HG2	10:N:78:TYR:CZ	2.43	0.53
10:N:15:LEU:HD12	10:N:137:LYS:HG2	1.89	0.53
10:N:30:ILE:O	10:N:34:LEU:HB2	2.09	0.53
15:S:64:GLU:HA	15:S:67:ARG:HB2	1.89	0.53
27:4:68:ARG:HA	27:4:68:ARG:NE	2.23	0.53
34:a:536:C:H2'	34:a:537:G:H8	1.72	0.53
34:a:1318:A:H5''	52:s:3:ARG:HH21	1.72	0.53
41:h:101:PRO:HG3	41:h:133:LEU:HD11	1.89	0.53
42:i:26:VAL:HG13	42:i:61:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:l:117:ARG:NH2	45:l:124:LYS:HB2	2.24	0.53
50:q:45:HIS:HB2	50:q:65:ILE:HD13	1.89	0.53
51:r:69:THR:HA	51:r:72:ARG:HB2	1.91	0.53
56:y:300:VAL:C	56:y:347:GLY:CA	2.79	0.53
56:y:468:LYS:O	56:y:472:ARG:N	2.41	0.53
1:A:644:A:H4'	1:A:645:C:C5	2.43	0.53
1:A:1259:G:H2'	1:A:1260:G:H8	1.73	0.53
1:A:1803:A:O2'	3:D:259:THR:HG21	2.08	0.53
1:A:1943:U:OP1	56:y:581:LYS:NZ	2.28	0.53
2:B:17:C:N4	2:B:68:C:H42	2.01	0.53
3:D:89:SER:HB2	3:D:159:ALA:HB2	1.90	0.53
11:O:48:PRO:HB3	34:a:1422:G:H5'	1.90	0.53
34:a:9:G:N2	34:a:10:A:C4	2.76	0.53
33:w:44:G:H3'	33:w:45:U:C6	2.43	0.53
56:y:201:PHE:HD2	56:y:202:ASP:CB	2.21	0.53
1:A:491:G:H2'	1:A:492:A:C8	2.42	0.53
15:S:13:ARG:O	15:S:15:ARG:N	2.36	0.53
24:1:18:ILE:HG12	24:1:37:ILE:HG23	1.90	0.53
25:2:9:GLN:HE22	25:2:56:GLN:HB3	1.74	0.53
56:y:509:HIS:HB2	56:y:512:LYS:CE	2.35	0.53
56:y:509:HIS:CB	56:y:512:LYS:HE2	2.33	0.53
1:A:2521:C:O2'	1:A:2564:A:N3	2.41	0.53
37:d:177:ASP:HB3	37:d:182:LYS:HG2	1.89	0.53
38:e:41:VAL:HG23	38:e:67:VAL:HG13	1.90	0.53
50:q:53:LEU:HG	50:q:54:GLY:H	1.74	0.53
56:y:-66:VAL:HG22	56:y:-50:VAL:O	2.08	0.53
56:y:431:LYS:CB	56:y:462:ASP:OD1	2.56	0.53
1:A:271(A):A:H2	1:A:272(D):G:N3	2.07	0.53
1:A:924:C:H2'	1:A:925:C:C6	2.44	0.53
2:B:7:G:H4'	15:S:29:PHE:CD1	2.43	0.53
3:D:69:ARG:NH2	3:D:128:GLY:O	2.41	0.53
4:E:116:VAL:HG11	4:E:138:PRO:HB3	1.91	0.53
20:X:40:LYS:HG3	20:X:51:VAL:HG12	1.89	0.53
34:a:794:A:H2'	34:a:795:C:C6	2.43	0.53
34:a:858:G:O2'	34:a:859:A:H5''	2.09	0.53
34:a:1327:C:OP2	54:u:12:LYS:NZ	2.41	0.53
35:b:18:GLY:HA2	35:b:42:ILE:HG13	1.91	0.53
35:b:145:LEU:O	35:b:149:LEU:HB2	2.08	0.53
56:y:98:ALA:HA	56:y:127:HIS:CE1	2.43	0.53
56:y:107:VAL:O	56:y:136:ASN:CA	2.56	0.53
56:y:266:ALA:O	56:y:267:ALA:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:340:LEU:HD22	56:y:341:GLY:O	2.09	0.53
1:A:7:G:H4'	10:N:13:TRP:CH2	2.43	0.53
1:A:1020:A:N1	1:A:1141:U:O2'	2.38	0.53
1:A:2101:G:N2	1:A:2188:C:N3	2.53	0.53
1:A:2787:C:H1'	4:E:62:PRO:HG3	1.91	0.53
3:D:16:MET:HE1	3:D:208:LYS:HE3	1.91	0.53
7:H:76:VAL:C	7:H:78:GLY:H	2.16	0.53
13:Q:66:ILE:HG23	13:Q:104:PHE:HD2	1.74	0.53
21:Y:2:ARG:NH1	21:Y:4:LYS:HA	2.23	0.53
33:x:30:G:N2	40:g:144:MET:HE1	2.23	0.53
34:a:369:C:H6	34:a:369:C:H5'	1.72	0.53
35:b:59:GLU:HB2	35:b:221:LEU:HD21	1.91	0.53
46:m:86:CYS:HB2	52:s:74:PHE:CE1	2.43	0.53
51:r:21:LYS:HD3	51:r:57:GLY:HA3	1.90	0.53
51:r:36:ASN:CG	51:r:39:VAL:HB	2.34	0.53
56:y:68:TYR:CD1	56:y:70:ALA:CA	2.90	0.53
56:y:193:GLU:HA	56:y:221:ARG:CD	2.37	0.53
56:y:223:ARG:HH11	56:y:223:ARG:CG	2.21	0.53
56:y:379:LYS:H	56:y:406:LEU:CA	2.21	0.53
56:y:393:PRO:HB3	56:y:507:ILE:HD13	1.91	0.53
3:D:139:GLY:H	3:D:165:ILE:HB	1.73	0.53
33:x:38:A:H2'	33:x:39:PSU:H5''	1.91	0.53
34:a:729:A:H2'	34:a:730:G:H8	1.74	0.53
34:a:881:G:P	45:l:12:ARG:HH22	2.31	0.53
34:a:986:A:H2'	34:a:987:G:O4'	2.08	0.53
41:h:112:LEU:HA	41:h:134:ILE:HG12	1.90	0.53
56:y:68:TYR:C	56:y:68:TYR:HD1	2.17	0.53
56:y:410:VAL:CB	56:y:481:GLN:O	2.57	0.53
1:A:12:U:O2	1:A:12:U:H2'	2.09	0.53
1:A:464:U:H4'	30:7:5:TRP:CZ3	2.44	0.53
1:A:607:U:OP1	5:F:102:PRO:HA	2.09	0.53
1:A:828:U:O2'	1:A:829:A:H5'	2.08	0.53
1:A:1171:G:O6	1:A:1178:C:N3	2.41	0.53
1:A:1265:A:H8	1:A:1265:A:OP1	1.92	0.53
1:A:1882:C:H2'	1:A:1883:G:O4'	2.09	0.53
3:D:221:VAL:HG23	3:D:226:MET:HE3	1.89	0.53
6:G:77:ILE:HD12	6:G:82:LEU:HD11	1.91	0.53
13:Q:35:VAL:O	13:Q:129:THR:HG22	2.09	0.53
24:1:85:LEU:HD13	24:1:85:LEU:H	1.74	0.53
32:9:32:HIS:O	32:9:34:GLN:HG3	2.09	0.53
34:a:924:C:O2'	34:a:1502:A:N6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:r:51:LEU:HD22	51:r:55:ARG:HD3	1.91	0.53
56:y:215:LEU:N	56:y:215:LEU:CD1	2.72	0.53
56:y:221:ARG:HB3	56:y:257:GLU:HA	1.91	0.53
56:y:331:THR:N	56:y:346:CYS:HB3	2.24	0.53
56:y:403:GLU:O	56:y:403:GLU:HG2	2.08	0.53
1:A:1364:G:OP2	24:1:3:LYS:HG3	2.08	0.53
3:D:221:VAL:CG2	3:D:226:MET:HE3	2.38	0.53
4:E:92:THR:O	4:E:95:ILE:HG23	2.09	0.53
34:a:7:G:H5'	34:a:298:A:O4'	2.08	0.53
34:a:376:G:H5''	49:p:5:ARG:HB2	1.91	0.53
56:y:192:PRO:CB	56:y:258:ALA:H	2.22	0.53
56:y:310:SER:N	56:y:311:GLY:CA	2.72	0.53
56:y:355:GLU:O	56:y:359:GLU:HB2	2.07	0.53
56:y:499:GLU:O	56:y:500:VAL:C	2.51	0.53
1:A:390:A:H4'	1:A:391:G:H5'	1.91	0.53
1:A:1041:C:H42	1:A:1114:G:H22	1.57	0.53
3:D:65:ILE:HD11	3:D:92:ILE:HG21	1.91	0.53
13:Q:65:PHE:HB2	13:Q:105:GLU:HB2	1.91	0.53
14:R:12:ARG:HD2	14:R:20:LEU:HD22	1.91	0.53
22:Z:108:PRO:HB3	22:Z:144:LEU:HB2	1.91	0.53
23:O:50:ASN:ND2	23:O:81:VAL:O	2.34	0.53
34:a:265:G:H5'	50:q:64:PRO:O	2.09	0.53
34:a:1446:U:H4'	34:a:1447:A:C8	2.44	0.53
35:b:97:TRP:CZ2	35:b:102:LEU:HD12	2.44	0.53
38:e:18:ARG:HG2	38:e:19:MET:H	1.73	0.53
38:e:31:LEU:HD22	38:e:43:LEU:HD11	1.91	0.53
41:h:13:ILE:O	41:h:17:THR:HG23	2.09	0.53
56:y:-66:VAL:HG23	56:y:-50:VAL:HG13	1.91	0.53
56:y:12:PHE:HD2	56:y:12:PHE:N	2.05	0.53
56:y:24:THR:HG21	61:y:703:GDP:H5''	1.90	0.53
1:A:86:C:H42	1:A:96:G:H1	1.57	0.52
1:A:278:A:O2'	1:A:279:C:OP1	2.25	0.52
1:A:1131:G:C4	10:N:75:TYR:HB2	2.44	0.52
1:A:2406:U:H2'	1:A:2406:U:OP2	2.09	0.52
15:S:66:ALA:HA	15:S:69:VAL:HG12	1.92	0.52
19:W:24:ILE:O	19:W:26:GLY:N	2.42	0.52
20:X:67:GLY:O	20:X:69:TYR:N	2.34	0.52
35:b:16:HIS:O	35:b:18:GLY:N	2.41	0.52
37:d:107:ARG:HG2	37:d:173:TRP:CH2	2.45	0.52
50:q:13:ASP:CG	50:q:14:LYS:N	2.67	0.52
56:y:214:TYR:CA	56:y:215:LEU:HD12	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:G:H1	1:A:102:G:HO2'	1.55	0.52
1:A:105:C:H2'	1:A:106:C:H6	1.74	0.52
1:A:2748:A:N3	7:H:63:SER:HB3	2.24	0.52
2:B:43:C:OP1	27:4:2:LYS:HB2	2.10	0.52
6:G:5:VAL:HG23	6:G:8:LYS:HB2	1.92	0.52
21:Y:31:LEU:HD12	21:Y:36:ALA:O	2.09	0.52
23:0:23:VAL:HG13	23:0:26:TYR:CE2	2.44	0.52
34:a:41:G:H2'	34:a:42:G:H8	1.73	0.52
34:a:1014:A:H2'	34:a:1015:A:C8	2.44	0.52
39:f:10:LEU:HB3	39:f:59:TYR:HB3	1.91	0.52
56:y:414:ILE:CG2	56:y:476:SER:O	2.49	0.52
1:A:539:G:H2'	1:A:540:C:H6	1.75	0.52
1:A:582:G:H2'	1:A:583:G:C8	2.45	0.52
1:A:1442:G:H2'	1:A:1443:G:H8	1.74	0.52
1:A:2345:G:N3	1:A:2381:C:H2'	2.23	0.52
4:E:128:SER:OG	4:E:129:HIS:N	2.41	0.52
5:F:117:ARG:HA	5:F:120:GLU:OE1	2.08	0.52
7:H:109:PHE:HE2	7:H:152:ARG:NH2	2.03	0.52
27:4:53:GLU:HG3	27:4:55:ARG:H	1.73	0.52
28:5:32:PRO:HB3	28:5:37:LYS:HE2	1.91	0.52
29:6:9:LEU:N	29:6:23:THR:O	2.34	0.52
34:a:154:C:H2'	34:a:155:C:H6	1.74	0.52
34:a:356:A:N3	34:a:368:U:O2'	2.40	0.52
34:a:620:C:C2	37:d:135:LEU:HG	2.44	0.52
34:a:1048:G:OP1	47:n:4:LYS:HB2	2.09	0.52
34:a:1352:C:OP1	62:a:3514:HOH:O	2.19	0.52
33:w:44:G:H3'	33:w:45:U:H6	1.74	0.52
56:y:369:LEU:HD22	56:y:370:ILE:H	0.70	0.52
1:A:141:A:H8	1:A:1408:C:O2'	1.91	0.52
1:A:587:C:OP2	12:P:21:ARG:NH2	2.38	0.52
1:A:613:G:O2'	1:A:614(C):A:N1	2.40	0.52
1:A:653:A:H2'	1:A:654:A:O4'	2.09	0.52
1:A:1105:U:H2'	1:A:1106:G:H8	1.75	0.52
1:A:1178:C:H2'	1:A:1179:C:H6	1.75	0.52
1:A:1301:A:O2'	1:A:1303:G:N7	2.40	0.52
1:A:2279:G:O6	23:0:14:ARG:HD2	2.09	0.52
1:A:2537:U:H2'	1:A:2538:C:C6	2.45	0.52
13:Q:34:LEU:HD11	13:Q:129:THR:HB	1.91	0.52
18:V:21:ARG:HA	18:V:93:GLU:HA	1.91	0.52
34:a:933:G:O6	40:g:3:ARG:NH2	2.42	0.52
34:a:1031:G:H2'	34:a:1032:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:m:23:TYR:CD2	46:m:70:LEU:HD13	2.45	0.52
56:y:372:THR:CG2	56:y:373:ALA:N	2.73	0.52
1:A:588:U:H1'	5:F:90:PHE:CD1	2.44	0.52
1:A:844:C:H3'	1:A:845:G:N2	2.24	0.52
1:A:2529:G:O6	32:9:31:LYS:NZ	2.41	0.52
11:O:17:ARG:HB2	11:O:45:GLU:HB3	1.91	0.52
15:S:58:LEU:CB	15:S:59:LYS:HB2	2.37	0.52
34:a:1280:A:C8	43:j:40:LEU:HD22	2.45	0.52
35:b:97:TRP:CH2	35:b:173:ALA:HA	2.45	0.52
56:y:200:ILE:CA	56:y:215:LEU:HB2	2.27	0.52
56:y:540:ALA:HB1	56:y:544:LYS:O	2.09	0.52
1:A:271(G):C:C2'	1:A:271(H):G:H5'	2.39	0.52
1:A:1417:C:H2'	1:A:1418:G:O4'	2.10	0.52
1:A:2284:C:OP1	29:6:3:SER:HB3	2.10	0.52
1:A:2285:C:OP2	29:6:6:ARG:NH1	2.42	0.52
3:D:147:LEU:HD13	3:D:155:LEU:HD11	1.92	0.52
19:W:45:TYR:HD2	19:W:46:PHE:HD1	1.58	0.52
40:g:137:LYS:O	40:g:141:VAL:HG23	2.10	0.52
46:m:2:ALA:HA	46:m:7:VAL:CB	2.40	0.52
56:y:340:LEU:N	56:y:340:LEU:CD1	2.73	0.52
1:A:292:C:H2'	1:A:293:U:H6	1.74	0.52
1:A:829:A:N7	1:A:2248:C:H5'	2.25	0.52
1:A:1062:G:H2'	1:A:1063:G:C8	2.44	0.52
1:A:2422:A:O4'	33:x:76:A:N6	2.43	0.52
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.45	0.52
6:G:39:ILE:HG23	6:G:157:ILE:HG12	1.91	0.52
7:H:24:VAL:HG11	7:H:72:ILE:HD11	1.92	0.52
7:H:76:VAL:O	7:H:78:GLY:N	2.43	0.52
9:K:65:PHE:H	9:K:65:PHE:HD2	1.58	0.52
33:x:41:C:H4'	40:g:143:ARG:HD2	1.91	0.52
34:a:975:A:O2'	47:n:32:SER:OG	2.18	0.52
49:p:40:ASP:OD1	49:p:42:ARG:N	2.41	0.52
1:A:193:U:C2	1:A:194:G:C8	2.98	0.52
1:A:296:C:O3'	21:Y:95:LYS:NZ	2.35	0.52
1:A:307:G:O5'	1:A:307:G:H8	1.93	0.52
1:A:773:U:O2'	3:D:48:ARG:HD3	2.10	0.52
1:A:1344:G:H5'	1:A:1384:A:N6	2.23	0.52
1:A:1776:G:H1	1:A:1788:C:H42	1.58	0.52
1:A:1932:A:H2'	1:A:1933:G:O4'	2.09	0.52
1:A:2136:C:O2'	1:A:2137:C:O4'	2.28	0.52
1:A:2287:A:N6	1:A:2344:U:N3	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:89:SER:HB2	3:D:159:ALA:CB	2.39	0.52
9:K:72:PRO:HG2	9:K:77:LEU:HD21	1.92	0.52
26:3:9:VAL:HG12	26:3:32:GLN:HE22	1.75	0.52
50:q:6:LEU:HD23	50:q:23:VAL:HG21	1.91	0.52
1:A:600:G:H2'	1:A:601:C:C6	2.45	0.52
1:A:1680:U:C2'	1:A:1681:G:H5'	2.40	0.52
1:A:1911:U:H2'	1:A:1918:A:N1	2.25	0.52
1:A:2850:A:N7	1:A:2868:A:O2'	2.38	0.52
9:K:55:VAL:HG22	9:K:57:ILE:HG13	1.91	0.52
13:Q:56:ARG:HB2	13:Q:56:ARG:HH11	1.75	0.52
34:a:1437:C:H2'	34:a:1438:G:C8	2.44	0.52
35:b:122:PHE:N	35:b:123:ALA:O	2.43	0.52
36:c:34:LEU:HG	36:c:38:ARG:HE	1.74	0.52
36:c:191:THR:CG2	36:c:196:LEU:HD23	2.40	0.52
39:f:12:PRO:HG3	39:f:57:GLN:O	2.10	0.52
50:q:14:LYS:HB2	50:q:14:LYS:NZ	2.25	0.52
56:y:-47:LYS:O	56:y:-44:TYR:N	2.42	0.52
56:y:8:ARG:O	56:y:9:ILE:CB	2.57	0.52
1:A:336:C:HO2'	21:Y:35:TYR:HH	1.58	0.52
1:A:571:A:C8	1:A:2030:A:N6	2.78	0.52
1:A:1379:A:H4'	1:A:1380:G:OP2	2.09	0.52
1:A:2105:C:N3	1:A:2184:G:O6	2.43	0.52
1:A:2758:A:C2	1:A:2759:G:H1'	2.45	0.52
4:E:163:GLU:HG2	4:E:164:ARG:N	2.25	0.52
34:a:489:C:H2'	34:a:490:G:H8	1.75	0.52
34:a:958:A:N6	52:s:77:THR:O	2.41	0.52
42:i:18:PHE:HB2	42:i:62:TYR:HB3	1.92	0.52
50:q:21:VAL:HG11	50:q:59:ILE:HD12	1.92	0.52
56:y:64:VAL:O	56:y:79:HIS:HA	2.10	0.52
1:A:307:G:H2'	1:A:309:G:N7	2.26	0.51
1:A:399:G:OP2	62:A:3780:HOH:O	2.19	0.51
1:A:557:U:H2'	1:A:558:G:C8	2.45	0.51
1:A:958:U:H4'	62:A:3713:HOH:O	2.10	0.51
1:A:1820:U:O2	3:D:201:HIS:HB3	2.09	0.51
1:A:2385:C:H2'	1:A:2386:C:C6	2.45	0.51
11:O:15:GLY:HA2	11:O:47:ILE:HD11	1.92	0.51
13:Q:109:VAL:CG1	13:Q:113:GLN:HB3	2.39	0.51
16:T:29:ARG:NH1	16:T:87:ASP:OD2	2.43	0.51
21:Y:75:ILE:HD13	21:Y:82:PRO:HA	1.92	0.51
22:Z:11:GLU:N	22:Z:13:GLU:OE1	2.38	0.51
35:b:213:LEU:O	35:b:217:ARG:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:417:PRO:C	56:y:446:LYS:O	2.52	0.51
56:y:512:LYS:O	56:y:513:ALA:C	2.52	0.51
1:A:1959:G:C6	1:A:1960:A:C5	2.98	0.51
1:A:2572:A:N7	4:E:144:ARG:HD2	2.24	0.51
7:H:118:PRO:HD2	7:H:121:ILE:HB	1.92	0.51
11:O:34:THR:OG1	11:O:35:VAL:N	2.42	0.51
24:1:2:SER:HB2	24:1:43:TYR:HD2	1.74	0.51
34:a:22:G:H4'	34:a:885:G:C8	2.45	0.51
34:a:404:U:H5'	37:d:122:ARG:HD3	1.92	0.51
38:e:110:LEU:HD13	38:e:118:ILE:HG21	1.92	0.51
41:h:21:LYS:O	41:h:65:TYR:OH	2.12	0.51
56:y:-21:GLU:O	56:y:-18:ILE:HG13	2.10	0.51
56:y:105:LEU:HD11	56:y:107:VAL:HG23	1.92	0.51
56:y:166:ALA:CA	56:y:173:GLY:H	2.23	0.51
1:A:666:G:C5	1:A:667:U:C5	2.98	0.51
1:A:1257:C:H2'	1:A:1258:C:C6	2.45	0.51
1:A:1794:U:H2'	1:A:1795:C:H6	1.75	0.51
1:A:1827:C:OP2	3:D:222:ARG:NH1	2.44	0.51
1:A:1933:G:H22	1:A:1968:G:H1'	1.76	0.51
1:A:2445:G:OP1	5:F:74:ARG:NH2	2.39	0.51
3:D:67:PHE:HB3	3:D:153:ALA:H	1.75	0.51
10:N:23:LEU:HA	10:N:60:ILE:HD11	1.93	0.51
22:Z:124:ILE:HG12	22:Z:125:LEU:N	2.22	0.51
34:a:1198:G:O2'	43:j:55:LYS:HE2	2.10	0.51
36:c:58:GLU:CB	43:j:92:THR:HG21	2.38	0.51
36:c:73:PRO:O	36:c:77:ILE:HG12	2.11	0.51
39:f:76:ALA:HA	39:f:79:LEU:HB2	1.91	0.51
33:w:19:G:N2	33:w:57:G:H1'	2.25	0.51
56:y:417:PRO:CB	56:y:446:LYS:HB3	2.20	0.51
1:A:338:G:H2'	1:A:339:U:H6	1.75	0.51
1:A:954:G:H4'	13:Q:13:GLN:HE21	1.75	0.51
1:A:1095:A:H2'	1:A:1096:A:C8	2.45	0.51
1:A:1385:G:O6	1:A:1403:C:N4	2.43	0.51
1:A:1504:C:H2'	1:A:1505:C:C6	2.45	0.51
1:A:1882:C:H5''	24:1:26:ARG:HH21	1.75	0.51
1:A:1918:A:O2'	1:A:1920:C:N4	2.43	0.51
1:A:2303:G:N3	6:G:132:ASN:ND2	2.57	0.51
5:F:102:PRO:HB2	5:F:105:VAL:HG23	1.91	0.51
6:G:45:GLU:C	6:G:47:LYS:H	2.17	0.51
9:K:98:ARG:HA	9:K:136:VAL:HG23	1.91	0.51
13:Q:75:THR:HG23	13:Q:88:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:49:HIS:HA	17:U:52:ARG:HB3	1.93	0.51
33:x:13:C:H2'	33:x:14:A:C8	2.46	0.51
34:a:164:U:H2'	34:a:165:C:C6	2.45	0.51
34:a:1114:C:H2'	34:a:1115:C:H6	1.76	0.51
34:a:1423:G:H2'	34:a:1424:C:H6	1.75	0.51
35:b:17:PHE:HD1	35:b:18:GLY:H	1.58	0.51
35:b:192:SER:O	35:b:194:PRO:HD3	2.10	0.51
40:g:64:GLN:HE21	40:g:68:ASN:HD21	1.58	0.51
51:r:21:LYS:HB3	51:r:24:ALA:HB3	1.91	0.51
56:y:12:PHE:N	56:y:12:PHE:CD2	2.73	0.51
56:y:105:LEU:HD12	56:y:134:VAL:H	1.75	0.51
56:y:109:ALA:O	56:y:144:ARG:N	2.43	0.51
1:A:143:G:H1'	20:X:37:THR:CG2	2.34	0.51
1:A:192:C:OP1	62:A:3781:HOH:O	2.19	0.51
1:A:814:C:H2'	1:A:815:C:H6	1.75	0.51
1:A:1051:G:N2	1:A:1108:U:O4	2.43	0.51
1:A:1786:A:C4	1:A:1938:A:C6	2.99	0.51
1:A:2252:G:H2'	1:A:2253:G:H8	1.75	0.51
1:A:2627:G:N2	1:A:2777:G:OP2	2.43	0.51
1:A:2839:G:H5'	14:R:46:GLY:HA2	1.93	0.51
9:K:75:SER:O	9:K:75:SER:OG	2.27	0.51
12:P:38:GLN:HE21	12:P:45:LEU:HD23	1.74	0.51
34:a:1119:C:H2'	34:a:1120:G:H8	1.75	0.51
42:i:16:ARG:HD3	42:i:64:THR:HG21	1.92	0.51
1:A:250:G:H5'	12:P:60:MET:HE1	1.92	0.51
1:A:1356:G:N2	1:A:1376:C:C2	2.78	0.51
1:A:2678:C:H2'	1:A:2679:A:C8	2.46	0.51
2:B:39:A:O2'	2:B:46:A:N1	2.42	0.51
3:D:261:LYS:HZ2	3:D:263:ARG:HB2	1.76	0.51
4:E:49:LEU:CD2	4:E:81:ILE:HG12	2.41	0.51
5:F:164:ARG:HA	5:F:167:ALA:HB3	1.93	0.51
12:P:2:LYS:HE3	12:P:4:SER:OG	2.11	0.51
20:X:72:LYS:HG2	20:X:73:ARG:O	2.10	0.51
34:a:162:A:H5''	34:a:163:C:OP2	2.11	0.51
34:a:254:G:OP1	50:q:66:SER:OG	2.26	0.51
34:a:835:U:OP1	51:r:64:ARG:NH1	2.44	0.51
34:a:1112:C:N3	36:c:178:LEU:N	2.40	0.51
1:A:1047:G:H4'	1:A:1047:G:OP1	2.09	0.51
1:A:1778:U:H2'	1:A:1784:A:N6	2.26	0.51
1:A:2168:G:N2	1:A:2171:A:H62	2.08	0.51
1:A:2529:G:H5''	1:A:2530:A:H5''	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:GLU:HB2	3:D:92:ILE:CD1	2.40	0.51
3:D:92:ILE:HD13	3:D:104:TYR:CD2	2.45	0.51
7:H:87:LEU:HD13	7:H:148:ILE:HG21	1.93	0.51
13:Q:43:THR:O	13:Q:46:GLN:N	2.43	0.51
22:Z:104:PHE:CE2	22:Z:119:GLU:HB3	2.45	0.51
31:8:61:LEU:O	31:8:62:LEU:HD23	2.11	0.51
33:x:28:G:H2'	33:x:29:G:C8	2.46	0.51
34:a:227:G:O2'	49:p:62:VAL:HG21	2.10	0.51
34:a:983:A:H5'	34:a:984:C:OP2	2.10	0.51
34:a:1053:G:H3'	34:a:1054:C:H5'	1.91	0.51
34:a:1346:A:OP1	42:i:120:ARG:NH1	2.44	0.51
34:a:1512:U:H2'	34:a:1513:A:C8	2.46	0.51
56:y:137:LYS:C	56:y:139:ASP:N	2.68	0.51
56:y:214:TYR:C	56:y:215:LEU:CD1	2.82	0.51
56:y:304:GLY:HA3	56:y:306:TYR:CE2	2.43	0.51
56:y:409:TYR:HA	56:y:455:PRO:HA	1.92	0.51
56:y:474:TYR:O	56:y:475:ALA:HB3	2.10	0.51
56:y:518:ARG:NH2	56:y:522:ASP:CA	2.73	0.51
1:A:242:G:H5''	31:8:64:TYR:CE2	2.45	0.51
1:A:582:G:C6	1:A:583:G:C6	2.98	0.51
1:A:642:G:H21	1:A:646:A:H2	1.58	0.51
1:A:1021:A:O2'	1:A:1123:C:H5''	2.11	0.51
1:A:1499:C:H2'	1:A:1500:G:C8	2.45	0.51
1:A:2079:U:H3	1:A:2241:A:H61	1.58	0.51
1:A:2427:C:H5''	1:A:2428:G:OP1	2.11	0.51
1:A:2576:G:OP1	62:A:3734:HOH:O	2.19	0.51
3:D:43:ARG:HA	3:D:48:ARG:O	2.10	0.51
3:D:154:LYS:NZ	62:D:402:HOH:O	2.35	0.51
5:F:34:TRP:CH2	12:P:8:PRO:HB3	2.46	0.51
6:G:105:LYS:HE3	6:G:143:GLU:OE1	2.11	0.51
20:X:8:ILE:HD12	20:X:43:VAL:HG23	1.92	0.51
31:8:16:ILE:HD11	31:8:59:LYS:HG2	1.92	0.51
43:j:54:PHE:CD2	43:j:55:LYS:HG2	2.45	0.51
43:j:81:THR:C	43:j:83:GLU:H	2.19	0.51
46:m:8:GLU:CB	46:m:9:ILE:HA	2.41	0.51
56:y:71:LYS:O	56:y:72:ASP:C	2.53	0.51
56:y:193:GLU:HG3	56:y:193:GLU:O	2.09	0.51
56:y:566:ASP:CG	56:y:568:THR:HG22	2.35	0.51
1:A:1478:G:N3	1:A:1479:G:C8	2.78	0.51
1:A:2436:G:C5	1:A:2437:U:C5	2.99	0.51
1:A:2439:A:O2'	1:A:2600:A:OP1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:38:VAL:O	9:K:42:ASN:HB2	2.11	0.51
14:R:12:ARG:HB2	14:R:17:ARG:HB2	1.92	0.51
16:T:77:PRO:HB2	16:T:80:SER:HB2	1.93	0.51
34:a:91:C:H2'	34:a:92:C:C5	2.46	0.51
34:a:643:C:H4'	41:h:31:PHE:CE2	2.45	0.51
34:a:738:C:OP1	39:f:2:ARG:NH1	2.44	0.51
34:a:1029:C:H2'	34:a:1030(A):G:C8	2.45	0.51
34:a:1053:G:C3'	34:a:1054:C:H5'	2.41	0.51
37:d:70:ILE:HG21	37:d:75:PHE:HD1	1.75	0.51
38:e:144:THR:H	38:e:147:ASP:HB2	1.76	0.51
56:y:318:ASP:O	56:y:321:GLU:N	2.43	0.51
56:y:433:GLY:C	56:y:453:GLU:O	2.54	0.51
1:A:1078:U:H5''	1:A:1079:C:OP1	2.11	0.51
1:A:2105:C:H2'	1:A:2106:G:O4'	2.11	0.51
1:A:2318:G:O2'	1:A:2319:G:OP1	2.24	0.51
6:G:89:GLY:C	6:G:90:LEU:HD23	2.36	0.51
35:b:98:LEU:HG	35:b:101:MET:HE3	1.93	0.51
37:d:148:VAL:HG21	37:d:181:MET:HE2	1.93	0.51
56:y:166:ALA:CA	56:y:173:GLY:N	2.73	0.51
1:A:848:G:H2'	1:A:849:A:C8	2.46	0.50
1:A:956:G:H8	13:Q:14:ARG:HH21	1.59	0.50
1:A:1070:A:H5'	1:A:1072:C:OP2	2.11	0.50
1:A:1607:C:N4	1:A:1621:U:H2'	2.26	0.50
1:A:1633:G:O5'	1:A:1633:G:H8	1.94	0.50
6:G:120:LEU:HB2	6:G:179:PRO:O	2.11	0.50
16:T:28:VAL:O	16:T:46:GLU:HA	2.12	0.50
19:W:68:ARG:O	19:W:110:LYS:N	2.41	0.50
27:4:48:ARG:HA	27:4:48:ARG:NE	2.25	0.50
34:a:299:G:H2'	34:a:300:A:C8	2.46	0.50
34:a:330:C:H2'	34:a:331:G:H5'	1.92	0.50
34:a:1004:A:H5''	34:a:1025:U:C4	2.46	0.50
34:a:1120:G:H2'	34:a:1121:U:C6	2.45	0.50
34:a:1309:G:OP1	46:m:92:HIS:HE1	1.93	0.50
53:t:60:GLU:HG3	53:t:81:LYS:HD2	1.93	0.50
56:y:5:ASN:HA	56:y:8:ARG:CB	2.41	0.50
56:y:137:LYS:C	56:y:139:ASP:H	2.17	0.50
56:y:504:LEU:HD22	56:y:599:ALA:O	2.11	0.50
1:A:359:A:H2'	1:A:360:G:H5'	1.93	0.50
1:A:1273:U:H4'	1:A:1275:A:OP2	2.11	0.50
1:A:1422:G:H1'	1:A:1495:A:H61	1.76	0.50
1:A:2032:G:O2'	4:E:145:LYS:HE3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:274:ARG:HB2	3:D:275:LYS:CB	2.40	0.50
16:T:35:LYS:HD3	16:T:37:GLY:N	2.26	0.50
26:3:5:LYS:HE3	26:3:34:GLU:OE1	2.11	0.50
33:x:50:U:H2'	33:x:51:U:C6	2.46	0.50
34:a:1368:G:OP2	42:i:112:LYS:HG3	2.11	0.50
35:b:114:ARG:NH1	35:b:141:GLU:OE1	2.43	0.50
35:b:195:ASP:OD2	35:b:195:ASP:N	2.34	0.50
46:m:29:ARG:HD3	46:m:64:TRP:CD2	2.46	0.50
56:y:180:ALA:O	56:y:183:GLN:HG3	2.10	0.50
56:y:492:VAL:HB	56:y:506:PHE:CZ	2.46	0.50
56:y:531:GLN:O	56:y:533:PHE:N	2.44	0.50
1:A:26:G:OP1	19:W:80:PRO:HB3	2.11	0.50
1:A:906:G:HO2'	13:Q:67:ARG:HH21	1.54	0.50
1:A:1845:G:H1	1:A:1895:C:H42	1.59	0.50
4:E:12:THR:HG21	16:T:11:GLU:HG2	1.93	0.50
5:F:184:TYR:O	5:F:188:ARG:HB2	2.12	0.50
7:H:69:ARG:HE	7:H:73:ALA:HB2	1.76	0.50
13:Q:84:GLY:O	13:Q:85:LYS:HB2	2.11	0.50
17:U:106:PHE:HA	17:U:109:LEU:HD12	1.93	0.50
24:1:56:GLN:NE2	24:1:87:PRO:HD3	2.26	0.50
34:a:545:C:H5''	37:d:72:GLU:HG2	1.93	0.50
34:a:624:C:H2'	34:a:625:G:C8	2.46	0.50
34:a:1030(C):G:H2'	34:a:1030(D):A:C8	2.46	0.50
34:a:1476:G:H2'	34:a:1477:C:H6	1.76	0.50
36:c:6:HIS:ND1	47:n:49:HIS:HB3	2.27	0.50
37:d:119:GLN:HG2	37:d:123:HIS:CD2	2.46	0.50
37:d:202:LEU:HA	37:d:205:GLU:HG3	1.93	0.50
50:q:95:TYR:CD1	50:q:98:LEU:HD22	2.47	0.50
33:w:8:4SU:O5'	33:w:8:4SU:H6	2.11	0.50
56:y:497:HIS:HA	56:y:536:PRO:HB2	1.93	0.50
1:A:234:C:H2'	1:A:235:U:O4'	2.12	0.50
1:A:271(O):C:H2'	1:A:271(P):C:C6	2.45	0.50
1:A:845:G:N2	1:A:845:G:OP2	2.32	0.50
1:A:1036:G:H1	1:A:1119:C:N4	2.02	0.50
1:A:1167:U:H2'	1:A:1168:G:C8	2.46	0.50
1:A:1487:G:H2'	1:A:1488:G:H8	1.76	0.50
1:A:1974:C:C4	1:A:1975:G:N7	2.79	0.50
1:A:2735:G:H2'	1:A:2736:G:H8	1.77	0.50
3:D:154:LYS:C	3:D:155:LEU:HD12	2.36	0.50
11:O:71:ARG:O	11:O:74:GLY:N	2.43	0.50
34:a:1001(A):G:H2'	34:a:1002:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1466:C:H2'	34:a:1467:G:O4'	2.11	0.50
38:e:6:PHE:HD1	38:e:36:ASP:HB3	1.76	0.50
42:i:23:ASN:OD1	42:i:23:ASN:N	2.35	0.50
56:y:-40:TYR:HE1	56:y:-36:ARG:CZ	2.24	0.50
56:y:426:GLN:O	56:y:429:GLN:HB3	2.12	0.50
1:A:34:C:O2'	1:A:35:G:OP1	2.30	0.50
1:A:117:G:H5''	1:A:118:A:OP2	2.12	0.50
1:A:245:G:O2'	1:A:384:U:O2	2.23	0.50
1:A:300:A:H1'	1:A:319:C:H1'	1.92	0.50
1:A:981:A:C8	1:A:982:C:C5	2.99	0.50
1:A:1177:A:H3'	1:A:1178:C:C6	2.47	0.50
1:A:1335:U:OP1	20:X:65:ARG:HD3	2.11	0.50
1:A:2790:A:O2'	1:A:2791:C:H5	1.94	0.50
3:D:68:LYS:HD2	3:D:70:TRP:CZ2	2.46	0.50
29:6:13:CYS:HB2	29:6:49:HIS:CE1	2.46	0.50
34:a:17:U:H2'	34:a:18:C:H6	1.75	0.50
34:a:1132:C:H2'	34:a:1133:G:C8	2.47	0.50
42:i:103:THR:HG22	42:i:104:ARG:N	2.26	0.50
51:r:21:LYS:HG2	51:r:22:VAL:H	1.75	0.50
56:y:216:ARG:HG2	56:y:218:PHE:H	1.74	0.50
56:y:537:ILE:O	56:y:549:ALA:CA	2.59	0.50
1:A:1139:G:H5'	10:N:23:LEU:HD21	1.92	0.50
1:A:2025:C:P	4:E:149:ARG:HH21	2.35	0.50
3:D:161:THR:H	3:D:196:VAL:HB	1.76	0.50
6:G:58:GLN:HE21	6:G:58:GLN:H	1.60	0.50
14:R:22:ARG:HD3	14:R:69:ASP:O	2.11	0.50
19:W:15:ARG:HH21	28:5:20:ARG:HE	1.58	0.50
25:2:29:LYS:HG2	25:2:57:ILE:HD13	1.92	0.50
26:3:36:VAL:C	26:3:37:LEU:HG	2.35	0.50
33:x:68:C:C2'	33:x:69:G:H5'	2.40	0.50
34:a:219:C:H2'	34:a:220:G:O4'	2.11	0.50
34:a:619:U:N3	37:d:134:ASP:OD1	2.42	0.50
39:f:97:PHE:HD1	51:r:31:LEU:HD21	1.77	0.50
51:r:52:PRO:O	51:r:56:THR:HG23	2.11	0.50
33:w:72:C:C2'	33:w:73:A:H5'	2.42	0.50
1:A:411:G:C5	12:P:72:PRO:HB3	2.45	0.50
1:A:447:A:C4	1:A:473:G:N7	2.80	0.50
1:A:1614:A:N1	19:W:93:ALA:HB2	2.27	0.50
1:A:1970:A:OP2	62:A:3782:HOH:O	2.20	0.50
1:A:2139:C:H42	1:A:2152:G:H1	1.60	0.50
2:B:106:G:C2	2:B:107:G:C8	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:101:LEU:HD12	5:F:102:PRO:CD	2.36	0.50
24:1:17:SER:HB2	24:1:40:ARG:HG2	1.94	0.50
34:a:1255:G:HO2'	34:a:1258:G:HO2'	1.54	0.50
34:a:1437:C:H2'	34:a:1438:G:H8	1.76	0.50
50:q:64:PRO:HA	50:q:70:ARG:HG2	1.92	0.50
56:y:18:VAL:HA	61:y:703:GDP:O3B	2.12	0.50
56:y:299:PRO:O	56:y:377:VAL:HG11	2.12	0.50
1:A:487:C:O2	19:W:53:SER:OG	2.30	0.50
1:A:627:A:H4'	1:A:628:G:OP1	2.11	0.50
1:A:1339:G:N3	62:A:3834:HOH:O	2.34	0.50
1:A:1385:G:H1'	1:A:1386:C:C6	2.46	0.50
1:A:1652:A:C2'	1:A:1653:G:H5'	2.41	0.50
1:A:2697:G:C2	1:A:2711:A:C2	3.00	0.50
2:B:12:C:H2'	23:0:73:GLY:HA3	1.94	0.50
2:B:63:G:H2'	2:B:64:C:H6	1.75	0.50
7:H:86:GLU:O	7:H:165:ALA:HB2	2.12	0.50
10:N:15:LEU:HB2	10:N:135:PRO:HB2	1.94	0.50
17:U:25:TRP:O	17:U:28:ARG:HB2	2.11	0.50
17:U:52:ARG:O	17:U:55:ARG:HG3	2.12	0.50
34:a:652:U:O2'	34:a:653:A:OP2	2.23	0.50
35:b:21:ARG:HB3	35:b:38:GLY:O	2.12	0.50
38:e:102:ALA:HA	38:e:120:THR:OG1	2.10	0.50
38:e:143:ARG:NH1	41:h:77:GLU:OE2	2.43	0.50
39:f:68:PRO:HB2	39:f:71:ARG:HB2	1.92	0.50
42:i:111:ARG:HG3	42:i:111:ARG:O	2.12	0.50
56:y:-46:PRO:O	56:y:-42:ARG:HB2	2.12	0.50
56:y:138:ILE:CG1	56:y:167:SER:HB2	2.41	0.50
56:y:142:ASN:ND2	56:y:142:ASN:O	2.44	0.50
56:y:411:LYS:CA	56:y:453:GLU:CA	2.85	0.50
56:y:418:GLU:HG3	56:y:419:GLU:H	1.77	0.50
1:A:570:G:H2'	1:A:2030:A:C6	2.47	0.50
1:A:1439:A:C2	1:A:1553:A:C5	3.00	0.50
2:B:40:U:C5	27:4:2:LYS:HG3	2.46	0.50
17:U:8:VAL:HG23	17:U:11:ARG:HH21	1.76	0.50
28:5:20:ARG:HA	28:5:23:HIS:CD2	2.46	0.50
34:a:678:U:H2'	34:a:679:C:C6	2.46	0.50
34:a:864:A:H2'	34:a:865:A:C8	2.47	0.50
34:a:1497:G:C2'	34:a:1498:U:H5'	2.41	0.50
36:c:180:ALA:O	36:c:181:ASN:HB3	2.11	0.50
45:l:53:ARG:HG2	45:l:93:LEU:HD11	1.92	0.50
1:A:285:C:H2'	1:A:286:C:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:A:OP1	1:A:561:G:N2	2.36	0.49
1:A:1988:C:C2	1:A:1989:G:C8	3.00	0.49
1:A:2849:U:H4'	1:A:2868:A:C2	2.47	0.49
7:H:3:ARG:HH11	7:H:3:ARG:CG	2.22	0.49
9:K:48:MET:SD	9:K:72:PRO:HD3	2.52	0.49
12:P:93:GLY:O	12:P:123:LEU:HD22	2.11	0.49
12:P:101:VAL:HA	12:P:106:LEU:HB3	1.94	0.49
34:a:411:A:OP2	37:d:25:ARG:NH2	2.45	0.49
34:a:955:U:O2'	52:s:83:HIS:HD2	1.95	0.49
38:e:11:ILE:HG21	38:e:105:VAL:HG13	1.94	0.49
42:i:32:ASP:OD2	42:i:34:ASN:HB2	2.12	0.49
56:y:13:SER:OG	56:y:103:VAL:HG12	2.12	0.49
56:y:25:LEU:O	56:y:29:ILE:N	2.45	0.49
1:A:182:A:N3	1:A:433:C:O2'	2.36	0.49
1:A:290:G:H1	1:A:350:U:H3	1.59	0.49
1:A:1495:A:H2'	1:A:1496:A:C8	2.46	0.49
1:A:2233:U:H2'	1:A:2234:G:C8	2.47	0.49
5:F:46:ARG:HB3	5:F:48:THR:HG23	1.93	0.49
12:P:47:ASP:OD2	12:P:50:ARG:NH2	2.44	0.49
17:U:75:ASN:OD1	17:U:78:THR:N	2.39	0.49
27:4:61:ARG:HH21	27:4:63:TYR:HD2	1.59	0.49
33:x:25:C:C2	33:x:26:A:C8	3.00	0.49
34:a:1423:G:H2'	34:a:1424:C:C6	2.48	0.49
35:b:24:TRP:CD1	35:b:24:TRP:N	2.79	0.49
35:b:84:GLU:OE2	35:b:216:SER:HB3	2.13	0.49
40:g:75:VAL:HG11	40:g:86:GLN:HB3	1.94	0.49
41:h:60:ARG:HH11	41:h:60:ARG:HB2	1.76	0.49
44:k:98:LEU:O	44:k:101:SER:HB3	2.12	0.49
56:y:105:LEU:CD1	56:y:107:VAL:HG23	2.41	0.49
1:A:90:U:O2'	1:A:92:A:O4'	2.31	0.49
1:A:361:G:C2'	1:A:362:U:H5'	2.42	0.49
1:A:380:U:H5'	24:1:18:ILE:HD12	1.93	0.49
1:A:741:G:O2'	1:A:1676:A:OP1	2.28	0.49
1:A:1055:G:H1	1:A:1104:C:H42	1.59	0.49
1:A:1278:A:OP1	14:R:36:THR:HG23	2.12	0.49
1:A:1424:G:H2'	1:A:1425:G:O4'	2.12	0.49
1:A:1796:U:H2'	1:A:1797:C:C6	2.47	0.49
1:A:2232:U:P	24:1:40:ARG:HH12	2.35	0.49
1:A:2369:A:H2'	1:A:2370:G:C8	2.47	0.49
3:D:146:GLU:HA	3:D:152:GLY:O	2.12	0.49
6:G:50:ALA:C	6:G:52:ILE:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:62:LEU:CD1	18:V:95:LEU:HB2	2.42	0.49
19:W:57:ASN:OD1	19:W:57:ASN:N	2.46	0.49
46:m:3:ARG:HH11	46:m:3:ARG:HB2	1.76	0.49
56:y:105:LEU:C	56:y:105:LEU:CD1	2.84	0.49
1:A:149:A:H2'	1:A:150:C:O4'	2.12	0.49
1:A:910:A:N1	1:A:2277:G:H1'	2.27	0.49
1:A:1056:G:H5''	1:A:1057:A:O4'	2.12	0.49
1:A:1792:G:H2'	1:A:1793:C:H6	1.76	0.49
1:A:2093:G:C6	1:A:2225:A:C8	3.00	0.49
4:E:4:ILE:HG12	4:E:28:ALA:HB1	1.93	0.49
10:N:67:LEU:HA	10:N:87:LEU:HD13	1.93	0.49
26:3:7:LYS:HE3	26:3:32:GLN:HE21	1.76	0.49
34:a:1363:C:H5'	34:a:1363(A):A:O5'	2.11	0.49
36:c:12:LEU:HD11	47:n:51:GLY:HA2	1.94	0.49
37:d:142:PRO:HA	37:d:185:PHE:HD1	1.76	0.49
41:h:103:VAL:HG12	41:h:104:ARG:HB2	1.95	0.49
48:o:40:SER:O	48:o:44:LYS:HG3	2.13	0.49
50:q:57:VAL:HG12	50:q:76:LEU:HA	1.95	0.49
56:y:62:SER:O	56:y:63:ALA:HB3	2.11	0.49
1:A:674:G:O2'	5:F:74:ARG:HD3	2.12	0.49
1:A:724:U:H2'	1:A:725:G:O4'	2.12	0.49
1:A:1253:A:N7	62:A:3837:HOH:O	2.35	0.49
1:A:2319:G:H22	15:S:3:ARG:HD2	1.77	0.49
3:D:36:PRO:HA	3:D:61:LEU:HD12	1.95	0.49
4:E:30:PRO:HB3	4:E:92:THR:HG22	1.95	0.49
6:G:65:GLY:HA3	27:4:9:LEU:HD21	1.94	0.49
6:G:111:LEU:HB2	6:G:112:PRO:HD3	1.95	0.49
11:O:89:ASN:C	11:O:91:LEU:H	2.20	0.49
15:S:102:ALA:O	15:S:105:ALA:N	2.45	0.49
34:a:108:G:N1	53:t:15:ARG:HG3	2.27	0.49
34:a:403:C:OP1	37:d:137:SER:OG	2.31	0.49
34:a:860:A:OP2	62:a:3515:HOH:O	2.20	0.49
34:a:1014:A:C2	52:s:34:TRP:CE2	3.00	0.49
35:b:29:ALA:C	35:b:31:TYR:H	2.20	0.49
39:f:44:GLY:HA2	39:f:59:TYR:CE1	2.48	0.49
50:q:22:LEU:HD12	50:q:23:VAL:H	1.76	0.49
56:y:-36:ARG:N	56:y:-35:GLY:HA3	2.28	0.49
1:A:272(I):U:H2'	1:A:272(J):C:H6	1.76	0.49
1:A:1164:G:C6	1:A:1165:U:C4	3.01	0.49
1:A:1504:C:H2'	1:A:1505:C:H6	1.77	0.49
1:A:1878:G:H2'	1:A:1879:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2518:A:H2'	1:A:2518:A:N3	2.27	0.49
62:A:4142:HOH:O	17:U:50:ARG:HB2	2.12	0.49
12:P:97:PRO:HD3	12:P:126:VAL:O	2.12	0.49
13:Q:110:THR:OG1	13:Q:113:GLN:HB2	2.12	0.49
20:X:51:VAL:HG21	20:X:81:VAL:HB	1.95	0.49
29:6:40:CYS:HB3	29:6:43:CYS:HB2	1.93	0.49
34:a:232:G:H2'	34:a:233:C:H6	1.77	0.49
34:a:1412:C:H2'	34:a:1413:A:C8	2.46	0.49
37:d:178:VAL:C	37:d:180:GLY:H	2.19	0.49
52:s:28:LYS:HB2	52:s:29:ARG:CA	2.42	0.49
56:y:188:PRO:HB2	56:y:216:ARG:CZ	2.38	0.49
56:y:531:GLN:CD	56:y:590:VAL:HG23	2.37	0.49
1:A:41:C:C2	1:A:438:G:N2	2.81	0.49
1:A:197:A:N6	1:A:2430:A:H2'	2.28	0.49
1:A:528:A:C8	1:A:528:A:C3'	2.96	0.49
1:A:1500:G:O2'	3:D:100:GLY:O	2.26	0.49
1:A:1820:U:O4	3:D:199:ALA:HB1	2.13	0.49
1:A:2199:A:H3'	1:A:2200:C:H6	1.78	0.49
1:A:2502:G:H5''	1:A:2503:A:H5''	1.94	0.49
1:A:2556:C:H2'	1:A:2557:G:O4'	2.12	0.49
3:D:220:HIS:C	3:D:220:HIS:CD2	2.89	0.49
4:E:105:THR:OG1	4:E:199:ARG:NH2	2.45	0.49
8:J:116:ILE:O	8:J:123:GLU:N	2.44	0.49
15:S:34:HIS:CD2	15:S:54:LEU:HD13	2.48	0.49
33:x:35:A:H8	33:x:35:A:H5''	1.77	0.49
34:a:779:C:H2'	34:a:780:A:O4'	2.13	0.49
34:a:1001(A):G:C2	34:a:1002:G:C5	3.00	0.49
34:a:1029:C:H1'	34:a:1030:C:OP1	2.12	0.49
34:a:1176:A:H2'	34:a:1177:G:C8	2.48	0.49
37:d:19:LEU:HD23	37:d:67:ILE:HG13	1.95	0.49
56:y:23:SER:O	56:y:26:ALA:N	2.45	0.49
56:y:86:HIS:ND1	56:y:86:HIS:N	2.60	0.49
1:A:322:A:C3'	5:F:169:ASN:HD21	2.24	0.49
1:A:1205:U:H4'	1:A:1206:G:OP2	2.12	0.49
1:A:2096:U:P	1:A:2096:U:O4'	2.70	0.49
1:A:2137:C:H2'	1:A:2138:C:H5''	1.94	0.49
1:A:2870:C:H2'	1:A:2871:C:O4'	2.13	0.49
4:E:9:VAL:HG13	4:E:25:VAL:HG12	1.95	0.49
8:J:130:THR:C	8:J:132:ASP:H	2.21	0.49
12:P:128:HIS:CE1	12:P:148:LEU:HD21	2.48	0.49
14:R:13:HIS:CE1	14:R:16:HIS:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:98:G:C6	34:a:99:U:C4	3.00	0.49
34:a:461:A:O2'	34:a:470:C:H5''	2.12	0.49
34:a:723:U:O2'	34:a:724:G:H5'	2.12	0.49
34:a:1129:C:H4'	34:a:1130:A:OP2	2.12	0.49
34:a:1162:C:N4	34:a:1174:G:H1	2.11	0.49
37:d:67:ILE:HG22	37:d:68:TYR:CD2	2.47	0.49
47:n:14:PRO:HB2	47:n:16:PHE:O	2.12	0.49
52:s:27:GLU:HB2	52:s:28:LYS:CD	2.41	0.49
56:y:301:VAL:O	56:y:302:PHE:O	2.31	0.49
56:y:579:GLU:HB2	56:y:583:ARG:HH21	1.78	0.49
1:A:782:A:O2'	3:D:225:ALA:O	2.28	0.49
1:A:1019:U:H3	1:A:1142(A):A:N6	2.05	0.49
1:A:1515:G:H4'	1:A:1556:C:O2'	2.13	0.49
1:A:1780:A:OP1	62:A:3783:HOH:O	2.20	0.49
1:A:2377:A:H2'	1:A:2378:A:C8	2.47	0.49
9:K:134:MET:HG3	9:K:136:VAL:HG12	1.94	0.49
16:T:30:VAL:HG22	16:T:86:ILE:HG12	1.95	0.49
17:U:24:TYR:HB2	17:U:29:SER:HB3	1.94	0.49
24:l:15:ALA:O	24:l:40:ARG:HG3	2.13	0.49
34:a:431:A:H2'	34:a:432:A:O4'	2.12	0.49
34:a:629:G:H2'	34:a:630:G:O4'	2.13	0.49
36:c:108:ASN:HD21	36:c:144:SER:HB3	1.77	0.49
38:e:8:GLU:HA	38:e:34:VAL:HA	1.94	0.49
44:k:54:ARG:HA	44:k:57:THR:HG23	1.94	0.49
1:A:13:A:N1	1:A:525:U:H2'	2.28	0.49
1:A:1412:A:H2'	1:A:1413:G:H8	1.74	0.49
1:A:1553:A:O2'	1:A:1554:A:C8	2.65	0.49
1:A:1987:G:H2'	1:A:1988:C:H6	1.78	0.49
1:A:2423:U:H4'	1:A:2424:C:O5'	2.12	0.49
1:A:2767:C:C2	1:A:2768:C:C5	3.01	0.49
1:A:2885:C:O2'	28:5:34:PRO:HG3	2.13	0.49
4:E:12:THR:HG22	4:E:13:ARG:N	2.24	0.49
25:2:13:ALA:O	25:2:16:LEU:HB2	2.12	0.49
34:a:989:C:HO2'	34:a:1017:G:HO2'	1.61	0.49
34:a:1054:C:H4'	34:a:1054:C:OP2	2.12	0.49
35:b:97:TRP:HZ2	35:b:102:LEU:HD12	1.78	0.49
37:d:105:VAL:HG13	37:d:110:PHE:HB2	1.95	0.49
38:e:45:PHE:CZ	38:e:129:ILE:HD11	2.48	0.49
39:f:97:PHE:N	51:r:30:ASP:OD1	2.44	0.49
40:g:50:ILE:HD11	40:g:58:PRO:HB3	1.95	0.49
56:y:12:PHE:O	56:y:13:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:H1'	1:A:319:C:C1'	2.43	0.48
1:A:537:C:H2'	1:A:538:G:C8	2.47	0.48
1:A:570:G:H2'	1:A:2030:A:C5	2.49	0.48
1:A:586:A:H5'	5:F:89:VAL:HG21	1.94	0.48
1:A:1174:A:H4'	1:A:1175:U:OP1	2.11	0.48
1:A:2122:U:H2'	1:A:2123:G:C8	2.45	0.48
1:A:2876:G:H4'	16:T:2:ASN:ND2	2.28	0.48
4:E:47:VAL:O	4:E:80:GLU:HA	2.12	0.48
7:H:10:PRO:HB2	7:H:12:PRO:HD3	1.95	0.48
16:T:105:LEU:HB2	16:T:110:ILE:HG12	1.95	0.48
17:U:40:PHE:CD2	18:V:75:PHE:CD2	3.01	0.48
28:5:51:TYR:HE1	28:5:56:LYS:HE2	1.78	0.48
34:a:667:G:H4'	48:o:51:HIS:CE1	2.47	0.48
34:a:1114:C:H2'	34:a:1115:C:C6	2.48	0.48
36:c:175:LEU:HD21	36:c:201:TYR:CE2	2.48	0.48
42:i:103:THR:HG22	42:i:104:ARG:H	1.77	0.48
51:r:67:ALA:HA	51:r:70:ILE:HG13	1.95	0.48
56:y:166:ALA:C	56:y:173:GLY:H	2.20	0.48
1:A:66:C:O2	1:A:89:G:N2	2.46	0.48
1:A:1207:C:H2'	1:A:1208:C:C6	2.48	0.48
1:A:1430:C:H2'	1:A:1431:U:C6	2.48	0.48
1:A:1518:U:H2'	1:A:1519:G:O4'	2.13	0.48
1:A:1530:C:H42	1:A:1539:G:H1	1.61	0.48
1:A:2040:C:H2'	1:A:2041:U:C6	2.48	0.48
1:A:2293:C:H5''	15:S:89:ARG:HH21	1.77	0.48
62:A:3883:HOH:O	4:E:144:ARG:HD3	2.12	0.48
5:F:39:TRP:CE3	5:F:101:LEU:HD23	2.48	0.48
5:F:118:ALA:O	5:F:120:GLU:N	2.46	0.48
22:Z:99:TYR:CZ	22:Z:125:LEU:HD13	2.48	0.48
24:1:2:SER:HB2	24:1:43:TYR:CD2	2.48	0.48
33:x:44:G:H8	33:x:44:G:OP2	1.95	0.48
33:x:58:A:O2'	33:x:60:U:H5	1.96	0.48
35:b:215:LEU:O	35:b:219:VAL:HG23	2.13	0.48
41:h:78:GLN:HE21	41:h:78:GLN:HB2	1.42	0.48
42:i:104:ARG:O	42:i:106:ALA:N	2.46	0.48
56:y:201:PHE:N	56:y:215:LEU:HA	2.27	0.48
56:y:393:PRO:O	56:y:394:ALA:C	2.55	0.48
56:y:449:GLU:CG	56:y:450:LEU:H	2.24	0.48
1:A:250:G:OP1	31:8:13:ARG:NH2	2.46	0.48
1:A:1062:G:H1	1:A:1076:C:N4	2.10	0.48
1:A:1120:G:H2'	1:A:1121:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2024:G:H2'	1:A:2025:C:C6	2.48	0.48
4:E:2:LYS:HA	4:E:84:PHE:CD2	2.48	0.48
12:P:63:PRO:HB2	31:8:30:ARG:NH2	2.28	0.48
16:T:56:GLY:O	16:T:59:THR:HG23	2.13	0.48
22:Z:138:GLU:H	22:Z:156:LYS:NZ	2.04	0.48
23:0:42:GLY:O	23:0:57:PHE:CG	2.67	0.48
24:1:23:LYS:HB3	24:1:29:GLY:HA3	1.95	0.48
34:a:1504:G:OP1	34:a:1507:A:H4'	2.14	0.48
36:c:152:ILE:HG23	36:c:167:TRP:HB3	1.96	0.48
41:h:87:SER:HB2	41:h:133:LEU:O	2.13	0.48
45:l:83:VAL:HG21	45:l:100:ILE:HG23	1.94	0.48
46:m:85:GLY:CA	46:m:86:CYS:HB3	2.42	0.48
52:s:44:MET:O	52:s:47:HIS:HB2	2.14	0.48
56:y:28:ARG:O	56:y:31:GLU:CG	2.54	0.48
56:y:77:VAL:C	56:y:78:PHE:HD1	2.21	0.48
1:A:372:G:O2'	1:A:373:U:OP2	2.31	0.48
1:A:528:A:H2	1:A:2043:C:H4'	1.77	0.48
1:A:1025:G:C4	1:A:1135:C:H1'	2.48	0.48
2:B:69:G:O6	62:B:302:HOH:O	2.19	0.48
4:E:120:TRP:CE3	4:E:155:LYS:HD3	2.48	0.48
5:F:123:LEU:HD12	5:F:124:LEU:H	1.78	0.48
6:G:80:PHE:N	6:G:80:PHE:CD1	2.80	0.48
7:H:27:LYS:HE2	7:H:27:LYS:HB3	1.62	0.48
9:K:119:ASP:HB3	9:K:122:ALA:H	1.77	0.48
13:Q:66:ILE:HG23	13:Q:104:PHE:CD2	2.49	0.48
18:V:24:LYS:HA	18:V:92:THR:OG1	2.12	0.48
20:X:31:HIS:O	20:X:77:LYS:HD3	2.13	0.48
25:2:7:ARG:O	25:2:11:GLU:HG3	2.13	0.48
34:a:302:G:N3	34:a:556:C:H4'	2.28	0.48
34:a:375:U:C4	34:a:376:G:N7	2.81	0.48
34:a:815:A:N7	34:a:1509:C:O2'	2.36	0.48
34:a:1427:U:C2	34:a:1474:G:N2	2.82	0.48
47:n:33:VAL:HA	47:n:40:CYS:HA	1.95	0.48
48:o:55:GLY:O	48:o:59:MET:HG3	2.13	0.48
52:s:28:LYS:HB2	52:s:29:ARG:HA	1.94	0.48
56:y:19:ASP:HA	61:y:703:GDP:O5'	2.12	0.48
56:y:463:PHE:O	56:y:467:LEU:N	2.46	0.48
1:A:2025:C:H5'	4:E:149:ARG:NH2	2.28	0.48
1:A:2582:G:C2	1:A:2583:G:C8	3.00	0.48
4:E:120:TRP:CD1	4:E:155:LYS:HB3	2.48	0.48
6:G:61:ALA:HB2	6:G:68:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:86:ARG:NH1	21:Y:100:ALA:HA	2.29	0.48
24:1:58:ILE:HD11	24:1:87:PRO:HA	1.96	0.48
24:1:67:ILE:N	24:1:68:PRO:HD2	2.27	0.48
35:b:88:ALA:HB2	35:b:219:VAL:HG13	1.96	0.48
56:y:-67:LYS:HA	56:y:-67:LYS:HE3	1.95	0.48
1:A:301:G:H1'	1:A:302:C:C6	2.49	0.48
1:A:645:C:H2'	1:A:645:C:O2	2.13	0.48
1:A:793:A:OP2	1:A:2072:G:H5'	2.14	0.48
1:A:1394:U:H4'	1:A:1603:A:H4'	1.96	0.48
1:A:1548:C:H2'	1:A:1549:C:C6	2.47	0.48
3:D:20:ASP:OD1	3:D:20:ASP:N	2.32	0.48
3:D:146:GLU:HG2	3:D:152:GLY:C	2.37	0.48
34:a:93:G:C2'	34:a:96:U:H5'	2.44	0.48
34:a:114:U:O2'	34:a:115:G:H5'	2.14	0.48
35:b:155:LEU:HA	35:b:156:LYS:CD	2.36	0.48
39:f:26:ILE:O	39:f:30:LEU:HG	2.13	0.48
56:y:566:ASP:HB3	56:y:569:ARG:CG	2.34	0.48
1:A:536:A:H5'	17:U:53:ARG:HD3	1.95	0.48
1:A:1114:G:H2'	1:A:1115:G:C8	2.48	0.48
1:A:2819:G:H2'	1:A:2821:A:N7	2.28	0.48
3:D:200:ASP:OD2	3:D:203:ASN:ND2	2.47	0.48
14:R:56:LYS:NZ	14:R:94:TYR:OH	2.47	0.48
14:R:87:TYR:OH	14:R:116:LEU:HB3	2.14	0.48
18:V:52:VAL:O	18:V:54:GLY:N	2.40	0.48
21:Y:79:CYS:HB3	21:Y:102:CYS:HB3	1.95	0.48
23:0:28:GLY:HA2	23:0:66:VAL:HG12	1.96	0.48
25:2:1:MET:HG3	25:2:5:GLU:HB2	1.95	0.48
34:a:679:C:N3	34:a:712:A:C2	2.82	0.48
42:i:89:ASN:O	42:i:91:ASP:N	2.46	0.48
42:i:126:SER:O	42:i:128:ARG:N	2.40	0.48
48:o:36:ILE:HD12	48:o:63:ARG:HD3	1.94	0.48
56:y:89:PHE:O	56:y:90:THR:CG2	2.62	0.48
1:A:143(A):C:H2'	1:A:144:C:H6	1.78	0.48
1:A:686:G:N2	1:A:788:A:H61	2.12	0.48
1:A:1227:G:OP1	17:U:13:LYS:HE3	2.13	0.48
1:A:1494:A:C2	1:A:1495:A:C4	3.01	0.48
1:A:1797:C:O3'	3:D:259:THR:HG22	2.13	0.48
1:A:1957:C:O2'	1:A:1985:G:H1'	2.13	0.48
1:A:2096:U:H2'	1:A:2097:C:C6	2.48	0.48
1:A:2420:C:P	31:8:33:ASN:H	2.35	0.48
1:A:2590:A:H5''	3:D:239:ARG:HE	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:G:C2	2:B:62:C:C2	3.01	0.48
2:B:68:C:H2'	2:B:69:G:H8	1.78	0.48
4:E:183:LEU:HD21	16:T:10:VAL:HG11	1.95	0.48
17:U:43:GLY:HA3	62:U:301:HOH:O	2.12	0.48
34:a:559:A:OP1	38:e:126:ARG:NH2	2.46	0.48
34:a:790:A:N6	34:a:1498:U:OP1	2.46	0.48
34:a:1070:U:OP1	38:e:18:ARG:NH2	2.40	0.48
34:a:1071:C:H2'	34:a:1072:G:H8	1.79	0.48
35:b:174:VAL:O	35:b:178:ARG:HB2	2.13	0.48
37:d:9:CYS:O	37:d:12:CYS:N	2.44	0.48
48:o:66:LEU:HD12	48:o:66:LEU:HA	1.67	0.48
54:u:5:ASP:O	54:u:11:GLY:HA3	2.13	0.48
56:y:537:ILE:HB	56:y:549:ALA:HB1	1.81	0.48
1:A:275:G:C8	1:A:275:G:O5'	2.67	0.48
1:A:528:A:C2	1:A:2043:C:H4'	2.49	0.48
1:A:1127:A:H2'	1:A:1128:A:H5''	1.95	0.48
1:A:1434:A:H2'	1:A:1435:G:C8	2.48	0.48
1:A:2018:G:H2'	1:A:2019:A:H8	1.78	0.48
4:E:116:VAL:O	4:E:122:PHE:HB2	2.14	0.48
11:O:9:GLU:OE1	11:O:18:LYS:HE2	2.13	0.48
14:R:54:LEU:O	14:R:57:ARG:N	2.46	0.48
25:2:16:LEU:HD21	25:2:20:GLU:HB2	1.96	0.48
28:5:41:PRO:HG2	28:5:44:THR:HG21	1.95	0.48
31:8:53:PRO:O	31:8:57:ARG:HG3	2.14	0.48
34:a:1496:C:H2'	34:a:1497:G:O4'	2.14	0.48
34:a:1499:A:C1'	34:a:1520:G:H5'	2.43	0.48
35:b:102:LEU:O	35:b:105:PHE:HB2	2.14	0.48
37:d:18:LYS:HG2	59:d:501:SF4:S1	2.54	0.48
40:g:41:ARG:HB3	40:g:41:ARG:HH11	1.79	0.48
49:p:39:TYR:CE2	49:p:41:PRO:HB3	2.48	0.48
1:A:186:G:H1	1:A:210:C:H42	1.62	0.48
1:A:423:A:H5''	1:A:424:G:C5'	2.44	0.48
1:A:634:C:H2'	1:A:635:C:C6	2.48	0.48
1:A:1823:G:OP1	3:D:54:ARG:NH1	2.38	0.48
1:A:2133:G:O2'	1:A:2156:G:O6	2.31	0.48
3:D:24:ILE:HD11	3:D:91:ARG:HE	1.79	0.48
5:F:12:LEU:HB2	5:F:124:LEU:HD11	1.95	0.48
5:F:161:GLU:O	5:F:165:ARG:HD3	2.13	0.48
7:H:5:GLY:HA3	7:H:65:HIS:CD2	2.49	0.48
10:N:67:LEU:HB3	10:N:88:GLU:HG3	1.96	0.48
18:V:16:PRO:HA	18:V:96:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:86:SER:O	24:1:90:ILE:HG13	2.14	0.48
27:4:14:ILE:HG12	27:4:31:ILE:HB	1.95	0.48
34:a:485:G:O2'	34:a:486:U:OP2	2.31	0.48
38:e:75:THR:HG23	38:e:76:ILE:O	2.14	0.48
39:f:94:GLN:HE22	51:r:72:ARG:HH22	1.61	0.48
41:h:119:LEU:HD13	41:h:123:GLU:HB3	1.96	0.48
46:m:68:GLY:HA2	46:m:71:ARG:HD2	1.95	0.48
52:s:50:ALA:HA	52:s:58:VAL:O	2.14	0.48
56:y:136:ASN:CG	56:y:137:LYS:N	2.66	0.48
56:y:310:SER:N	56:y:311:GLY:HA2	2.28	0.48
56:y:554:LEU:C	56:y:556:LYS:N	2.72	0.48
1:A:252:G:P	12:P:50:ARG:HH12	2.37	0.47
1:A:468:G:H2'	1:A:469:G:O4'	2.14	0.47
1:A:1986:A:H2'	1:A:1987:G:H8	1.79	0.47
1:A:2097:C:H2'	1:A:2098:U:O4'	2.14	0.47
1:A:2529:G:H5''	1:A:2530:A:C5'	2.44	0.47
1:A:2615:U:C2	28:5:7:PRO:HA	2.49	0.47
2:B:6:C:H2'	2:B:7:G:H5''	1.96	0.47
4:E:177:PRO:O	4:E:180:ASN:N	2.46	0.47
17:U:57:PHE:O	17:U:60:LEU:N	2.46	0.47
24:1:62:VAL:HG13	24:1:63:ALA:O	2.14	0.47
34:a:145:G:H1	34:a:177:C:H42	1.62	0.47
34:a:411:A:O2'	34:a:413:G:H5'	2.13	0.47
34:a:721:G:H4'	34:a:722:A:O4'	2.14	0.47
34:a:1039:C:H2'	34:a:1040:U:C6	2.49	0.47
56:y:-64:LEU:C	56:y:-63:LEU:HD23	2.39	0.47
56:y:214:TYR:HA	56:y:215:LEU:HD12	1.95	0.47
1:A:211:A:H2'	1:A:212:G:O4'	2.14	0.47
1:A:848:G:C4	1:A:933:A:H8	2.32	0.47
1:A:911:A:H5''	1:A:912:C:C5'	2.43	0.47
1:A:1477:A:N6	1:A:1478:G:O6	2.47	0.47
1:A:1695:G:H1'	3:D:8:PRO:O	2.14	0.47
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.13	0.47
1:A:2639:A:H1'	1:A:2778:A:C2	2.50	0.47
1:A:2708:G:H2'	1:A:2709:G:H8	1.79	0.47
12:P:38:GLN:HE21	12:P:45:LEU:HA	1.79	0.47
17:U:76:TYR:CZ	17:U:80:ILE:HG13	2.49	0.47
34:a:189(D):C:O5'	34:a:189(D):C:H6	1.97	0.47
34:a:1027:C:N3	34:a:1034:G:C6	2.83	0.47
34:a:1117:G:H5''	42:i:104:ARG:NH2	2.30	0.47
34:a:1314:C:OP1	52:s:6:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:93:VAL:HG21	35:b:97:TRP:CD1	2.49	0.47
1:A:604:G:H2'	1:A:605:C:C6	2.47	0.47
1:A:614:U:H5'	1:A:614(C):A:N6	2.29	0.47
1:A:950:G:C6	1:A:951:C:C4	3.02	0.47
1:A:1116:C:H2'	1:A:1117:G:O4'	2.14	0.47
1:A:1388:G:H2'	1:A:1389:G:H8	1.79	0.47
1:A:1459:G:C6	1:A:1461:G:C5	3.02	0.47
1:A:2361:A:OP2	31:8:26:LYS:NZ	2.35	0.47
1:A:2590:A:O2'	1:A:2591:C:H5'	2.14	0.47
1:A:2729:G:H2'	1:A:2730:C:C6	2.49	0.47
1:A:2850:A:C2	1:A:2851:A:C4	3.02	0.47
3:D:70:TRP:CE2	3:D:150:LYS:HG3	2.49	0.47
3:D:223:GLY:O	3:D:225:ALA:N	2.47	0.47
3:D:242:ARG:O	3:D:244:ARG:HG2	2.15	0.47
4:E:100:GLU:O	4:E:172:VAL:HG23	2.14	0.47
4:E:111:ARG:HG3	4:E:160:TYR:CD1	2.49	0.47
5:F:89:VAL:HG12	5:F:90:PHE:N	2.29	0.47
8:J:54:ALA:HA	8:J:85:ASP:HA	1.95	0.47
19:W:65:LEU:HD12	19:W:65:LEU:H	1.80	0.47
22:Z:92:SER:OG	22:Z:93:ASP:N	2.44	0.47
34:a:522:C:H2'	34:a:523:A:H5'	1.96	0.47
34:a:767:A:H2'	34:a:768:A:O4'	2.14	0.47
37:d:111:ALA:HA	37:d:161:ASN:HD22	1.80	0.47
40:g:26:PHE:HD1	40:g:101:LEU:HD13	1.78	0.47
56:y:140:LEU:HB2	61:y:703:GDP:HN21	1.80	0.47
56:y:188:PRO:HB2	56:y:216:ARG:HH22	1.73	0.47
56:y:200:ILE:N	56:y:215:LEU:CB	2.68	0.47
56:y:518:ARG:NH1	56:y:548:ARG:HH12	2.11	0.47
1:A:1208:C:C2	1:A:1209:G:C8	3.02	0.47
1:A:1422:G:C1'	1:A:1495:A:H61	2.27	0.47
1:A:2232:U:OP1	24:1:40:ARG:NH1	2.47	0.47
4:E:4:ILE:HG13	4:E:5:LEU:N	2.28	0.47
6:G:47:LYS:HD3	6:G:81:LYS:O	2.14	0.47
6:G:80:PHE:N	6:G:80:PHE:HD1	2.11	0.47
6:G:155:MET:HE2	6:G:155:MET:HB3	1.80	0.47
10:N:36:GLY:C	10:N:38:HIS:H	2.22	0.47
10:N:110:GLY:O	10:N:114:ARG:HG3	2.14	0.47
12:P:77:ARG:O	12:P:79:ARG:NE	2.48	0.47
15:S:10:ARG:HG2	15:S:91:PRO:HA	1.97	0.47
20:X:44:GLU:HG2	20:X:49:VAL:O	2.14	0.47
22:Z:22:GLY:O	22:Z:41:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:32:LEU:HD23	25:2:32:LEU:HA	1.69	0.47
31:8:25:MET:HE1	31:8:45:GLY:O	2.15	0.47
33:x:22:G:C8	33:x:46:7MG:O6	2.67	0.47
34:a:664:G:H22	34:a:741:G:H1	1.61	0.47
34:a:977:A:H2'	34:a:978:A:H5''	1.97	0.47
34:a:1235:U:H2'	34:a:1236:A:O4'	2.14	0.47
34:a:1433:A:C4	34:a:1468:A:C2	3.03	0.47
47:n:23:ARG:HH11	47:n:30:ALA:HB2	1.80	0.47
52:s:45:VAL:HA	52:s:62:ILE:HG22	1.96	0.47
56:y:68:TYR:C	56:y:70:ALA:N	2.72	0.47
56:y:201:PHE:CE2	56:y:214:TYR:CB	2.97	0.47
1:A:28:A:O2'	1:A:583:G:H5'	2.15	0.47
1:A:1792:G:H2'	1:A:1793:C:C6	2.50	0.47
1:A:1818:U:H2'	3:D:157:ARG:HG3	1.96	0.47
1:A:1930:G:O2'	1:A:1968:G:O6	2.28	0.47
1:A:2736:G:C2	1:A:2737:G:C8	3.03	0.47
5:F:103:LYS:O	5:F:106:ARG:HG2	2.14	0.47
5:F:182:ASN:ND2	5:F:185:ASP:OD2	2.45	0.47
6:G:133:LEU:HD21	6:G:157:ILE:HB	1.96	0.47
12:P:31:ALA:O	12:P:32:THR:OG1	2.31	0.47
12:P:100:LEU:HA	12:P:100:LEU:HD23	1.60	0.47
13:Q:32:TYR:CE2	13:Q:133:ARG:HG3	2.50	0.47
14:R:21:TYR:HB3	14:R:47:PHE:CD1	2.48	0.47
17:U:104:GLN:OE1	17:U:105:VAL:HG23	2.14	0.47
27:4:63:TYR:N	27:4:63:TYR:CD1	2.82	0.47
34:a:1206:G:O4'	36:c:194:GLY:HA2	2.14	0.47
43:j:70:ARG:HD3	43:j:70:ARG:HA	1.67	0.47
56:y:190:GLY:O	56:y:191:ASP:C	2.58	0.47
1:A:978:G:C2	1:A:986:C:C2	3.03	0.47
1:A:1416:G:H1	1:A:1582:C:N4	2.00	0.47
2:B:89:G:H2'	2:B:90:A:C8	2.50	0.47
5:F:155:LEU:HD12	5:F:174:VAL:HB	1.96	0.47
12:P:138:LEU:HD23	12:P:145:PRO:HG3	1.96	0.47
14:R:12:ARG:HB3	14:R:16:HIS:HB3	1.95	0.47
14:R:22:ARG:NE	14:R:69:ASP:HA	2.29	0.47
14:R:65:LEU:O	14:R:68:ARG:HG3	2.15	0.47
15:S:11:LYS:HG2	15:S:91:PRO:HD3	1.97	0.47
15:S:74:ALA:HA	15:S:110:LEU:HD11	1.96	0.47
17:U:88:ILE:HD13	17:U:109:LEU:CD2	2.41	0.47
27:4:59:PHE:CA	27:4:61:ARG:H	2.20	0.47
29:6:40:CYS:O	29:6:44:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:9:14:CYS:HA	32:9:27:CYS:HB2	1.96	0.47
33:x:15:G:C6	33:x:48:C:O2	2.68	0.47
34:a:580:U:H2'	34:a:581:G:O4'	2.14	0.47
34:a:953:G:H2'	34:a:954:G:O4'	2.15	0.47
37:d:32:ALA:HB3	59:d:501:SF4:S3	2.54	0.47
37:d:111:ALA:HB2	37:d:120:LEU:HD12	1.96	0.47
37:d:150:GLU:CG	37:d:151:LYS:H	2.28	0.47
42:i:121:ARG:NH1	42:i:122:ALA:O	2.47	0.47
48:o:33:THR:HG23	48:o:63:ARG:NH1	2.29	0.47
48:o:67:LEU:HD23	48:o:78:TYR:HE1	1.80	0.47
53:t:57:ARG:HH22	53:t:100:ILE:HD12	1.79	0.47
56:y:26:ALA:O	56:y:29:ILE:N	2.46	0.47
56:y:68:TYR:CE2	56:y:178:LEU:C	2.91	0.47
56:y:101:GLU:HA	56:y:129:HIS:HE1	1.73	0.47
56:y:200:ILE:C	56:y:215:LEU:HA	2.36	0.47
56:y:223:ARG:NH1	56:y:223:ARG:CG	2.77	0.47
56:y:382:LEU:O	56:y:385:GLY:O	2.32	0.47
1:A:58:G:N2	1:A:70:G:C4	2.83	0.47
1:A:126:A:C6	1:A:127:A:N1	2.83	0.47
1:A:945:A:N6	62:A:3884:HOH:O	2.47	0.47
1:A:1361:G:H2'	1:A:1362:C:H6	1.79	0.47
1:A:2148:G:H2'	1:A:2149:G:H8	1.80	0.47
1:A:2162:G:H2'	1:A:2163:C:C6	2.50	0.47
1:A:2648:C:H2'	1:A:2649:U:C6	2.50	0.47
3:D:183:ARG:HE	3:D:183:ARG:HB2	1.39	0.47
12:P:65:ARG:HD3	12:P:66:GLY:N	2.29	0.47
24:1:3:LYS:HB3	24:1:4:VAL:HG13	1.97	0.47
34:a:160:A:H2'	34:a:161:A:O4'	2.14	0.47
34:a:253:U:H2'	34:a:254:G:H8	1.80	0.47
34:a:572:A:H5'	34:a:573:A:OP2	2.15	0.47
34:a:926:G:H3'	34:a:1505:G:N2	2.26	0.47
34:a:1158:C:H5	34:a:1181:G:H1	1.58	0.47
34:a:1299:A:N3	34:a:1299:A:H5''	2.29	0.47
34:a:1329:A:P	46:m:28:ALA:HB3	2.54	0.47
35:b:178:ARG:HG2	41:h:72:PRO:HA	1.96	0.47
38:e:51:VAL:O	38:e:55:VAL:HG23	2.14	0.47
39:f:83:ASP:O	39:f:84:ASN:ND2	2.48	0.47
44:k:97:ALA:O	44:k:101:SER:HB2	2.15	0.47
49:p:2:VAL:HA	49:p:23:ASP:HA	1.97	0.47
52:s:12:ASP:HB3	52:s:14:HIS:CD2	2.49	0.47
53:t:93:GLU:OE2	53:t:93:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:t:100:ILE:HB	53:t:101:GLY:H	1.44	0.47
56:y:118:LEU:O	56:y:121:PHE:HB3	2.15	0.47
56:y:246:THR:N	56:y:249:GLY:O	2.47	0.47
56:y:348:PHE:O	56:y:350:GLY:N	2.48	0.47
1:A:476:G:H4'	1:A:502:A:N1	2.29	0.47
1:A:517:C:OP1	28:5:16:ARG:NH2	2.48	0.47
1:A:1239:G:H2'	1:A:1240:U:O4'	2.15	0.47
1:A:1478:G:O2'	1:A:1558:A:H2	1.98	0.47
1:A:1791:A:O2'	3:D:207:GLY:N	2.48	0.47
1:A:2028:U:H2'	1:A:2029:G:O4'	2.14	0.47
1:A:2334:G:C4	15:S:12:PHE:CD1	3.03	0.47
1:A:2512:C:H2'	1:A:2513:G:O4'	2.15	0.47
1:A:2660:A:H2'	1:A:2661:G:C8	2.50	0.47
1:A:2815:C:O2	28:5:43:HIS:HE1	1.98	0.47
1:A:2851:A:H8	1:A:2851:A:O5'	1.97	0.47
19:W:20:VAL:HG21	19:W:43:GLY:HA3	1.96	0.47
22:Z:5:LEU:HD22	22:Z:6:LYS:H	1.80	0.47
22:Z:17:ALA:HA	22:Z:20:ARG:NH1	2.29	0.47
23:0:38:VAL:HG23	23:0:59:LEU:HB2	1.97	0.47
32:9:28:GLU:O	32:9:30:PRO:HD3	2.15	0.47
35:b:162:ILE:HG13	35:b:184:VAL:HG23	1.97	0.47
40:g:18:TYR:HB3	40:g:59:LEU:HD12	1.96	0.47
41:h:100:ILE:H	41:h:100:ILE:HG12	1.51	0.47
48:o:23:GLY:O	48:o:28:GLN:HG3	2.15	0.47
50:q:90:ILE:HD13	50:q:90:ILE:HA	1.82	0.47
52:s:3:ARG:NH1	52:s:7:LYS:HB3	2.29	0.47
56:y:121:PHE:HD1	56:y:156:LEU:HD12	1.71	0.47
56:y:509:HIS:HB2	56:y:512:LYS:HB2	1.97	0.47
1:A:1297:C:O2'	1:A:1302:A:N1	2.41	0.47
1:A:1798:U:H5'	3:D:259:THR:CG2	2.45	0.47
1:A:2840:C:H5''	14:R:53:HIS:CD2	2.50	0.47
5:F:12:LEU:HB3	5:F:126:VAL:HG12	1.97	0.47
6:G:73:ALA:HB3	6:G:85:GLY:N	2.30	0.47
7:H:3:ARG:NE	7:H:3:ARG:HA	2.30	0.47
27:4:61:ARG:HG3	27:4:62:ARG:O	2.15	0.47
33:x:57:G:H2'	33:x:58:A:H5'	1.97	0.47
34:a:392:G:H2'	34:a:393:A:H8	1.79	0.47
34:a:974:A:P	47:n:29:ARG:HH22	2.38	0.47
34:a:1003:G:N1	34:a:1004:A:N3	2.63	0.47
34:a:1049:U:OP1	47:n:3:ARG:HG3	2.14	0.47
35:b:23:ARG:NH2	35:b:191:ASP:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:27:LYS:HD3	35:b:193:ASP:OD1	2.15	0.47
36:c:11:ARG:HD3	36:c:15:THR:CG2	2.44	0.47
44:k:120:ARG:NH1	44:k:126:ARG:HD2	2.30	0.47
48:o:6:GLU:H	48:o:6:GLU:CD	2.23	0.47
33:w:66:U:H2'	33:w:67:C:O4'	2.15	0.47
56:y:12:PHE:CD2	56:y:12:PHE:C	2.91	0.47
56:y:28:ARG:CB	56:y:28:ARG:NH1	2.73	0.47
56:y:183:GLN:HG3	56:y:184:ARG:H	1.78	0.47
1:A:652(F):G:H1	1:A:652(S):C:N4	2.13	0.47
1:A:848:G:N9	1:A:933:A:H8	2.13	0.47
1:A:1176:G:H1'	1:A:1177:A:C5'	2.45	0.47
1:A:1221(A):C:H2'	1:A:1222:C:C6	2.48	0.47
1:A:1459:G:H2'	1:A:1461:G:O5'	2.15	0.47
1:A:1664:A:C2	11:O:1:MET:HE1	2.39	0.47
1:A:1721:G:H3'	1:A:1722:A:H5''	1.97	0.47
3:D:35:LYS:HB2	3:D:35:LYS:HE3	1.69	0.47
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.45	0.47
5:F:7:TYR:OH	5:F:119:ARG:HD3	2.15	0.47
7:H:98:LEU:HD21	7:H:123:PHE:HB3	1.96	0.47
11:O:63:VAL:HG23	11:O:84:ALA:HA	1.95	0.47
20:X:57:LEU:N	20:X:57:LEU:HD12	2.30	0.47
31:8:52:LYS:HG3	31:8:53:PRO:CD	2.44	0.47
34:a:26:A:H5''	34:a:27:G:OP2	2.15	0.47
34:a:115:G:H1	34:a:312:C:H42	1.63	0.47
34:a:233:C:H2'	34:a:234:C:C6	2.45	0.47
34:a:502:G:P	45:l:118:SER:HG	2.31	0.47
34:a:1027:C:O2	34:a:1034:G:C2	2.68	0.47
34:a:1130:A:OP2	34:a:1130:A:H3'	2.15	0.47
35:b:19:HIS:HE1	35:b:206:ASP:OD1	1.98	0.47
35:b:98:LEU:HB2	35:b:101:MET:HG3	1.97	0.47
36:c:56:ASP:O	36:c:66:VAL:HA	2.15	0.47
37:d:114:ARG:HH11	37:d:114:ARG:HG3	1.80	0.47
40:g:50:ILE:HD11	40:g:58:PRO:HA	1.97	0.47
48:o:32:LEU:HD13	48:o:63:ARG:HB2	1.97	0.47
53:t:73:HIS:CG	53:t:74:LYS:H	2.33	0.47
1:A:625:G:N7	12:P:107:LYS:NZ	2.60	0.46
1:A:1079:C:O5'	9:K:132:ARG:NH2	2.48	0.46
1:A:1801:G:OP2	3:D:154:LYS:NZ	2.35	0.46
1:A:2582:G:H2'	1:A:2582:G:N3	2.29	0.46
5:F:32:LEU:O	5:F:32:LEU:HD23	2.15	0.46
6:G:27:ASN:C	6:G:29:TRP:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:137:LYS:HD3	10:N:138:LEU:N	2.29	0.46
12:P:126:VAL:HG22	12:P:146:VAL:HB	1.97	0.46
17:U:44:ASN:N	17:U:44:ASN:OD1	2.46	0.46
22:Z:119:GLU:OE2	22:Z:122:ARG:NH1	2.48	0.46
25:2:10:LEU:HB3	25:2:14:ARG:NH1	2.30	0.46
33:x:58:A:N6	33:x:61:C:C2	2.83	0.46
34:a:253:U:H2'	34:a:254:G:C8	2.51	0.46
34:a:452:A:N7	34:a:480:U:N3	2.62	0.46
34:a:1039:C:H2'	34:a:1040:U:H6	1.80	0.46
35:b:175:ARG:HG2	35:b:175:ARG:NH1	2.22	0.46
37:d:18:LYS:HG3	37:d:33:MET:HG2	1.97	0.46
41:h:68:ARG:HG3	41:h:69:ARG:N	2.31	0.46
42:i:3:GLN:OE1	42:i:20:ARG:NE	2.41	0.46
42:i:118:LYS:O	42:i:119:ALA:HB3	2.14	0.46
52:s:23:ASN:HA	52:s:27:GLU:CG	2.45	0.46
56:y:15:ILE:HD12	56:y:103:VAL:CB	2.45	0.46
56:y:98:ALA:CA	56:y:127:HIS:CE1	2.99	0.46
56:y:427:LEU:HD12	56:y:427:LEU:O	2.14	0.46
1:A:397:G:O2'	1:A:2230:G:N2	2.47	0.46
1:A:1256:G:H1'	5:F:82:ILE:HD11	1.97	0.46
1:A:1381:G:C6	1:A:1382:G:C5	3.03	0.46
1:A:2335:A:C8	1:A:2337:G:C5	3.03	0.46
1:A:2343:C:H2'	1:A:2344:U:C6	2.49	0.46
12:P:2:LYS:HZ3	12:P:2:LYS:HB2	1.79	0.46
22:Z:54:HIS:HB3	22:Z:101:PRO:HD3	1.96	0.46
22:Z:160:GLY:N	22:Z:161:VAL:HB	2.30	0.46
34:a:8:A:N6	37:d:209:ARG:HB3	2.29	0.46
34:a:472:A:H3'	34:a:473:G:H8	1.80	0.46
34:a:684:A:C1'	44:k:38:ASN:HD22	2.28	0.46
34:a:691:G:H2'	34:a:692:U:C6	2.50	0.46
34:a:745:C:H2'	34:a:746:A:H8	1.77	0.46
34:a:1473:A:O2'	34:a:1474:G:H5'	2.15	0.46
40:g:113:GLU:HG2	40:g:119:ARG:HG2	1.98	0.46
50:q:95:TYR:HD1	50:q:98:LEU:HD22	1.80	0.46
52:s:37:ARG:H	52:s:37:ARG:HG3	1.43	0.46
33:w:68:C:H2'	33:w:69:G:C8	2.51	0.46
56:y:21:GLY:HA2	56:y:24:THR:OG1	2.15	0.46
56:y:277:GLY:HA3	56:y:293:GLY:H	1.79	0.46
1:A:82:G:N2	1:A:103:A:OP2	2.40	0.46
1:A:181:A:C2	1:A:182:A:C4	3.03	0.46
1:A:1055:G:H2'	1:A:1056:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:C:C5	1:A:1569:A:H5''	2.51	0.46
1:A:1885:A:H2'	1:A:1886:C:O4'	2.16	0.46
1:A:2021:C:OP1	28:5:12:SER:OG	2.22	0.46
1:A:2107:C:N3	1:A:2182:G:N2	2.63	0.46
1:A:2135:A:H61	1:A:2156:G:H1'	1.81	0.46
1:A:2405:G:O2'	1:A:2406:U:OP1	2.22	0.46
1:A:2661:G:C6	1:A:2662:A:C2	3.03	0.46
1:A:2680:C:OP2	4:E:111:ARG:NH2	2.47	0.46
2:B:78:A:C2	2:B:100:A:C4	3.04	0.46
7:H:87:LEU:N	7:H:131:VAL:O	2.48	0.46
14:R:63:ARG:HH21	14:R:77:ARG:HA	1.80	0.46
16:T:94:ALA:HB1	16:T:99:LEU:HD21	1.96	0.46
33:x:5:G:H2'	33:x:6:G:C8	2.51	0.46
34:a:1118:C:OP1	42:i:9:ARG:HD2	2.16	0.46
34:a:1162:C:H42	34:a:1174:G:H1	1.63	0.46
34:a:1302:U:OP1	46:m:13:LYS:HE3	2.16	0.46
36:c:15:THR:HG21	36:c:181:ASN:HA	1.97	0.46
45:l:7:ILE:HG21	50:q:34:LYS:HB2	1.96	0.46
46:m:87:TYR:O	46:m:91:ARG:HG2	2.15	0.46
48:o:39:LEU:HB3	48:o:56:LEU:HD12	1.96	0.46
51:r:55:ARG:HB3	51:r:55:ARG:NH1	2.29	0.46
56:y:192:PRO:O	56:y:220:GLY:O	2.33	0.46
1:A:195:A:H5''	12:P:46:LYS:NZ	2.30	0.46
1:A:265:A:H1'	1:A:266:G:O4'	2.16	0.46
1:A:1052:C:O2'	1:A:1053:C:OP1	2.24	0.46
1:A:1264:G:C6	1:A:1265:A:N6	2.84	0.46
1:A:1292:U:H2'	1:A:1293:C:C6	2.50	0.46
1:A:1366:A:C4	1:A:1367:A:C8	3.03	0.46
1:A:1469:A:H2'	1:A:1470:G:O4'	2.16	0.46
1:A:1509(A):A:H2'	1:A:1509(B):A:O4'	2.15	0.46
1:A:1572:A:H5'	62:A:4010:HOH:O	2.16	0.46
1:A:1802:A:H8	1:A:1802:A:O5'	1.99	0.46
1:A:2114:A:H2'	1:A:2115:G:H5'	1.97	0.46
1:A:2230:G:H2'	1:A:2231:C:H6	1.78	0.46
1:A:2493:U:H2'	1:A:2494:G:O4'	2.15	0.46
5:F:165:ARG:H	5:F:167:ALA:H	1.62	0.46
9:K:112:MET:C	9:K:114:ASP:H	2.23	0.46
10:N:68:GLU:O	10:N:70:LYS:N	2.47	0.46
10:N:75:TYR:CE2	10:N:77:GLY:HA2	2.50	0.46
13:Q:21:THR:OG1	13:Q:23:GLY:O	2.33	0.46
34:a:407:G:H2'	34:a:408:A:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:794:A:C5	34:a:795:C:C4	3.03	0.46
34:a:1071:C:H2'	34:a:1072:G:C8	2.50	0.46
35:b:100:GLY:O	35:b:104:ASN:N	2.47	0.46
41:h:97:VAL:O	41:h:100:ILE:HG12	2.15	0.46
45:l:7:ILE:O	45:l:11:VAL:HG23	2.16	0.46
50:q:20:THR:HG21	50:q:41:LYS:HE2	1.98	0.46
56:y:81:ILE:N	56:y:81:ILE:CD1	2.73	0.46
56:y:223:ARG:HG2	56:y:223:ARG:HH11	1.79	0.46
56:y:373:ALA:CB	56:y:374:PRO:CA	2.90	0.46
1:A:2310:A:H2'	1:A:2311:A:H5''	1.98	0.46
1:A:2331:G:C6	1:A:2332:U:C4	3.04	0.46
1:A:2436:G:C6	1:A:2437:U:C4	3.03	0.46
1:A:2684:U:OP2	16:T:53:ARG:NH1	2.48	0.46
1:A:2859:G:H2'	1:A:2860:A:C8	2.51	0.46
4:E:152:LYS:HG2	10:N:78:TYR:CE1	2.51	0.46
6:G:114:ILE:HG12	6:G:140:ILE:HD13	1.98	0.46
10:N:42:TRP:CE3	17:U:63:VAL:HG11	2.50	0.46
10:N:42:TRP:HD1	10:N:48:MET:CE	2.28	0.46
11:O:71:ARG:O	11:O:73:ASP:N	2.49	0.46
12:P:84:ASN:HB2	12:P:87:ASP:OD2	2.16	0.46
12:P:144:GLU:HA	12:P:145:PRO:HD3	1.78	0.46
23:O:27:GLU:HG3	23:O:68:GLU:HA	1.98	0.46
34:a:45:U:H2'	34:a:46:G:C8	2.51	0.46
34:a:93:G:H2'	34:a:96:U:H5'	1.98	0.46
34:a:629:G:H3'	34:a:630:G:H5''	1.96	0.46
34:a:1435:G:H2'	34:a:1436:U:C6	2.51	0.46
45:l:6:THR:HG23	45:l:9:GLN:OE1	2.15	0.46
45:l:24:VAL:O	45:l:24:VAL:CG1	2.64	0.46
48:o:26:GLU:H	48:o:26:GLU:HG2	1.48	0.46
49:p:9:PHE:CE1	49:p:18:ARG:HD2	2.50	0.46
56:y:65:ARG:CA	56:y:78:PHE:O	2.64	0.46
56:y:417:PRO:HD2	56:y:420:TYR:HD2	1.80	0.46
1:A:40:C:N4	1:A:438:G:H1	2.10	0.46
1:A:860:U:H1'	1:A:2268:A:H5'	1.97	0.46
1:A:875:G:H2'	1:A:876:C:O4'	2.16	0.46
1:A:1315:C:H2'	1:A:1316:U:C6	2.51	0.46
1:A:1429:G:H2'	1:A:1430:C:C6	2.51	0.46
1:A:1442:G:H2'	1:A:1443:G:C8	2.50	0.46
1:A:2451:A:O2'	33:w:76:A:O2'	2.09	0.46
1:A:2554:U:H2'	1:A:2555:U:H6	1.80	0.46
2:B:78:A:H2'	2:B:79:C:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:32:PRO:HA	20:X:77:LYS:CD	2.46	0.46
22:Z:80:ARG:HH11	22:Z:80:ARG:HB2	1.80	0.46
34:a:280:C:O2	50:q:38:ARG:HD2	2.15	0.46
34:a:598:U:H2'	34:a:599:C:C6	2.51	0.46
34:a:1109:C:C2	34:a:1110:A:C8	3.03	0.46
34:a:1128:C:H5''	42:i:16:ARG:HH12	1.81	0.46
34:a:1457:G:P	53:t:39:LYS:HZ1	2.39	0.46
34:a:1481:U:H2'	34:a:1482:G:C8	2.51	0.46
35:b:121:LEU:HG	35:b:127:ILE:HD13	1.97	0.46
35:b:154:LEU:HD13	35:b:154:LEU:HA	1.71	0.46
37:d:20:TYR:HD2	37:d:26:CYS:HB3	1.81	0.46
38:e:148:VAL:O	38:e:151:LEU:N	2.21	0.46
40:g:62:PHE:O	40:g:65:ALA:HB3	2.15	0.46
41:h:10:LEU:HD22	41:h:83:ILE:HD11	1.96	0.46
47:n:13:THR:HG22	47:n:14:PRO:HD2	1.96	0.46
33:w:6:G:O2'	33:w:7:A:H5'	2.15	0.46
1:A:248:G:H5''	1:A:386:G:N2	2.31	0.46
1:A:579:G:H2'	1:A:580:C:C6	2.51	0.46
1:A:2436:G:O2'	1:A:2598:A:N1	2.46	0.46
62:A:3760:HOH:O	12:P:56:SER:N	2.45	0.46
11:O:97:ARG:HA	11:O:117:LEU:HD22	1.97	0.46
16:T:64:ARG:NH1	16:T:103:ARG:HA	2.31	0.46
17:U:19:LYS:HG2	17:U:22:LYS:HE3	1.98	0.46
17:U:92:ARG:HA	17:U:95:LEU:HB2	1.98	0.46
34:a:712:A:N6	34:a:713:G:C6	2.84	0.46
39:f:89:MET:HE1	51:r:72:ARG:HB3	1.98	0.46
41:h:40:ALA:HB2	41:h:45:ILE:HG13	1.98	0.46
44:k:20:TYR:CE1	44:k:83:ILE:HD12	2.50	0.46
48:o:32:LEU:HD22	48:o:59:MET:HB3	1.98	0.46
56:y:15:ILE:HD12	56:y:103:VAL:CG2	2.46	0.46
56:y:108:ASP:HA	56:y:137:LYS:HG2	1.97	0.46
56:y:228:ILE:HD12	56:y:228:ILE:O	2.15	0.46
1:A:105:C:O2'	21:Y:1:MET:HA	2.16	0.46
1:A:530:G:O4'	1:A:530:G:N3	2.47	0.46
1:A:652(E):G:O6	1:A:652(S):C:N4	2.48	0.46
1:A:1491:G:N2	1:A:1500:G:H1'	2.31	0.46
1:A:2261:C:OP1	23:O:17:GLN:HB2	2.16	0.46
1:A:2267:A:H5''	1:A:2268:A:C5'	2.46	0.46
14:R:104:ARG:HD2	14:R:107:ASP:OD1	2.16	0.46
33:x:48:C:OP1	33:x:48:C:H2'	2.16	0.46
34:a:551:U:H2'	34:a:552:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:734:G:H21	51:r:75:ILE:HD11	1.81	0.46
34:a:1050:G:N3	34:a:1050:G:H2'	2.30	0.46
34:a:1317:C:H5''	34:a:1318:A:OP2	2.15	0.46
42:i:34:ASN:O	42:i:38:GLN:HB3	2.16	0.46
44:k:34:ASP:HB3	44:k:40:ILE:HD11	1.96	0.46
33:w:18:G:H4'	33:w:60:U:C5	2.51	0.46
56:y:21:GLY:O	56:y:24:THR:N	2.49	0.46
56:y:97:LEU:CB	56:y:127:HIS:CE1	2.99	0.46
56:y:201:PHE:HD2	56:y:202:ASP:N	2.14	0.46
56:y:295:ARG:CB	56:y:296:PRO:CD	2.94	0.46
56:y:300:VAL:O	56:y:346:CYS:O	2.34	0.46
56:y:320:LEU:O	56:y:324:LYS:N	2.44	0.46
56:y:594:GLN:HG3	56:y:595:GLU:OE2	2.16	0.46
1:A:272(I):U:H2'	1:A:272(J):C:C6	2.50	0.46
1:A:568:U:H5'	1:A:945:A:N1	2.31	0.46
1:A:990:A:N6	1:A:1186:G:H1'	2.31	0.46
1:A:1742:G:H2'	1:A:1743:C:O4'	2.15	0.46
1:A:2048:G:C6	1:A:2049:G:C5	3.04	0.46
1:A:2590:A:H2'	1:A:2591:C:H6	1.80	0.46
1:A:2815:C:O2'	28:5:43:HIS:ND1	2.46	0.46
3:D:275:LYS:HD2	3:D:276:LYS:H	1.80	0.46
10:N:48:MET:O	10:N:48:MET:HE3	2.16	0.46
16:T:2:ASN:HB3	16:T:5:ALA:HB3	1.98	0.46
16:T:48:ILE:O	16:T:64:ARG:N	2.43	0.46
20:X:63:LYS:O	20:X:64:LYS:HD3	2.16	0.46
20:X:92:LEU:C	20:X:94:GLY:N	2.67	0.46
22:Z:133:ILE:O	22:Z:135:GLU:HG3	2.15	0.46
25:2:22:GLU:O	25:2:25:VAL:HG12	2.16	0.46
32:9:15:LYS:HB3	32:9:26:ILE:HD12	1.98	0.46
33:x:2:C:H42	33:x:71:G:H1	1.63	0.46
34:a:262:A:N6	34:a:263:A:N6	2.64	0.46
34:a:374:A:C6	34:a:375:U:C4	3.04	0.46
34:a:633:G:H2'	34:a:634:C:C6	2.51	0.46
34:a:1112:C:O2	36:c:179:ARG:HG2	2.16	0.46
34:a:1189:C:P	43:j:51:ARG:HH22	2.38	0.46
37:d:114:ARG:HH11	37:d:114:ARG:CG	2.29	0.46
39:f:67:MET:HB2	39:f:68:PRO:HD2	1.98	0.46
41:h:4:ASP:CG	41:h:85:ARG:HH11	2.24	0.46
42:i:41:VAL:HG23	42:i:42:ARG:H	1.81	0.46
52:s:14:HIS:O	52:s:18:LYS:HG3	2.15	0.46
1:A:306:U:H2'	1:A:307:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:G:C8	30:7:37:LYS:HG2	2.51	0.46
1:A:1064:C:H5''	9:K:86:LYS:HB2	1.97	0.46
1:A:1090:U:C2	1:A:1102:C:H1'	2.51	0.46
1:A:2168:G:N1	1:A:2171:A:N7	2.64	0.46
1:A:2298:A:H2'	1:A:2299:G:O4'	2.15	0.46
1:A:2562:U:H1'	11:O:23:ARG:HH11	1.79	0.46
1:A:2771:C:H2'	1:A:2772:C:C6	2.51	0.46
1:A:2851:A:H2'	1:A:2852:G:O4'	2.16	0.46
3:D:73:VAL:C	3:D:75:ILE:H	2.22	0.46
3:D:109:ASP:N	3:D:195:ALA:O	2.37	0.46
11:O:37:ASP:OD1	11:O:109:LYS:NZ	2.49	0.46
11:O:39:ILE:HD12	11:O:41:ALA:HB2	1.98	0.46
13:Q:2:LEU:H	13:Q:2:LEU:HD12	1.80	0.46
19:W:48:ALA:O	19:W:52:GLU:HB2	2.16	0.46
22:Z:98:MET:HE2	22:Z:98:MET:HB2	1.78	0.46
34:a:236:G:H2'	34:a:237:C:C6	2.51	0.46
34:a:311:C:H2'	34:a:312:C:O4'	2.16	0.46
34:a:435:C:O2'	34:a:436:C:H5'	2.15	0.46
34:a:652:U:C4	34:a:752:G:N3	2.84	0.46
34:a:1226:C:C5	46:m:104:ARG:HA	2.51	0.46
34:a:1253:G:OP1	43:j:44:VAL:HG21	2.16	0.46
35:b:54:THR:HG22	35:b:58:ILE:HD11	1.98	0.46
35:b:104:ASN:O	35:b:108:ILE:HG12	2.16	0.46
40:g:14:PRO:HA	40:g:21:VAL:HG12	1.97	0.46
40:g:80:VAL:HG12	40:g:83:ALA:H	1.81	0.46
45:l:93:LEU:HA	45:l:94:PRO:HD2	1.79	0.46
49:p:60:LEU:HD22	49:p:60:LEU:HA	1.81	0.46
50:q:60:ILE:HG12	50:q:61:GLU:N	2.31	0.46
33:w:48:C:H2'	33:w:59:U:H1'	1.98	0.46
56:y:105:LEU:HD13	56:y:105:LEU:O	2.16	0.46
56:y:581:LYS:HA	56:y:581:LYS:HD3	1.76	0.46
1:A:271(G):C:H2'	1:A:271(H):G:H5'	1.98	0.45
1:A:1783:A:C2	1:A:2588:G:O4'	2.69	0.45
1:A:2199:A:H5''	1:A:2200:C:C5	2.51	0.45
1:A:2359:C:H2'	1:A:2360:A:C8	2.51	0.45
1:A:2677:G:H2'	1:A:2678:C:H6	1.81	0.45
1:A:2744:G:H1'	1:A:2761:G:N2	2.31	0.45
2:B:33:G:H2'	2:B:34:U:C6	2.51	0.45
9:K:34:ILE:H	9:K:34:ILE:HG12	1.55	0.45
14:R:72:ASP:OD1	14:R:75:LEU:HB2	2.16	0.45
15:S:30:ARG:HG2	15:S:31:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:29:TYR:CB	22:Z:34:ASN:HD22	2.24	0.45
22:Z:57:ILE:O	22:Z:69:THR:OG1	2.33	0.45
34:a:122:G:H8	34:a:122:G:OP1	1.99	0.45
34:a:722:A:O2'	34:a:723:U:H2'	2.16	0.45
34:a:1030(C):G:H2'	34:a:1030(D):A:H8	1.80	0.45
34:a:1058:G:H2'	34:a:1059:C:O4'	2.16	0.45
34:a:1486:G:H5'	34:a:1487:G:OP2	2.16	0.45
37:d:205:GLU:OE1	38:e:100:VAL:N	2.46	0.45
52:s:23:ASN:OD1	52:s:47:HIS:HE1	1.98	0.45
56:y:28:ARG:CD	56:y:168:GLY:O	2.63	0.45
56:y:471:SER:O	56:y:472:ARG:CB	2.62	0.45
1:A:607:U:H5	1:A:619:G:C5	2.34	0.45
1:A:631:A:N3	1:A:2415:G:O2'	2.38	0.45
1:A:903:C:H2'	1:A:904:C:C6	2.50	0.45
1:A:1090:U:O2	1:A:1102:C:H1'	2.16	0.45
1:A:2123:G:N2	1:A:2176:A:H1'	2.32	0.45
1:A:2141:G:H22	1:A:2149:G:H22	1.64	0.45
9:K:37:PHE:O	9:K:41:PHE:HB3	2.15	0.45
15:S:78:LEU:C	15:S:80:LEU:H	2.24	0.45
22:Z:110:GLY:O	22:Z:113:ALA:HB3	2.15	0.45
33:x:6:G:C6	33:x:7:A:C5	3.05	0.45
34:a:370:C:H2'	34:a:371:G:H8	1.81	0.45
34:a:598:U:H2'	34:a:599:C:H6	1.81	0.45
34:a:983:A:H3'	34:a:983:A:N3	2.31	0.45
34:a:1193:G:H8	34:a:1193:G:H5''	1.82	0.45
36:c:22:TRP:CD1	36:c:59:ARG:HD2	2.51	0.45
41:h:111:ILE:H	41:h:111:ILE:HG12	1.57	0.45
44:k:92:GLU:OE1	51:r:87:ARG:NH1	2.50	0.45
45:l:60:LEU:HD21	45:l:66:VAL:HG22	1.99	0.45
46:m:30:ALA:O	46:m:34:LEU:HD23	2.16	0.45
49:p:28:ARG:HG3	49:p:29:ASP:N	2.32	0.45
50:q:34:LYS:HG2	50:q:35:VAL:N	2.31	0.45
51:r:33:ASP:OD2	51:r:36:ASN:HB2	2.16	0.45
1:A:136:G:C2	1:A:137:C:C6	3.05	0.45
1:A:207:A:H2'	1:A:208:C:O4'	2.17	0.45
1:A:1079:C:H4'	9:K:132:ARG:NH2	2.31	0.45
1:A:1477:A:C6	1:A:1478:G:C6	3.04	0.45
1:A:1499:C:H2'	1:A:1500:G:H8	1.80	0.45
1:A:2330:G:H4'	23:0:44:ARG:NH1	2.30	0.45
1:A:2419:U:O2'	1:A:2420:C:H5'	2.16	0.45
1:A:2552:U:H2'	1:A:2554:U:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:LYS:HD2	3:D:70:TRP:CH2	2.51	0.45
3:D:130:ALA:C	3:D:131:LEU:HD12	2.41	0.45
3:D:133:LEU:HB3	3:D:173:VAL:HG11	1.97	0.45
4:E:119:ARG:HG2	4:E:160:TYR:CG	2.51	0.45
22:Z:24:LEU:HD11	22:Z:86:VAL:CG2	2.46	0.45
22:Z:29:TYR:HB3	22:Z:34:ASN:ND2	2.24	0.45
23:0:27:GLU:HB2	23:0:69:PHE:HD1	1.81	0.45
33:x:7:A:HO2'	33:x:49:C:H5'	1.76	0.45
34:a:63:C:H5''	34:a:383:A:H61	1.80	0.45
35:b:16:HIS:HB2	35:b:210:SER:HB2	1.98	0.45
36:c:104:GLN:C	36:c:104:GLN:HE21	2.23	0.45
36:c:110:ASN:O	36:c:141:VAL:HG22	2.15	0.45
40:g:37:ASN:O	40:g:41:ARG:HG3	2.17	0.45
40:g:46:ALA:O	40:g:50:ILE:HG23	2.17	0.45
42:i:44:VAL:HA	42:i:45:ALA:HA	1.58	0.45
43:j:81:THR:HA	43:j:84:GLN:HG3	1.98	0.45
45:l:60:LEU:HD11	45:l:85:ILE:HG12	1.97	0.45
56:y:348:PHE:O	56:y:349:LEU:C	2.59	0.45
1:A:85:G:H8	1:A:85:G:H5''	1.81	0.45
1:A:247:G:C8	1:A:249:C:C6	3.04	0.45
1:A:467:G:P	30:7:33:ARG:HH12	2.40	0.45
1:A:1176:G:N3	1:A:1177:A:H5'	2.30	0.45
1:A:1386:C:H2'	1:A:1387:C:C6	2.52	0.45
1:A:1496:A:H8	1:A:1496:A:O5'	1.98	0.45
1:A:1845:G:H1	1:A:1895:C:N4	2.13	0.45
1:A:2469:A:H4'	13:Q:56:ARG:CG	2.46	0.45
1:A:2663:G:C6	1:A:2664:G:C4	3.04	0.45
5:F:53:THR:HG23	5:F:55:GLY:H	1.81	0.45
9:K:20:ALA:HA	9:K:21:PRO:HD3	1.81	0.45
12:P:87:ASP:O	12:P:90:ARG:HG2	2.16	0.45
15:S:102:ALA:O	15:S:104:GLY:N	2.49	0.45
17:U:111:GLU:O	17:U:114:LYS:HB2	2.17	0.45
22:Z:8:TYR:HB2	22:Z:38:TYR:CE2	2.51	0.45
34:a:109:A:H2'	34:a:326:G:N2	2.31	0.45
34:a:271:C:O5'	34:a:271:C:H6	1.98	0.45
34:a:1228:C:H6	34:a:1228:C:H5''	1.81	0.45
35:b:28:PHE:CE1	35:b:190:THR:HA	2.50	0.45
35:b:155:LEU:HB3	35:b:157:ARG:H	1.82	0.45
37:d:19:LEU:CD2	37:d:67:ILE:HG13	2.46	0.45
37:d:64:LEU:HB2	37:d:198:VAL:HG11	1.97	0.45
39:f:29:ALA:O	39:f:32:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:w:73:A:C5	56:y:572:LYS:HB2	2.51	0.45
56:y:80:LEU:C	56:y:81:ILE:HD12	2.40	0.45
1:A:432:A:H2'	1:A:433:C:C6	2.52	0.45
1:A:443:A:H1'	1:A:1201:C:O4'	2.15	0.45
1:A:484:C:N4	1:A:496:G:H1	2.14	0.45
1:A:556:G:C5	1:A:557:U:C4	3.04	0.45
1:A:1266:G:OP2	28:5:19:ARG:HD2	2.16	0.45
1:A:2038:G:C6	1:A:2039:C:C4	3.04	0.45
1:A:2259:G:C2	1:A:2282:G:C6	3.05	0.45
3:D:13:ARG:HD2	3:D:13:ARG:HA	1.66	0.45
3:D:33:LEU:O	3:D:64:ILE:HG13	2.16	0.45
5:F:110:LEU:HD23	5:F:110:LEU:HA	1.76	0.45
6:G:43:LEU:HB3	6:G:44:GLY:H	1.61	0.45
13:Q:71:ASP:OD1	13:Q:71:ASP:N	2.49	0.45
14:R:60:LEU:O	14:R:63:ARG:N	2.49	0.45
30:7:8:ASN:HB3	30:7:11:LYS:HB3	1.98	0.45
34:a:78:G:H4'	34:a:79:G:OP1	2.16	0.45
34:a:631:G:OP2	34:a:631:G:H8	1.99	0.45
34:a:1060:C:C4	36:c:2:GLY:HA3	2.52	0.45
34:a:1314:C:H2'	34:a:1315:U:H6	1.80	0.45
34:a:1328:C:H2'	34:a:1329:A:O4'	2.16	0.45
38:e:148:VAL:O	38:e:150:ARG:N	2.49	0.45
40:g:8:GLU:H	40:g:8:GLU:HG2	1.48	0.45
56:y:122:TYR:O	56:y:123:MET:O	2.34	0.45
1:A:588:U:H1'	5:F:90:PHE:CG	2.52	0.45
1:A:1041:C:H42	1:A:1114:G:H1	1.63	0.45
1:A:1264:G:N7	1:A:1265:A:C5	2.84	0.45
1:A:1434:A:C2	1:A:1435:G:C5	3.05	0.45
1:A:2189:U:H2'	1:A:2190:G:C8	2.52	0.45
9:K:78:ILE:HG13	9:K:99:ILE:HG13	1.99	0.45
9:K:115:LEU:HB2	9:K:116:ASN:H	1.48	0.45
17:U:11:ARG:O	17:U:15:LYS:HB2	2.16	0.45
25:2:46:GLN:HB3	25:2:48:HIS:CE1	2.51	0.45
27:4:46:GLN:C	27:4:48:ARG:H	2.23	0.45
34:a:43:C:H2'	34:a:44:G:O4'	2.17	0.45
34:a:652:U:C2	34:a:752:G:N2	2.85	0.45
34:a:977:A:N6	34:a:1224:G:O5'	2.49	0.45
36:c:101:LEU:HD12	36:c:101:LEU:HA	1.75	0.45
38:e:8:GLU:HB3	38:e:34:VAL:HG23	1.98	0.45
40:g:89:MET:HE3	40:g:90:GLU:H	1.80	0.45
41:h:17:THR:O	41:h:20:TYR:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:l:97:ARG:HB2	45:l:98:TYR:CE2	2.51	0.45
45:l:104:VAL:HG12	45:l:105:TYR:CG	2.52	0.45
1:A:527:C:OP1	62:A:3786:HOH:O	2.21	0.45
1:A:595:C:H2'	1:A:596:G:O4'	2.17	0.45
1:A:652(E):G:C2	1:A:652(U):G:C2	3.05	0.45
1:A:816:C:O2'	62:A:3785:HOH:O	2.21	0.45
1:A:1384:A:N3	1:A:1405:U:H1'	2.31	0.45
1:A:2303:G:O2'	6:G:132:ASN:HB2	2.17	0.45
1:A:2420:C:OP1	31:8:33:ASN:N	2.50	0.45
1:A:2630:G:O2'	1:A:2892:A:O2'	2.13	0.45
1:A:2675:A:H2'	1:A:2676:C:O4'	2.16	0.45
3:D:145:VAL:HB	3:D:155:LEU:HB2	1.98	0.45
10:N:75:TYR:CZ	10:N:77:GLY:HA2	2.52	0.45
15:S:93:LYS:O	15:S:95:HIS:N	2.49	0.45
17:U:28:ARG:HH11	17:U:38:THR:HG23	1.81	0.45
23:0:32:ARG:HE	23:0:32:ARG:HB3	1.53	0.45
33:x:53:G:N1	33:x:61:C:N4	2.38	0.45
34:a:1003:G:C2'	34:a:1004:A:H4'	2.46	0.45
49:p:38:TYR:CE2	49:p:50:LYS:HB2	2.51	0.45
52:s:27:GLU:H	52:s:27:GLU:HG3	1.46	0.45
56:y:121:PHE:CD1	56:y:156:LEU:CD1	2.87	0.45
56:y:504:LEU:CD2	56:y:599:ALA:O	2.63	0.45
56:y:559:LEU:HD21	56:y:570:LYS:O	2.17	0.45
1:A:92:A:C8	1:A:93:G:C8	3.05	0.45
1:A:248:G:H5'	1:A:250:G:N7	2.31	0.45
1:A:652(F):G:H1	1:A:652(S):C:H42	1.65	0.45
1:A:831:G:N2	12:P:53:GLY:O	2.49	0.45
1:A:954:G:H4'	13:Q:13:GLN:NE2	2.30	0.45
1:A:1164:G:C5	1:A:1165:U:C4	3.04	0.45
1:A:1968:G:H5''	62:A:4154:HOH:O	2.17	0.45
5:F:39:TRP:CD2	5:F:101:LEU:HD23	2.52	0.45
6:G:145:THR:H	6:G:148:MET:HE2	1.81	0.45
9:K:30:HIS:CD2	9:K:65:PHE:HB3	2.52	0.45
15:S:92:TYR:HB2	15:S:98:VAL:HG21	1.98	0.45
22:Z:70:LEU:HD11	22:Z:98:MET:HE3	1.98	0.45
23:0:40:GLN:HE21	23:0:57:PHE:HB3	1.82	0.45
25:2:26:ARG:NH1	25:2:26:ARG:HB2	2.32	0.45
33:x:19:G:N2	33:x:56:C:N3	2.64	0.45
34:a:892:A:C6	34:a:893:C:C4	3.04	0.45
34:a:1036:G:H3'	34:a:1037:C:H6	1.82	0.45
43:j:57:LYS:HG3	43:j:57:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:q:84:LEU:O	50:q:87:LYS:N	2.49	0.45
33:w:76:A:H4'	33:w:76:A:OP1	2.16	0.45
56:y:-16:ALA:O	56:y:-12:ARG:HB2	2.16	0.45
56:y:201:PHE:CE2	56:y:214:TYR:HB2	2.51	0.45
56:y:201:PHE:CZ	56:y:214:TYR:HB3	2.52	0.45
56:y:228:ILE:C	56:y:228:ILE:CD1	2.85	0.45
56:y:286:PRO:O	56:y:287:THR:C	2.60	0.45
56:y:479:TYR:CG	56:y:479:TYR:O	2.69	0.45
56:y:497:HIS:CD2	56:y:497:HIS:O	2.70	0.45
1:A:307:G:H21	1:A:330:A:N6	2.15	0.45
1:A:831:G:C6	1:A:832:G:C5	3.05	0.45
1:A:2121:G:N2	1:A:2177:C:N3	2.58	0.45
1:A:2267:A:H5''	1:A:2268:A:H5'	1.99	0.45
4:E:67:PHE:CD2	4:E:74:PRO:HA	2.51	0.45
9:K:109:LYS:HA	9:K:112:MET:SD	2.56	0.45
20:X:67:GLY:C	20:X:69:TYR:N	2.75	0.45
22:Z:24:LEU:HD11	22:Z:86:VAL:HG23	1.98	0.45
22:Z:100:VAL:HA	22:Z:101:PRO:HD3	1.85	0.45
22:Z:157:LEU:HD11	22:Z:163:LEU:HD13	1.98	0.45
33:x:2:C:N4	33:x:71:G:H1	2.14	0.45
34:a:161:A:N1	34:a:347:G:O2'	2.49	0.45
34:a:512:U:H1'	37:d:42:GLN:HE22	1.82	0.45
34:a:1025:U:H5'	34:a:1026:G:OP1	2.17	0.45
35:b:75:LYS:O	35:b:77:ALA:N	2.43	0.45
35:b:120:ALA:O	35:b:121:LEU:HB3	2.16	0.45
41:h:51:VAL:HB	41:h:52:ASP:H	1.46	0.45
53:t:8:ARG:O	53:t:9:ASN:HB3	2.17	0.45
56:y:100:VAL:C	56:y:129:HIS:NE2	2.75	0.45
56:y:121:PHE:O	56:y:122:TYR:C	2.56	0.45
56:y:598:LEU:HA	56:y:598:LEU:HD23	1.73	0.45
1:A:215:G:O3'	1:A:216:A:H4'	2.16	0.45
1:A:572:A:H3'	1:A:573:G:O4'	2.16	0.45
1:A:1182:A:H2'	1:A:1183:G:O4'	2.17	0.45
1:A:1583:A:O2'	1:A:1586:A:N6	2.50	0.45
1:A:1721:G:N3	1:A:1721:G:H5''	2.31	0.45
1:A:2257:U:H2'	1:A:2258:C:C6	2.51	0.45
1:A:2291:U:O2'	1:A:2374:C:O2	2.32	0.45
3:D:92:ILE:HA	3:D:107:ALA:H	1.82	0.45
3:D:182:LEU:HB3	3:D:271:ILE:HB	1.98	0.45
10:N:94:HIS:HB3	10:N:96:GLU:OE1	2.17	0.45
12:P:3:LEU:HA	12:P:3:LEU:HD12	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:32:THR:HG22	18:V:60:GLU:HB2	1.99	0.45
34:a:189(K):U:H2'	34:a:189(L):G:C8	2.52	0.45
34:a:293:G:C6	34:a:294:U:C4	3.05	0.45
34:a:708:C:O2'	34:a:709:G:H5'	2.17	0.45
34:a:892:A:C5	34:a:893:C:C4	3.05	0.45
34:a:974:A:OP1	47:n:29:ARG:NH2	2.44	0.45
34:a:1003:G:N3	34:a:1004:A:H1'	2.32	0.45
34:a:1342:C:H2'	34:a:1343:G:C8	2.52	0.45
39:f:4:TYR:HB2	39:f:65:VAL:HG23	1.99	0.45
40:g:4:ARG:HB2	40:g:5:ARG:H	1.52	0.45
40:g:49:ILE:C	40:g:51:GLN:H	2.26	0.45
43:j:9:ARG:NH2	43:j:95:GLU:OE1	2.49	0.45
46:m:54:VAL:O	46:m:58:GLU:N	2.43	0.45
46:m:64:TRP:HB2	46:m:66:LEU:HD21	1.99	0.45
46:m:85:GLY:N	46:m:86:CYS:HB3	2.32	0.45
46:m:108:ARG:CZ	46:m:114:ARG:HB3	2.46	0.45
47:n:40:CYS:O	47:n:42:ILE:N	2.50	0.45
48:o:71:GLN:HE21	48:o:71:GLN:HB2	1.59	0.45
52:s:28:LYS:HB3	52:s:28:LYS:HE3	1.61	0.45
56:y:363:ARG:HB3	56:y:363:ARG:CZ	2.47	0.45
56:y:418:GLU:CA	56:y:446:LYS:HG2	2.45	0.45
1:A:392:C:H5''	1:A:409:C:H5''	1.99	0.44
1:A:480:A:H2'	1:A:480:A:N3	2.32	0.44
1:A:602:G:N2	1:A:655:A:C8	2.73	0.44
1:A:1047:G:H21	1:A:1111:A:N6	2.15	0.44
1:A:1204:A:H5'	1:A:1206:G:H1'	1.99	0.44
1:A:1250:G:OP2	12:P:21:ARG:NH1	2.50	0.44
1:A:1316:U:H2'	1:A:1317:A:C8	2.52	0.44
1:A:1403:C:H2'	1:A:1404:C:H6	1.82	0.44
1:A:1773:A:C5	1:A:1829:A:H1'	2.51	0.44
1:A:1773:A:N7	1:A:1829:A:H1'	2.32	0.44
1:A:1859:A:H2'	1:A:1860:G:O4'	2.17	0.44
1:A:1914:C:H2'	1:A:1915:U:C6	2.52	0.44
1:A:2014:A:C2	1:A:2015:A:N1	2.85	0.44
2:B:39:A:O2'	2:B:40:U:H5'	2.16	0.44
9:K:30:HIS:HB3	9:K:32:ALA:HB2	1.99	0.44
9:K:90:LYS:HB2	9:K:93:ARG:NH2	2.32	0.44
10:N:103:VAL:O	10:N:106:MET:N	2.41	0.44
12:P:116:GLY:N	12:P:134:ALA:HB2	2.32	0.44
12:P:131:SER:O	12:P:133:SER:N	2.50	0.44
13:Q:61:GLY:HA2	22:Z:177:PRO:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:35:LYS:NZ	16:T:38:ASN:HA	2.27	0.44
20:X:32:PRO:HA	20:X:77:LYS:HD3	1.99	0.44
22:Z:20:ARG:CZ	22:Z:20:ARG:HB2	2.46	0.44
33:x:71:G:H2'	33:x:72:C:C6	2.52	0.44
34:a:472:A:H5''	34:a:473:G:OP2	2.17	0.44
34:a:885:G:O2'	34:a:914:A:N1	2.45	0.44
39:f:82:ARG:HB3	39:f:85:VAL:HG23	1.99	0.44
41:h:59:LEU:HD23	41:h:59:LEU:HA	1.78	0.44
45:l:25:PRO:HD2	45:l:98:TYR:OH	2.16	0.44
53:t:67:ALA:HB2	53:t:77:ALA:HB2	1.99	0.44
56:y:12:PHE:HE2	56:y:80:LEU:HA	1.82	0.44
56:y:444:ALA:O	56:y:447:ARG:N	2.50	0.44
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.27	0.44
1:A:545:G:N2	1:A:546:C:H5	2.14	0.44
1:A:613:G:C6	1:A:614:U:N3	2.85	0.44
1:A:614(B):G:H5''	1:A:614(C):A:OP1	2.17	0.44
1:A:902:C:H2'	1:A:903:C:C6	2.52	0.44
1:A:978:G:C2	1:A:986:C:N3	2.86	0.44
1:A:1137:G:N2	10:N:105:GLY:O	2.50	0.44
1:A:1221(A):C:C2	1:A:1229:G:C2	3.06	0.44
1:A:1355:G:H8	1:A:1355:G:O5'	2.00	0.44
1:A:1975:G:C2	1:A:1976:U:C2	3.05	0.44
1:A:2018:G:H2'	1:A:2019:A:C8	2.53	0.44
1:A:2126:A:N6	1:A:2163:C:H4'	2.33	0.44
1:A:2195:C:H2'	1:A:2196:C:H6	1.82	0.44
6:G:17:PRO:HA	6:G:20:ILE:HD12	1.98	0.44
7:H:7:LEU:HA	7:H:8:PRO:HD2	1.70	0.44
7:H:126:PRO:HB2	7:H:127:GLU:H	1.60	0.44
11:O:89:ASN:C	11:O:91:LEU:N	2.75	0.44
21:Y:9:LYS:HA	21:Y:10:GLY:HA2	1.74	0.44
34:a:148:G:H2'	34:a:149:A:C8	2.49	0.44
34:a:422:C:H4'	34:a:423:G:O5'	2.17	0.44
34:a:959:A:H61	52:s:78:ARG:HA	1.82	0.44
34:a:1416:G:C2	34:a:1485:U:O2	2.70	0.44
35:b:71:VAL:HG12	35:b:170:GLU:HG3	1.98	0.44
36:c:22:TRP:CB	36:c:59:ARG:HB2	2.48	0.44
36:c:109:PRO:C	36:c:111:LEU:H	2.25	0.44
37:d:177:ASP:OD1	37:d:180:GLY:HA3	2.17	0.44
44:k:74:ALA:C	44:k:76:GLY:H	2.25	0.44
46:m:20:THR:HA	46:m:25:ILE:HG22	1.98	0.44
48:o:4:THR:HB	48:o:6:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:138:ILE:CG1	56:y:167:SER:CB	2.95	0.44
56:y:372:THR:HG22	56:y:373:ALA:H	1.83	0.44
56:y:468:LYS:O	56:y:469:SER:C	2.60	0.44
1:A:259:G:O2'	1:A:621:A:O2'	2.25	0.44
1:A:578:A:O2'	17:U:33:ARG:NH2	2.51	0.44
1:A:1094:U:H3'	1:A:1095:A:H5''	1.99	0.44
1:A:1395:A:H4'	1:A:1397:U:C5	2.52	0.44
1:A:1568:G:H4'	3:D:59:LYS:HB3	1.99	0.44
1:A:1572:A:H2'	1:A:1573:G:O4'	2.16	0.44
1:A:1592:C:H2'	1:A:1593:G:H8	1.82	0.44
1:A:2107:C:H2'	1:A:2108:C:O4'	2.18	0.44
1:A:2199:A:H3'	1:A:2200:C:C6	2.52	0.44
1:A:2478:A:H1'	1:A:2528:U:O2'	2.16	0.44
3:D:106:ILE:O	3:D:106:ILE:HG12	2.16	0.44
3:D:140:THR:O	3:D:165:ILE:HG12	2.18	0.44
3:D:166:GLN:HE22	3:D:176:ARG:NH2	2.15	0.44
3:D:177:LEU:HD11	3:D:183:ARG:HG2	2.00	0.44
4:E:177:PRO:O	4:E:179:GLU:N	2.50	0.44
5:F:53:THR:O	5:F:57:VAL:HG23	2.18	0.44
5:F:178:PRO:HG2	5:F:179:GLU:OE1	2.17	0.44
5:F:183:VAL:O	5:F:187:VAL:HG23	2.17	0.44
9:K:69:THR:C	9:K:70:LYS:HD2	2.43	0.44
10:N:4:TYR:O	17:U:64:ARG:NH2	2.48	0.44
10:N:96:GLU:O	10:N:100:GLU:HG3	2.16	0.44
15:S:36:TYR:N	15:S:36:TYR:CD1	2.83	0.44
16:T:35:LYS:HZ3	16:T:37:GLY:HA2	1.83	0.44
16:T:114:LEU:HD23	16:T:114:LEU:HA	1.80	0.44
21:Y:5:MET:HB3	21:Y:6:HIS:H	1.58	0.44
27:4:10:VAL:HG22	27:4:26:SER:O	2.18	0.44
29:6:36:LEU:HD23	29:6:36:LEU:HA	1.73	0.44
30:7:1:MET:HE2	30:7:1:MET:HB3	1.87	0.44
34:a:1203:C:H2'	34:a:1204:A:C8	2.51	0.44
35:b:24:TRP:CZ3	35:b:26:PRO:HA	2.52	0.44
35:b:111:ARG:HG2	35:b:111:ARG:HH11	1.82	0.44
38:e:34:VAL:HG12	38:e:42:GLY:O	2.17	0.44
45:l:45:PRO:HB3	45:l:92:ASP:HB3	1.99	0.44
52:s:42:PRO:O	52:s:45:VAL:HG22	2.17	0.44
56:y:167:SER:OG	56:y:170:THR:CB	2.65	0.44
56:y:230:ILE:CG1	56:y:234:GLY:O	2.64	0.44
56:y:277:GLY:HA3	56:y:293:GLY:N	2.33	0.44
1:A:118:A:N7	1:A:119:A:C8	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:C:H2'	1:A:173:G:H8	1.82	0.44
3:D:165:ILE:HD13	3:D:175:LEU:HD21	2.00	0.44
4:E:199:ARG:HG3	4:E:200:GLU:O	2.17	0.44
10:N:42:TRP:HA	10:N:48:MET:SD	2.58	0.44
10:N:138:LEU:HD23	10:N:138:LEU:HA	1.78	0.44
14:R:67:LEU:HD12	14:R:76:VAL:HG21	1.98	0.44
16:T:19:LEU:HD13	16:T:86:ILE:HD12	1.98	0.44
17:U:38:THR:O	17:U:41:ALA:HB3	2.17	0.44
17:U:66:ASN:CG	17:U:76:TYR:HB2	2.43	0.44
22:Z:111:VAL:HG13	22:Z:115:GLY:O	2.17	0.44
23:O:25:ARG:HA	23:O:25:ARG:HD2	1.72	0.44
34:a:1040:U:C2	34:a:1041:A:C8	3.05	0.44
42:i:54:ASP:N	42:i:54:ASP:OD2	2.50	0.44
45:l:34:ARG:O	45:l:61:THR:HG23	2.17	0.44
48:o:39:LEU:HD13	48:o:56:LEU:HB2	1.99	0.44
51:r:58:LEU:HG	51:r:62:GLU:HB3	1.99	0.44
55:v:14:A:C4	55:v:15:A:C8	3.05	0.44
56:y:100:VAL:C	56:y:129:HIS:HE2	2.25	0.44
56:y:121:PHE:C	56:y:121:PHE:CD2	2.94	0.44
56:y:417:PRO:HD2	56:y:420:TYR:CD2	2.53	0.44
1:A:583:G:H2'	1:A:584:C:H6	1.82	0.44
1:A:603:A:H3'	12:P:90:ARG:NH2	2.32	0.44
1:A:895:U:H5''	1:A:895:U:H6	1.83	0.44
1:A:977:G:C5	1:A:987:G:C2	3.05	0.44
1:A:1275:A:H2	1:A:1295:C:O2	2.01	0.44
1:A:1359:A:N3	1:A:1359:A:H5'	2.32	0.44
1:A:1434:A:H61	1:A:1558:A:N6	2.10	0.44
1:A:1629:U:H2'	1:A:1630:G:C8	2.53	0.44
1:A:2222:G:C4	1:A:2223:G:C8	3.06	0.44
2:B:116:G:H2'	2:B:117:G:C8	2.53	0.44
3:D:145:VAL:HG12	3:D:146:GLU:O	2.18	0.44
4:E:107:THR:HA	4:E:163:GLU:O	2.18	0.44
24:1:72:GLU:O	24:1:75:GLU:HB2	2.17	0.44
25:2:17:SER:HB3	25:2:20:GLU:OE2	2.18	0.44
34:a:232:G:C5	34:a:233:C:C4	3.06	0.44
34:a:658:G:C6	34:a:659:U:C4	3.05	0.44
34:a:743:U:O2'	34:a:744:C:H5'	2.17	0.44
34:a:1288:A:N1	34:a:1371:G:H1'	2.33	0.44
34:a:1299:A:C6	34:a:1301:U:O2	2.70	0.44
34:a:1314:C:H2'	34:a:1315:U:C6	2.53	0.44
50:q:11:VAL:O	50:q:12:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:100:VAL:O	56:y:129:HIS:NE2	2.50	0.44
56:y:121:PHE:O	56:y:125:LEU:N	2.25	0.44
56:y:164:ILE:O	56:y:165:PHE:CD1	2.71	0.44
1:A:456:C:C4	20:X:69:TYR:CE2	3.05	0.44
1:A:1027:A:C2	1:A:2488:A:H5'	2.52	0.44
1:A:1309:G:OP1	30:7:9:ARG:HB2	2.18	0.44
1:A:2054:A:C2	1:A:2616:C:C2	3.05	0.44
1:A:2339:G:H2'	1:A:2340:G:C8	2.53	0.44
1:A:2574:G:H2'	1:A:2575:C:C6	2.53	0.44
1:A:2744:G:C2	1:A:2761:G:C4	3.06	0.44
12:P:84:ASN:N	12:P:87:ASP:OD2	2.43	0.44
18:V:16:PRO:HB3	18:V:97:LYS:O	2.18	0.44
34:a:583:A:H2'	34:a:584:G:O4'	2.17	0.44
34:a:862:C:C2'	34:a:863:U:H5'	2.47	0.44
34:a:1127:G:H1'	34:a:1147:C:H42	1.83	0.44
34:a:1180:A:OP1	42:i:103:THR:HG23	2.18	0.44
35:b:44:LEU:HA	35:b:47:THR:HB	2.00	0.44
37:d:150:GLU:C	37:d:152:SER:H	2.26	0.44
37:d:173:TRP:CE3	37:d:189:PRO:HG3	2.53	0.44
41:h:91:ARG:HG3	45:l:7:ILE:HG13	1.99	0.44
41:h:111:ILE:HG13	41:h:135:CYS:SG	2.57	0.44
50:q:6:LEU:O	50:q:58:GLU:HA	2.17	0.44
52:s:3:ARG:HD3	52:s:8:GLY:O	2.18	0.44
52:s:80:TYR:O	52:s:81:ARG:HB2	2.18	0.44
56:y:113:VAL:CG2	56:y:117:THR:CG2	2.91	0.44
56:y:154:GLU:C	56:y:154:GLU:CD	2.85	0.44
56:y:223:ARG:CG	56:y:255:ALA:CA	2.96	0.44
56:y:398:ASP:C	56:y:400:THR:N	2.75	0.44
56:y:414:ILE:HG12	56:y:476:SER:O	2.18	0.44
1:A:975:C:OP2	1:A:975:C:H4'	2.17	0.44
1:A:1442:G:H1	1:A:1549:C:H42	1.64	0.44
1:A:1653:G:H3'	14:R:2:ARG:HD3	1.99	0.44
1:A:1833:U:H2'	1:A:1834:U:C6	2.47	0.44
1:A:2055:C:OP1	28:5:8:LYS:NZ	2.31	0.44
1:A:2320:A:H2'	1:A:2320:A:N3	2.33	0.44
1:A:2471:C:H2'	1:A:2472:G:O4'	2.18	0.44
4:E:144:ARG:HB3	4:E:145:LYS:H	1.60	0.44
8:J:33:PRO:O	8:J:37:THR:N	2.50	0.44
12:P:3:LEU:HD12	12:P:6:LEU:HD12	1.99	0.44
17:U:83:LEU:HD12	17:U:113:ALA:HB2	2.00	0.44
34:a:658:G:C5	34:a:659:U:C5	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1082:G:H2'	34:a:1083:U:O4'	2.18	0.44
34:a:1157:A:H5'	34:a:1158:C:C2	2.53	0.44
39:f:80:ARG:HG2	39:f:88:VAL:CG2	2.46	0.44
41:h:104:ARG:O	41:h:105:ARG:HB2	2.18	0.44
41:h:120:THR:HG23	41:h:123:GLU:CD	2.43	0.44
44:k:99:GLN:C	44:k:101:SER:H	2.24	0.44
52:s:49:ILE:HG21	52:s:71:LEU:HD21	1.99	0.44
56:y:33:THR:HG22	56:y:68:TYR:HA	2.00	0.44
56:y:479:TYR:O	56:y:479:TYR:CD2	2.70	0.44
1:A:330:A:H2	1:A:1210:A:H2'	1.83	0.44
1:A:598:G:H2'	1:A:599:G:O4'	2.17	0.44
1:A:701:G:H1	1:A:731:C:H42	1.65	0.44
1:A:1289:C:H2'	1:A:1290:C:H6	1.83	0.44
1:A:1354:A:N7	1:A:1355:G:C4	2.86	0.44
1:A:2505:G:O6	1:A:2576:G:H2'	2.18	0.44
1:A:2810:A:N6	1:A:2891:G:O2'	2.43	0.44
6:G:41:GLN:HB3	6:G:43:LEU:HD22	1.99	0.44
7:H:54:ARG:HH21	7:H:57:ASP:HA	1.81	0.44
9:K:6:ALA:HB2	9:K:59:ILE:HG22	2.00	0.44
10:N:126:PRO:HG2	10:N:127:ASP:OD2	2.18	0.44
21:Y:79:CYS:CB	21:Y:102:CYS:HB3	2.48	0.44
22:Z:103:ARG:O	22:Z:138:GLU:HA	2.17	0.44
22:Z:157:LEU:HD22	22:Z:161:VAL:HG13	2.00	0.44
24:1:13:ILE:HG12	24:1:42:GLN:HB2	2.00	0.44
25:2:46:GLN:O	25:2:49:LYS:HB2	2.18	0.44
36:c:70:VAL:O	36:c:106:VAL:N	2.47	0.44
36:c:71:ALA:HB2	36:c:115:LEU:HD21	1.99	0.44
40:g:146:GLU:OE1	40:g:149:ARG:HD2	2.18	0.44
48:o:82:ILE:HB	48:o:87:ILE:HG22	2.00	0.44
49:p:58:TYR:O	49:p:61:SER:HB3	2.18	0.44
50:q:48:GLU:O	50:q:49:GLU:C	2.60	0.44
56:y:311:GLY:C	56:y:312:ASP:CG	2.85	0.44
1:A:634:C:H2'	1:A:635:C:H6	1.81	0.44
1:A:864:G:C6	1:A:865:C:N4	2.86	0.44
1:A:1344:G:H5'	1:A:1384:A:C6	2.53	0.44
1:A:2054:A:H2'	28:5:8:LYS:HE3	2.00	0.44
1:A:2098:U:H2'	1:A:2099:U:C6	2.53	0.44
1:A:2461:C:H42	1:A:2489:G:H1	1.66	0.44
1:A:2821:A:C2	1:A:2822:G:C4	3.06	0.44
4:E:168:MET:O	4:E:170:LEU:N	2.50	0.44
5:F:149:ASP:OD2	5:F:149:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:121:ASN:HA	6:G:122:PRO:HD3	1.66	0.44
7:H:124:GLU:O	7:H:126:PRO:HD3	2.18	0.44
9:K:93:ARG:HG3	22:Z:112:ARG:O	2.18	0.44
11:O:1:MET:HG2	11:O:32:TYR:CD2	2.52	0.44
13:Q:43:THR:HA	13:Q:94:VAL:HA	1.99	0.44
16:T:16:ARG:HD3	16:T:18:ASP:OD1	2.18	0.44
33:x:4:C:H3'	33:x:5:G:H5''	2.00	0.44
34:a:427:U:OP1	37:d:13:ARG:NH2	2.50	0.44
34:a:551:U:H2'	34:a:552:U:C6	2.53	0.44
34:a:1285:A:H4'	34:a:1286:A:O5'	2.17	0.44
40:g:104:LEU:O	40:g:108:ALA:N	2.48	0.44
49:p:3:LYS:O	49:p:21:VAL:HA	2.18	0.44
56:y:131:ILE:HD12	56:y:158:LEU:HD21	1.98	0.44
56:y:303:ALA:C	56:y:345:ARG:HA	2.43	0.44
1:A:491:G:H2'	1:A:492:A:H8	1.83	0.43
1:A:517:C:O2'	19:W:18:ARG:NH2	2.50	0.43
1:A:627:A:N1	1:A:636:G:O2'	2.47	0.43
1:A:902:C:H2'	1:A:903:C:H6	1.83	0.43
1:A:1398:C:H2'	1:A:1399:C:H6	1.82	0.43
1:A:2339:G:H2'	1:A:2340:G:H8	1.83	0.43
1:A:2519:U:C6	1:A:2542:A:N6	2.86	0.43
62:A:4142:HOH:O	17:U:51:LYS:HG2	2.18	0.43
3:D:242:ARG:C	3:D:244:ARG:H	2.25	0.43
9:K:33:ASN:ND2	9:K:36:GLU:HB2	2.33	0.43
10:N:67:LEU:O	10:N:88:GLU:N	2.45	0.43
11:O:64:ARG:NH2	11:O:99:PHE:O	2.51	0.43
14:R:99:LYS:HA	14:R:112:ALA:HA	2.00	0.43
27:4:16:CYS:SG	27:4:17:GLY:N	2.91	0.43
33:x:36:A:H2'	33:x:37:MIA:O4'	2.18	0.43
34:a:76:C:N3	34:a:93:G:O6	2.51	0.43
34:a:1120:G:H2'	34:a:1121:U:H6	1.82	0.43
36:c:52:LEU:HA	36:c:69:HIS:O	2.17	0.43
38:e:69:VAL:HA	38:e:70:PRO:HD2	1.50	0.43
38:e:118:ILE:HG12	38:e:119:LEU:N	2.33	0.43
52:s:22:LEU:HA	52:s:22:LEU:HD23	1.65	0.43
56:y:535:VAL:N	56:y:551:VAL:O	2.35	0.43
1:A:143:G:O2'	20:X:37:THR:HB	2.18	0.43
1:A:1187:G:OP2	62:A:3788:HOH:O	2.21	0.43
1:A:1257:C:OP1	5:F:72:ARG:NH2	2.51	0.43
1:A:1314:C:C2	1:A:1315:C:C5	3.07	0.43
1:A:1430:C:H2'	1:A:1431:U:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450(A):C:N4	1:A:1451:C:H41	2.16	0.43
1:A:1487:G:H2'	1:A:1488:G:C8	2.53	0.43
1:A:2123:G:C4	1:A:2124:G:C8	3.05	0.43
1:A:2816:C:O2	1:A:2883:A:O2'	2.31	0.43
11:O:68:GLU:O	11:O:68:GLU:HG2	2.17	0.43
17:U:104:GLN:CD	17:U:104:GLN:H	2.26	0.43
17:U:107:ALA:O	17:U:111:GLU:HG2	2.18	0.43
21:Y:28:LYS:HE2	21:Y:28:LYS:HB3	1.75	0.43
23:O:15:ASP:OD1	23:O:16:SER:N	2.50	0.43
33:x:23:A:H2'	33:x:24:G:C8	2.53	0.43
34:a:381:C:H2'	34:a:382:A:O4'	2.17	0.43
34:a:514:C:H42	34:a:537:G:H1	1.66	0.43
34:a:1038:C:H2'	34:a:1039:C:O4'	2.18	0.43
38:e:151:LEU:HD13	38:e:151:LEU:HA	1.58	0.43
39:f:78:GLU:O	39:f:81:ILE:HG22	2.18	0.43
41:h:122:ARG:NH1	41:h:125:ARG:HB3	2.33	0.43
46:m:67:GLU:O	46:m:70:LEU:N	2.51	0.43
56:y:16:ALA:HB2	56:y:106:VAL:O	2.18	0.43
56:y:392:ASN:ND2	56:y:393:PRO:HD2	2.26	0.43
1:A:57:C:H2'	1:A:58:G:O4'	2.18	0.43
1:A:590:A:OP1	5:F:95:ARG:NH1	2.51	0.43
1:A:681:G:H2'	1:A:682:G:O4'	2.18	0.43
1:A:847:U:H5'	62:A:3722:HOH:O	2.18	0.43
1:A:2205:C:O2	1:A:2220:G:C2	2.71	0.43
1:A:2790:A:O2'	1:A:2791:C:C5	2.67	0.43
3:D:242:ARG:C	3:D:244:ARG:N	2.77	0.43
7:H:32:GLU:H	7:H:32:GLU:CD	2.26	0.43
13:Q:1:MET:HB2	62:Q:301:HOH:O	2.18	0.43
18:V:32:THR:HG22	18:V:60:GLU:HA	2.00	0.43
21:Y:92:ASN:N	21:Y:93:GLY:HA2	2.33	0.43
22:Z:179:ASP:HB3	22:Z:182:LYS:H	1.83	0.43
33:x:62:C:H2'	33:x:63:G:C8	2.50	0.43
34:a:264:U:H6	34:a:264:U:O5'	2.01	0.43
34:a:805:C:N4	34:a:806:C:H41	2.16	0.43
34:a:982:U:H4'	34:a:983:A:O4'	2.18	0.43
34:a:1062:U:H2'	34:a:1063:C:C6	2.53	0.43
34:a:1119:C:H2'	34:a:1120:G:C8	2.53	0.43
34:a:1237:C:O3'	34:a:1300:G:N2	2.49	0.43
40:g:45:ASP:O	40:g:49:ILE:HG13	2.17	0.43
42:i:89:ASN:HD22	42:i:89:ASN:C	2.27	0.43
56:y:398:ASP:O	56:y:401:ARG:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:G:C6	1:A:25:U:C4	3.07	0.43
1:A:213:A:H2'	1:A:214:G:O4'	2.18	0.43
1:A:804:A:H5''	1:A:805:G:OP1	2.19	0.43
1:A:1102:C:H2'	1:A:1103:A:C8	2.53	0.43
1:A:2690:C:N4	1:A:2713:A:H1'	2.33	0.43
1:A:2887:U:H2'	1:A:2888:C:C6	2.53	0.43
6:G:64:THR:HB	6:G:94:LEU:HD21	2.00	0.43
6:G:170:ARG:HH21	6:G:180:PHE:CB	2.32	0.43
27:4:58:ARG:HD3	52:s:65:ASN:O	2.18	0.43
33:x:54:5MU:H72	33:x:55:PSU:O2	2.18	0.43
34:a:109:A:C6	34:a:326:G:C6	3.07	0.43
34:a:607:A:H2'	34:a:608:A:H8	1.83	0.43
34:a:661:G:N2	34:a:745:C:O2	2.51	0.43
34:a:1303:C:C2'	34:a:1304:G:H5'	2.48	0.43
34:a:1456:G:C3'	34:a:1457:G:H5'	2.49	0.43
34:a:1463:C:H2'	34:a:1464:G:H8	1.83	0.43
35:b:152:PHE:O	35:b:154:LEU:N	2.51	0.43
43:j:39:PRO:HA	43:j:70:ARG:HD3	2.00	0.43
48:o:5:LYS:O	48:o:9:GLN:HG2	2.18	0.43
56:y:18:VAL:O	56:y:19:ASP:CB	2.66	0.43
56:y:307:PRO:HA	56:y:369:LEU:HG	2.00	0.43
56:y:468:LYS:C	56:y:470:VAL:N	2.74	0.43
1:A:125:G:H4'	1:A:126:A:OP2	2.19	0.43
1:A:150:C:H2'	1:A:151:C:C6	2.53	0.43
1:A:586:A:OP2	62:A:3787:HOH:O	2.21	0.43
1:A:947:G:N2	1:A:971:C:C2	2.86	0.43
1:A:2347:C:H5	1:A:2382:G:C4	2.36	0.43
1:A:2604:U:H2'	1:A:2605:U:H6	1.83	0.43
3:D:231:HIS:ND1	3:D:232:PRO:HD2	2.33	0.43
15:S:28:VAL:CG1	15:S:101:LEU:HD22	2.49	0.43
16:T:42:ILE:HD13	16:T:42:ILE:HA	1.78	0.43
18:V:72:VAL:HG13	18:V:85:LYS:HB3	1.99	0.43
21:Y:69:ALA:O	21:Y:71:LYS:N	2.51	0.43
22:Z:52:SER:HG	22:Z:53:ILE:N	2.11	0.43
26:3:3:ARG:HB2	26:3:60:GLU:HB3	2.00	0.43
33:x:3:C:H2'	33:x:4:C:O4'	2.18	0.43
34:a:838:G:H8	34:a:838:G:O5'	2.02	0.43
34:a:1016:A:H2'	34:a:1017:G:O4'	2.17	0.43
34:a:1108:G:H5'	36:c:176:HIS:CD2	2.53	0.43
34:a:1120:G:O2'	34:a:1121:U:H5'	2.17	0.43
34:a:1427:U:O2	34:a:1474:G:N2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:16:ARG:HH12	36:c:183:ASP:HA	1.83	0.43
39:f:10:LEU:HD12	39:f:10:LEU:HA	1.72	0.43
53:t:10:LEU:HB3	53:t:11:SER:H	1.50	0.43
53:t:16:HIS:HA	53:t:19:SER:HB3	2.00	0.43
56:y:554:LEU:HD23	56:y:554:LEU:H	1.83	0.43
1:A:515:A:H2'	62:A:3937:HOH:O	2.17	0.43
1:A:565:C:H2'	1:A:566:U:O4'	2.18	0.43
1:A:1216:G:P	17:U:12:ARG:HH21	2.42	0.43
1:A:1540:U:O4	1:A:1541:G:N1	2.51	0.43
1:A:1843:C:H5'	3:D:253:GLN:HE22	1.82	0.43
1:A:2455:G:H2'	1:A:2456:C:H6	1.83	0.43
1:A:2745:C:H2'	1:A:2746:U:C6	2.54	0.43
2:B:17:C:H42	2:B:68:C:N4	2.09	0.43
3:D:126:GLN:HB3	3:D:129:ASN:ND2	2.34	0.43
3:D:137:PRO:O	3:D:140:THR:HG23	2.18	0.43
7:H:86:GLU:HA	7:H:132:ARG:HA	2.01	0.43
12:P:45:LEU:HD23	12:P:45:LEU:HA	1.56	0.43
12:P:100:LEU:O	12:P:105:LEU:HB2	2.17	0.43
14:R:97:VAL:HG22	14:R:114:VAL:HG13	1.99	0.43
20:X:89:ILE:HG22	20:X:92:LEU:N	2.34	0.43
22:Z:107:THR:HA	22:Z:108:PRO:HD3	1.87	0.43
33:x:57:G:H2'	33:x:58:A:C5'	2.48	0.43
34:a:115:G:H4'	34:a:116:A:O5'	2.18	0.43
34:a:592:G:H2'	34:a:593:G:C8	2.49	0.43
34:a:598:U:H4'	41:h:94:TYR:CD1	2.52	0.43
34:a:604:G:C6	34:a:605:U:C4	3.06	0.43
34:a:909:A:H2'	34:a:910:C:O4'	2.19	0.43
34:a:977:A:H1'	34:a:982:U:O4	2.18	0.43
34:a:1035:A:H2'	34:a:1036:G:O4'	2.18	0.43
40:g:100:ALA:O	40:g:104:LEU:HD22	2.18	0.43
43:j:59:SER:O	43:j:60:ARG:HD3	2.18	0.43
56:y:230:ILE:HD11	56:y:234:GLY:O	2.16	0.43
56:y:303:ALA:HB1	56:y:392:ASN:CG	2.37	0.43
1:A:249:C:HO2'	12:P:64:LYS:HZ2	1.56	0.43
1:A:354:G:H2'	1:A:355:G:H8	1.84	0.43
1:A:365:C:O5'	1:A:365:C:H6	2.01	0.43
1:A:1464:C:H2'	1:A:1465:G:C8	2.53	0.43
1:A:1766:U:C2	1:A:1767:C:C5	3.07	0.43
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.50	0.43
1:A:1859:A:H3'	1:A:1860:G:H8	1.84	0.43
1:A:2364:C:H2'	1:A:2365:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2704:C:H2'	1:A:2705:A:O4'	2.19	0.43
3:D:232:PRO:HB3	3:D:244:ARG:CZ	2.49	0.43
4:E:36:ARG:NH1	4:E:85:ASN:ND2	2.67	0.43
4:E:152:LYS:HE3	4:E:152:LYS:HB2	1.90	0.43
5:F:17:ARG:NH1	5:F:19:GLU:HG3	2.29	0.43
5:F:20:LEU:HD22	5:F:21:ALA:N	2.28	0.43
5:F:198:ALA:O	5:F:201:VAL:HG22	2.19	0.43
13:Q:135:ASP:HB3	13:Q:136:ALA:H	1.42	0.43
16:T:52:ILE:HG12	16:T:61:PHE:HB3	2.00	0.43
27:4:15:ILE:HD12	27:4:32:TYR:CE1	2.54	0.43
28:5:51:TYR:CE1	28:5:56:LYS:HG2	2.53	0.43
31:8:40:GLU:O	31:8:44:LYS:HG3	2.19	0.43
34:a:105:G:H2'	34:a:106:C:C6	2.54	0.43
34:a:591:U:H2'	34:a:592:G:H8	1.83	0.43
34:a:1196:U:H3	36:c:162:GLN:HE22	1.66	0.43
34:a:1269:A:H2	34:a:1312:G:N3	2.17	0.43
35:b:122:PHE:HA	35:b:123:ALA:HA	1.83	0.43
40:g:51:GLN:C	40:g:53:LYS:H	2.26	0.43
40:g:138:LYS:HD3	40:g:142:GLU:OE1	2.18	0.43
41:h:122:ARG:HA	41:h:122:ARG:HD2	1.25	0.43
46:m:49:THR:OG1	46:m:52:GLU:HG3	2.19	0.43
56:y:-38:LEU:HB3	56:y:-37:PRO:HD3	2.01	0.43
56:y:358:GLN:O	56:y:361:LEU:HB2	2.18	0.43
56:y:497:HIS:O	56:y:497:HIS:CG	2.70	0.43
1:A:298:G:OP1	21:Y:87:LYS:N	2.42	0.43
1:A:415:A:H2'	1:A:416:C:O4'	2.19	0.43
1:A:463:G:N1	1:A:467:G:C6	2.86	0.43
1:A:1107:G:N3	1:A:1107:G:H2'	2.33	0.43
1:A:2031:A:C6	1:A:2498:C:H1'	2.53	0.43
1:A:2628:C:H1'	1:A:2781:A:C4	2.54	0.43
1:A:2646:C:OP2	1:A:2732:G:O2'	2.25	0.43
2:B:96:U:H2'	2:B:97:G:C8	2.54	0.43
11:O:71:ARG:HA	11:O:72:PRO:HD2	1.63	0.43
12:P:101:VAL:HG22	12:P:106:LEU:HD12	2.00	0.43
27:4:37:SER:HB2	27:4:43:TYR:CE1	2.53	0.43
29:6:10:LEU:HD12	29:6:54:ILE:HA	2.01	0.43
34:a:251:G:H4'	34:a:252:U:C5'	2.49	0.43
34:a:679:C:C2	34:a:712:A:H2	2.36	0.43
34:a:913:A:H4'	34:a:914:A:O5'	2.19	0.43
34:a:1060:C:OP1	47:n:45:ARG:NH2	2.49	0.43
37:d:22:LYS:HB3	37:d:22:LYS:HE3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:118:ILE:HG12	38:e:119:LEU:H	1.83	0.43
49:p:1:MET:HG2	49:p:2:VAL:N	2.34	0.43
50:q:92:ARG:HD3	50:q:92:ARG:HA	1.77	0.43
56:y:138:ILE:HG22	56:y:145:PRO:HB3	2.01	0.43
56:y:413:THR:HG21	56:y:449:GLU:OE2	2.19	0.43
56:y:518:ARG:NH1	56:y:548:ARG:NH1	2.66	0.43
56:y:526:GLU:H	56:y:526:GLU:CD	2.27	0.43
1:A:300:A:H1'	1:A:319:C:O4'	2.19	0.43
1:A:455:C:H6	1:A:455:C:H2'	1.62	0.43
1:A:583:G:C4	1:A:584:C:C5	3.07	0.43
1:A:621:A:H5'	1:A:622:G:OP2	2.19	0.43
1:A:666:G:C5	1:A:667:U:H5	2.37	0.43
1:A:868:U:C4	1:A:869:G:N7	2.87	0.43
1:A:997:G:OP1	17:U:92:ARG:HG2	2.19	0.43
1:A:1286:A:C6	1:A:1329:U:C2	3.07	0.43
1:A:1540:U:H2'	1:A:1541:G:O4'	2.19	0.43
1:A:2739:U:O2'	1:A:2740:A:H5'	2.19	0.43
1:A:2747:G:N2	1:A:2748:A:H62	2.16	0.43
1:A:2817:G:C2	1:A:2818:G:H1'	2.53	0.43
2:B:18:G:H2'	2:B:19:G:C8	2.52	0.43
3:D:16:MET:HE3	3:D:16:MET:HB2	1.60	0.43
3:D:143:HIS:HB2	3:D:156:ALA:O	2.19	0.43
6:G:136:ARG:H	6:G:136:ARG:HG3	1.69	0.43
7:H:26:VAL:HG12	7:H:79:VAL:HG21	2.01	0.43
9:K:38:VAL:HG12	9:K:42:ASN:HD22	1.83	0.43
12:P:27:HIS:HB3	12:P:32:THR:CG2	2.48	0.43
17:U:34:LYS:HA	17:U:34:LYS:HD2	1.51	0.43
23:0:39:ARG:NH1	23:0:58:THR:OG1	2.51	0.43
29:6:21:TYR:CZ	29:6:38:LYS:HG2	2.53	0.43
32:9:17:ILE:HD12	32:9:17:ILE:HA	1.88	0.43
34:a:78:G:C6	34:a:91:C:N4	2.84	0.43
34:a:106:C:O2	34:a:379:C:H4'	2.19	0.43
34:a:453:A:C5	34:a:454:C:C4	3.07	0.43
34:a:750:G:N3	34:a:751:U:C6	2.87	0.43
34:a:881:G:H2'	34:a:882:C:O4'	2.19	0.43
36:c:111:LEU:HD21	36:c:144:SER:HB2	2.01	0.43
37:d:206:PHE:CD1	37:d:206:PHE:C	2.97	0.43
38:e:91:LEU:HD12	38:e:120:THR:HG22	2.01	0.43
39:f:35:ALA:O	39:f:37:VAL:N	2.51	0.43
40:g:115:ARG:H	40:g:115:ARG:HG2	1.58	0.43
56:y:179:GLU:O	56:y:182:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:250:LEU:H	56:y:250:LEU:CD1	2.27	0.43
56:y:428:LEU:HD23	56:y:428:LEU:HA	1.82	0.43
56:y:537:ILE:C	56:y:549:ALA:O	2.55	0.43
1:A:353:G:H2'	1:A:354:G:C8	2.52	0.43
1:A:559:G:H22	17:U:49:HIS:CE1	2.37	0.43
1:A:709:U:H2'	1:A:710:G:O4'	2.18	0.43
1:A:858:U:OP2	23:0:77:ARG:NH2	2.52	0.43
1:A:1866:C:H2'	1:A:1876:A:O4'	2.19	0.43
1:A:2389:G:H5''	1:A:2390:U:O4'	2.19	0.43
1:A:2820:A:P	14:R:2:ARG:HH22	2.42	0.43
1:A:2844:G:H2'	1:A:2845:G:O4'	2.18	0.43
1:A:2887:U:O2'	1:A:2888:C:H5'	2.18	0.43
17:U:44:ASN:ND2	18:V:75:PHE:O	2.52	0.43
22:Z:59:LEU:HD12	22:Z:69:THR:HG21	2.00	0.43
23:0:49:LYS:O	23:0:50:ASN:HB2	2.19	0.43
33:x:22:G:N7	33:x:46:7MG:C6	2.87	0.43
34:a:839:U:O2	34:a:839:U:H2'	2.19	0.43
34:a:990:C:O2'	34:a:991:U:H5'	2.19	0.43
39:f:33:TYR:HA	39:f:71:ARG:HH11	1.84	0.43
42:i:28:VAL:HG12	42:i:29:ASN:HB2	2.00	0.43
49:p:73:LEU:HD23	49:p:73:LEU:HA	1.84	0.43
33:w:17:C:H4'	33:w:18:G:H5''	2.01	0.43
33:w:24:G:H2'	33:w:25:C:C6	2.54	0.43
56:y:67:THR:HA	56:y:76:TYR:O	2.19	0.43
56:y:77:VAL:C	56:y:78:PHE:CD1	2.97	0.43
56:y:306:TYR:CD2	56:y:344:PHE:N	2.87	0.43
1:A:675:A:OP1	5:F:63:LYS:HD2	2.19	0.42
1:A:692:C:O2'	1:A:693:C:H5'	2.18	0.42
1:A:1207:C:H2'	1:A:1208:C:H6	1.84	0.42
1:A:1434:A:C5	1:A:1560:G:N2	2.87	0.42
1:A:1434:A:N6	1:A:1558:A:H62	2.13	0.42
1:A:1684:C:H2'	1:A:1685:C:C6	2.54	0.42
1:A:2115:G:H4'	1:A:2166:G:N2	2.34	0.42
1:A:2678:C:H2'	1:A:2679:A:H8	1.84	0.42
1:A:2820:A:C4	14:R:4:LEU:HD11	2.54	0.42
1:A:2864:G:H2'	1:A:2865:U:O4'	2.19	0.42
7:H:3:ARG:CZ	7:H:4:ILE:H	2.32	0.42
7:H:98:LEU:HD23	7:H:125:VAL:HG23	2.01	0.42
12:P:19:VAL:CG2	12:P:31:ALA:HB1	2.49	0.42
15:S:24:LEU:O	15:S:85:VAL:HG22	2.19	0.42
18:V:59:ALA:HB2	18:V:96:ILE:HD13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:40:ARG:HG3	24:l:40:ARG:H	1.69	0.42
34:a:106:C:H2'	34:a:107:G:O4'	2.19	0.42
34:a:109:A:H4'	34:a:110:C:OP2	2.18	0.42
34:a:426:G:OP1	37:d:38:TYR:OH	2.31	0.42
34:a:583:A:N6	34:a:758:G:O2'	2.52	0.42
34:a:926:G:C6	34:a:1505:G:C6	3.06	0.42
35:b:155:LEU:CB	35:b:157:ARG:H	2.32	0.42
37:d:61:LYS:HE2	37:d:62:GLN:HG2	2.00	0.42
37:d:158:ILE:O	37:d:162:LEU:HB2	2.18	0.42
43:j:34:VAL:HA	43:j:73:ASP:O	2.19	0.42
49:p:21:VAL:HG12	49:p:34:GLU:O	2.19	0.42
33:w:44:G:N3	33:w:44:G:H2'	2.32	0.42
56:y:87:VAL:HG12	56:y:88:ASP:CA	2.45	0.42
56:y:241:LYS:N	56:y:265:VAL:HG23	2.12	0.42
1:A:272:G:H1	1:A:404:C:H42	1.67	0.42
1:A:471:A:N1	20:X:68:ARG:NH1	2.60	0.42
1:A:608:A:C2	1:A:609:A:C4	3.07	0.42
1:A:1413:G:H2'	1:A:1414:G:C8	2.52	0.42
1:A:1509(A):A:H3'	1:A:1509(B):A:H8	1.84	0.42
1:A:1637:A:H4'	1:A:2711:A:O2'	2.18	0.42
1:A:1652:A:H2'	1:A:1653:G:H5'	2.00	0.42
1:A:2358:G:H22	12:P:55:ARG:HH12	1.67	0.42
6:G:73:ALA:HB3	6:G:85:GLY:H	1.84	0.42
6:G:126:ASP:HB2	6:G:130:ASN:O	2.19	0.42
7:H:94:TYR:CD1	7:H:107:VAL:HA	2.54	0.42
9:K:12:LEU:HD11	9:K:23:VAL:HG22	2.01	0.42
13:Q:80:GLU:HB2	56:y:567:VAL:HG23	2.01	0.42
19:W:66:GLU:C	19:W:68:ARG:H	2.26	0.42
21:Y:5:MET:HE2	21:Y:32:PRO:HA	2.00	0.42
33:x:5:G:C2	33:x:6:G:C4	3.07	0.42
34:a:1118:C:H1'	34:a:1179:A:C5	2.54	0.42
35:b:109:SER:O	35:b:112:VAL:HB	2.19	0.42
37:d:188:LEU:HA	37:d:189:PRO:HD3	1.89	0.42
40:g:23:VAL:O	40:g:27:ILE:HG12	2.19	0.42
43:j:46:ARG:HB3	43:j:46:ARG:NH1	2.33	0.42
53:t:77:ALA:O	53:t:81:LYS:HG3	2.18	0.42
56:y:230:ILE:CG2	56:y:279:THR:O	2.65	0.42
56:y:509:HIS:O	56:y:513:ALA:N	2.36	0.42
1:A:392:C:H2'	1:A:393:C:C6	2.53	0.42
1:A:438:G:H2'	1:A:440:G:H8	1.84	0.42
1:A:569:U:C4	1:A:570:G:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:U:H2'	1:A:658:C:C6	2.54	0.42
1:A:990:A:C6	1:A:1186:G:H1'	2.54	0.42
1:A:1009:A:P	10:N:37:LYS:HZ1	2.36	0.42
1:A:1281:G:H5''	1:A:1281:G:H8	1.83	0.42
1:A:1381:G:C5	1:A:1382:G:N7	2.87	0.42
1:A:1680:U:H2'	1:A:1681:G:H5'	2.01	0.42
1:A:1688:U:H1'	1:A:1701:A:C6	2.54	0.42
1:A:2104:G:H1	1:A:2185:C:N4	2.15	0.42
1:A:2773:C:H5''	4:E:164:ARG:HG2	2.01	0.42
3:D:177:LEU:O	3:D:180:GLY:N	2.41	0.42
6:G:133:LEU:CD2	6:G:157:ILE:HB	2.50	0.42
12:P:101:VAL:HG22	12:P:106:LEU:HB3	2.01	0.42
19:W:107:LEU:HA	19:W:107:LEU:HD12	1.84	0.42
23:O:40:GLN:NE2	23:O:43:THR:HA	2.34	0.42
26:3:8:LEU:HD23	26:3:23:LEU:HD11	2.00	0.42
33:x:13:C:H2'	33:x:14:A:H8	1.82	0.42
34:a:1030(A):G:N2	34:a:1030(D):A:OP2	2.51	0.42
34:a:1258:G:O2'	34:a:1259:C:H5'	2.20	0.42
34:a:1325:C:O2'	34:a:1326:C:H5'	2.18	0.42
34:a:1325:C:OP1	54:u:6:ARG:NH2	2.52	0.42
40:g:91:VAL:CG1	40:g:96:GLN:HG3	2.49	0.42
45:l:33:ARG:HB3	45:l:60:LEU:HD12	2.01	0.42
46:m:11:ARG:O	46:m:12:ASN:HB2	2.19	0.42
48:o:39:LEU:C	48:o:41:GLU:H	2.28	0.42
56:y:226:ASP:OD2	56:y:227:ARG:O	2.37	0.42
56:y:250:LEU:N	56:y:250:LEU:CD1	2.73	0.42
56:y:507:ILE:HG23	56:y:507:ILE:O	2.20	0.42
1:A:250:G:C6	1:A:251:A:C6	3.07	0.42
1:A:322:A:H1'	1:A:339:U:O2	2.19	0.42
1:A:410:G:N2	1:A:2407:G:C5	2.87	0.42
1:A:528:A:O2'	1:A:529:A:H5'	2.20	0.42
1:A:646:A:H2'	1:A:647:G:O4'	2.20	0.42
1:A:839:U:O2'	1:A:1191:G:N3	2.52	0.42
1:A:922:U:H1'	23:O:26:TYR:CD1	2.54	0.42
1:A:1208:C:C4	1:A:1209:G:N7	2.87	0.42
1:A:1241:A:C2	1:A:1242:A:C4	3.08	0.42
1:A:1426:G:H8	1:A:1426:G:O5'	2.02	0.42
1:A:1767:C:C2	1:A:1768:U:C6	3.08	0.42
1:A:2013:A:C2	1:A:2014:A:C4	3.07	0.42
1:A:2684:U:H2'	1:A:2685:G:O4'	2.18	0.42
1:A:2758:A:H2'	1:A:2759:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:13:ARG:HD3	16:T:58:ASN:ND2	2.31	0.42
7:H:7:LEU:HD23	7:H:69:ARG:HH12	1.84	0.42
7:H:162:ILE:C	7:H:163:TYR:HD1	2.27	0.42
9:K:17:ALA:HB3	9:K:38:VAL:HG13	2.01	0.42
10:N:42:TRP:O	17:U:64:ARG:NH1	2.52	0.42
18:V:6:LYS:HD2	18:V:9:GLY:HA2	2.02	0.42
18:V:29:PRO:HA	18:V:61:VAL:HG23	2.01	0.42
21:Y:3:VAL:HG21	21:Y:32:PRO:O	2.19	0.42
23:O:63:VAL:O	23:O:81:VAL:HG11	2.20	0.42
24:1:95:LEU:HD13	24:1:95:LEU:HA	1.89	0.42
25:2:1:MET:HE3	25:2:5:GLU:HB3	2.01	0.42
27:4:1:MET:HG2	27:4:6:HIS:CD2	2.54	0.42
34:a:35:G:H21	45:l:118:SER:HB2	1.84	0.42
34:a:138:G:H2'	34:a:139:G:O4'	2.19	0.42
34:a:235:C:H2'	34:a:236:G:H8	1.84	0.42
34:a:689:C:H2'	34:a:690:G:O4'	2.19	0.42
34:a:718:G:N2	51:r:49:LYS:HE2	2.35	0.42
34:a:1003:G:N2	34:a:1038:C:C4	2.88	0.42
40:g:5:ARG:C	40:g:7:ALA:H	2.26	0.42
40:g:79:ARG:HB3	40:g:80:VAL:H	1.51	0.42
46:m:64:TRP:O	46:m:66:LEU:HG	2.19	0.42
47:n:10:ALA:HB2	47:n:23:ARG:HH21	1.84	0.42
56:y:11:ASN:OD1	56:y:79:HIS:HB2	2.19	0.42
56:y:213:PRO:HD2	56:y:264:LEU:O	2.02	0.42
56:y:230:ILE:HG22	56:y:279:THR:CA	2.49	0.42
1:A:71:A:H4'	1:A:72:U:H5''	2.02	0.42
1:A:196:A:C2	12:P:51:PHE:HZ	2.37	0.42
1:A:300:A:N3	1:A:319:C:H1'	2.34	0.42
1:A:764:A:H2	3:D:219:PRO:HG3	1.83	0.42
1:A:1023:U:OP2	62:A:3737:HOH:O	2.22	0.42
1:A:1064:C:H4'	9:K:89:HIS:HD2	1.85	0.42
1:A:1257:C:H2'	1:A:1258:C:H6	1.84	0.42
1:A:1320:C:O2'	1:A:1329:U:OP1	2.31	0.42
1:A:1406:U:H2'	1:A:1407:C:H6	1.84	0.42
1:A:1682:G:H2'	1:A:1683:C:C6	2.55	0.42
1:A:2262:U:OP1	1:A:2387:U:O2'	2.34	0.42
3:D:79:VAL:HG12	3:D:113:VAL:HA	2.02	0.42
9:K:28:GLY:C	9:K:30:HIS:N	2.75	0.42
21:Y:86:ARG:HH12	21:Y:100:ALA:HA	1.83	0.42
22:Z:13:GLU:O	22:Z:15:PRO:HD3	2.19	0.42
26:3:30:ARG:NH1	26:3:33:GLN:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:109:A:H3'	34:a:110:C:H5'	2.02	0.42
34:a:587:G:C2	34:a:755:G:C5	3.07	0.42
34:a:1275:A:C6	34:a:1276:G:C5	3.08	0.42
34:a:1401:G:C2	34:a:1402:C:H1'	2.54	0.42
36:c:50:ALA:O	36:c:70:VAL:HG13	2.19	0.42
39:f:53:ALA:C	39:f:54:LYS:HD2	2.44	0.42
40:g:38:LEU:O	40:g:42:ILE:HD12	2.19	0.42
45:l:124:LYS:HA	45:l:125:PRO:HD2	1.57	0.42
53:t:47:GLY:HA2	53:t:48:LYS:C	2.44	0.42
56:y:25:LEU:C	56:y:28:ARG:HB3	2.37	0.42
56:y:62:SER:N	56:y:82:ASP:CB	2.83	0.42
1:A:112:U:H2'	1:A:113:G:O4'	2.19	0.42
1:A:406:G:H5''	1:A:407:G:OP2	2.19	0.42
1:A:797:C:C2	1:A:798:G:C8	3.08	0.42
1:A:879:G:H2'	1:A:880:G:O4'	2.19	0.42
1:A:1067:A:H8	1:A:1067:A:OP1	2.03	0.42
1:A:1754:C:H2'	1:A:1755:A:O4'	2.20	0.42
1:A:1816:G:H8	3:D:62:TYR:CZ	2.37	0.42
1:A:2135:A:N6	1:A:2156:G:H1'	2.35	0.42
1:A:2838:G:C6	1:A:2839:G:N7	2.88	0.42
3:D:66:ASP:HB2	3:D:103:ARG:HD2	2.00	0.42
4:E:6:GLY:O	4:E:195:LEU:HA	2.19	0.42
4:E:86:PRO:C	4:E:88:GLY:H	2.28	0.42
14:R:41:ALA:O	14:R:42:LYS:C	2.63	0.42
20:X:89:ILE:CG2	20:X:91:ALA:HB3	2.49	0.42
22:Z:145:GLU:O	22:Z:148:ASP:HB2	2.20	0.42
23:0:23:VAL:CG1	23:0:26:TYR:HE2	2.33	0.42
29:6:12:GLU:HB2	29:6:19:ARG:HD2	2.01	0.42
30:7:31:LEU:HA	30:7:31:LEU:HD23	1.64	0.42
33:x:18:G:N2	33:x:58:A:C8	2.88	0.42
34:a:105:G:C6	34:a:106:C:C4	3.07	0.42
34:a:436:C:O2'	34:a:437:U:P	2.78	0.42
34:a:564:C:O2'	41:h:91:ARG:NH2	2.52	0.42
34:a:737:A:H2'	34:a:738:C:H6	1.84	0.42
34:a:815:A:C2	34:a:1529:G:C4	3.08	0.42
34:a:1027:C:O2	34:a:1027:C:H2'	2.18	0.42
34:a:1124:G:O2'	34:a:1145:C:N4	2.53	0.42
34:a:1144:G:O2'	34:a:1145:C:H5'	2.19	0.42
34:a:1422:G:O2'	34:a:1423:G:H5'	2.20	0.42
35:b:180:LEU:HD23	35:b:180:LEU:HA	1.66	0.42
36:c:112:SER:O	36:c:116:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:130:VAL:H	36:c:130:VAL:HG23	1.62	0.42
36:c:164:ARG:HG2	36:c:165:THR:N	2.32	0.42
40:g:78:ARG:HG3	40:g:156:TRP:CE3	2.54	0.42
41:h:132:GLU:HG2	41:h:134:ILE:HD13	2.01	0.42
46:m:52:GLU:HG2	46:m:55:ARG:HH21	1.83	0.42
48:o:77:ARG:O	48:o:81:LEU:HB2	2.19	0.42
56:y:15:ILE:HD12	56:y:103:VAL:HG21	2.02	0.42
56:y:559:LEU:HG	56:y:574:LEU:HD21	2.00	0.42
1:A:768:G:C4	1:A:769:G:C8	3.08	0.42
1:A:776:G:H4'	1:A:777:A:O5'	2.20	0.42
1:A:1009:A:H5''	17:U:63:VAL:CG2	2.49	0.42
1:A:1192:G:OP2	12:P:17:LYS:NZ	2.49	0.42
1:A:2305:A:H2'	1:A:2306:C:O4'	2.20	0.42
1:A:2513:G:H2'	1:A:2514:U:C6	2.55	0.42
2:B:50:G:H5''	15:S:61:ASN:HD22	1.85	0.42
2:B:77:U:C2'	2:B:78:A:H5'	2.50	0.42
4:E:132:HIS:O	4:E:134:ILE:HG23	2.20	0.42
10:N:1:MET:HE2	10:N:1:MET:HB2	1.91	0.42
31:8:41:ILE:HA	31:8:41:ILE:HD12	1.74	0.42
34:a:126:G:OP1	34:a:605:U:O2'	2.34	0.42
34:a:130:A:O2'	34:a:131:C:O5'	2.33	0.42
34:a:1004:A:N6	34:a:1035:A:N7	2.67	0.42
34:a:1118:C:H2'	34:a:1119:C:O4'	2.19	0.42
34:a:1346:A:C8	40:g:10:ARG:NH2	2.88	0.42
34:a:1374:A:OP1	40:g:36:LYS:NZ	2.52	0.42
35:b:16:HIS:HB2	35:b:210:SER:CB	2.50	0.42
35:b:20:GLU:O	35:b:40:HIS:HB2	2.20	0.42
35:b:42:ILE:HD12	35:b:203:GLY:HA2	2.01	0.42
35:b:172:ILE:H	35:b:172:ILE:HG13	1.48	0.42
36:c:3:ASN:N	36:c:3:ASN:OD1	2.52	0.42
37:d:64:LEU:O	37:d:65:ARG:C	2.60	0.42
37:d:158:ILE:H	37:d:158:ILE:HG12	1.48	0.42
45:l:24:VAL:HG22	45:l:98:TYR:HE1	1.83	0.42
48:o:18:PHE:HB2	48:o:19:PRO:HD2	2.02	0.42
56:y:214:TYR:O	56:y:215:LEU:CB	2.67	0.42
56:y:374:PRO:HD2	56:y:374:PRO:O	2.20	0.42
1:A:154:G:C6	1:A:154(A):C:N4	2.88	0.42
1:A:451:C:H4'	5:F:52:LYS:HE2	2.01	0.42
1:A:669:G:O2'	1:A:670:A:H5'	2.19	0.42
1:A:871:U:H5''	13:Q:69:PHE:CZ	2.55	0.42
1:A:1167:U:C2	1:A:1183:G:N2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1804:C:O5'	1:A:1804:C:H6	2.03	0.42
1:A:2070:G:C2	1:A:2442:C:C2	3.08	0.42
1:A:2248:C:C2'	1:A:2249:U:H5'	2.50	0.42
1:A:2813:A:H2'	1:A:2814:C:O4'	2.19	0.42
3:D:206:LEU:HD23	3:D:211:ARG:NE	2.34	0.42
3:D:261:LYS:NZ	3:D:263:ARG:HB2	2.34	0.42
5:F:162:LEU:HD13	5:F:162:LEU:HA	1.83	0.42
7:H:40:GLU:H	7:H:40:GLU:HG3	1.67	0.42
10:N:22:THR:O	10:N:24:GLY:N	2.53	0.42
10:N:112:LEU:C	10:N:114:ARG:N	2.77	0.42
11:O:122:LEU:HD12	16:T:72:VAL:HG11	2.02	0.42
12:P:47:ASP:HA	12:P:48:PRO:HD2	1.76	0.42
22:Z:144:LEU:HD11	22:Z:150:LEU:HD23	2.02	0.42
25:2:32:LEU:HD21	25:2:50:ILE:HG23	2.01	0.42
32:9:3:VAL:HA	32:9:35:ARG:O	2.19	0.42
33:x:7:A:C6	33:x:49:C:C4	3.07	0.42
34:a:656:C:O2'	48:o:28:GLN:NE2	2.53	0.42
34:a:1288:A:H2'	34:a:1289:A:O4'	2.19	0.42
35:b:51:LEU:HG	35:b:201:ILE:HG23	2.01	0.42
39:f:30:LEU:O	39:f:34:GLY:N	2.53	0.42
40:g:18:TYR:HD2	40:g:59:LEU:HD12	1.83	0.42
42:i:99:LEU:HD22	42:i:101:PHE:CZ	2.54	0.42
45:l:69:TYR:O	45:l:100:ILE:HB	2.20	0.42
45:l:75:HIS:ND1	45:l:77:LEU:HB2	2.35	0.42
1:A:26:G:C6	1:A:27:G:N1	2.88	0.42
1:A:83:G:HO2'	1:A:102:G:N2	2.18	0.42
1:A:185:U:H4'	1:A:218:A:H4'	2.02	0.42
1:A:581:C:OP1	17:U:33:ARG:HG2	2.20	0.42
1:A:784:A:C8	1:A:792:G:C5	3.08	0.42
1:A:887:A:H2	1:A:889:C:H5''	1.85	0.42
1:A:1136:G:H2'	1:A:1136:G:N3	2.34	0.42
1:A:1264:G:OP1	28:5:19:ARG:NH2	2.50	0.42
1:A:1791:A:H3'	1:A:1792:G:H8	1.85	0.42
1:A:1996:C:H4'	1:A:1997:G:OP1	2.19	0.42
1:A:2304:G:H5'	1:A:2305:A:OP2	2.20	0.42
1:A:2685:G:P	16:T:51:ARG:HH22	2.42	0.42
1:A:2727:G:O2'	11:O:70:LYS:HE3	2.20	0.42
3:D:206:LEU:HA	3:D:211:ARG:HH21	1.85	0.42
7:H:98:LEU:HD13	7:H:102:ALA:O	2.19	0.42
9:K:93:ARG:CZ	9:K:94:GLU:HB2	2.49	0.42
12:P:81:GLN:HG2	12:P:106:LEU:CD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:21:TYR:OH	14:R:43:GLU:HG2	2.20	0.42
17:U:28:ARG:HG2	17:U:38:THR:OG1	2.20	0.42
18:V:43:GLU:HB2	18:V:44:LYS:H	1.69	0.42
19:W:85:VAL:HG13	19:W:93:ALA:HB1	2.02	0.42
34:a:265:G:N2	34:a:267:C:H5'	2.34	0.42
34:a:825:G:C6	34:a:826:C:C4	3.07	0.42
34:a:1145:C:H4'	34:a:1146:A:O5'	2.20	0.42
34:a:1205:U:H2'	34:a:1206:G:C8	2.55	0.42
35:b:100:GLY:N	35:b:176:GLU:OE2	2.45	0.42
38:e:59:GLY:O	38:e:62:ALA:HB3	2.19	0.42
40:g:12:LEU:H	40:g:12:LEU:HD12	1.85	0.42
41:h:20:TYR:CE1	41:h:76:PRO:HG2	2.54	0.42
49:p:19:ILE:CD1	49:p:36:ILE:HG13	2.48	0.42
52:s:30:LEU:HD11	52:s:50:ALA:HB2	2.02	0.42
56:y:100:VAL:O	56:y:129:HIS:CE1	2.72	0.42
56:y:138:ILE:HG12	56:y:167:SER:HB3	2.02	0.42
56:y:299:PRO:O	56:y:377:VAL:CG1	2.67	0.42
56:y:300:VAL:O	56:y:301:VAL:C	2.62	0.42
1:A:72:U:OP2	20:X:1:MET:N	2.53	0.42
1:A:143(A):C:O2'	1:A:144:C:H5'	2.20	0.42
1:A:584:C:O2	1:A:584:C:H2'	2.19	0.42
1:A:1406:U:H2'	1:A:1407:C:C6	2.55	0.42
1:A:1464:C:H2'	1:A:1465:G:H8	1.85	0.42
1:A:2039:C:H2'	1:A:2040:C:H6	1.84	0.42
1:A:2061:G:C2	1:A:2063:C:C4	3.08	0.42
1:A:2680:C:O2'	1:A:2681:C:H5'	2.20	0.42
3:D:92:ILE:HD13	3:D:104:TYR:CE2	2.55	0.42
3:D:224:ALA:H	3:D:233:HIS:HB3	1.84	0.42
4:E:119:ARG:HD2	4:E:120:TRP:CD1	2.55	0.42
9:K:24:GLY:O	9:K:28:GLY:N	2.53	0.42
9:K:30:HIS:CE1	9:K:59:ILE:HB	2.55	0.42
16:T:27:THR:O	16:T:89:VAL:HG22	2.20	0.42
17:U:13:LYS:HE2	17:U:13:LYS:HB3	1.90	0.42
23:O:53:MET:HE2	23:O:53:MET:HB3	1.85	0.42
24:1:89:GLU:H	24:1:89:GLU:HG2	1.50	0.42
27:4:59:PHE:N	27:4:60:GLN:HB3	2.35	0.42
28:5:23:HIS:CD2	28:5:23:HIS:N	2.88	0.42
30:7:12:ARG:HG2	30:7:46:VAL:HG11	2.01	0.42
34:a:544:G:H2'	34:a:545:C:O4'	2.20	0.42
34:a:860:A:H2'	34:a:861:G:O4'	2.20	0.42
34:a:872:A:C4	34:a:874:G:N7	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1126:U:P	34:a:1281:U:O2	2.78	0.42
35:b:155:LEU:HA	35:b:156:LYS:CB	2.50	0.42
37:d:59:ARG:O	37:d:63:LYS:N	2.50	0.42
37:d:201:GLN:O	37:d:204:ILE:HB	2.20	0.42
38:e:48:ALA:HB3	38:e:54:ALA:HB2	2.02	0.42
39:f:62:TRP:C	39:f:63:TYR:HD2	2.28	0.42
42:i:118:LYS:HB3	42:i:121:ARG:HB3	2.02	0.42
47:n:23:ARG:NH1	47:n:30:ALA:HB2	2.34	0.42
52:s:41:VAL:O	52:s:44:MET:HB2	2.19	0.42
56:y:26:ALA:O	56:y:27:ASP:C	2.62	0.42
56:y:68:TYR:HE1	56:y:70:ALA:HA	1.78	0.42
1:A:139(A):G:N1	20:X:44:GLU:OE1	2.50	0.41
1:A:564:C:H1'	17:U:37:GLU:OE1	2.20	0.41
1:A:571:A:C8	1:A:2030:A:C6	3.08	0.41
1:A:1491:G:C6	1:A:1500:G:C2	3.07	0.41
1:A:1652:A:OP1	14:R:8:ARG:HD3	2.20	0.41
1:A:2044:C:C2	1:A:2625:G:N2	2.87	0.41
1:A:2421:G:H5'	1:A:2422:A:OP2	2.19	0.41
1:A:2503:A:N3	1:A:2503:A:H2'	2.35	0.41
1:A:2586:C:O5'	1:A:2586:C:H6	2.03	0.41
4:E:2:LYS:HA	4:E:84:PHE:CE2	2.55	0.41
5:F:116:ASP:OD2	12:P:1:MET:HB3	2.20	0.41
7:H:76:VAL:C	7:H:78:GLY:N	2.78	0.41
15:S:99:LYS:O	15:S:102:ALA:HB3	2.19	0.41
15:S:105:ALA:HB1	15:S:110:LEU:HD13	2.00	0.41
16:T:23:ARG:HG3	16:T:120:ARG:CZ	2.50	0.41
19:W:15:ARG:NH2	28:5:20:ARG:HE	2.18	0.41
19:W:79:GLY:C	19:W:100:THR:HG22	2.44	0.41
22:Z:119:GLU:H	22:Z:119:GLU:HG3	1.51	0.41
27:4:40:HIS:HA	27:4:41:PRO:HD3	1.92	0.41
33:x:5:G:C6	33:x:6:G:C6	3.08	0.41
33:x:24:G:C6	33:x:25:C:C4	3.08	0.41
34:a:839:U:O2'	34:a:840:C:OP1	2.35	0.41
34:a:957:U:O2	34:a:959:A:C8	2.73	0.41
34:a:1202:G:O4'	47:n:29:ARG:HD2	2.19	0.41
35:b:8:LYS:O	35:b:9:GLU:HB3	2.20	0.41
35:b:17:PHE:CD1	35:b:18:GLY:N	2.88	0.41
35:b:24:TRP:H	35:b:24:TRP:HD1	1.63	0.41
38:e:20:GLN:NE2	38:e:25:ARG:HH22	2.17	0.41
39:f:10:LEU:CB	39:f:59:TYR:HB3	2.49	0.41
42:i:10:ARG:O	42:i:11:LYS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:k:122:LYS:HB3	44:k:123:LYS:H	1.48	0.41
45:l:28:LYS:N	45:l:29:GLY:HA2	2.35	0.41
48:o:25:THR:O	48:o:28:GLN:HB2	2.20	0.41
48:o:74:ASP:HB3	48:o:77:ARG:HG2	2.02	0.41
51:r:76:LEU:HD12	51:r:76:LEU:HA	1.79	0.41
56:y:96:ALA:HA	56:y:201:PHE:HB2	2.01	0.41
56:y:134:VAL:HG12	56:y:135:ILE:N	2.35	0.41
56:y:372:THR:CG2	56:y:373:ALA:H	2.33	0.41
1:A:28:A:H1'	1:A:513:A:C2	2.55	0.41
1:A:65:C:H2'	1:A:66:C:C6	2.55	0.41
1:A:338:G:C4	1:A:339:U:C6	3.07	0.41
1:A:686:G:H5''	30:7:11:LYS:HE2	2.01	0.41
1:A:1168:G:C2	1:A:1182:A:C2	3.08	0.41
1:A:1171:G:C3'	1:A:1173:G:H5'	2.50	0.41
1:A:1517:G:C6	1:A:1518:U:C4	3.08	0.41
1:A:1773:A:H2'	1:A:1774:C:O4'	2.20	0.41
1:A:1978:A:H2'	1:A:1979:C:O4'	2.19	0.41
1:A:1983:C:H4'	1:A:2606:C:H4'	2.03	0.41
1:A:2129:C:H2'	1:A:2130:U:O4'	2.20	0.41
1:A:2250:G:H8	1:A:2497:A:OP2	2.04	0.41
1:A:2270:G:H2'	1:A:2271:G:H8	1.83	0.41
1:A:2291:U:O2'	1:A:2374:C:H1'	2.20	0.41
1:A:2373:G:C6	1:A:2374:C:N4	2.88	0.41
1:A:2576:G:O2'	1:A:2579:C:OP2	2.24	0.41
1:A:2723:C:OP1	4:E:109:LYS:HD3	2.21	0.41
1:A:2889:C:O2	1:A:2889:C:H2'	2.21	0.41
3:D:152:GLY:O	3:D:154:LYS:HG2	2.20	0.41
3:D:223:GLY:O	3:D:226:MET:N	2.48	0.41
4:E:10:GLY:HA2	4:E:192:ASN:OD1	2.20	0.41
4:E:117:MET:O	4:E:118:LYS:HB3	2.19	0.41
7:H:164:TYR:HD2	7:H:164:TYR:HA	1.73	0.41
15:S:69:VAL:HG13	15:S:101:LEU:HD12	2.02	0.41
17:U:81:HIS:CD2	17:U:84:LYS:HD3	2.55	0.41
22:Z:136:PHE:HD2	22:Z:136:PHE:HA	1.72	0.41
22:Z:176:PRO:HA	22:Z:177:PRO:HD3	1.82	0.41
24:1:51:VAL:HG12	24:1:58:ILE:O	2.20	0.41
27:4:63:TYR:N	27:4:64:GLY:HA2	2.34	0.41
31:8:58:ILE:O	31:8:61:LEU:HB2	2.20	0.41
33:x:5:G:H2'	33:x:6:G:H8	1.85	0.41
33:x:6:G:C6	33:x:7:A:C6	3.08	0.41
34:a:170:U:O2'	34:a:171:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:291:C:C2'	34:a:292:G:H5'	2.49	0.41
34:a:392:G:H2'	34:a:393:A:C8	2.55	0.41
34:a:447:G:H2'	34:a:485:G:H22	1.83	0.41
34:a:1107:C:C4	34:a:1108:G:C8	3.09	0.41
34:a:1312:G:N7	52:s:2:PRO:HG2	2.35	0.41
34:a:1446:U:OP1	34:a:1447:A:N6	2.53	0.41
35:b:196:LEU:HA	35:b:196:LEU:HD22	1.76	0.41
40:g:16:LEU:HG	42:i:45:ALA:H	1.85	0.41
42:i:70:LYS:O	42:i:74:ILE:HG13	2.20	0.41
42:i:108:VAL:HG12	42:i:109:VAL:H	1.84	0.41
42:i:128:ARG:NH1	33:w:35:A:OP2	2.53	0.41
43:j:45:ARG:HG2	43:j:47:PHE:CZ	2.55	0.41
56:y:302:PHE:O	56:y:303:ALA:HB3	2.21	0.41
1:A:84:A:C5'	21:Y:8:LYS:HG2	2.49	0.41
1:A:438:G:H2'	1:A:440:G:C8	2.54	0.41
1:A:565:C:C4	1:A:566:U:C5	3.07	0.41
1:A:675:A:H4'	5:F:67:GLN:OE1	2.20	0.41
1:A:1144:G:C6	1:A:1145:C:N4	2.88	0.41
1:A:1352:U:O2'	1:A:1353:A:H5'	2.20	0.41
1:A:1500:G:N2	3:D:99:ASP:O	2.51	0.41
1:A:2023:G:H4'	1:A:2617:C:O3'	2.20	0.41
1:A:2309:A:N6	1:A:2310:A:C6	2.88	0.41
1:A:2373:G:C6	1:A:2374:C:C4	3.08	0.41
1:A:2406:U:N3	12:P:72:PRO:HD2	2.35	0.41
1:A:2883:A:H5''	1:A:2884:U:H5'	2.02	0.41
6:G:22:ARG:NH2	6:G:175:LEU:HD11	2.32	0.41
7:H:101:ARG:NH2	7:H:121:ILE:O	2.53	0.41
8:J:85:ASP:O	8:J:87:VAL:N	2.54	0.41
10:N:18:ALA:O	10:N:19:GLU:HB2	2.20	0.41
10:N:112:LEU:C	10:N:114:ARG:H	2.28	0.41
15:S:61:ASN:OD1	15:S:64:GLU:HG3	2.20	0.41
19:W:15:ARG:HH21	28:5:20:ARG:NE	2.18	0.41
19:W:23:LEU:HD11	28:5:27:PRO:HD3	2.02	0.41
22:Z:137:ILE:HG23	22:Z:156:LYS:HE3	2.01	0.41
22:Z:150:LEU:O	22:Z:171:ILE:HG12	2.20	0.41
22:Z:156:LYS:HD2	22:Z:157:LEU:H	1.85	0.41
24:1:70:VAL:O	24:1:74:VAL:HG23	2.20	0.41
27:4:69:LYS:HE2	27:4:69:LYS:HB3	1.86	0.41
28:5:51:TYR:HA	28:5:55:ARG:O	2.19	0.41
28:5:58:LEU:O	28:5:60:VAL:N	2.53	0.41
33:x:68:C:C4	33:x:69:G:N7	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:109:A:C3'	34:a:110:C:H5'	2.50	0.41
34:a:453:A:C6	34:a:454:C:C4	3.08	0.41
34:a:509:A:C8	34:a:509:A:C3'	3.03	0.41
34:a:526:C:H5'	34:a:527:G:OP2	2.20	0.41
34:a:584:G:OP1	50:q:91:ARG:NH2	2.53	0.41
34:a:1128:C:H1'	34:a:1130:A:N7	2.36	0.41
34:a:1516:G:H2'	34:a:1518:A:OP2	2.21	0.41
34:a:1521:G:H1'	62:a:3521:HOH:O	2.20	0.41
35:b:72:GLY:HA3	35:b:81:VAL:HG21	2.02	0.41
36:c:159:GLY:HA2	36:c:193:TYR:CD2	2.55	0.41
37:d:8:VAL:HG11	37:d:22:LYS:HG3	2.02	0.41
39:f:1:MET:HA	39:f:67:MET:O	2.20	0.41
42:i:69:GLY:O	42:i:71:SER:N	2.53	0.41
44:k:120:ARG:HA	44:k:121:PRO:HD3	1.94	0.41
50:q:34:LYS:HG2	50:q:35:VAL:H	1.85	0.41
56:y:140:LEU:HD12	61:y:703:GDP:HN22	1.84	0.41
56:y:194:ALA:O	56:y:220:GLY:HA2	2.21	0.41
1:A:392:C:H2'	1:A:393:C:H6	1.85	0.41
1:A:483:A:H2'	1:A:484:C:O4'	2.21	0.41
1:A:827:U:H5'	1:A:828:U:O5'	2.19	0.41
1:A:1676:A:H2'	1:A:1677:A:O4'	2.19	0.41
1:A:2206:G:H5'	1:A:2207:G:N7	2.35	0.41
1:A:2506:U:C6	1:A:2507:C:H5	2.39	0.41
1:A:2531:A:H2	1:A:2658:C:O2	2.03	0.41
1:A:2861:G:C2	1:A:2862:G:C8	3.08	0.41
6:G:25:TYR:CE2	6:G:31:VAL:HA	2.55	0.41
6:G:99:MET:HE2	6:G:99:MET:HB2	1.67	0.41
10:N:100:GLU:HG2	10:N:122:VAL:HG21	2.03	0.41
10:N:115:ARG:O	10:N:115:ARG:HG3	2.21	0.41
11:O:43:VAL:HG12	11:O:54:GLU:HA	2.03	0.41
15:S:52:SER:C	15:S:54:LEU:N	2.78	0.41
16:T:7:ILE:HD13	16:T:7:ILE:HA	1.88	0.41
18:V:51:VAL:HB	18:V:53:GLU:H	1.84	0.41
33:x:20:U:C4'	33:x:21:A:H5'	2.50	0.41
33:x:49:C:H2'	33:x:50:U:H6	1.85	0.41
34:a:154:C:H2'	34:a:155:C:C6	2.53	0.41
34:a:436:C:O2'	34:a:437:U:OP2	2.35	0.41
34:a:460:G:O6	34:a:470:C:H5'	2.20	0.41
34:a:565:U:C4	34:a:566:G:C5	3.09	0.41
34:a:1028:C:N4	34:a:1033:G:C6	2.85	0.41
34:a:1124:G:H4'	43:j:38:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:20:GLN:HE21	38:e:25:ARG:HH22	1.69	0.41
38:e:38:GLN:HE21	38:e:38:GLN:HB2	1.53	0.41
38:e:78:HIS:HA	41:h:105:ARG:HG3	2.03	0.41
42:i:16:ARG:HH11	42:i:64:THR:HG21	1.86	0.41
42:i:128:ARG:HD3	33:w:35:A:OP1	2.21	0.41
43:j:55:LYS:HE3	43:j:56:HIS:CE1	2.56	0.41
43:j:81:THR:C	43:j:83:GLU:N	2.79	0.41
54:u:5:ASP:OD1	54:u:7:ARG:N	2.48	0.41
56:y:107:VAL:O	56:y:136:ASN:HB3	2.16	0.41
56:y:223:ARG:CB	56:y:224:PRO:HD3	2.48	0.41
56:y:557:ASP:OD2	56:y:557:ASP:N	2.53	0.41
1:A:118:A:N3	1:A:178:G:H1'	2.35	0.41
1:A:293:U:H5''	1:A:294:A:OP2	2.21	0.41
1:A:1144:G:H2'	1:A:1145:C:C6	2.56	0.41
1:A:1355:G:C6	1:A:1356:G:C5	3.08	0.41
1:A:1439:A:N3	1:A:1553:A:C6	2.89	0.41
1:A:1478:G:H2'	1:A:1479:G:C8	2.46	0.41
1:A:2072:G:C5	1:A:2073:C:C5	3.08	0.41
1:A:2099:U:H2'	1:A:2100:G:C8	2.55	0.41
1:A:2224:G:H4'	1:A:2226:C:O2	2.21	0.41
1:A:2812:G:N2	1:A:2889:C:C2	2.88	0.41
2:B:57:A:H1'	6:G:29:TRP:HB2	2.02	0.41
3:D:99:ASP:OD2	3:D:99:ASP:N	2.54	0.41
3:D:176:ARG:HA	3:D:181:GLU:O	2.21	0.41
3:D:179:SER:O	3:D:275:LYS:HB2	2.21	0.41
4:E:37:ARG:HD2	4:E:44:TYR:CZ	2.56	0.41
6:G:45:GLU:H	6:G:45:GLU:HG2	1.71	0.41
7:H:38:SER:OG	7:H:40:GLU:HG3	2.20	0.41
9:K:13:PRO:HG3	9:K:52:ILE:HG12	2.02	0.41
9:K:32:ALA:O	9:K:34:ILE:N	2.53	0.41
12:P:81:GLN:HG3	12:P:82:GLY:N	2.30	0.41
16:T:19:LEU:HD23	16:T:19:LEU:HA	1.78	0.41
17:U:97:ASP:O	17:U:101:ARG:HG3	2.21	0.41
21:Y:6:HIS:CD2	21:Y:7:VAL:HG23	2.56	0.41
34:a:103:C:OP2	53:t:14:LYS:HD2	2.21	0.41
34:a:585:G:H2'	34:a:586:C:O4'	2.19	0.41
34:a:946:A:C2	34:a:1236:A:C2	3.07	0.41
35:b:180:LEU:O	35:b:181:PHE:HB2	2.20	0.41
37:d:120:LEU:HD23	37:d:120:LEU:HA	1.77	0.41
37:d:178:VAL:C	37:d:180:GLY:N	2.77	0.41
41:h:39:LEU:HB3	41:h:45:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:m:15:VAL:O	46:m:19:LEU:HD23	2.21	0.41
51:r:51:LEU:HD22	51:r:55:ARG:HH11	1.86	0.41
51:r:66:LEU:HD11	51:r:70:ILE:HD11	2.03	0.41
56:y:17:HIS:CD2	56:y:114:GLU:HB2	2.55	0.41
1:A:77:C:OP1	25:2:59:ARG:HD3	2.21	0.41
1:A:77:C:H42	1:A:109:G:H1	1.67	0.41
1:A:247:G:C8	1:A:249:C:C5	3.08	0.41
1:A:250:G:P	31:8:13:ARG:HH21	2.43	0.41
1:A:301:G:C4	1:A:302:C:C5	3.09	0.41
1:A:370:G:H4'	1:A:371:A:OP2	2.20	0.41
1:A:894:C:H2'	1:A:895:U:O4'	2.20	0.41
1:A:1006:C:H1'	10:N:106:MET:HB3	2.01	0.41
1:A:1097:U:H2'	1:A:1098:A:H5'	2.03	0.41
1:A:1452:A:O2'	1:A:1453:U:H2'	2.19	0.41
3:D:161:THR:O	3:D:196:VAL:HG23	2.20	0.41
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.41	0.41
7:H:10:PRO:C	7:H:12:PRO:HD3	2.45	0.41
9:K:12:LEU:HA	9:K:13:PRO:HD3	1.76	0.41
20:X:89:ILE:HG23	20:X:91:ALA:HB3	2.02	0.41
22:Z:53:ILE:HG22	22:Z:71:VAL:HB	2.02	0.41
34:a:229:U:H2'	34:a:230:G:C8	2.56	0.41
34:a:601:C:H2'	34:a:602:A:C8	2.56	0.41
34:a:668:G:O4'	48:o:49:ASP:HB2	2.19	0.41
34:a:719:C:H1'	51:r:49:LYS:CG	2.51	0.41
34:a:922:G:C6	34:a:923:A:C6	3.09	0.41
36:c:113:ALA:O	36:c:114:PRO:C	2.64	0.41
36:c:153:VAL:HG12	36:c:157:ILE:HD11	2.03	0.41
36:c:157:ILE:HG21	36:c:164:ARG:NH1	2.36	0.41
37:d:20:TYR:CD2	37:d:26:CYS:HB3	2.55	0.41
39:f:46:ARG:HB3	39:f:60:PHE:CE1	2.56	0.41
42:i:9:ARG:HG2	42:i:14:VAL:HG22	2.03	0.41
43:j:16:LEU:HD11	43:j:70:ARG:HB2	2.01	0.41
49:p:60:LEU:O	49:p:61:SER:C	2.64	0.41
53:t:16:HIS:O	53:t:19:SER:HB3	2.20	0.41
56:y:424:LEU:C	56:y:424:LEU:CD1	2.93	0.41
1:A:34:C:H2'	1:A:35:G:C5'	2.46	0.41
1:A:464:U:H2'	1:A:465:G:O4'	2.20	0.41
1:A:904:C:H2'	1:A:905:U:H6	1.85	0.41
1:A:980:A:N3	1:A:2037:G:O2'	2.48	0.41
1:A:1139:G:OP1	10:N:101:HIS:ND1	2.43	0.41
1:A:1149:G:H2'	1:A:1150:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:C:H2'	1:A:1290:C:C6	2.55	0.41
1:A:1668:A:H4'	1:A:1669:A:O5'	2.20	0.41
1:A:1838:C:C5	1:A:1899:G:C2	3.09	0.41
1:A:2243:U:H2'	1:A:2244:U:C6	2.55	0.41
1:A:2491:U:H6	1:A:2491:U:H5''	1.86	0.41
5:F:34:TRP:HA	12:P:6:LEU:HD22	2.03	0.41
6:G:50:ALA:O	6:G:53:LEU:HD23	2.21	0.41
7:H:94:TYR:CG	7:H:107:VAL:HG12	2.55	0.41
17:U:61:TRP:O	17:U:64:ARG:N	2.54	0.41
22:Z:150:LEU:HD13	22:Z:150:LEU:HA	1.77	0.41
34:a:519:C:H2'	34:a:520:A:O4'	2.20	0.41
34:a:585:G:H1'	34:a:879:C:H5''	2.02	0.41
34:a:727:G:C6	34:a:731:G:C6	3.09	0.41
34:a:1058:G:H2'	34:a:1059:C:C6	2.55	0.41
34:a:1215:G:C6	34:a:1216:G:N7	2.89	0.41
35:b:47:THR:HA	35:b:202:PRO:HG2	2.03	0.41
36:c:12:LEU:HD11	47:n:51:GLY:CA	2.50	0.41
37:d:206:PHE:C	37:d:208:SER:H	2.28	0.41
38:e:20:GLN:HE21	38:e:25:ARG:NH2	2.18	0.41
39:f:10:LEU:N	39:f:59:TYR:O	2.52	0.41
41:h:37:ARG:NH1	41:h:41:ARG:HH22	2.19	0.41
42:i:43:ALA:O	42:i:46:ALA:N	2.54	0.41
45:l:24:VAL:N	45:l:25:PRO:HD3	2.35	0.41
47:n:60:SER:O	47:n:61:TRP:HB3	2.19	0.41
56:y:410:VAL:HA	56:y:481:GLN:O	2.20	0.41
56:y:595:GLU:O	56:y:598:LEU:HB2	2.21	0.41
1:A:151:C:H2'	1:A:152:G:C8	2.56	0.41
1:A:234:C:H2'	1:A:235:U:C6	2.56	0.41
1:A:715:G:C2	48:o:56:LEU:HD21	2.56	0.41
1:A:1062:G:N2	1:A:1076:C:N3	2.66	0.41
1:A:1063:G:H8	1:A:1063:G:O5'	2.04	0.41
1:A:1707:G:H2'	1:A:1708:C:C6	2.56	0.41
1:A:1813:G:N3	3:D:50:THR:OG1	2.53	0.41
1:A:2367:G:H2'	1:A:2368:C:H6	1.86	0.41
1:A:2747:G:O6	1:A:2755:C:H5''	2.20	0.41
1:A:2869:G:H2'	1:A:2870:C:O4'	2.20	0.41
4:E:52:LEU:HA	4:E:53:PRO:HD2	1.78	0.41
6:G:107:LEU:O	27:4:43:TYR:OH	2.39	0.41
7:H:76:VAL:HG12	7:H:77:LYS:N	2.36	0.41
8:J:97:ALA:C	8:J:99:SER:H	2.29	0.41
10:N:10:GLU:OE2	10:N:11:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:70:PRO:HA	13:Q:95:ALA:HB2	2.02	0.41
17:U:36:ARG:HD2	17:U:40:PHE:CZ	2.55	0.41
24:1:40:ARG:HE	24:1:40:ARG:HB2	1.30	0.41
25:2:31:GLU:O	25:2:35:LEU:HG	2.21	0.41
26:3:26:LEU:HB2	26:3:28:LEU:HD12	2.03	0.41
34:a:16:A:C2'	34:a:17:U:H5'	2.50	0.41
34:a:293:G:C5	34:a:294:U:C5	3.09	0.41
34:a:436:C:H6	34:a:436:C:H2'	1.67	0.41
34:a:833:U:H2'	34:a:834:C:H6	1.82	0.41
34:a:1157:A:C2	34:a:1181:G:C5	3.09	0.41
41:h:81:HIS:N	41:h:138:TRP:O	2.53	0.41
46:m:14:ARG:HB3	46:m:41:PRO:O	2.21	0.41
46:m:96:LEU:O	46:m:110:ARG:NH1	2.41	0.41
50:q:48:GLU:C	50:q:50:LYS:N	2.78	0.41
50:q:50:LYS:HD2	50:q:51:TYR:CE2	2.56	0.41
56:y:72:ASP:OD1	56:y:74:GLU:N	2.54	0.41
1:A:686:G:H1'	30:7:6:GLN:O	2.21	0.41
1:A:691:C:H2'	1:A:692:C:H6	1.85	0.41
1:A:881:G:H2'	1:A:882:G:O4'	2.21	0.41
1:A:911:A:H2'	13:Q:9:TYR:OH	2.21	0.41
1:A:1130:U:O2	4:E:149:ARG:NH2	2.53	0.41
1:A:2074:U:H2'	1:A:2075:U:H6	1.82	0.41
1:A:2343:C:O2'	1:A:2373:G:H4'	2.21	0.41
1:A:2418:A:H2'	1:A:2419:U:C6	2.55	0.41
1:A:2485:G:H5''	13:Q:46:GLN:HE21	1.86	0.41
1:A:2536:G:C6	1:A:2537:U:C4	3.09	0.41
1:A:2782:G:N2	1:A:2783:G:H1'	2.36	0.41
1:A:2794:C:C2	1:A:2802:G:N2	2.82	0.41
2:B:88:C:H2'	2:B:89:G:O4'	2.19	0.41
3:D:164:GLN:HE21	3:D:164:GLN:HB3	1.66	0.41
5:F:21:ALA:O	5:F:23:ASP:N	2.52	0.41
5:F:206:ILE:H	5:F:206:ILE:HG12	1.56	0.41
6:G:47:LYS:CG	6:G:48:GLU:H	2.33	0.41
7:H:3:ARG:NH1	7:H:5:GLY:H	2.14	0.41
10:N:62:VAL:CG1	10:N:66:LYS:HD2	2.51	0.41
11:O:23:ARG:HG3	11:O:24:VAL:N	2.36	0.41
11:O:25:LEU:HB2	11:O:38:VAL:O	2.21	0.41
11:O:111:PHE:O	11:O:115:VAL:HG23	2.21	0.41
12:P:109:GLY:C	12:P:110:TYR:HD1	2.28	0.41
13:Q:98:LYS:HA	13:Q:99:PRO:HD3	1.96	0.41
16:T:124:ASP:C	16:T:126:ALA:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:5:MET:HE3	21:Y:30:VAL:CG1	2.49	0.41
21:Y:46:LYS:HD3	21:Y:60:PHE:CD2	2.55	0.41
24:1:74:VAL:HB	24:1:75:GLU:OE2	2.21	0.41
25:2:16:LEU:CD2	25:2:20:GLU:HB2	2.51	0.41
25:2:21:LEU:HD23	25:2:21:LEU:HA	1.67	0.41
27:4:40:HIS:O	27:4:42:PHE:N	2.53	0.41
28:5:36:CYS:SG	28:5:38:ALA:HB3	2.61	0.41
28:5:40:LYS:HE2	28:5:40:LYS:HB2	1.80	0.41
30:7:11:LYS:O	30:7:15:THR:OG1	2.24	0.41
31:8:23:VAL:HG11	31:8:47:LYS:HD3	2.02	0.41
31:8:30:ARG:HD3	31:8:30:ARG:HA	1.70	0.41
34:a:16:A:H2'	34:a:17:U:H5'	2.02	0.41
34:a:46:G:O2'	34:a:365:U:O2	2.37	0.41
34:a:110:C:H2'	34:a:111:G:O4'	2.21	0.41
34:a:235:C:O2'	34:a:236:G:H5'	2.21	0.41
34:a:556:C:H2'	34:a:557:G:O4'	2.20	0.41
34:a:604:G:C6	34:a:605:U:N3	2.89	0.41
34:a:609:A:OP1	49:p:18:ARG:NH2	2.44	0.41
34:a:938:A:N6	34:a:939:G:C6	2.88	0.41
34:a:1129:C:O5'	34:a:1130:A:H5'	2.21	0.41
34:a:1234:C:H2'	34:a:1235:U:C6	2.56	0.41
34:a:1318:A:OP1	52:s:3:ARG:NH2	2.54	0.41
34:a:1416:G:H2'	34:a:1417:G:O4'	2.21	0.41
34:a:1529:G:H4'	34:a:1530:G:OP2	2.21	0.41
37:d:190:ASP:O	37:d:192:GLU:N	2.54	0.41
38:e:85:GLY:C	38:e:87:SER:H	2.28	0.41
39:f:5:GLU:HG2	39:f:62:TRP:HE1	1.86	0.41
39:f:30:LEU:HD23	39:f:75:LEU:HD11	2.03	0.41
41:h:97:VAL:HG23	41:h:129:VAL:O	2.20	0.41
44:k:18:ARG:HB2	44:k:33:THR:OG1	2.20	0.41
44:k:65:ALA:HB2	44:k:94:ALA:HB1	2.03	0.41
46:m:59:TYR:HE2	46:m:63:THR:HG1	1.64	0.41
48:o:57:LEU:HD23	48:o:57:LEU:HA	1.88	0.41
49:p:4:ILE:HB	49:p:66:PRO:HA	2.02	0.41
33:w:61:C:O2'	33:w:62:C:H5'	2.21	0.41
56:y:-39:LEU:HB3	56:y:-33:ALA:HB3	2.02	0.41
56:y:62:SER:O	56:y:63:ALA:CB	2.69	0.41
56:y:299:PRO:HB2	56:y:300:VAL:CA	2.50	0.41
56:y:392:ASN:HA	56:y:393:PRO:HD3	1.50	0.41
56:y:417:PRO:O	56:y:418:GLU:HG2	2.21	0.41
56:y:418:GLU:HB3	56:y:446:LYS:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:y:440:TYR:HA	56:y:448:VAL:HA	2.03	0.41
56:y:479:TYR:CD2	56:y:479:TYR:N	2.89	0.41
1:A:66:C:C2	1:A:89:G:C2	3.09	0.41
1:A:185:U:H2'	1:A:186:G:C8	2.56	0.41
1:A:947:G:N3	1:A:984:A:H2	2.18	0.41
1:A:1067:A:N3	56:y:429:GLN:OE1	2.53	0.41
1:A:1265:A:C8	1:A:1267:U:C2	3.09	0.41
1:A:1270:C:H4'	1:A:1325:G:N7	2.36	0.41
1:A:1754:C:OP2	16:T:113:LYS:HE3	2.21	0.41
1:A:1952:A:N3	11:O:22:ILE:HD12	2.36	0.41
1:A:2061:G:N3	1:A:2063:C:C5	2.89	0.41
1:A:2478:A:OP1	32:9:31:LYS:HD3	2.21	0.41
2:B:9:G:C5	2:B:113:G:C6	3.09	0.41
3:D:43:ARG:HG3	3:D:49:ILE:HG13	2.02	0.41
7:H:33:LEU:HB3	7:H:34:GLU:H	1.67	0.41
18:V:89:GLN:HA	18:V:90:PRO:HD3	1.88	0.41
21:Y:28:LYS:HD2	21:Y:40:GLU:HA	2.03	0.41
22:Z:152:ALA:HB1	22:Z:163:LEU:HD21	2.03	0.41
24:1:90:ILE:O	24:1:94:LEU:HD12	2.21	0.41
33:x:5:G:O6	33:x:67:C:N4	2.54	0.41
34:a:320:C:H2'	34:a:321:A:O4'	2.21	0.41
34:a:728:A:H2'	34:a:729:A:C8	2.56	0.41
34:a:1276:G:H2'	34:a:1277:C:O4'	2.20	0.41
35:b:47:THR:O	35:b:51:LEU:HB2	2.21	0.41
36:c:141:VAL:HG11	36:c:202:ILE:HG12	2.03	0.41
37:d:112:VAL:HG12	37:d:116:GLN:OE1	2.21	0.41
39:f:19:LEU:HD11	39:f:59:TYR:CZ	2.56	0.41
42:i:19:LEU:HD23	42:i:19:LEU:HA	1.93	0.41
42:i:41:VAL:O	42:i:43:ALA:N	2.54	0.41
42:i:69:GLY:O	42:i:70:LYS:C	2.64	0.41
43:j:98:ILE:H	43:j:98:ILE:HD12	1.86	0.41
44:k:33:THR:HG22	44:k:39:PRO:HA	2.03	0.41
46:m:88:ARG:HG3	46:m:98:VAL:HG13	2.03	0.41
56:y:304:GLY:CA	56:y:306:TYR:CZ	2.83	0.41
56:y:398:ASP:C	56:y:400:THR:H	2.29	0.41
1:A:1434:A:O2'	1:A:1435:G:H5'	2.21	0.40
1:A:2140:C:O2	1:A:2151:G:N1	2.36	0.40
1:A:2199:A:H2'	1:A:2199:A:N3	2.35	0.40
1:A:2338:G:N2	1:A:2339:G:C4	2.88	0.40
1:A:2486:G:H2'	1:A:2487:G:O4'	2.21	0.40
1:A:2638:G:P	4:E:82:ARG:HH22	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:81:ALA:HA	3:D:113:VAL:CG1	2.51	0.40
6:G:99:MET:HG3	6:G:100:TRP:N	2.36	0.40
7:H:24:VAL:HG13	7:H:37:VAL:HG21	2.04	0.40
9:K:53:VAL:HA	9:K:54:PRO:HD3	1.92	0.40
10:N:128:HIS:C	10:N:130:HIS:H	2.29	0.40
12:P:84:ASN:HB3	12:P:85:LEU:H	1.63	0.40
15:S:62:LYS:HG3	15:S:97:ARG:HD2	2.03	0.40
16:T:29:ARG:HB3	16:T:87:ASP:HB2	2.04	0.40
19:W:12:ILE:HG13	19:W:42:ARG:NH1	2.37	0.40
19:W:68:ARG:HB3	19:W:109:GLU:HG2	2.02	0.40
21:Y:19:LYS:HD3	21:Y:20:TYR:CE1	2.56	0.40
23:0:11:ARG:O	23:0:14:ARG:NH2	2.47	0.40
27:4:17:GLY:C	27:4:19:GLY:H	2.29	0.40
32:9:29:ASN:HA	32:9:30:PRO:HD3	1.90	0.40
34:a:540:G:H2'	34:a:541:G:O4'	2.21	0.40
34:a:688:G:C5	34:a:700:G:C2	3.09	0.40
34:a:793:U:O4	34:a:1517:G:H5''	2.20	0.40
34:a:891:U:O2'	34:a:892:A:H5'	2.22	0.40
34:a:1027:C:O2	34:a:1028:C:N4	2.43	0.40
34:a:1132:C:H2'	34:a:1133:G:H8	1.86	0.40
34:a:1305:G:N2	34:a:1331:G:H1'	2.35	0.40
34:a:1343:G:H2'	34:a:1344:C:C6	2.56	0.40
35:b:133:LYS:O	35:b:137:ARG:HB2	2.21	0.40
36:c:97:LYS:H	36:c:97:LYS:HG2	1.64	0.40
36:c:114:PRO:O	36:c:118:GLN:HG2	2.21	0.40
37:d:28:SER:OG	37:d:31:CYS:N	2.54	0.40
38:e:122:GLU:O	38:e:126:ARG:NH1	2.53	0.40
44:k:44:SER:OG	44:k:47:VAL:HG23	2.21	0.40
46:m:12:ASN:O	46:m:44:ARG:HD2	2.21	0.40
46:m:19:LEU:HB3	46:m:25:ILE:HG21	2.02	0.40
49:p:23:ASP:O	49:p:24:ALA:C	2.64	0.40
51:r:59:SER:H	51:r:62:GLU:HB2	1.86	0.40
53:t:34:LYS:HB2	53:t:34:LYS:HE3	1.71	0.40
56:y:33:THR:HB	56:y:67:THR:O	2.21	0.40
56:y:230:ILE:HG13	56:y:234:GLY:C	2.46	0.40
1:A:485:C:H2'	1:A:486:C:C6	2.56	0.40
1:A:1138:G:H1'	10:N:105:GLY:O	2.21	0.40
1:A:1141:U:H4'	1:A:1142(A):A:O4'	2.21	0.40
1:A:1142(A):A:C4	1:A:1144:G:C8	3.09	0.40
1:A:1288:U:O2'	1:A:1647:G:N2	2.54	0.40
1:A:1548:C:H2'	1:A:1549:C:H6	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:U:H5'	3:D:259:THR:HG22	2.03	0.40
1:A:2058:A:C6	1:A:2059:A:N6	2.89	0.40
1:A:2079:U:H3	1:A:2241:A:N6	2.19	0.40
1:A:2099:U:H1'	1:A:2191:G:H22	1.86	0.40
1:A:2133:G:C2	1:A:2157:G:C5	3.09	0.40
1:A:2277:G:C6	1:A:2278:A:N7	2.90	0.40
1:A:2752:C:H2'	1:A:2753:A:O4'	2.21	0.40
3:D:175:LEU:HD23	3:D:175:LEU:HA	1.57	0.40
3:D:206:LEU:HD22	3:D:211:ARG:HB3	2.03	0.40
4:E:181:LEU:HD11	16:T:6:LEU:HD23	2.02	0.40
5:F:154:VAL:N	5:F:172:TRP:O	2.38	0.40
7:H:121:ILE:HD13	7:H:121:ILE:HA	1.99	0.40
9:K:103:GLN:HA	9:K:106:GLU:HG2	2.03	0.40
10:N:36:GLY:HA3	10:N:48:MET:CE	2.50	0.40
13:Q:34:LEU:HD12	13:Q:34:LEU:HA	1.81	0.40
20:X:60:ARG:HH12	30:7:47:ARG:HH22	1.69	0.40
21:Y:39:VAL:HB	21:Y:42:VAL:HG21	2.03	0.40
22:Z:166:SER:HA	22:Z:167:PRO:HD3	1.95	0.40
23:0:43:THR:O	23:0:43:THR:OG1	2.39	0.40
31:8:61:LEU:C	31:8:63:PRO:HD3	2.47	0.40
33:x:18:G:O6	33:x:55:PSU:H1'	2.21	0.40
34:a:189(K):U:H2'	34:a:189(L):G:H8	1.86	0.40
34:a:568:G:O6	45:l:5:PRO:HD3	2.21	0.40
34:a:978:A:C5	34:a:1319:A:C2	3.10	0.40
34:a:1072:G:C5	34:a:1073:U:C4	3.09	0.40
34:a:1084:G:H1'	34:a:1103:C:H41	1.86	0.40
35:b:187:LEU:HD13	35:b:205:ASP:HB3	2.02	0.40
35:b:230:VAL:HG22	35:b:231:GLU:H	1.86	0.40
43:j:38:ILE:HA	43:j:39:PRO:HD3	1.98	0.40
44:k:82:VAL:HG23	44:k:107:SER:O	2.20	0.40
1:A:556:G:C6	1:A:557:U:C4	3.10	0.40
1:A:781:A:N1	1:A:1776:G:O2'	2.47	0.40
1:A:1388:G:H1	1:A:1399:C:H42	1.69	0.40
1:A:1434:A:H2'	1:A:1435:G:H8	1.87	0.40
1:A:1826:G:OP2	3:D:222:ARG:HB3	2.21	0.40
1:A:2057:A:O2'	1:A:2058:A:H5'	2.21	0.40
1:A:2126:A:H4'	1:A:2127:G:O5'	2.20	0.40
1:A:2135:A:N7	1:A:2136:C:N4	2.69	0.40
1:A:2370:G:C6	1:A:2371:G:C6	3.09	0.40
9:K:70:LYS:HB3	9:K:71:THR:H	1.61	0.40
9:K:115:LEU:O	9:K:116:ASN:ND2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:1:MET:H1	10:N:1:MET:HG3	1.76	0.40
10:N:54:VAL:HB	10:N:122:VAL:HG13	2.04	0.40
11:O:64:ARG:NH1	11:O:81:ASP:OD2	2.54	0.40
12:P:115:LEU:HA	12:P:131:SER:OG	2.21	0.40
14:R:39:PRO:O	14:R:40:LYS:C	2.65	0.40
16:T:19:LEU:HA	16:T:20:PRO:HD2	1.67	0.40
17:U:109:LEU:O	17:U:110:VAL:C	2.64	0.40
30:7:43:THR:HA	30:7:44:PRO:HD3	1.99	0.40
34:a:115:G:C2	34:a:313:A:C2	3.09	0.40
34:a:132:C:O2'	34:a:133:U:H5'	2.21	0.40
34:a:137:C:H42	34:a:226:G:H1	1.67	0.40
34:a:373:A:H1'	34:a:481:G:N3	2.36	0.40
34:a:604:G:H2'	34:a:605:U:O4'	2.21	0.40
34:a:665:A:N3	34:a:732:C:H2'	2.37	0.40
34:a:680:C:C2	34:a:711:G:N2	2.89	0.40
34:a:684:A:N3	44:k:39:PRO:HG2	2.37	0.40
34:a:1035:A:H2'	34:a:1036:G:H8	1.87	0.40
34:a:1106:G:O2'	34:a:1107:C:H5'	2.21	0.40
35:b:61:LEU:HD22	35:b:61:LEU:HA	1.92	0.40
35:b:128:GLU:HA	35:b:135:GLN:OE1	2.21	0.40
36:c:130:VAL:HG12	36:c:134:ILE:CD1	2.52	0.40
40:g:29:LYS:HD2	40:g:29:LYS:HA	1.88	0.40
46:m:82:MET:HG2	46:m:93:ARG:HG3	2.04	0.40
47:n:29:ARG:HH21	47:n:32:SER:HB2	1.86	0.40
50:q:26:GLN:NE2	50:q:37:LYS:HE3	2.36	0.40
56:y:21:GLY:CA	56:y:24:THR:OG1	2.69	0.40
56:y:121:PHE:CE1	56:y:158:LEU:HD21	2.56	0.40
56:y:302:PHE:O	56:y:303:ALA:CB	2.70	0.40
1:A:365:C:H2'	1:A:366:C:O4'	2.21	0.40
1:A:906:G:H5''	1:A:907:U:OP2	2.20	0.40
1:A:926:A:H2'	1:A:927:G:H8	1.87	0.40
1:A:1051:G:C6	1:A:1052:C:C4	3.10	0.40
1:A:1173:G:H2'	1:A:1173:G:OP2	2.22	0.40
1:A:1234:U:H2'	1:A:1235:G:O4'	2.22	0.40
1:A:1689:A:H62	1:A:1698:A:H2	1.68	0.40
1:A:1987:G:N3	1:A:1988:C:C6	2.90	0.40
1:A:2697:G:H2'	1:A:2698:U:O4'	2.21	0.40
1:A:2774:C:H2'	1:A:2775:A:O4'	2.22	0.40
3:D:160:GLY:HA3	3:D:199:ALA:HA	2.03	0.40
6:G:31:VAL:HA	6:G:32:PRO:HD2	1.88	0.40
16:T:54:ARG:HG2	16:T:54:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:U:8:VAL:CG2	17:U:11:ARG:HH21	2.34	0.40
18:V:25:LEU:HD22	18:V:26:ASP:N	2.30	0.40
19:W:95:ILE:HG23	19:W:95:ILE:HD12	1.87	0.40
24:1:76:ARG:H	24:1:76:ARG:HG3	1.72	0.40
34:a:428:G:OP2	37:d:10:ARG:NH1	2.53	0.40
34:a:502:G:H2'	34:a:503:C:O4'	2.21	0.40
34:a:522:C:C2'	34:a:523:A:H5'	2.51	0.40
34:a:553:A:H5''	45:l:24:VAL:HG11	2.03	0.40
34:a:602:A:H2'	34:a:603:U:O4'	2.21	0.40
34:a:641:U:HO2'	34:a:642:A:P	2.42	0.40
34:a:1015:A:H1'	34:a:1218:C:O2'	2.22	0.40
34:a:1071:C:OP1	38:e:27:ARG:NH2	2.55	0.40
34:a:1129:C:H4'	34:a:1130:A:H5'	2.03	0.40
34:a:1410:G:N2	34:a:1491:G:C4	2.89	0.40
34:a:1501:C:N3	34:a:1504:G:C6	2.90	0.40
34:a:1531:A:N3	34:a:1531:A:H5''	2.37	0.40
35:b:112:VAL:O	35:b:115:LEU:HB3	2.22	0.40
35:b:152:PHE:C	35:b:154:LEU:H	2.30	0.40
36:c:148:GLY:HA3	36:c:172:ARG:O	2.21	0.40
37:d:89:THR:O	37:d:90:GLY:C	2.64	0.40
39:f:18:GLN:HA	39:f:21:LEU:HB2	2.04	0.40
39:f:44:GLY:HA2	39:f:59:TYR:CE2	2.57	0.40
44:k:33:THR:HG22	44:k:39:PRO:N	2.37	0.40
44:k:86:GLY:O	44:k:91:ARG:HD3	2.21	0.40
46:m:56:LEU:HD23	46:m:56:LEU:HA	1.80	0.40
56:y:398:ASP:O	56:y:401:ARG:N	2.53	0.40
1:A:27:G:N2	1:A:512:G:H1'	2.36	0.40
1:A:45:C:H5''	1:A:215:G:H8	1.87	0.40
1:A:862:G:H2'	1:A:863:A:O4'	2.21	0.40
1:A:1022:G:C6	1:A:1141:U:C5	3.09	0.40
1:A:1421:G:O2'	1:A:1494:A:N6	2.54	0.40
1:A:1451:C:N4	1:A:1459:G:H1	2.15	0.40
1:A:1673:U:N3	1:A:1675:C:O4'	2.53	0.40
1:A:1792:G:C4	1:A:1793:C:C5	3.10	0.40
1:A:2083:G:H8	1:A:2083:G:O5'	2.03	0.40
1:A:2631:G:O2'	1:A:2810:A:N1	2.50	0.40
4:E:117:MET:O	4:E:119:ARG:N	2.50	0.40
9:K:21:PRO:HA	9:K:23:VAL:N	2.37	0.40
10:N:108:PRO:O	10:N:113:GLY:HA3	2.22	0.40
17:U:75:ASN:OD1	17:U:78:THR:OG1	2.26	0.40
22:Z:144:LEU:HD11	22:Z:150:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:9:2:LYS:HE2	32:9:31:LYS:O	2.22	0.40
34:a:189:G:C6	34:a:189(L):G:C6	3.10	0.40
34:a:923:A:H8	34:a:923:A:O5'	2.04	0.40
34:a:1121:U:H2'	34:a:1122:U:O4'	2.22	0.40
34:a:1278:U:H3'	34:a:1278:U:H6	1.87	0.40
34:a:1468:A:H5''	34:a:1469:G:OP2	2.22	0.40
35:b:19:HIS:CG	35:b:20:GLU:H	2.37	0.40
35:b:103:THR:HA	35:b:180:LEU:HD11	2.04	0.40
36:c:70:VAL:C	36:c:106:VAL:HG23	2.46	0.40
36:c:156:ARG:HD3	36:c:193:TYR:O	2.22	0.40
37:d:15:GLU:HG2	37:d:63:LYS:HA	2.02	0.40
39:f:68:PRO:HG2	39:f:71:ARG:HD2	2.04	0.40
39:f:69:GLU:O	39:f:72:VAL:HG12	2.22	0.40
56:y:435:LEU:HD13	56:y:452:TYR:CE1	2.55	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	
3	D	273/276 (99%)	233 (85%)	26 (10%)	14 (5%)	1	6
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	1	6
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	1	4
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	1	4
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	1	4
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0	0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	1	2
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	1	4
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1	2
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	2	11
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	4	17
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	0	1
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	16	44
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	1	5
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	0	1
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	0	1
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	0	1
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	0	1
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1	2
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	9	30
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	3
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	8	28
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	12
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0	0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	0	1
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	2	10
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	5	21
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	3	15
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	0	1
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	2	10
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	1	6
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	1	4
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	0	2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	4	17
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	8	28
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1	2
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	0	1
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	2	9
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	0	1
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	5
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	5	19
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	4	17
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	1	3
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	2	8
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	0	1
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	0	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	1	4
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	1	4

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	14	ARG
3	D	224	ALA
4	E	195	LEU
5	F	89	VAL
5	F	130	ALA
5	F	136	THR
5	F	168	ARG
5	F	169	ASN
6	G	28	VAL
6	G	47	LYS
6	G	115	ARG
6	G	150	ASP
7	H	80	SER
8	J	7	VAL
8	J	53	VAL
8	J	56	ASN
8	J	74	LEU
8	J	77	PRO
8	J	80	VAL
8	J	93	LEU
8	J	99	SER
8	J	100	ASN

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Mol	Chain	Res	Type
8	J	107	VAL
8	J	128	LEU
9	K	7	VAL
9	K	115	LEU
10	N	23	LEU
10	N	37	LYS
10	N	69	GLN
11	O	72	PRO
12	P	45	LEU
13	Q	59	ARG
13	Q	134	ARG
13	Q	135	ASP
16	T	55	ASN
17	U	86	ALA
19	W	25	ARG
19	W	36	LEU
19	W	57	ASN
20	X	18	TYR
20	X	19	ALA
20	X	77	LYS
21	Y	5	MET
21	Y	6	HIS
22	Z	161	VAL
22	Z	177	PRO
22	Z	179	ASP
22	Z	182	LYS
22	Z	184	ALA
24	1	76	ARG
24	1	77	ALA
26	3	13	ILE
27	4	51	ASP
30	7	46	VAL
35	b	9	GLU
35	b	12	GLU
35	b	17	PHE
35	b	23	ARG
35	b	77	ALA
35	b	165	VAL
37	d	150	GLU
37	d	179	GLU
37	d	200	GLU
38	e	72	GLN

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Mol	Chain	Res	Type
39	f	36	ARG
41	h	51	VAL
42	i	95	LYS
42	i	105	ASP
42	i	118	LYS
43	j	34	VAL
43	j	87	THR
44	k	122	LYS
46	m	7	VAL
46	m	8	GLU
47	n	3	ARG
47	n	41	ARG
48	o	19	PRO
49	p	67	THR
50	q	17	LYS
50	q	34	LYS
50	q	49	GLU
50	q	53	LEU
52	s	27	GLU
53	t	9	ASN
53	t	10	LEU
53	t	11	SER
53	t	46	GLU
53	t	47	GLY
53	t	100	ILE
56	y	-67	LYS
56	y	-59	GLU
56	y	9	ILE
56	y	63	ALA
56	y	89	PHE
56	y	138	ILE
56	y	153	GLU
56	y	213	PRO
56	y	244	VAL
56	y	280	ILE
56	y	281	THR
56	y	373	ALA
56	y	402	ILE
56	y	437	ASN
56	y	438	MET
56	y	487	GLY
56	y	555	ARG

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Mol	Chain	Res	Type
56	y	600	VAL
3	D	3	VAL
3	D	90	ALA
3	D	110	GLY
3	D	127	VAL
3	D	241	PRO
4	E	2	LYS
4	E	151	TYR
5	F	119	ARG
5	F	160	ASN
6	G	116	ASP
7	H	76	VAL
7	H	77	LYS
7	H	92	ILE
7	H	126	PRO
8	J	21	GLN
8	J	73	GLY
8	J	101	PRO
8	J	104	ILE
8	J	120	LYS
9	K	33	ASN
10	N	19	GLU
11	O	5	GLN
12	P	23	PRO
12	P	42	SER
12	P	132	LYS
13	Q	136	ALA
15	S	13	ARG
15	S	14	VAL
15	S	57	LYS
15	S	88	ASP
15	S	102	ALA
15	S	103	GLU
17	U	79	PHE
18	V	24	LYS
18	V	54	GLY
18	V	55	ALA
19	W	67	ASP
20	X	66	LEU
20	X	68	ARG
20	X	93	GLU
21	Y	70	SER

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Mol	Chain	Res	Type
21	Y	105	ALA
22	Z	154	ASP
22	Z	183	LEU
24	1	10	LYS
27	4	18	CYS
27	4	45	GLY
27	4	60	GLN
27	4	62	ARG
27	4	68	ARG
28	5	21	SER
28	5	35	GLU
29	6	33	LYS
35	b	8	LYS
35	b	24	TRP
35	b	131	PRO
35	b	204	ASN
35	b	227	GLY
35	b	232	PRO
36	c	22	TRP
36	c	130	VAL
37	d	5	ILE
37	d	10	ARG
37	d	151	LYS
38	e	68	GLU
38	e	85	GLY
38	e	148	VAL
38	e	149	GLU
39	f	70	ASP
40	g	7	ALA
41	h	54	ASP
42	i	42	ARG
42	i	54	ASP
42	i	88	TYR
42	i	126	SER
42	i	127	LYS
43	j	27	ALA
43	j	36	GLY
43	j	77	PRO
43	j	82	ILE
44	k	103	LEU
45	l	14	GLY
46	m	68	GLY

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Mol	Chain	Res	Type
46	m	85	GLY
49	p	46	PRO
50	q	3	LYS
50	q	54	GLY
51	r	36	ASN
52	s	14	HIS
52	s	30	LEU
52	s	71	LEU
53	t	65	LYS
53	t	99	LEU
56	y	13	SER
56	y	167	SER
56	y	215	LEU
56	y	286	PRO
56	y	301	VAL
56	y	446	LYS
56	y	486	PRO
3	D	219	PRO
4	E	52	LEU
4	E	162	ALA
5	F	165	ARG
5	F	206	ILE
6	G	43	LEU
6	G	46	ALA
6	G	55	LYS
7	H	34	GLU
7	H	65	HIS
7	H	174	GLY
8	J	23	SER
8	J	30	GLN
8	J	61	LEU
8	J	69	PRO
8	J	91	LYS
9	K	11	GLN
9	K	73	PRO
9	K	87	GLY
10	N	22	THR
13	Q	60	ARG
14	R	45	ARG
14	R	93	GLY
15	S	59	LYS
15	S	79	ALA

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Mol	Chain	Res	Type
17	U	54	LYS
17	U	98	LEU
18	V	45	THR
18	V	97	LYS
19	W	27	LYS
19	W	56	ALA
19	W	66	GLU
22	Z	93	ASP
22	Z	155	LEU
22	Z	158	PRO
27	4	55	ARG
29	6	34	LEU
35	b	20	GLU
35	b	36	ARG
35	b	76	GLN
36	c	79	ARG
37	d	26	CYS
37	d	172	PRO
37	d	191	ARG
39	f	5	GLU
39	f	62	TRP
39	f	64	GLN
39	f	71	ARG
42	i	70	LYS
42	i	99	LEU
45	l	121	GLY
45	l	125	PRO
46	m	3	ARG
46	m	49	THR
47	n	32	SER
51	r	32	ARG
56	y	86	HIS
56	y	90	THR
56	y	267	ALA
4	E	72	VAL
5	F	67	GLN
5	F	194	MET
8	J	84	GLU
9	K	16	LYS
11	O	29	ASN
12	P	97	PRO
12	P	122	PRO

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Mol	Chain	Res	Type
15	S	84	GLN
15	S	94	TYR
17	U	87	GLY
18	V	43	GLU
20	X	2	LYS
21	Y	2	ARG
21	Y	54	LYS
22	Z	160	GLY
26	3	22	ALA
27	4	43	TYR
27	4	46	GLN
28	5	24	ALA
28	5	37	LYS
35	b	30	ARG
35	b	35	GLU
35	b	122	PHE
35	b	153	ARG
36	c	99	VAL
36	c	100	ALA
38	e	9	LYS
38	e	73	ASN
39	f	51	PRO
40	g	80	VAL
43	j	78	ASN
45	l	19	ARG
46	m	40	ASN
52	s	29	ARG
53	t	66	ALA
56	y	-17	ARG
56	y	417	PRO
56	y	560	ALA
3	D	223	GLY
4	E	57	LYS
4	E	73	GLU
4	E	128	SER
5	F	22	ALA
6	G	109	VAL
6	G	177	GLY
8	J	85	ASP
8	J	90	ALA
8	J	124	ALA
10	N	2	LYS

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Mol	Chain	Res	Type
10	N	40	PRO
10	N	65	LYS
12	P	10	PRO
12	P	78	PRO
14	R	28	LEU
15	S	15	ARG
18	V	100	ARG
19	W	28	SER
19	W	51	LEU
19	W	59	VAL
21	Y	58	GLY
21	Y	69	ALA
22	Z	157	LEU
23	0	48	GLY
24	1	9	GLY
24	1	83	GLU
25	2	67	LYS
27	4	47	GLN
28	5	59	GLU
32	9	36	GLN
36	c	3	ASN
36	c	66	VAL
37	d	175	SER
39	f	96	PRO
40	g	50	ILE
43	j	83	GLU
44	k	100	ALA
46	m	67	GLU
46	m	101	GLN
48	o	79	ARG
52	s	12	ASP
56	y	-36	ARG
56	y	137	LYS
56	y	303	ALA
56	y	500	VAL
56	y	594	GLN
3	D	144	ALA
4	E	178	GLU
8	J	86	PRO
9	K	24	GLY
11	O	35	VAL
24	1	51	VAL

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Mol	Chain	Res	Type
27	4	41	PRO
38	e	39	GLY
43	j	37	PRO
51	r	60	ALA
52	s	76	PRO
56	y	448	VAL
6	G	149	VAL
9	K	23	VAL
12	P	47	ASP
21	Y	15	VAL
21	Y	27	VAL
36	c	108	ASN
56	y	-37	PRO
3	D	106	ILE
3	D	137	PRO
3	D	178	PRO
7	H	17	VAL
17	U	8	VAL
18	V	9	GLY
22	Z	27	VAL
44	k	105	VAL
46	m	38	GLY
20	X	94	GLY
21	Y	72	VAL
53	t	102	GLY
56	y	-48	VAL
7	H	4	ILE
8	J	68	LEU
8	J	129	PRO
9	K	21	PRO
18	V	79	VAL
35	b	159	PRO
45	l	24	VAL
52	s	42	PRO
3	D	74	GLY
22	Z	68	PRO
40	g	130	GLY
12	P	72	PRO
35	b	125	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
3	D	215/218 (99%)	164 (76%)	51 (24%)	1	2
4	E	164/166 (99%)	134 (82%)	30 (18%)	2	6
5	F	160/162 (99%)	128 (80%)	32 (20%)	1	4
6	G	143/156 (92%)	106 (74%)	37 (26%)	0	2
7	H	144/148 (97%)	111 (77%)	33 (23%)	1	3
9	K	104/111 (94%)	81 (78%)	23 (22%)	1	3
10	N	118/119 (99%)	90 (76%)	28 (24%)	1	2
11	O	100/100 (100%)	85 (85%)	15 (15%)	3	10
12	P	115/116 (99%)	93 (81%)	22 (19%)	1	5
13	Q	111/111 (100%)	92 (83%)	19 (17%)	2	7
14	R	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	S	87/88 (99%)	71 (82%)	16 (18%)	1	6
16	T	115/127 (91%)	94 (82%)	21 (18%)	2	6
17	U	93/94 (99%)	72 (77%)	21 (23%)	1	3
18	V	80/82 (98%)	62 (78%)	18 (22%)	1	3
19	W	90/92 (98%)	70 (78%)	20 (22%)	1	3
20	X	77/78 (99%)	63 (82%)	14 (18%)	2	6
21	Y	85/91 (93%)	68 (80%)	17 (20%)	1	4
22	Z	156/179 (87%)	118 (76%)	38 (24%)	1	2
23	0	59/67 (88%)	50 (85%)	9 (15%)	3	9
24	1	80/83 (96%)	60 (75%)	20 (25%)	0	2
25	2	65/67 (97%)	51 (78%)	14 (22%)	1	3
26	3	51/52 (98%)	39 (76%)	12 (24%)	1	3
27	4	60/63 (95%)	46 (77%)	14 (23%)	1	3
28	5	51/52 (98%)	40 (78%)	11 (22%)	1	3
29	6	51/52 (98%)	38 (74%)	13 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	7	42/42 (100%)	33 (79%)	9 (21%)	1	4
31	8	53/55 (96%)	46 (87%)	7 (13%)	4	13
32	9	34/34 (100%)	30 (88%)	4 (12%)	5	17
35	b	193/220 (88%)	142 (74%)	51 (26%)	0	2
36	c	142/188 (76%)	120 (84%)	22 (16%)	2	9
37	d	169/181 (93%)	126 (75%)	43 (25%)	0	2
38	e	113/123 (92%)	80 (71%)	33 (29%)	0	1
39	f	83/90 (92%)	65 (78%)	18 (22%)	1	3
40	g	118/127 (93%)	91 (77%)	27 (23%)	1	3
41	h	114/119 (96%)	90 (79%)	24 (21%)	1	4
42	i	90/99 (91%)	72 (80%)	18 (20%)	1	4
43	j	65/92 (71%)	46 (71%)	19 (29%)	0	1
44	k	82/99 (83%)	70 (85%)	12 (15%)	3	10
45	l	97/109 (89%)	82 (84%)	15 (16%)	2	9
46	m	89/101 (88%)	70 (79%)	19 (21%)	1	4
47	n	49/50 (98%)	32 (65%)	17 (35%)	0	0
48	o	78/80 (98%)	64 (82%)	14 (18%)	2	6
49	p	69/74 (93%)	55 (80%)	14 (20%)	1	4
50	q	94/97 (97%)	73 (78%)	21 (22%)	1	3
51	r	59/77 (77%)	44 (75%)	15 (25%)	0	2
52	s	68/80 (85%)	50 (74%)	18 (26%)	0	2
53	t	69/82 (84%)	57 (83%)	12 (17%)	2	7
54	u	18/22 (82%)	15 (83%)	3 (17%)	2	7
56	y	289/560 (52%)	189 (65%)	100 (35%)	0	0
All	All	4952/5576 (89%)	3847 (78%)	1105 (22%)	1	3

All (1105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3	VAL
3	D	13	ARG
3	D	20	ASP
3	D	22	SER
3	D	25	THR

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Mol	Chain	Res	Type
3	D	27	THR
3	D	32	SER
3	D	34	VAL
3	D	37	LEU
3	D	38	LYS
3	D	39	LYS
3	D	50	THR
3	D	51	VAL
3	D	61	LEU
3	D	85	ASP
3	D	87	ASN
3	D	94	LEU
3	D	98	VAL
3	D	102	LYS
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	109	ASP
3	D	111	LEU
3	D	117	VAL
3	D	118	VAL
3	D	122	ASP
3	D	125	ILE
3	D	138	VAL
3	D	148	GLU
3	D	150	LYS
3	D	157	ARG
3	D	161	THR
3	D	164	GLN
3	D	165	ILE
3	D	169	GLU
3	D	171	ASP
3	D	173	VAL
3	D	183	ARG
3	D	200	ASP
3	D	205	VAL
3	D	212	SER
3	D	215	LEU
3	D	217	ARG
3	D	221	VAL
3	D	222	ARG
3	D	229	VAL

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Mol	Chain	Res	Type
3	D	257	LEU
3	D	260	ARG
3	D	267	SER
3	D	274	ARG
4	E	2	LYS
4	E	4	ILE
4	E	9	VAL
4	E	13	ARG
4	E	21	VAL
4	E	23	VAL
4	E	33	VAL
4	E	48	GLN
4	E	49	LEU
4	E	72	VAL
4	E	73	GLU
4	E	77	ILE
4	E	82	ARG
4	E	87	GLU
4	E	93	VAL
4	E	119	ARG
4	E	134	ILE
4	E	144	ARG
4	E	146	THR
4	E	149	ARG
4	E	152	LYS
4	E	154	LYS
4	E	165	VAL
4	E	170	LEU
4	E	173	VAL
4	E	179	GLU
4	E	181	LEU
4	E	184	VAL
4	E	195	LEU
4	E	196	VAL
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU
5	F	33	LEU
5	F	35	GLU
5	F	38	ARG
5	F	44	ARG
5	F	51	THR

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Mol	Chain	Res	Type
5	F	53	THR
5	F	64	ILE
5	F	84	VAL
5	F	104	LYS
5	F	106	ARG
5	F	112	MET
5	F	132	VAL
5	F	148	LEU
5	F	152	GLU
5	F	157	VAL
5	F	162	LEU
5	F	164	ARG
5	F	165	ARG
5	F	169	ASN
5	F	170	LEU
5	F	171	PRO
5	F	175	THR
5	F	183	VAL
5	F	192	LEU
5	F	196	LEU
5	F	197	ASP
5	F	200	GLU
5	F	205	ARG
5	F	206	ILE
6	G	5	VAL
6	G	7	LEU
6	G	9	ARG
6	G	19	LEU
6	G	22	ARG
6	G	28	VAL
6	G	30	GLU
6	G	31	VAL
6	G	34	LEU
6	G	43	LEU
6	G	45	GLU
6	G	58	GLN
6	G	62	LEU
6	G	80	PHE
6	G	81	LYS
6	G	82	LEU
6	G	90	LEU
6	G	91	ARG

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Mol	Chain	Res	Type
6	G	99	MET
6	G	101	ILE
6	G	109	VAL
6	G	120	LEU
6	G	123	ASN
6	G	124	SER
6	G	135	LEU
6	G	136	ARG
6	G	139	LEU
6	G	143	GLU
6	G	148	MET
6	G	150	ASP
6	G	153	ARG
6	G	159	VAL
6	G	161	THR
6	G	164	GLU
6	G	165	THR
6	G	170	ARG
6	G	173	LEU
7	H	3	ARG
7	H	4	ILE
7	H	6	ARG
7	H	13	LYS
7	H	15	VAL
7	H	16	SER
7	H	17	VAL
7	H	23	ARG
7	H	24	VAL
7	H	27	LYS
7	H	32	GLU
7	H	37	VAL
7	H	40	GLU
7	H	41	MET
7	H	43	VAL
7	H	45	VAL
7	H	46	GLU
7	H	47	GLU
7	H	49	VAL
7	H	50	VAL
7	H	62	LYS
7	H	69	ARG
7	H	72	ILE

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Mol	Chain	Res	Type
7	H	79	VAL
7	H	86	GLU
7	H	88	LEU
7	H	95	ARG
7	H	98	LEU
7	H	106	THR
7	H	107	VAL
7	H	127	GLU
7	H	164	TYR
7	H	175	LYS
9	K	2	LYS
9	K	4	VAL
9	K	11	GLN
9	K	23	VAL
9	K	30	HIS
9	K	34	ILE
9	K	35	MET
9	K	38	VAL
9	K	57	ILE
9	K	59	ILE
9	K	62	ASP
9	K	65	PHE
9	K	75	SER
9	K	79	ARG
9	K	86	LYS
9	K	95	LYS
9	K	96	VAL
9	K	115	LEU
9	K	116	ASN
9	K	117	THR
9	K	119	ASP
9	K	136	VAL
9	K	138	VAL
10	N	1	MET
10	N	2	LYS
10	N	17	ASP
10	N	23	LEU
10	N	28	THR
10	N	30	ILE
10	N	34	LEU
10	N	38	HIS
10	N	39	ARG

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Mol	Chain	Res	Type
10	N	48	MET
10	N	67	LEU
10	N	68	GLU
10	N	70	LYS
10	N	87	LEU
10	N	90	MET
10	N	97	ARG
10	N	99	LEU
10	N	106	MET
10	N	109	LYS
10	N	115	ARG
10	N	120	LEU
10	N	122	VAL
10	N	127	ASP
10	N	131	GLN
10	N	133	GLN
10	N	137	LYS
10	N	138	LEU
10	N	140	VAL
11	O	3	GLN
11	O	8	LEU
11	O	10	VAL
11	O	14	THR
11	O	23	ARG
11	O	24	VAL
11	O	57	VAL
11	O	61	VAL
11	O	63	VAL
11	O	66	LYS
11	O	69	ILE
11	O	91	LEU
11	O	108	GLU
11	O	114	ILE
11	O	115	VAL
12	P	2	LYS
12	P	16	ARG
12	P	19	VAL
12	P	27	HIS
12	P	30	THR
12	P	40	SER
12	P	50	ARG
12	P	57	THR

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Mol	Chain	Res	Type
12	P	58	THR
12	P	59	LEU
12	P	65	ARG
12	P	70	GLN
12	P	71	VAL
12	P	74	GLU
12	P	81	GLN
12	P	96	THR
12	P	105	LEU
12	P	106	LEU
12	P	115	LEU
12	P	132	LYS
12	P	135	LEU
12	P	148	LEU
13	Q	7	MET
13	Q	21	THR
13	Q	31	ASP
13	Q	42	ILE
13	Q	45	GLN
13	Q	52	VAL
13	Q	56	ARG
13	Q	63	LYS
13	Q	66	ILE
13	Q	72	LYS
13	Q	75	THR
13	Q	82	ARG
13	Q	89	ASN
13	Q	109	VAL
13	Q	112	GLU
13	Q	129	THR
13	Q	131	ILE
13	Q	135	ASP
13	Q	138	ASP
14	R	15	SER
14	R	18	LEU
14	R	28	LEU
14	R	29	LEU
14	R	30	THR
14	R	36	THR
14	R	38	VAL
14	R	40	LYS
14	R	44	LEU

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Mol	Chain	Res	Type
14	R	51	LEU
14	R	60	LEU
14	R	65	LEU
14	R	66	VAL
14	R	67	LEU
14	R	75	LEU
14	R	77	ARG
14	R	79	LEU
14	R	91	GLN
14	R	100	LEU
14	R	113	LEU
14	R	114	VAL
14	R	118	GLU
15	S	8	GLU
15	S	14	VAL
15	S	15	ARG
15	S	19	LYS
15	S	20	ARG
15	S	28	VAL
15	S	36	TYR
15	S	41	ASP
15	S	43	GLU
15	S	48	LEU
15	S	49	VAL
15	S	52	SER
15	S	53	SER
15	S	63	THR
15	S	80	LEU
15	S	85	VAL
16	T	7	ILE
16	T	9	LEU
16	T	17	THR
16	T	18	ASP
16	T	23	ARG
16	T	31	SER
16	T	34	VAL
16	T	40	THR
16	T	44	ASP
16	T	49	VAL
16	T	54	ARG
16	T	57	PHE
16	T	58	ASN

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Mol	Chain	Res	Type
16	T	59	THR
16	T	75	ILE
16	T	78	LEU
16	T	93	ARG
16	T	96	ARG
16	T	118	ARG
16	T	123	GLN
16	T	124	ASP
17	U	8	VAL
17	U	11	ARG
17	U	17	ILE
17	U	18	LEU
17	U	20	LEU
17	U	33	ARG
17	U	34	LYS
17	U	36	ARG
17	U	55	ARG
17	U	56	ASP
17	U	63	VAL
17	U	64	ARG
17	U	71	GLN
17	U	74	LEU
17	U	78	THR
17	U	85	LYS
17	U	92	ARG
17	U	95	LEU
17	U	101	ARG
17	U	104	GLN
17	U	112	ARG
18	V	6	LYS
18	V	7	THR
18	V	13	ARG
18	V	14	VAL
18	V	18	LEU
18	V	20	LEU
18	V	25	LEU
18	V	33	VAL
18	V	35	LEU
18	V	38	LEU
18	V	46	VAL
18	V	51	VAL
18	V	70	ILE

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Mol	Chain	Res	Type
18	V	71	LEU
18	V	72	VAL
18	V	73	SER
18	V	95	LEU
18	V	99	ILE
19	W	8	ARG
19	W	10	VAL
19	W	11	ARG
19	W	16	LYS
19	W	19	LEU
19	W	20	VAL
19	W	27	LYS
19	W	37	ARG
19	W	39	THR
19	W	47	VAL
19	W	51	LEU
19	W	52	GLU
19	W	57	ASN
19	W	65	LEU
19	W	67	ASP
19	W	86	LEU
19	W	92	ARG
19	W	100	THR
19	W	107	LEU
19	W	111	HIS
20	X	2	LYS
20	X	9	LEU
20	X	23	GLU
20	X	27	THR
20	X	43	VAL
20	X	49	VAL
20	X	51	VAL
20	X	56	THR
20	X	57	LEU
20	X	68	ARG
20	X	72	LYS
20	X	76	ARG
20	X	80	ILE
20	X	92	LEU
21	Y	7	VAL
21	Y	9	LYS
21	Y	21	LYS

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Mol	Chain	Res	Type
21	Y	28	LYS
21	Y	30	VAL
21	Y	31	LEU
21	Y	38	ILE
21	Y	43	ASN
21	Y	61	ILE
21	Y	62	GLU
21	Y	72	VAL
21	Y	79	CYS
21	Y	84	ARG
21	Y	85	VAL
21	Y	90	LEU
21	Y	91	GLU
21	Y	98	VAL
22	Z	11	GLU
22	Z	19	ARG
22	Z	24	LEU
22	Z	27	VAL
22	Z	33	LEU
22	Z	37	VAL
22	Z	39	VAL
22	Z	41	LEU
22	Z	56	VAL
22	Z	58	VAL
22	Z	61	LEU
22	Z	67	LEU
22	Z	70	LEU
22	Z	72	ARG
22	Z	76	LEU
22	Z	80	ARG
22	Z	81	ARG
22	Z	86	VAL
22	Z	96	VAL
22	Z	100	VAL
22	Z	102	LEU
22	Z	107	THR
22	Z	111	VAL
22	Z	119	GLU
22	Z	122	ARG
22	Z	124	ILE
22	Z	132	ASN
22	Z	136	PHE

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Mol	Chain	Res	Type
22	Z	139	VAL
22	Z	141	VAL
22	Z	149	SER
22	Z	150	LEU
22	Z	156	LYS
22	Z	161	VAL
22	Z	163	LEU
22	Z	170	THR
22	Z	179	ASP
22	Z	185	GLU
23	0	11	ARG
23	0	19	LYS
23	0	25	ARG
23	0	32	ARG
23	0	41	ARG
23	0	44	ARG
23	0	62	LEU
23	0	63	VAL
23	0	66	VAL
24	1	2	SER
24	1	4	VAL
24	1	10	LYS
24	1	14	VAL
24	1	19	GLN
24	1	20	ARG
24	1	21	ARG
24	1	38	SER
24	1	40	ARG
24	1	46	LEU
24	1	57	GLU
24	1	59	THR
24	1	62	VAL
24	1	69	LYS
24	1	75	GLU
24	1	80	LEU
24	1	85	LEU
24	1	89	GLU
24	1	94	LEU
24	1	98	LEU
25	2	3	LEU
25	2	4	SER
25	2	16	LEU

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Mol	Chain	Res	Type
25	2	25	VAL
25	2	32	LEU
25	2	34	GLU
25	2	45	SER
25	2	47	ASN
25	2	49	LYS
25	2	51	ARG
25	2	52	ASP
25	2	62	THR
25	2	65	ASN
25	2	70	GLN
26	3	4	LEU
26	3	9	VAL
26	3	30	ARG
26	3	33	GLN
26	3	37	LEU
26	3	40	THR
26	3	49	LYS
26	3	53	LEU
26	3	54	VAL
26	3	56	VAL
26	3	57	GLU
26	3	59	VAL
27	4	8	LYS
27	4	20	ASN
27	4	22	ILE
27	4	23	GLU
27	4	26	SER
27	4	43	TYR
27	4	49	PHE
27	4	50	VAL
27	4	58	ARG
27	4	59	PHE
27	4	63	TYR
27	4	65	ASP
27	4	68	ARG
27	4	69	LYS
28	5	6	VAL
28	5	8	LYS
28	5	11	THR
28	5	25	LEU
28	5	26	THR

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Mol	Chain	Res	Type
28	5	29	THR
28	5	35	GLU
28	5	37	LYS
28	5	40	LYS
28	5	48	GLU
28	5	57	VAL
29	6	3	SER
29	6	4	GLU
29	6	6	ARG
29	6	13	CYS
29	6	23	THR
29	6	27	LYS
29	6	28	ARG
29	6	34	LEU
29	6	36	LEU
29	6	38	LYS
29	6	46	HIS
29	6	48	VAL
29	6	52	VAL
30	7	1	MET
30	7	9	ARG
30	7	14	LYS
30	7	23	ARG
30	7	24	THR
30	7	41	ARG
30	7	43	THR
30	7	46	VAL
30	7	49	ARG
31	8	14	VAL
31	8	23	VAL
31	8	32	LEU
31	8	41	ILE
31	8	42	ARG
31	8	52	LYS
31	8	56	GLU
32	9	9	ARG
32	9	17	ILE
32	9	22	ARG
32	9	26	ILE
35	b	8	LYS
35	b	9	GLU
35	b	10	LEU

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Mol	Chain	Res	Type
35	b	11	LEU
35	b	15	VAL
35	b	16	HIS
35	b	17	PHE
35	b	20	GLU
35	b	21	ARG
35	b	24	TRP
35	b	35	GLU
35	b	40	HIS
35	b	41	ILE
35	b	44	LEU
35	b	51	LEU
35	b	53	ARG
35	b	61	LEU
35	b	73	THR
35	b	79	ASP
35	b	80	ILE
35	b	87	ARG
35	b	94	ASN
35	b	96	ARG
35	b	97	TRP
35	b	107	THR
35	b	109	SER
35	b	119	GLU
35	b	127	ILE
35	b	136	VAL
35	b	139	LYS
35	b	154	LEU
35	b	155	LEU
35	b	156	LYS
35	b	168	THR
35	b	169	LYS
35	b	172	ILE
35	b	175	ARG
35	b	185	ILE
35	b	187	LEU
35	b	189	ASP
35	b	190	THR
35	b	195	ASP
35	b	196	LEU
35	b	200	ILE
35	b	206	ASP

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Mol	Chain	Res	Type
35	b	208	ILE
35	b	213	LEU
35	b	217	ARG
35	b	221	LEU
35	b	223	ILE
35	b	229	VAL
36	c	3	ASN
36	c	12	LEU
36	c	15	THR
36	c	37	GLN
36	c	49	SER
36	c	52	LEU
36	c	70	VAL
36	c	91	LEU
36	c	97	LYS
36	c	104	GLN
36	c	115	LEU
36	c	132	ARG
36	c	134	ILE
36	c	138	VAL
36	c	150	LYS
36	c	152	ILE
36	c	153	VAL
36	c	165	THR
36	c	188	LEU
36	c	191	THR
36	c	192	THR
36	c	195	VAL
37	d	3	ARG
37	d	5	ILE
37	d	8	VAL
37	d	13	ARG
37	d	19	LEU
37	d	21	LEU
37	d	22	LYS
37	d	31	CYS
37	d	33	MET
37	d	52	SER
37	d	53	ASP
37	d	57	ARG
37	d	58	LEU
37	d	59	ARG

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Mol	Chain	Res	Type
37	d	66	ARG
37	d	67	ILE
37	d	70	ILE
37	d	76	ARG
37	d	85	LYS
37	d	86	LYS
37	d	91	SER
37	d	97	LEU
37	d	107	ARG
37	d	108	LEU
37	d	112	VAL
37	d	113	SER
37	d	114	ARG
37	d	135	LEU
37	d	139	ARG
37	d	141	ARG
37	d	148	VAL
37	d	150	GLU
37	d	158	ILE
37	d	162	LEU
37	d	163	GLU
37	d	168	ARG
37	d	170	VAL
37	d	178	VAL
37	d	186	LEU
37	d	188	LEU
37	d	190	ASP
37	d	196	LEU
37	d	201	GLN
38	e	8	GLU
38	e	14	ARG
38	e	20	GLN
38	e	31	LEU
38	e	38	GLN
38	e	41	VAL
38	e	47	LYS
38	e	51	VAL
38	e	53	LEU
38	e	67	VAL
38	e	71	LEU
38	e	75	THR
38	e	79	GLU

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Mol	Chain	Res	Type
38	e	80	ILE
38	e	81	GLU
38	e	82	VAL
38	e	87	SER
38	e	89	ILE
38	e	91	LEU
38	e	92	LYS
38	e	98	THR
38	e	107	ARG
38	e	116	THR
38	e	121	LYS
38	e	123	LEU
38	e	126	ARG
38	e	129	ILE
38	e	135	THR
38	e	143	ARG
38	e	144	THR
38	e	147	ASP
38	e	151	LEU
38	e	152	ARG
39	f	9	VAL
39	f	10	LEU
39	f	15	ASP
39	f	16	GLN
39	f	25	ILE
39	f	36	ARG
39	f	43	LEU
39	f	65	VAL
39	f	69	GLU
39	f	72	VAL
39	f	73	ASN
39	f	74	ASP
39	f	75	LEU
39	f	79	LEU
39	f	85	VAL
39	f	86	ARG
39	f	98	LEU
39	f	100	ASN
40	g	4	ARG
40	g	8	GLU
40	g	12	LEU
40	g	16	LEU

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Mol	Chain	Res	Type
40	g	21	VAL
40	g	22	LEU
40	g	24	THR
40	g	32	ARG
40	g	41	ARG
40	g	42	ILE
40	g	56	GLN
40	g	57	GLU
40	g	70	LYS
40	g	75	VAL
40	g	90	GLU
40	g	92	SER
40	g	94	ARG
40	g	97	GLN
40	g	101	LEU
40	g	104	LEU
40	g	113	GLU
40	g	114	ARG
40	g	115	ARG
40	g	126	ASP
40	g	131	LYS
40	g	138	LYS
40	g	144	MET
41	h	2	LEU
41	h	3	THR
41	h	6	ILE
41	h	10	LEU
41	h	19	VAL
41	h	26	VAL
41	h	54	ASP
41	h	56	LYS
41	h	59	LEU
41	h	60	ARG
41	h	63	LEU
41	h	68	ARG
41	h	75	ARG
41	h	78	GLN
41	h	84	ARG
41	h	87	SER
41	h	88	LYS
41	h	91	ARG
41	h	100	ILE

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Mol	Chain	Res	Type
41	h	104	ARG
41	h	111	ILE
41	h	120	THR
41	h	122	ARG
41	h	137	VAL
42	i	14	VAL
42	i	23	ASN
42	i	25	LYS
42	i	26	VAL
42	i	27	THR
42	i	41	VAL
42	i	54	ASP
42	i	56	LEU
42	i	64	THR
42	i	66	ARG
42	i	81	ILE
42	i	83	ARG
42	i	97	LYS
42	i	99	LEU
42	i	108	VAL
42	i	109	VAL
42	i	120	ARG
42	i	128	ARG
43	j	13	HIS
43	j	16	LEU
43	j	19	SER
43	j	21	GLN
43	j	34	VAL
43	j	35	SER
43	j	38	ILE
43	j	44	VAL
43	j	46	ARG
43	j	65	LEU
43	j	67	THR
43	j	70	ARG
43	j	71	LEU
43	j	72	VAL
43	j	89	ASP
43	j	92	THR
43	j	96	ILE
43	j	98	ILE
43	j	100	THR

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Mol	Chain	Res	Type
44	k	14	VAL
44	k	16	SER
44	k	51	LYS
44	k	62	GLN
44	k	82	VAL
44	k	83	ILE
44	k	105	VAL
44	k	109	VAL
44	k	110	ASP
44	k	114	VAL
44	k	119	CYS
44	k	126	ARG
45	l	6	THR
45	l	24	VAL
45	l	27	LEU
45	l	33	ARG
45	l	41	ARG
45	l	44	THR
45	l	52	LEU
45	l	54	LYS
45	l	55	VAL
45	l	57	LYS
45	l	66	VAL
45	l	67	THR
45	l	84	LEU
45	l	97	ARG
45	l	100	ILE
46	m	3	ARG
46	m	4	ILE
46	m	11	ARG
46	m	15	VAL
46	m	25	ILE
46	m	48	LEU
46	m	49	THR
46	m	54	VAL
46	m	56	LEU
46	m	70	LEU
46	m	73	GLU
46	m	78	ILE
46	m	80	ARG
46	m	82	MET
46	m	86	CYS

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Mol	Chain	Res	Type
46	m	110	ARG
46	m	114	ARG
46	m	115	LYS
46	m	120	LYS
47	n	3	ARG
47	n	6	LEU
47	n	7	ILE
47	n	9	LYS
47	n	13	THR
47	n	15	LYS
47	n	16	PHE
47	n	17	LYS
47	n	18	VAL
47	n	22	THR
47	n	29	ARG
47	n	31	ARG
47	n	32	SER
47	n	33	VAL
47	n	41	ARG
47	n	44	LEU
47	n	46	GLU
48	o	17	ARG
48	o	26	GLU
48	o	35	ARG
48	o	38	ARG
48	o	39	LEU
48	o	42	HIS
48	o	56	LEU
48	o	66	LEU
48	o	71	GLN
48	o	77	ARG
48	o	82	ILE
48	o	83	GLU
48	o	84	LYS
48	o	87	ILE
49	p	2	VAL
49	p	3	LYS
49	p	8	ARG
49	p	19	ILE
49	p	20	VAL
49	p	27	LYS
49	p	28	ARG

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Mol	Chain	Res	Type
49	p	31	LYS
49	p	40	ASP
49	p	45	THR
49	p	50	LYS
49	p	60	LEU
49	p	61	SER
49	p	67	THR
50	q	9	VAL
50	q	14	LYS
50	q	15	MET
50	q	16	GLN
50	q	25	ARG
50	q	34	LYS
50	q	35	VAL
50	q	36	ILE
50	q	49	GLU
50	q	57	VAL
50	q	59	ILE
50	q	60	ILE
50	q	63	ARG
50	q	65	ILE
50	q	68	ARG
50	q	72	ARG
50	q	74	LEU
50	q	78	GLU
50	q	86	GLU
50	q	90	ILE
50	q	96	GLU
51	r	26	LEU
51	r	31	LEU
51	r	32	ARG
51	r	33	ASP
51	r	39	VAL
51	r	46	GLU
51	r	49	LYS
51	r	55	ARG
51	r	58	LEU
51	r	68	LYS
51	r	70	ILE
51	r	75	ILE
51	r	76	LEU
51	r	84	LYS

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Mol	Chain	Res	Type
51	r	85	LEU
52	s	4	SER
52	s	6	LYS
52	s	12	ASP
52	s	22	LEU
52	s	27	GLU
52	s	28	LYS
52	s	31	ILE
52	s	32	LYS
52	s	37	ARG
52	s	38	SER
52	s	39	THR
52	s	41	VAL
52	s	48	THR
52	s	56	GLN
52	s	63	THR
52	s	65	ASN
52	s	76	PRO
52	s	79	THR
53	t	8	ARG
53	t	10	LEU
53	t	19	SER
53	t	50	GLU
53	t	56	MET
53	t	62	LEU
53	t	80	ARG
53	t	84	LEU
53	t	89	ARG
53	t	92	LEU
53	t	93	GLU
53	t	100	ILE
54	u	12	LYS
54	u	18	TYR
54	u	24	ARG
56	y	-68	MET
56	y	-67	LYS
56	y	-64	LEU
56	y	-63	LEU
56	y	-62	GLU
56	y	-57	LEU
56	y	-54	VAL
56	y	-51	VAL

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Mol	Chain	Res	Type
56	y	-50	VAL
56	y	-36	ARG
56	y	-32	VAL
56	y	-29	THR
56	y	-28	GLU
56	y	-25	LEU
56	y	-18	ILE
56	y	-11	LEU
56	y	-8	ARG
56	y	-7	LYS
56	y	0	LYS
56	y	4	GLU
56	y	7	SER
56	y	12	PHE
56	y	28	ARG
56	y	34	HIS
56	y	68	TYR
56	y	75	GLU
56	y	81	ILE
56	y	83	THR
56	y	103	VAL
56	y	105	LEU
56	y	108	ASP
56	y	114	GLU
56	y	117	THR
56	y	127	HIS
56	y	129	HIS
56	y	142	ASN
56	y	154	GLU
56	y	167	SER
56	y	170	THR
56	y	182	VAL
56	y	183	GLN
56	y	193	GLU
56	y	211	VAL
56	y	215	LEU
56	y	219	GLU
56	y	221	ARG
56	y	223	ARG
56	y	228	ILE
56	y	230	ILE
56	y	250	LEU

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Mol	Chain	Res	Type
56	y	265	VAL
56	y	292	PRO
56	y	312	ASP
56	y	335	GLU
56	y	338	THR
56	y	340	LEU
56	y	351	LEU
56	y	358	GLN
56	y	359	GLU
56	y	360	ARG
56	y	361	LEU
56	y	363	ARG
56	y	369	LEU
56	y	375	SER
56	y	377	VAL
56	y	392	ASN
56	y	412	LEU
56	y	413	THR
56	y	423	SER
56	y	424	LEU
56	y	429	GLN
56	y	434	ARG
56	y	436	VAL
56	y	440	TYR
56	y	461	TYR
56	y	462	ASP
56	y	469	SER
56	y	479	TYR
56	y	493	ASN
56	y	505	THR
56	y	506	PHE
56	y	507	ILE
56	y	509	HIS
56	y	512	LYS
56	y	531	GLN
56	y	532	LEU
56	y	533	PHE
56	y	534	GLU
56	y	544	LYS
56	y	545	ILE
56	y	548	ARG
56	y	550	THR

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Mol	Chain	Res	Type
56	y	551	VAL
56	y	557	ASP
56	y	568	THR
56	y	570	LYS
56	y	584	LEU
56	y	587	ILE
56	y	592	VAL
56	y	602	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	164	GLN
3	D	166	GLN
3	D	203	ASN
3	D	220	HIS
3	D	253	GLN
4	E	85	ASN
4	E	192	ASN
5	F	69	HIS
5	F	169	ASN
6	G	41	GLN
6	G	58	GLN
7	H	65	HIS
9	K	29	GLN
9	K	30	HIS
9	K	42	ASN
9	K	89	HIS
10	N	8	GLN
11	O	3	GLN
11	O	29	ASN
12	P	128	HIS
13	Q	13	GLN
13	Q	45	GLN
13	Q	57	HIS
13	Q	123	HIS
14	R	50	HIS
14	R	91	GLN
15	S	34	HIS
16	T	58	ASN
16	T	84	GLN
17	U	72	HIS

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Mol	Chain	Res	Type
18	V	80	GLN
20	X	31	HIS
22	Z	34	ASN
22	Z	50	GLN
22	Z	73	GLN
22	Z	132	ASN
23	0	17	GLN
23	0	40	GLN
24	1	56	GLN
25	2	9	GLN
25	2	47	ASN
25	2	65	ASN
26	3	19	GLN
26	3	32	GLN
27	4	20	ASN
27	4	40	HIS
28	5	22	HIS
29	6	29	ASN
31	8	35	GLN
32	9	29	ASN
32	9	36	GLN
35	b	19	HIS
35	b	45	GLN
35	b	94	ASN
36	c	102	ASN
36	c	104	GLN
36	c	110	ASN
36	c	136	GLN
36	c	162	GLN
36	c	181	ASN
37	d	42	GLN
37	d	45	GLN
37	d	77	ASN
37	d	123	HIS
38	e	20	GLN
38	e	38	GLN
38	e	73	ASN
38	e	141	GLN
39	f	73	ASN
39	f	94	GLN
39	f	100	ASN
40	g	28	ASN

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Mol	Chain	Res	Type
40	g	64	GLN
40	g	86	GLN
41	h	78	GLN
41	h	82	HIS
42	i	89	ASN
42	i	124	GLN
43	j	56	HIS
44	k	38	ASN
44	k	62	GLN
45	l	99	HIS
46	m	12	ASN
46	m	92	HIS
48	o	28	GLN
48	o	71	GLN
49	p	16	HIS
49	p	76	GLN
50	q	26	GLN
52	s	14	HIS
52	s	47	HIS
52	s	56	GLN
52	s	65	ASN
52	s	83	HIS
53	t	16	HIS
53	t	75	ASN
56	y	17	HIS
56	y	20	HIS
56	y	127	HIS
56	y	142	ASN
56	y	183	GLN
56	y	426	GLN
56	y	577	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	643 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0
33	w	75/76 (98%)	23 (30%)	0
33	x	72/76 (94%)	38 (52%)	0
34	a	1493/1521 (98%)	311 (20%)	0
55	v	6/18 (33%)	1 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4630/4728 (97%)	1034 (22%)	38 (0%)

All (1034) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	15	G
1	A	22	C
1	A	23	G
1	A	28	A
1	A	35	G
1	A	41	C
1	A	45	C
1	A	49	A
1	A	51	G
1	A	54	G
1	A	55	G
1	A	61	G
1	A	64	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	81	G
1	A	84	A
1	A	90	U
1	A	92	A
1	A	95	G
1	A	102	G
1	A	110	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	123	G
1	A	125	G
1	A	131	G
1	A	135	G
1	A	141	A
1	A	148	C
1	A	154(A)	C
1	A	181	A
1	A	182	A
1	A	196	A

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Mol	Chain	Res	Type
1	A	197	A
1	A	200	U
1	A	205	G
1	A	206	U
1	A	212	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	227	A
1	A	228	A
1	A	229	A
1	A	230	U
1	A	233	A
1	A	248	G
1	A	250	G
1	A	252	G
1	A	264	C
1	A	265	A
1	A	266	G
1	A	267	C
1	A	271(F)	C
1	A	271(H)	G
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	271(R)	G
1	A	271(Y)	U
1	A	272(A)	U
1	A	272(B)	G
1	A	272(G)	C
1	A	272(H)	C
1	A	274	G
1	A	279	C
1	A	294	A
1	A	296	C
1	A	299	A
1	A	310	A
1	A	311	A

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Mol	Chain	Res	Type
1	A	324	A
1	A	329	G
1	A	330	A
1	A	345	A
1	A	352	G
1	A	353	G
1	A	362	U
1	A	363	G
1	A	363(E)	U
1	A	366	C
1	A	384	U
1	A	385	C
1	A	386	G
1	A	396	G
1	A	404	C
1	A	405	U
1	A	406	G
1	A	407	G
1	A	408	G
1	A	411	G
1	A	420	C
1	A	423	A
1	A	434	U
1	A	435	C
1	A	444	C
1	A	448	U
1	A	451	C
1	A	455	C
1	A	457	A
1	A	470	A
1	A	471	A
1	A	472	A
1	A	481	G
1	A	491	G
1	A	504	U
1	A	505	A
1	A	508	G
1	A	509	C
1	A	530	G
1	A	531	C
1	A	532	A
1	A	536	A

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Mol	Chain	Res	Type
1	A	545	G
1	A	549	G
1	A	556	G
1	A	563	G
1	A	572	A
1	A	573	G
1	A	575	A
1	A	584	C
1	A	594	U
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(A)	U
1	A	614(B)	G
1	A	615	G
1	A	627	A
1	A	628	G
1	A	631	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	652(B)	A
1	A	652(E)	G
1	A	652(T)	C
1	A	652(U)	G
1	A	652(V)	C
1	A	654	A
1	A	668	G
1	A	669	G
1	A	670	A
1	A	684	G
1	A	686	G
1	A	694	U
1	A	695	G
1	A	717	G
1	A	730	C
1	A	738	G
1	A	746	A
1	A	747	U
1	A	752	A
1	A	753	C
1	A	764	A

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Mol	Chain	Res	Type
1	A	774	A
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	794	G
1	A	800	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	829	A
1	A	830	G
1	A	832	G
1	A	842	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	870	A
1	A	875	G
1	A	881	G
1	A	886	C
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	906	G
1	A	907	U
1	A	910	A
1	A	911	A
1	A	917	A
1	A	931	G
1	A	932	G
1	A	936	C
1	A	941	A

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Mol	Chain	Res	Type
1	A	945	A
1	A	946	G
1	A	953	A
1	A	957	A
1	A	959	A
1	A	961	C
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	976	C
1	A	982	C
1	A	983	A
1	A	996	A
1	A	1005	C
1	A	1008	C
1	A	1012	U
1	A	1013	C
1	A	1015	G
1	A	1017	G
1	A	1022	G
1	A	1025	G
1	A	1027	A
1	A	1033	U
1	A	1034	G
1	A	1036	G
1	A	1038	C
1	A	1041	C
1	A	1042	G
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1058	G
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1067	A
1	A	1070	A

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Mol	Chain	Res	Type
1	A	1073	A
1	A	1076	C
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1088	A
1	A	1089	G
1	A	1095	A
1	A	1109	C
1	A	1110	G
1	A	1111	A
1	A	1112	G
1	A	1115	G
1	A	1119	C
1	A	1124	C
1	A	1127	A
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1142(A)	A
1	A	1143	A
1	A	1149	G
1	A	1152	C
1	A	1155	A
1	A	1156	A
1	A	1157	G
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1206	G
1	A	1210	A
1	A	1211	U
1	A	1219	G
1	A	1220	A
1	A	1224	C

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Mol	Chain	Res	Type
1	A	1230	C
1	A	1236	G
1	A	1244	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1275	A
1	A	1300	U
1	A	1301	A
1	A	1308	A
1	A	1313	U
1	A	1320	C
1	A	1321	A
1	A	1329	U
1	A	1332	G
1	A	1342	A
1	A	1347	G
1	A	1359	A
1	A	1360	A
1	A	1363	C
1	A	1365	A
1	A	1369	G
1	A	1373	A
1	A	1378	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1398	C
1	A	1413	G
1	A	1416	G
1	A	1417	C
1	A	1420	U
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1436	G
1	A	1437	C
1	A	1445	A

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Mol	Chain	Res	Type
1	A	1450	G
1	A	1451	C
1	A	1455	G
1	A	1459	G
1	A	1460	A
1	A	1461	G
1	A	1467	C
1	A	1471	A
1	A	1481	U
1	A	1482	G
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1511	C
1	A	1523	U
1	A	1526	G
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1553	A
1	A	1554	A
1	A	1558	A
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1581	G
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1595	G
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1613	G
1	A	1617	C
1	A	1631(A)	A
1	A	1644	C

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Mol	Chain	Res	Type
1	A	1648	C
1	A	1649	G
1	A	1651	G
1	A	1654	A
1	A	1674	G
1	A	1695	G
1	A	1696	G
1	A	1700	A
1	A	1702	G
1	A	1705	G
1	A	1721	G
1	A	1722	A
1	A	1740	G
1	A	1745(A)	C
1	A	1746	G
1	A	1747	G
1	A	1756	G
1	A	1758	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1781	C
1	A	1791	A
1	A	1800	C
1	A	1802	A
1	A	1812	A
1	A	1816	G
1	A	1817	G
1	A	1820	U
1	A	1821	A
1	A	1828	G
1	A	1829	A
1	A	1838	C
1	A	1847	A
1	A	1877	A
1	A	1878	G
1	A	1889	A
1	A	1895	C
1	A	1900	A
1	A	1903	G
1	A	1906	G

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Mol	Chain	Res	Type
1	A	1913	A
1	A	1914	C
1	A	1920	C
1	A	1921	G
1	A	1929	G
1	A	1930	G
1	A	1934	C
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1941	C
1	A	1943	U
1	A	1955	U
1	A	1958	C
1	A	1960	A
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1983	C
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	G
1	A	2020	A
1	A	2021	C
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2035	G
1	A	2043	C
1	A	2049	G
1	A	2050	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A

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Mol	Chain	Res	Type
1	A	2063	C
1	A	2069	G
1	A	2070	G
1	A	2077	A
1	A	2087	G
1	A	2091	U
1	A	2096	U
1	A	2098	U
1	A	2105	C
1	A	2110	G
1	A	2111	C
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2119	A
1	A	2127	G
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2137	C
1	A	2138	C
1	A	2141	G
1	A	2142	C
1	A	2146	C
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2161	C
1	A	2166	G
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2172	U
1	A	2178	C
1	A	2182	G
1	A	2184	G
1	A	2186	G
1	A	2187	G
1	A	2188	C
1	A	2189	U

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Mol	Chain	Res	Type
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2201	C
1	A	2203	U
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2235	G
1	A	2238	G
1	A	2239	G
1	A	2243	U
1	A	2246	G
1	A	2251	G
1	A	2265	U
1	A	2268	A
1	A	2271	G
1	A	2273	A
1	A	2275	C
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2305	A
1	A	2307	G
1	A	2308	G
1	A	2311	A
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2322	A
1	A	2325	G
1	A	2334	G
1	A	2336	A
1	A	2338	G
1	A	2343	C
1	A	2345	G
1	A	2347	C
1	A	2350	C

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Mol	Chain	Res	Type
1	A	2374	C
1	A	2383	G
1	A	2385	C
1	A	2406	U
1	A	2408	U
1	A	2410	G
1	A	2414	G
1	A	2422	A
1	A	2424	C
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2447	G
1	A	2448	A
1	A	2460	U
1	A	2469	A
1	A	2471	C
1	A	2474	C
1	A	2476	A
1	A	2478	A
1	A	2482	G
1	A	2491	U
1	A	2498	C
1	A	2502	G
1	A	2503	A
1	A	2505	G
1	A	2507	C
1	A	2511	U
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2528	U
1	A	2529	G
1	A	2535	G
1	A	2545	G
1	A	2554	U
1	A	2564	A

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Mol	Chain	Res	Type
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2581	G
1	A	2582	G
1	A	2586	C
1	A	2602	A
1	A	2605	U
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2621	A
1	A	2629	A
1	A	2630	G
1	A	2639	A
1	A	2645	G
1	A	2654	A
1	A	2660	A
1	A	2663	G
1	A	2669	G
1	A	2679	A
1	A	2686	G
1	A	2689	U
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2751	G
1	A	2755	C
1	A	2757	A
1	A	2758	A
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2780	G

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Mol	Chain	Res	Type
1	A	2784	C
1	A	2790	A
1	A	2791	C
1	A	2792	G
1	A	2802	G
1	A	2811	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2831	G
1	A	2833	G
1	A	2835	A
1	A	2872	G
1	A	2880	C
1	A	2887	U
1	A	2889	C
1	A	2895	U
1	A	2897	U
2	B	7	G
2	B	9	G
2	B	10	C
2	B	13	A
2	B	24	G
2	B	25	A
2	B	35	U
2	B	40	U
2	B	42	C
2	B	44	G
2	B	45	A
2	B	56	G
2	B	73	A
2	B	77	U
2	B	78	A
2	B	110	G
2	B	119	G
2	B	120	A
33	x	2	C
33	x	4	C
33	x	5	G
33	x	7	A
33	x	9	A
33	x	10	G

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Mol	Chain	Res	Type
33	x	11	C
33	x	14	A
33	x	19	G
33	x	20	U
33	x	21	A
33	x	23	A
33	x	25	C
33	x	26	A
33	x	32	PSU
33	x	34	G
33	x	37	MIA
33	x	39	PSU
33	x	41	C
33	x	42	C
33	x	44	G
33	x	45	U
33	x	46	7MG
33	x	47	U
33	x	48	C
33	x	49	C
33	x	54	5MU
33	x	56	C
33	x	57	G
33	x	58	A
33	x	59	U
33	x	60	U
33	x	61	C
33	x	62	C
33	x	67	C
33	x	68	C
33	x	69	G
33	x	73	A
34	a	7	G
34	a	9	G
34	a	15	G
34	a	22	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A

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Mol	Chain	Res	Type
34	a	51	A
34	a	61	G
34	a	73	G
34	a	77	G
34	a	78	G
34	a	79	G
34	a	92	C
34	a	96	U
34	a	97	G
34	a	101	A
34	a	110	C
34	a	116	A
34	a	120	A
34	a	121	C
34	a	131	C
34	a	133	U
34	a	144	G
34	a	151	A
34	a	159	G
34	a	163	C
34	a	167	G
34	a	171	A
34	a	182	U
34	a	189(G)	G
34	a	194	C
34	a	197	A
34	a	202	U
34	a	203	U
34	a	204	U
34	a	216	G
34	a	232	G
34	a	236	G
34	a	247	G
34	a	251	G
34	a	253	U
34	a	266	G
34	a	267	C
34	a	280	C
34	a	289	G
34	a	291	C
34	a	305	G
34	a	306	G

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Mol	Chain	Res	Type
34	a	317	G
34	a	321	A
34	a	325	A
34	a	328	C
34	a	331	G
34	a	332	G
34	a	346	G
34	a	347	G
34	a	348	G
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	355	C
34	a	366	C
34	a	367	U
34	a	369	C
34	a	372	C
34	a	374	A
34	a	378	G
34	a	382	A
34	a	384	G
34	a	398	C
34	a	406	G
34	a	412	A
34	a	413	G
34	a	422	C
34	a	423	G
34	a	429	U
34	a	430	A
34	a	437	U
34	a	439	A
34	a	441	A
34	a	444	C
34	a	452	A
34	a	453	A
34	a	461	A
34	a	470	C
34	a	472	A
34	a	485	G
34	a	496	A
34	a	498	U

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Mol	Chain	Res	Type
34	a	505	G
34	a	506	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	518	C
34	a	525	C
34	a	527	G
34	a	532	A
34	a	533	A
34	a	546	G
34	a	547	A
34	a	559	A
34	a	561	U
34	a	562	C
34	a	564	C
34	a	565	U
34	a	572	A
34	a	573	A
34	a	576	G
34	a	577	G
34	a	596	C
34	a	597	G
34	a	607	A
34	a	630	G
34	a	631	G
34	a	641	U
34	a	653	A
34	a	661	G
34	a	665	A
34	a	666	G
34	a	687	A
34	a	688	G
34	a	693	G
34	a	697	U
34	a	702	A
34	a	704	A
34	a	707	C
34	a	718	G
34	a	723	U
34	a	731	G
34	a	734	G

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Mol	Chain	Res	Type
34	a	749	C
34	a	750	G
34	a	752	G
34	a	753	A
34	a	755	G
34	a	760	G
34	a	764	C
34	a	777	A
34	a	786	G
34	a	790	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	816	A
34	a	817	C
34	a	821	G
34	a	828	A
34	a	836	G
34	a	839	U
34	a	840	C
34	a	841	U
34	a	848	C
34	a	853	G
34	a	859	A
34	a	860	A
34	a	863	U
34	a	870	U
34	a	873	A
34	a	874	G
34	a	896	C
34	a	902	G
34	a	914	A
34	a	916	G
34	a	919	A
34	a	922	G
34	a	926	G
34	a	927	G
34	a	928	G
34	a	934	C
34	a	935	A
34	a	936	C

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Mol	Chain	Res	Type
34	a	938	A
34	a	960	U
34	a	961	U
34	a	968	A
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	984	C
34	a	993	G
34	a	997	U
34	a	998	G
34	a	1006	C
34	a	1009	G
34	a	1016	A
34	a	1024	G
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	C
34	a	1030	C
34	a	1030(A)	G
34	a	1030(B)	C
34	a	1030(C)	G
34	a	1032	G
34	a	1033	G
34	a	1036	G
34	a	1044	A
34	a	1053	G
34	a	1054	C
34	a	1055	A
34	a	1062	U
34	a	1064	G
34	a	1070	U
34	a	1090	U
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1103	C
34	a	1121	U
34	a	1124	G
34	a	1125	U

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Mol	Chain	Res	Type
34	a	1126	U
34	a	1127	G
34	a	1129	C
34	a	1130	A
34	a	1131	G
34	a	1137	C
34	a	1139	G
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1157	A
34	a	1159	U
34	a	1170	A
34	a	1181	G
34	a	1182	G
34	a	1183	A
34	a	1184	G
34	a	1193	G
34	a	1196	U
34	a	1197	G
34	a	1212	U
34	a	1213	A
34	a	1227	A
34	a	1236	A
34	a	1238	A
34	a	1250	A
34	a	1251	A
34	a	1253	G
34	a	1256	A
34	a	1257	U
34	a	1258	G
34	a	1259	C
34	a	1260	C
34	a	1268	A
34	a	1270	C
34	a	1273	G
34	a	1278	U
34	a	1279	A
34	a	1280	A
34	a	1281	U
34	a	1282	C
34	a	1287	A

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Mol	Chain	Res	Type
34	a	1299	A
34	a	1300	G
34	a	1302	U
34	a	1304	G
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1323	G
34	a	1338	G
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1364	U
34	a	1365	G
34	a	1370	G
34	a	1376	U
34	a	1379	G
34	a	1383	C
34	a	1392	G
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1411	C
34	a	1419	G
34	a	1442	G
34	a	1442(B)	A
34	a	1445	C
34	a	1446	U
34	a	1447	A
34	a	1452	C
34	a	1456	G
34	a	1457	G
34	a	1458	G
34	a	1486	G
34	a	1487	G
34	a	1497	G
34	a	1498	U
34	a	1502	A
34	a	1503	A
34	a	1504	G
34	a	1506	U

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Mol	Chain	Res	Type
34	a	1507	A
34	a	1517	G
34	a	1519	A
34	a	1520	G
34	a	1529	G
34	a	1530	G
34	a	1531	A
33	w	10	G
33	w	13	C
33	w	16	U
33	w	17	C
33	w	18	G
33	w	19	G
33	w	20	U
33	w	21	A
33	w	22	G
33	w	35	A
33	w	37	MIA
33	w	38	A
33	w	41	C
33	w	44	G
33	w	45	U
33	w	46	7MG
33	w	47	U
33	w	48	C
33	w	49	C
33	w	61	C
33	w	64	A
33	w	71	G
33	w	76	A
55	v	18	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	34	C
1	A	90	U
1	A	196	A
1	A	266	G
1	A	278	A
1	A	328	U
1	A	529	A

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Mol	Chain	Res	Type
1	A	685	A
1	A	746	A
1	A	752	A
1	A	774	A
1	A	895	U
1	A	1033	U
1	A	1052	C
1	A	1069	A
1	A	1078	U
1	A	1108	U
1	A	1145	C
1	A	1174	A
1	A	1176	G
1	A	1210	A
1	A	1300	U
1	A	1379	A
1	A	1529	G
1	A	1608	A
1	A	1617	C
1	A	1653	G
1	A	1992	G
1	A	2110	G
1	A	2132	U
1	A	2183	C
1	A	2187	G
1	A	2318	G
1	A	2428	G
1	A	2439	A
1	A	2611	U
1	A	2756	U
1	A	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	MIA	x	37	33	21,24,32	1.64	4 (19%)	30,35,47	1.99	7 (23%)
33	PSU	x	32	33	18,21,22	1.41	2 (11%)	21,30,33	1.93	4 (19%)
33	4SU	w	8	33	18,21,22	1.60	4 (22%)	25,30,33	2.15	5 (20%)
33	PSU	w	32	33	18,21,22	1.39	1 (5%)	21,30,33	1.89	5 (23%)
33	PSU	w	39	33	18,21,22	1.42	2 (11%)	21,30,33	2.38	4 (19%)
33	MIA	w	37	33	28,31,32	2.81	8 (28%)	38,44,47	3.21	11 (28%)
33	5MU	w	54	33	19,22,23	1.36	5 (26%)	27,32,35	2.03	6 (22%)
33	4SU	x	8	33	18,21,22	1.77	3 (16%)	25,30,33	2.33	6 (24%)
33	5MU	x	54	33	19,22,23	1.56	5 (26%)	27,32,35	2.04	6 (22%)
33	PSU	x	55	33	18,21,22	1.32	2 (11%)	21,30,33	2.10	5 (23%)
33	PSU	x	39	33	18,21,22	1.43	2 (11%)	21,30,33	1.87	5 (23%)
33	7MG	w	46	33	23,26,27	1.33	4 (17%)	27,39,42	2.72	8 (29%)
33	PSU	w	55	33	18,21,22	1.47	3 (16%)	21,30,33	2.23	5 (23%)
33	7MG	x	46	33	23,26,27	1.26	2 (8%)	27,39,42	3.06	9 (33%)

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
33	MIA	x	37	33	-	3/7/25/34	0/3/3/3
33	PSU	x	32	33	-	2/7/25/26	0/2/2/2
33	4SU	w	8	33	-	0/7/25/26	0/2/2/2
33	PSU	w	32	33	-	0/7/25/26	0/2/2/2
33	PSU	w	39	33	-	0/7/25/26	0/2/2/2
33	MIA	w	37	33	-	4/15/33/34	0/3/3/3
33	5MU	w	54	33	-	0/7/25/26	0/2/2/2
33	4SU	x	8	33	-	0/7/25/26	0/2/2/2
33	5MU	x	54	33	-	4/7/25/26	0/2/2/2
33	PSU	x	55	33	-	1/7/25/26	0/2/2/2
33	PSU	x	39	33	-	2/7/25/26	0/2/2/2
33	7MG	w	46	33	-	1/7/37/38	0/3/3/3
33	PSU	w	55	33	-	0/7/25/26	0/2/2/2
33	7MG	x	46	33	-	4/7/37/38	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	w	37	MIA	C2-S10	-9.46	1.67	1.75
33	w	37	MIA	C13-C14	7.43	1.54	1.32
33	x	37	MIA	C5-C4	5.21	1.48	1.39
33	w	37	MIA	C5-C4	5.08	1.48	1.39
33	x	8	4SU	C4-S4	-4.90	1.60	1.68
33	w	8	4SU	C4-S4	-4.44	1.60	1.68
33	w	32	PSU	C6-C5	4.20	1.39	1.35
33	w	39	PSU	C6-C5	4.15	1.39	1.35
33	x	39	PSU	C6-C5	4.03	1.39	1.35
33	x	32	PSU	C6-C5	3.82	1.39	1.35
33	w	46	7MG	C4-N9	-3.77	1.33	1.37
33	w	55	PSU	C6-C5	3.37	1.39	1.35
33	x	55	PSU	C6-C5	3.32	1.39	1.35
33	x	46	7MG	C5-C4	3.28	1.47	1.37
33	w	37	MIA	C4-N9	-3.21	1.31	1.37
33	x	54	5MU	C2-N1	3.18	1.43	1.38
33	w	55	PSU	C4-N3	-3.09	1.33	1.38
33	x	8	4SU	C4-N3	-2.99	1.34	1.37
33	x	54	5MU	C6-C5	2.97	1.39	1.34
33	x	8	4SU	C5-C4	-2.97	1.39	1.42
33	x	37	MIA	C5-C6	2.95	1.49	1.41
33	w	46	7MG	C5-C4	2.90	1.46	1.37
33	w	37	MIA	C5-C6	2.77	1.48	1.41
33	w	54	5MU	C6-C5	2.76	1.39	1.34
33	w	37	MIA	C2-N1	2.71	1.38	1.34
33	x	54	5MU	C4-N3	-2.71	1.33	1.38
33	w	37	MIA	C8-N7	2.67	1.36	1.31
33	w	37	MIA	C5-N7	-2.66	1.34	1.39
33	x	39	PSU	C4-N3	-2.65	1.33	1.38
33	x	32	PSU	C4-N3	-2.59	1.34	1.38
33	w	55	PSU	C2-N3	-2.57	1.33	1.37
33	w	54	5MU	C4-N3	-2.56	1.34	1.38
33	x	54	5MU	C4-C5	2.52	1.48	1.44
33	x	55	PSU	C4-N3	-2.46	1.34	1.38
33	x	46	7MG	C6-N1	-2.44	1.34	1.38
33	x	37	MIA	C8-N7	2.36	1.36	1.31
33	w	46	7MG	C6-N1	-2.28	1.34	1.38
33	w	8	4SU	C5-C4	-2.23	1.39	1.42
33	w	8	4SU	C4-N3	-2.21	1.35	1.37
33	w	54	5MU	C2-N3	-2.18	1.34	1.38
33	w	8	4SU	C2-N1	2.16	1.41	1.38
33	x	37	MIA	C5-N7	-2.12	1.35	1.39
33	w	54	5MU	C2-N1	2.11	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	w	46	7MG	C5-C6	2.10	1.48	1.43
33	x	54	5MU	C2-N3	-2.08	1.34	1.38
33	w	39	PSU	C4-C5	2.07	1.50	1.44
33	w	54	5MU	C4-C5	2.02	1.48	1.44

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	37	MIA	C11-S10-C2	-15.04	90.96	102.25
33	x	46	7MG	N9-C4-N3	10.87	141.39	125.46
33	w	46	7MG	N9-C4-N3	8.16	137.42	125.46
33	w	39	PSU	N1-C2-N3	6.98	122.53	115.17
33	x	8	4SU	C4-N3-C2	-6.96	120.64	127.31
33	w	55	PSU	N1-C2-N3	6.93	122.48	115.17
33	w	46	7MG	N9-C8-N7	-6.69	93.90	103.37
33	x	55	PSU	N1-C2-N3	6.58	122.11	115.17
33	x	46	7MG	C5-C4-N3	-6.35	116.21	128.13
33	w	37	MIA	C5-C4-N3	-6.20	120.65	127.18
33	w	8	4SU	C4-N3-C2	-6.14	121.43	127.31
33	x	32	PSU	N1-C2-N3	5.98	121.47	115.17
33	x	39	PSU	N1-C2-N3	5.88	121.37	115.17
33	x	37	MIA	C5-C4-N3	-5.72	118.84	126.72
33	x	8	4SU	C5-C4-N3	5.71	120.06	114.75
33	w	8	4SU	C5-C4-N3	5.39	119.77	114.75
33	w	32	PSU	N1-C2-N3	5.35	120.81	115.17
33	x	54	5MU	N3-C2-N1	5.28	121.77	114.89
33	w	54	5MU	N3-C2-N1	5.18	121.63	114.89
33	w	39	PSU	O2-C2-N1	-5.15	117.48	122.79
33	w	37	MIA	C12-C13-C14	-5.14	117.78	127.01
33	x	46	7MG	N9-C8-N7	-5.01	96.29	103.37
33	w	46	7MG	C5-C4-N3	-4.92	118.90	128.13
33	x	46	7MG	C2-N3-C4	4.83	120.61	112.30
33	w	54	5MU	C4-N3-C2	-4.77	121.09	127.34
33	w	55	PSU	C4-N3-C2	-4.73	119.85	126.37
33	x	54	5MU	C4-N3-C2	-4.72	121.15	127.34
33	w	46	7MG	C2-N3-C4	4.72	120.42	112.30
33	w	37	MIA	C16-C14-C13	-4.64	108.74	122.66
33	x	37	MIA	N3-C4-N9	4.63	135.04	127.17
33	w	8	4SU	C5-C4-S4	-4.38	119.31	124.31
33	w	39	PSU	C4-N3-C2	-4.29	120.46	126.37
33	w	54	5MU	O4-C4-C5	-4.29	120.01	124.92
33	x	8	4SU	C5-C4-S4	-4.28	119.42	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	54	5MU	C5-C4-N3	4.13	118.91	115.32
33	x	8	4SU	N3-C2-N1	4.12	120.25	114.89
33	w	32	PSU	C4-N3-C2	-4.11	120.71	126.37
33	x	32	PSU	C4-N3-C2	-4.06	120.77	126.37
33	x	55	PSU	C4-N3-C2	-4.06	120.77	126.37
33	x	55	PSU	O2-C2-N1	-3.99	118.68	122.79
33	x	39	PSU	C4-N3-C2	-3.82	121.11	126.37
33	x	54	5MU	C5-C4-N3	3.70	118.54	115.32
33	w	37	MIA	N6-C6-N1	3.64	123.21	118.33
33	x	37	MIA	C2-N3-C4	3.58	120.57	111.83
33	w	8	4SU	N3-C2-N1	3.56	119.53	114.89
33	x	37	MIA	C4-C5-N7	-3.54	106.53	110.58
33	x	54	5MU	O4-C4-C5	-3.52	120.89	124.92
33	w	37	MIA	C4-C5-N7	-3.45	106.63	110.58
33	w	37	MIA	N3-C4-N9	3.30	131.18	126.99
33	x	46	7MG	O6-C6-C5	-3.29	119.56	127.62
33	x	37	MIA	N3-C2-N1	-3.28	123.62	128.58
33	x	54	5MU	C5-C6-N1	-3.27	119.77	123.31
33	w	46	7MG	C5-C6-N1	3.26	116.68	110.94
33	w	39	PSU	C6-C5-C4	-3.26	115.97	118.17
33	w	55	PSU	O2-C2-N1	-3.25	119.44	122.79
33	x	46	7MG	C5-C6-N1	3.13	116.45	110.94
33	x	46	7MG	C5-C4-N9	-3.08	102.39	106.33
33	w	37	MIA	C6-C5-N7	3.04	135.74	132.43
33	x	54	5MU	O2-C2-N3	-2.82	116.28	121.49
33	x	32	PSU	O2-C2-N1	-2.75	119.95	122.79
33	w	46	7MG	C6-C5-N7	2.68	136.08	131.93
33	w	54	5MU	C5-C6-N1	-2.68	120.41	123.31
33	x	37	MIA	C5-N7-C8	2.62	107.57	103.45
33	w	8	4SU	O2-C2-N1	-2.57	119.44	122.80
33	w	37	MIA	C2-N3-C4	2.55	118.97	112.29
33	x	37	MIA	C4-N9-C8	2.54	108.40	105.74
33	w	55	PSU	C5-C6-N1	-2.53	118.63	122.14
33	w	37	MIA	C15-C14-C13	-2.45	115.31	122.66
33	w	32	PSU	C5-C6-N1	-2.45	118.75	122.14
33	w	46	7MG	C6-C5-C4	-2.41	118.17	122.40
33	x	8	4SU	O2-C2-N1	-2.39	119.69	122.80
33	w	54	5MU	O2-C2-N1	-2.32	119.77	122.80
33	x	55	PSU	C5-C6-N1	-2.24	119.04	122.14
33	w	32	PSU	O2-C2-N1	-2.23	120.49	122.79
33	x	39	PSU	O2-C2-N3	-2.22	117.92	121.86
33	x	39	PSU	C5-C6-N1	-2.21	119.08	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	x	8	4SU	C1'-N1-C2	2.20	121.54	117.59
33	w	37	MIA	C5-C4-N9	2.16	108.17	105.81
33	w	32	PSU	O4-C4-C5	-2.15	118.66	124.01
33	w	55	PSU	O2-C2-N3	-2.13	118.08	121.86
33	x	46	7MG	C4-C5-N7	2.12	107.88	105.38
33	x	32	PSU	C5-C6-N1	-2.11	119.22	122.14
33	w	46	7MG	C5-C4-N9	-2.09	103.65	106.33
33	x	46	7MG	O6-C6-N1	2.06	123.99	120.11
33	x	55	PSU	O4'-C1'-C2'	2.04	107.97	105.15
33	x	39	PSU	O2-C2-N1	-2.02	120.71	122.79

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	x	32	PSU	O4'-C4'-C5'-O5'
33	x	46	7MG	C4'-C5'-O5'-P
33	w	37	MIA	C5-C6-N6-C12
33	w	37	MIA	N1-C6-N6-C12
33	w	37	MIA	C12-C13-C14-C16
33	x	37	MIA	C3'-C4'-C5'-O5'
33	x	54	5MU	C3'-C4'-C5'-O5'
33	x	54	5MU	O4'-C4'-C5'-O5'
33	x	32	PSU	C3'-C4'-C5'-O5'
33	x	39	PSU	C3'-C4'-C5'-O5'
33	x	37	MIA	O4'-C4'-C5'-O5'
33	x	39	PSU	O4'-C4'-C5'-O5'
33	x	46	7MG	C2'-C1'-N9-C8
33	w	37	MIA	C4'-C5'-O5'-P
33	x	55	PSU	O4'-C1'-C5-C4
33	x	46	7MG	O4'-C1'-N9-C8
33	w	46	7MG	C2'-C1'-N9-C8
33	x	46	7MG	C3'-C4'-C5'-O5'
33	x	37	MIA	C4'-C5'-O5'-P
33	x	54	5MU	C2'-C1'-N1-C2
33	x	54	5MU	C2'-C1'-N1-C6

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	x	37	MIA	1	0
33	w	8	4SU	1	0
33	w	54	5MU	2	0
33	x	8	4SU	1	0
33	x	54	5MU	1	0
33	x	55	PSU	2	0
33	x	39	PSU	2	0
33	w	46	7MG	1	0
33	x	46	7MG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 915 ligands modelled in this entry, 912 are monoatomic - leaving 3 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	PHE	w	107	33	10,11,12	1.37	0	8,13,15	1.11	0
59	SF4	d	501	37	0,12,12	-	-	-		
61	GDP	y	703	57	29,30,30	1.31	4 (13%)	45,47,47	1.96	7 (15%)

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	PHE	w	107	33	-	2/5/6/8	0/1/1/1
61	GDP	y	703	57	-	1/16/32/32	0/3/3/3
59	SF4	d	501	37	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	y	703	GDP	C5-C4	3.32	1.47	1.38
61	y	703	GDP	PA-O3A	2.57	1.62	1.59
61	y	703	GDP	C6-N1	-2.55	1.34	1.38
61	y	703	GDP	C5-N7	-2.41	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	y	703	GDP	C5-C4-N3	-7.44	116.55	128.39
61	y	703	GDP	C2-N3-C4	5.59	121.93	112.30
61	y	703	GDP	N9-C4-N3	5.25	136.44	125.95
61	y	703	GDP	C4-C5-N7	-3.01	105.90	110.67
61	y	703	GDP	C6-C5-N7	2.91	135.58	130.29
61	y	703	GDP	C3'-C2'-C1'	2.35	105.91	101.46
61	y	703	GDP	C2-N1-C6	-2.06	121.37	125.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	w	107	PHE	CA-CB-CG-CD2
60	w	107	PHE	CA-CB-CG-CD1
61	y	703	GDP	C5'-O5'-PA-O1A

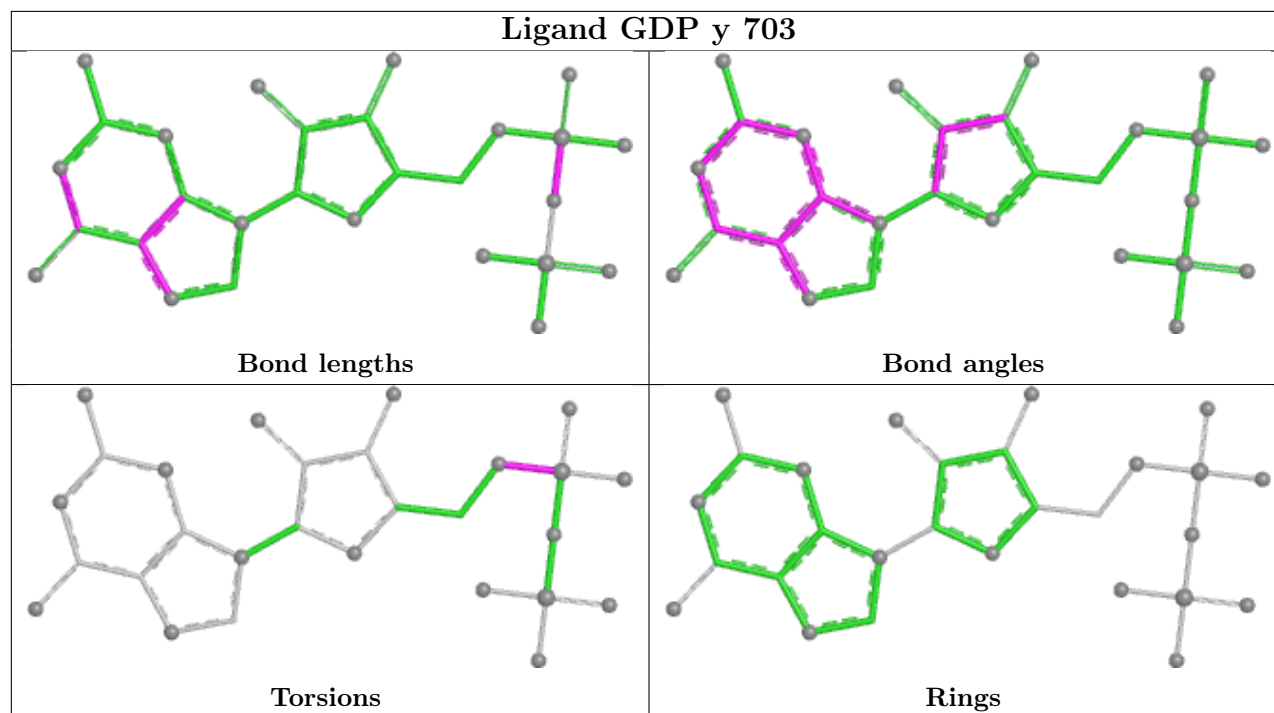
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	d	501	SF4	2	0
61	y	703	GDP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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	A	2873/2915 (98%)	-0.10	58 (2%) 65 56	35, 61, 175, 394	0
2	B	120/122 (98%)	0.18	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	0.27	3 (1%) 78 71	35, 56, 75, 108	0
4	E	204/206 (99%)	0.15	5 (2%) 58 48	34, 57, 77, 101	0
5	F	203/205 (99%)	0.43	8 (3%) 43 35	38, 70, 108, 135	0
6	G	181/182 (99%)	0.55	6 (3%) 49 40	68, 84, 106, 128	0
7	H	174/180 (96%)	0.76	10 (5%) 29 23	62, 96, 131, 154	0
8	J	130/173 (75%)	2.06	57 (43%) 0 0	129, 161, 183, 197	0
9	K	139/147 (94%)	2.46	84 (60%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	0.30	4 (2%) 53 45	47, 64, 93, 110	0
11	O	122/122 (100%)	0.02	0 100 100	37, 52, 68, 75	0
12	P	149/150 (99%)	0.71	9 (6%) 27 21	42, 81, 109, 116	0
13	Q	141/141 (100%)	0.40	0 100 100	44, 64, 80, 97	0
14	R	118/118 (100%)	0.45	3 (2%) 58 48	46, 66, 86, 102	0
15	S	110/112 (98%)	0.98	18 (16%) 4 3	75, 90, 102, 113	0
16	T	131/146 (89%)	0.20	4 (3%) 51 42	49, 61, 94, 113	0
17	U	116/118 (98%)	0.32	1 (0%) 81 75	42, 56, 75, 83	0
18	V	101/101 (100%)	0.34	0 100 100	41, 73, 93, 104	0
19	W	112/113 (99%)	0.37	1 (0%) 81 75	46, 62, 89, 128	0
20	X	95/96 (98%)	0.56	6 (6%) 26 20	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.66	7 (6%) 25 20	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.86	17 (9%) 14 12	68, 90, 114, 135	0
23	0	74/85 (87%)	0.58	3 (4%) 41 33	50, 67, 85, 105	0
24	1	97/98 (98%)	0.80	6 (6%) 26 21	48, 68, 104, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	70/72 (97%)	0.50	0 100 100	69, 86, 100, 109	0
26	3	59/60 (98%)	0.44	0 100 100	52, 68, 101, 116	0
27	4	69/71 (97%)	0.95	8 (11%) 9 8	80, 107, 150, 158	0
28	5	59/60 (98%)	0.17	2 (3%) 48 39	41, 63, 81, 100	0
29	6	53/54 (98%)	0.40	1 (1%) 66 58	62, 71, 85, 87	0
30	7	49/49 (100%)	0.45	4 (8%) 17 14	40, 49, 73, 96	0
31	8	64/65 (98%)	0.71	1 (1%) 70 62	51, 59, 65, 86	0
32	9	37/37 (100%)	0.88	4 (10%) 11 9	52, 63, 78, 88	0
33	w	69/76 (90%)	-0.41	1 (1%) 73 65	43, 73, 96, 137	0
33	x	67/76 (88%)	1.52	14 (20%) 2 2	94, 267, 283, 306	0
34	a	1496/1521 (98%)	-0.23	12 (0%) 82 77	37, 60, 119, 295	0
35	b	231/256 (90%)	0.61	18 (7%) 19 16	53, 84, 134, 165	0
36	c	206/239 (86%)	0.13	4 (1%) 66 58	50, 65, 88, 99	0
37	d	208/209 (99%)	0.42	8 (3%) 44 36	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.03	0 100 100	40, 55, 72, 107	0
39	f	100/101 (99%)	1.04	10 (10%) 12 10	74, 106, 138, 146	0
40	g	155/156 (99%)	0.30	9 (5%) 29 22	54, 73, 124, 156	0
41	h	137/138 (99%)	0.07	1 (0%) 84 79	47, 59, 72, 90	0
42	i	127/128 (99%)	0.48	6 (4%) 36 28	45, 70, 91, 102	0
43	j	96/105 (91%)	0.68	5 (5%) 33 26	42, 70, 119, 133	0
44	k	114/129 (88%)	0.47	6 (5%) 32 25	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.04	1 (0%) 82 77	39, 53, 68, 80	0
46	m	119/126 (94%)	0.28	1 (0%) 82 77	43, 72, 99, 111	0
47	n	60/61 (98%)	0.14	1 (1%) 69 61	42, 51, 66, 69	0
48	o	88/89 (98%)	0.51	4 (4%) 38 30	57, 74, 98, 107	0
49	p	82/88 (93%)	0.25	0 100 100	45, 57, 69, 85	0
50	q	99/105 (94%)	0.45	7 (7%) 22 17	50, 62, 80, 93	0
51	r	68/88 (77%)	0.54	2 (2%) 53 45	67, 85, 107, 116	0
52	s	83/93 (89%)	0.13	1 (1%) 76 69	45, 57, 76, 89	0
53	t	96/106 (90%)	0.59	6 (6%) 26 20	51, 65, 88, 96	0
54	u	23/27 (85%)	1.04	4 (17%) 4 3	54, 62, 69, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
55	v	7/18 (38%)	0.87	1 (14%) 6 5	49, 50, 130, 149	0
56	y	644/679 (94%)	1.93	272 (42%) 0 0	69, 151, 188, 213	0
All	All	11202/11638 (96%)	0.34	724 (6%) 25 20	34, 68, 168, 394	0

All (724) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	K	52	ILE	8.1
56	y	13	SER	7.9
56	y	209	GLN	7.9
9	K	22	PRO	6.9
8	J	51	LEU	6.7
9	K	12	LEU	6.6
56	y	513	ALA	6.1
56	y	330	LEU	6.1
56	y	264	LEU	6.0
56	y	599	ALA	6.0
56	y	416	THR	5.9
56	y	414	ILE	5.9
1	A	614(B)	G	5.9
56	y	93	VAL	5.9
9	K	9	LYS	5.8
8	J	50	ARG	5.7
33	x	34	G	5.7
9	K	120	LEU	5.7
24	1	2	SER	5.6
56	y	554	LEU	5.5
56	y	530	ARG	5.4
56	y	462	ASP	5.3
56	y	156	LEU	5.3
3	D	276	LYS	5.3
56	y	208	TYR	5.3
56	y	29	ILE	5.2
56	y	138	ILE	5.2
30	7	49	ARG	5.2
56	y	26	ALA	5.2
9	K	13	PRO	5.2
56	y	374	PRO	5.2
56	y	265	VAL	5.1
56	y	598	LEU	5.0
8	J	37	THR	5.0

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Mol	Chain	Res	Type	RSRZ
56	y	435	LEU	5.0
7	H	2	SER	4.9
56	y	180	ALA	4.9
56	y	596	ALA	4.9
9	K	93	ARG	4.7
56	y	525	ALA	4.7
1	A	1509	C	4.7
56	y	91	TYR	4.6
9	K	21	PRO	4.6
9	K	25	PRO	4.6
56	y	99	ALA	4.6
40	g	83	ALA	4.5
9	K	16	LYS	4.4
56	y	561	LYS	4.4
9	K	19	PRO	4.4
8	J	7	VAL	4.4
9	K	10	LEU	4.4
56	y	217	LEU	4.4
9	K	94	GLU	4.4
56	y	12	PHE	4.4
9	K	138	VAL	4.3
56	y	349	LEU	4.3
33	x	36	A	4.3
1	A	2145	C	4.3
56	y	177	ILE	4.3
43	j	73	ASP	4.2
56	y	206	ASP	4.2
15	S	7	TYR	4.2
56	y	274	VAL	4.2
8	J	84	GLU	4.2
40	g	85	TYR	4.2
9	K	8	VAL	4.2
56	y	563	TYR	4.1
9	K	17	ALA	4.1
43	j	32	ALA	4.1
15	S	3	ARG	4.1
56	y	461	TYR	4.1
8	J	110	GLY	4.1
8	J	111	LEU	4.0
33	x	35	A	4.0
56	y	302	PHE	4.0
15	S	13	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2146	C	4.0
6	G	35	GLU	4.0
56	y	205	TYR	4.0
37	d	154	ASN	4.0
39	f	98	LEU	4.0
56	y	124	ALA	3.9
56	y	469	SER	3.9
33	x	1	G	3.9
12	P	76	LYS	3.9
8	J	53	VAL	3.8
1	A	2178	C	3.8
8	J	62	ALA	3.8
56	y	109	ALA	3.8
56	y	225	GLY	3.8
56	y	471	SER	3.8
44	k	14	VAL	3.8
1	A	34	C	3.8
56	y	278	ASP	3.7
8	J	17	LEU	3.7
8	J	36	GLU	3.7
56	y	568	THR	3.7
50	q	98	LEU	3.7
8	J	103	GLY	3.7
56	y	456	PHE	3.7
56	y	510	ARG	3.7
56	y	299	PRO	3.7
56	y	529	PRO	3.7
40	g	84	ASN	3.7
56	y	164	ILE	3.7
8	J	49	ALA	3.7
56	y	90	THR	3.7
8	J	25	PHE	3.6
9	K	47	ASN	3.6
56	y	481	GLN	3.6
40	g	81	GLY	3.6
56	y	391	HIS	3.6
56	y	165	PHE	3.6
9	K	15	GLY	3.6
1	A	2165	G	3.6
3	D	230	ASP	3.6
35	b	134	GLU	3.5
56	y	410	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
56	y	450	LEU	3.5
8	J	29	TYR	3.5
56	y	415	PHE	3.5
4	E	195	LEU	3.5
33	x	18	G	3.5
56	y	373	ALA	3.5
8	J	99	SER	3.5
1	A	275	G	3.5
44	k	13	GLN	3.5
53	t	103	GLY	3.5
56	y	305	LEU	3.5
56	y	231	TYR	3.5
56	y	16	ALA	3.5
56	y	539	ALA	3.5
56	y	222	VAL	3.4
8	J	40	LEU	3.4
56	y	134	VAL	3.4
4	E	159	HIS	3.4
56	y	270	ASP	3.4
56	y	132	ILE	3.4
9	K	48	MET	3.4
9	K	23	VAL	3.4
40	g	79	ARG	3.4
56	y	436	VAL	3.4
8	J	54	ALA	3.4
9	K	51	ALA	3.4
8	J	109	SER	3.4
8	J	57	THR	3.4
56	y	590	VAL	3.3
56	y	562	CYS	3.3
9	K	74	ALA	3.3
30	7	48	LYS	3.3
56	y	452	TYR	3.3
15	S	20	ARG	3.3
9	K	108	ALA	3.3
4	E	113	PHE	3.3
8	J	8	GLU	3.3
7	H	77	LYS	3.3
8	J	89	ALA	3.3
9	K	107	ILE	3.3
56	y	368	SER	3.3
56	y	423	SER	3.3

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Mol	Chain	Res	Type	RSRZ
56	y	488	ASP	3.3
23	0	84	LEU	3.3
16	T	115	ARG	3.3
53	t	101	GLY	3.3
35	b	117	GLU	3.2
56	y	351	LEU	3.2
56	y	87	VAL	3.2
56	y	473	GLY	3.2
56	y	602	SER	3.2
1	A	2112	G	3.2
34	a	1126	U	3.2
56	y	437	ASN	3.2
56	y	516	MET	3.2
56	y	457	ALA	3.2
30	7	46	VAL	3.2
56	y	113	VAL	3.2
56	y	116	GLU	3.2
9	K	112	MET	3.2
56	y	92	GLU	3.2
9	K	34	ILE	3.2
21	Y	17	SER	3.2
56	y	489	LEU	3.2
12	P	114	ILE	3.2
54	u	18	TYR	3.1
56	y	409	TYR	3.1
12	P	15	ARG	3.1
56	y	88	ASP	3.1
9	K	109	LYS	3.1
9	K	18	THR	3.1
7	H	8	PRO	3.1
56	y	14	ILE	3.1
53	t	10	LEU	3.1
56	y	474	TYR	3.1
56	y	94	SER	3.1
56	y	597	PHE	3.1
3	D	275	LYS	3.1
56	y	211	VAL	3.1
9	K	127	ILE	3.1
56	y	355	GLU	3.1
1	A	2164	C	3.1
56	y	412	LEU	3.1
56	y	448	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
56	y	494	VAL	3.1
1	A	2182	G	3.1
33	x	15	G	3.1
44	k	126	ARG	3.1
56	y	236	GLU	3.1
9	K	68	VAL	3.0
27	4	50	VAL	3.0
56	y	490	VAL	3.0
53	t	9	ASN	3.0
27	4	61	ARG	3.0
34	a	1125	U	3.0
1	A	2181	G	3.0
9	K	20	ALA	3.0
56	y	517	ALA	3.0
9	K	96	VAL	3.0
22	Z	166	SER	3.0
9	K	57	ILE	3.0
48	o	20	GLY	3.0
56	y	104	LEU	3.0
56	y	428	LEU	3.0
9	K	123	ALA	3.0
40	g	80	VAL	3.0
56	y	496	VAL	3.0
56	y	15	ILE	3.0
9	K	77	LEU	3.0
9	K	105	LEU	3.0
56	y	145	PRO	3.0
56	y	372	THR	3.0
56	y	470	VAL	3.0
9	K	90	LYS	3.0
56	y	110	SER	3.0
9	K	26	ALA	3.0
56	y	115	ALA	3.0
56	y	166	ALA	3.0
56	y	371	ALA	3.0
15	S	14	VAL	3.0
35	b	122	PHE	3.0
9	K	101	TRP	2.9
8	J	116	ILE	2.9
9	K	83	GLY	2.9
56	y	493	ASN	2.9
33	x	30	G	2.9

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Mol	Chain	Res	Type	RSRZ
34	a	79	G	2.9
56	y	558	VAL	2.9
56	y	600	VAL	2.9
56	y	140	LEU	2.9
9	K	87	GLY	2.9
56	y	139	ASP	2.9
56	y	475	ALA	2.9
56	y	279	THR	2.9
15	S	10	ARG	2.9
22	Z	80	ARG	2.9
23	0	74	ARG	2.9
1	A	2104	G	2.9
20	X	9	LEU	2.9
20	X	1	MET	2.9
9	K	81	ALA	2.9
22	Z	27	VAL	2.9
56	y	106	VAL	2.9
15	S	9	ARG	2.9
56	y	427	LEU	2.9
56	y	504	LEU	2.9
36	c	159	GLY	2.9
6	G	29	TRP	2.9
34	a	630	G	2.9
35	b	132	LYS	2.9
56	y	160	ALA	2.9
56	y	62	SER	2.9
51	r	78	LEU	2.9
56	y	173	GLY	2.8
6	G	146	TYR	2.8
34	a	1129	C	2.8
44	k	75	TYR	2.8
9	K	104	VAL	2.8
56	y	18	VAL	2.8
40	g	82	GLY	2.8
8	J	13	LEU	2.8
5	F	49	ALA	2.8
8	J	52	PHE	2.8
56	y	460	LEU	2.8
1	A	2105	C	2.8
9	K	75	SER	2.8
9	K	80	LYS	2.8
1	A	2190	G	2.8

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Mol	Chain	Res	Type	RSRZ
6	G	26	GLN	2.8
9	K	85	GLU	2.8
7	H	43	VAL	2.8
35	b	7	VAL	2.8
39	f	97	PHE	2.8
5	F	181	LEU	2.8
9	K	84	LEU	2.8
44	k	111	ASP	2.8
56	y	411	LYS	2.8
39	f	96	PRO	2.8
35	b	126	GLU	2.7
46	m	2	ALA	2.7
56	y	553	ALA	2.7
56	y	378	TYR	2.7
27	4	62	ARG	2.7
9	K	136	VAL	2.7
56	y	130	VAL	2.7
56	y	182	VAL	2.7
32	9	15	LYS	2.7
8	J	28	ASN	2.7
8	J	47	ASN	2.7
56	y	287	THR	2.7
56	y	73	GLY	2.7
8	J	18	GLU	2.7
56	y	526	GLU	2.7
8	J	24	PHE	2.7
56	y	80	LEU	2.7
56	y	201	PHE	2.7
9	K	134	MET	2.7
33	x	31	A	2.7
33	x	33	U	2.7
9	K	132	ARG	2.7
24	1	20	ARG	2.7
8	J	85	ASP	2.7
56	y	167	SER	2.7
53	t	24	LEU	2.7
56	y	81	ILE	2.7
56	y	369	LEU	2.7
56	y	601	LEU	2.7
8	J	96	PHE	2.7
9	K	128	ALA	2.7
20	X	34	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	2177	C	2.7
8	J	48	GLY	2.7
35	b	131	PRO	2.7
56	y	296	PRO	2.7
1	A	614(A)	U	2.7
8	J	113	GLN	2.7
22	Z	118	GLN	2.7
56	y	207	ALA	2.6
56	y	454	ALA	2.6
34	a	1024	G	2.6
56	y	509	HIS	2.6
40	g	156	TRP	2.6
15	S	36	TYR	2.6
8	J	81	VAL	2.6
9	K	115	LEU	2.6
56	y	105	LEU	2.6
56	y	511	GLU	2.6
33	x	76	A	2.6
9	K	37	PHE	2.6
27	4	59	PHE	2.6
56	y	417	PRO	2.6
56	y	455	PRO	2.6
1	A	2138	C	2.6
10	N	140	VAL	2.6
22	Z	74	VAL	2.6
43	j	33	GLN	2.6
56	y	284	ASP	2.6
55	v	14	A	2.6
30	7	47	ARG	2.6
56	y	479	TYR	2.6
9	K	70	LYS	2.6
56	y	340	LEU	2.6
6	G	48	GLU	2.6
56	y	453	GLU	2.6
56	y	480	GLU	2.6
8	J	126	ALA	2.6
56	y	240	ASP	2.6
56	y	273	ASP	2.6
31	8	46	ARG	2.6
34	a	1447	A	2.6
22	Z	117	LEU	2.6
56	y	390	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
56	y	507	ILE	2.6
56	y	176	GLU	2.6
9	K	44	ALA	2.6
56	y	297	ALA	2.6
56	y	465	ASP	2.6
1	A	2183	C	2.5
8	J	78	SER	2.5
8	J	83	TYR	2.5
7	H	49	VAL	2.5
22	Z	165	VAL	2.5
28	5	60	VAL	2.5
35	b	136	VAL	2.5
56	y	535	VAL	2.5
50	q	96	GLU	2.5
56	y	413	THR	2.5
9	K	67	PHE	2.5
56	y	326	ASN	2.5
56	y	161	ASP	2.5
56	y	312	ASP	2.5
56	y	472	ARG	2.5
56	y	235	LYS	2.5
35	b	10	LEU	2.5
35	b	11	LEU	2.5
21	Y	1	MET	2.5
45	l	18	VAL	2.5
56	y	520	ILE	2.5
8	J	30	GLN	2.5
9	K	45	THR	2.5
56	y	332	PHE	2.5
56	y	267	ALA	2.5
56	y	444	ALA	2.5
37	d	209	ARG	2.5
56	y	345	ARG	2.5
1	A	2180	U	2.5
8	J	74	LEU	2.5
7	H	174	GLY	2.5
56	y	440	TYR	2.5
5	F	175	THR	2.5
9	K	66	THR	2.5
8	J	14	LYS	2.5
56	y	11	ASN	2.5
35	b	15	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
56	y	301	VAL	2.5
56	y	121	PHE	2.5
56	y	407	GLU	2.5
56	y	449	GLU	2.5
37	d	159	ARG	2.5
56	y	508	ALA	2.5
14	R	42	LYS	2.5
1	A	2101	G	2.5
1	A	2121	G	2.5
1	A	2160	G	2.5
21	Y	92	ASN	2.5
39	f	100	ASN	2.5
44	k	117	ASN	2.5
56	y	25	LEU	2.4
56	y	424	LEU	2.4
9	K	54	PRO	2.4
7	H	76	VAL	2.4
56	y	210	GLY	2.4
1	A	2113	U	2.4
34	a	90	U	2.4
9	K	121	GLU	2.4
39	f	95	GLU	2.4
56	y	74	GLU	2.4
9	K	40	ALA	2.4
21	Y	34	LYS	2.4
37	d	182	LYS	2.4
56	y	122	TYR	2.4
1	A	2137	C	2.4
1	A	2175	C	2.4
22	Z	34	ASN	2.4
8	J	112	LEU	2.4
48	o	57	LEU	2.4
56	y	-34	LEU	2.4
17	U	56	ASP	2.4
22	Z	57	ILE	2.4
56	y	131	ILE	2.4
56	y	459	ILE	2.4
9	K	133	SER	2.4
8	J	133	GLU	2.4
56	y	120	LYS	2.4
15	S	5	THR	2.4
56	y	79	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
56	y	537	ILE	2.4
12	P	73	GLY	2.4
56	y	551	VAL	2.4
1	A	2131	G	2.4
1	A	2166	G	2.4
12	P	74	GLU	2.4
8	J	20	ALA	2.4
22	Z	76	LEU	2.4
56	y	146	LEU	2.4
9	K	7	VAL	2.4
56	y	168	GLY	2.4
56	y	523	LYS	2.4
22	Z	2	GLU	2.4
56	y	337	SER	2.4
1	A	1537	G	2.4
1	A	2133	G	2.4
1	A	2144	U	2.4
9	K	69	THR	2.4
9	K	118	THR	2.4
56	y	313	TYR	2.4
51	r	31	LEU	2.4
56	y	325	LEU	2.4
43	j	76	ASN	2.3
56	y	376	VAL	2.3
9	K	92	GLY	2.3
9	K	102	GLU	2.3
56	y	458	GLU	2.3
56	y	275	GLN	2.3
33	x	14	A	2.3
15	S	32	LEU	2.3
56	y	250	LEU	2.3
56	y	367	LEU	2.3
56	y	9	ILE	2.3
56	y	587	ILE	2.3
9	K	95	LYS	2.3
56	y	576	LYS	2.3
9	K	55	VAL	2.3
37	d	153	ARG	2.3
53	t	22	ARG	2.3
56	y	204	VAL	2.3
9	K	65	PHE	2.3
42	i	18	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
52	s	12	ASP	2.3
56	y	531	GLN	2.3
1	A	886	C	2.3
4	E	151	TYR	2.3
20	X	8	ILE	2.3
56	y	144	ARG	2.3
9	K	5	VAL	2.3
56	y	261	VAL	2.3
56	y	348	PHE	2.3
1	A	2123	G	2.3
56	y	-55	ASP	2.3
43	j	85	LEU	2.3
56	y	183	GLN	2.3
21	Y	68	HIS	2.3
21	Y	71	LYS	2.3
56	y	71	LYS	2.3
56	y	512	LYS	2.3
56	y	253	THR	2.3
36	c	190	ARG	2.3
5	F	6	VAL	2.3
8	J	27	VAL	2.3
35	b	125	PRO	2.3
56	y	247	PRO	2.3
5	F	208	GLY	2.3
8	J	73	GLY	2.3
8	J	88	ALA	2.3
15	S	6	ALA	2.3
15	S	8	GLU	2.3
22	Z	119	GLU	2.3
36	c	161	GLU	2.3
37	d	149	ALA	2.3
8	J	106	GLN	2.3
56	y	524	LEU	2.3
9	K	125	ARG	2.3
56	y	292	PRO	2.3
1	A	1420	U	2.3
33	x	20	U	2.3
1	A	546	C	2.2
1	A	2143	C	2.2
8	J	6	ASN	2.2
56	y	98	ALA	2.2
56	y	560	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
24	1	98	LEU	2.2
39	f	55	ASP	2.2
42	i	105	ASP	2.2
10	N	43	THR	2.2
28	5	26	THR	2.2
7	H	50	VAL	2.2
1	A	2120	G	2.2
12	P	53	GLY	2.2
1	A	2585	U	2.2
15	S	37	ALA	2.2
56	y	63	ALA	2.2
56	y	329	ALA	2.2
12	P	6	LEU	2.2
39	f	10	LEU	2.2
56	y	361	LEU	2.2
1	A	2179	C	2.2
56	y	585	LYS	2.2
56	y	230	ILE	2.2
20	X	68	ARG	2.2
48	o	68	ARG	2.2
56	y	69	ARG	2.2
7	H	169	VAL	2.2
12	P	83	VAL	2.2
39	f	6	VAL	2.2
56	y	527	VAL	2.2
27	4	63	TYR	2.2
42	i	126	SER	2.2
56	y	291	TYR	2.2
54	u	2	GLY	2.2
56	y	266	ALA	2.2
56	y	468	LYS	2.2
1	A	1087	G	2.2
1	A	2116	G	2.2
1	A	2168	G	2.2
34	a	1131	G	2.2
42	i	2	GLU	2.2
56	y	503	ALA	2.2
1	A	90	U	2.2
9	K	116	ASN	2.2
14	R	68	ARG	2.2
42	i	3	GLN	2.2
54	u	24	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2161	C	2.2
9	K	4	VAL	2.2
56	y	7	SER	2.2
56	y	21	GLY	2.2
56	y	514	TYR	2.2
8	J	82	PHE	2.2
56	y	556	LYS	2.2
9	K	56	GLU	2.2
21	Y	29	GLU	2.2
29	6	2	ALA	2.2
35	b	237	ALA	2.2
50	q	24	GLU	2.2
56	y	333	GLU	2.2
56	y	268	ILE	2.2
1	A	1176	G	2.2
1	A	2334	G	2.2
34	a	1021	G	2.2
1	A	1046	A	2.2
19	W	22	ASP	2.2
1	A	2794	C	2.2
32	9	13	LYS	2.2
32	9	37	GLY	2.2
50	q	37	LYS	2.2
12	P	110	TYR	2.2
50	q	27	PHE	2.2
56	y	365	PHE	2.2
24	1	97	LEU	2.2
7	H	145	ALA	2.2
16	T	130	ALA	2.2
15	S	89	ARG	2.1
56	y	485	ARG	2.1
35	b	140	HIS	2.1
8	J	86	PRO	2.1
22	Z	1	MET	2.1
22	Z	140	ASP	2.1
1	A	887	A	2.1
1	A	2106	G	2.1
1	A	2115	G	2.1
1	A	2141	G	2.1
56	y	22	LYS	2.1
5	F	207	GLY	2.1
56	y	170	THR	2.1

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Mol	Chain	Res	Type	RSRZ
8	J	10	LEU	2.1
9	K	27	LEU	2.1
20	X	28	PHE	2.1
9	K	130	SER	2.1
16	T	131	ALA	2.1
22	Z	51	ALA	2.1
56	y	119	ALA	2.1
5	F	35	GLU	2.1
32	9	17	ILE	2.1
56	y	181	ILE	2.1
56	y	500	VAL	2.1
15	S	60	GLY	2.1
56	y	433	GLY	2.1
56	y	245	PHE	2.1
56	y	533	PHE	2.1
9	K	14	ALA	2.1
14	R	21	TYR	2.1
39	f	87	ARG	2.1
56	y	519	ALA	2.1
42	i	110	GLU	2.1
33	w	17	C	2.1
9	K	86	LYS	2.1
27	4	56	VAL	2.1
56	y	77	VAL	2.1
56	y	377	VAL	2.1
56	y	552	LYS	2.1
27	4	17	GLY	2.1
37	d	21	LEU	2.1
56	y	277	GLY	2.1
56	y	350	GLY	2.1
56	y	238	THR	2.1
35	b	97	TRP	2.1
40	g	76	ARG	2.1
8	J	97	ALA	2.1
47	n	2	ALA	2.1
56	y	482	ALA	2.1
56	y	203	SER	2.1
8	J	95	GLN	2.1
1	A	2110	G	2.1
5	F	112	MET	2.1
34	a	1030(B)	C	2.1
56	y	464	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
56	y	276	VAL	2.1
10	N	11	PRO	2.1
23	0	47	PRO	2.1
56	y	136	ASN	2.1
15	S	54	LEU	2.1
37	d	155	LEU	2.1
41	h	2	LEU	2.1
56	y	158	LEU	2.1
56	y	532	LEU	2.1
34	a	723	U	2.1
56	y	463	PHE	2.1
16	T	107	ASP	2.1
24	1	59	THR	2.1
56	y	233	THR	2.1
56	y	328	ALA	2.1
39	f	63	TYR	2.1
56	y	322	LYS	2.0
8	J	38	HIS	2.0
9	K	89	HIS	2.0
56	y	497	HIS	2.0
1	A	652(B)	A	2.0
8	J	80	VAL	2.0
8	J	94	VAL	2.0
33	x	38	A	2.0
56	y	186	PRO	2.0
1	A	2136	C	2.0
35	b	149	LEU	2.0
56	y	142	ASN	2.0
35	b	17	PHE	2.0
35	b	137	ARG	2.0
56	y	555	ARG	2.0
56	y	565	GLY	2.0
36	c	84	ILE	2.0
4	E	204	ALA	2.0
9	K	46	ALA	2.0
22	Z	127	LYS	2.0
24	1	92	LYS	2.0
50	q	69	LYS	2.0
9	K	11	GLN	2.0
50	q	26	GLN	2.0
56	y	421	VAL	2.0
56	y	567	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	2176	A	2.0
6	G	33	ARG	2.0
10	N	115	ARG	2.0
15	S	16	ASN	2.0
15	S	17	ARG	2.0
27	4	68	ARG	2.0
48	o	63	ARG	2.0
9	K	41	PHE	2.0
54	u	11	GLY	2.0
33	x	2	C	2.0
8	J	12	THR	2.0
56	y	547	ALA	2.0
9	K	50	ASP	2.0
1	A	1047	G	2.0
1	A	2152	G	2.0
22	Z	29	TYR	2.0
56	y	64	VAL	2.0
56	y	103	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
33	7MG	x	46	24/25	0.18	0.17	275,282,285,287	0
33	5MU	x	54	21/22	0.29	0.14	275,282,283,285	0
33	PSU	x	55	20/21	0.37	0.15	274,285,289,293	0
33	PSU	x	32	20/21	0.47	0.18	188,202,216,216	0
33	MIA	x	37	22/30	0.51	0.20	204,221,237,241	0
33	4SU	x	8	20/21	0.58	0.12	263,275,277,277	0
33	PSU	x	39	20/21	0.65	0.14	175,193,200,201	0
33	7MG	w	46	24/25	0.85	0.10	59,76,103,118	0
33	MIA	w	37	29/30	0.92	0.11	46,55,61,64	0
33	4SU	w	8	20/21	0.92	0.07	56,58,64,64	0
33	PSU	w	55	20/21	0.92	0.07	75,83,85,86	0
33	5MU	w	54	21/22	0.94	0.08	67,77,82,84	0
33	PSU	w	39	20/21	0.96	0.07	41,50,55,56	0
33	PSU	w	32	20/21	0.96	0.09	40,46,49,51	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
57	MG	A	3157	1/1	0.15	0.28	118,118,118,118	0
57	MG	x	3001	1/1	0.16	0.18	237,237,237,237	0
57	MG	x	3003	1/1	0.25	0.17	215,215,215,215	0
57	MG	A	3435	1/1	0.26	0.20	95,95,95,95	0
57	MG	A	3608	1/1	0.32	0.21	108,108,108,108	0
57	MG	0	101	1/1	0.48	0.20	73,73,73,73	0
57	MG	A	3576	1/1	0.50	0.20	89,89,89,89	0
57	MG	A	3186	1/1	0.51	0.26	90,90,90,90	0
57	MG	A	3057	1/1	0.52	0.15	56,56,56,56	0
57	MG	A	3282	1/1	0.54	0.15	66,66,66,66	0
57	MG	A	3408	1/1	0.55	0.20	98,98,98,98	0
57	MG	A	3607	1/1	0.58	0.23	90,90,90,90	0
57	MG	B	207	1/1	0.59	0.21	103,103,103,103	0
57	MG	A	3554	1/1	0.59	0.21	74,74,74,74	0
57	MG	A	3265	1/1	0.59	0.12	61,61,61,61	0
57	MG	A	3625	1/1	0.59	0.24	84,84,84,84	0
57	MG	A	3354	1/1	0.61	0.20	101,101,101,101	0
57	MG	A	3564	1/1	0.62	0.20	75,75,75,75	0
57	MG	A	3569	1/1	0.64	0.12	85,85,85,85	0
57	MG	A	3572	1/1	0.64	0.16	70,70,70,70	0
57	MG	A	3549	1/1	0.64	0.32	75,75,75,75	0
57	MG	A	3216	1/1	0.64	0.18	62,62,62,62	0
57	MG	A	3011	1/1	0.64	0.22	79,79,79,79	0
57	MG	A	3361	1/1	0.66	0.20	84,84,84,84	0
57	MG	A	3560	1/1	0.67	0.14	79,79,79,79	0
57	MG	A	3002	1/1	0.67	0.11	50,50,50,50	0
57	MG	A	3158	1/1	0.67	0.35	97,97,97,97	0
57	MG	A	3532	1/1	0.68	0.20	66,66,66,66	0
57	MG	A	3240	1/1	0.68	0.25	79,79,79,79	0
57	MG	A	3319	1/1	0.68	0.16	31,31,31,31	0
57	MG	A	3357	1/1	0.69	0.14	69,69,69,69	0
57	MG	a	3459	1/1	0.69	0.13	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B	214	1/1	0.70	0.22	83,83,83,83	0
57	MG	a	3371	1/1	0.70	0.21	65,65,65,65	0
57	MG	a	3392	1/1	0.70	0.22	65,65,65,65	0
57	MG	U	203	1/1	0.70	0.18	67,67,67,67	0
57	MG	A	3281	1/1	0.71	0.13	57,57,57,57	0
57	MG	A	3603	1/1	0.71	0.14	82,82,82,82	0
57	MG	f	201	1/1	0.71	0.20	92,92,92,92	0
57	MG	A	3600	1/1	0.72	0.19	64,64,64,64	0
57	MG	A	3040	1/1	0.72	0.11	58,58,58,58	0
57	MG	A	3605	1/1	0.72	0.14	70,70,70,70	0
57	MG	A	3441	1/1	0.72	0.12	73,73,73,73	0
57	MG	a	3369	1/1	0.72	0.20	60,60,60,60	0
57	MG	A	3059	1/1	0.72	0.17	66,66,66,66	0
57	MG	A	3571	1/1	0.72	0.13	89,89,89,89	0
57	MG	a	3419	1/1	0.72	0.19	72,72,72,72	0
57	MG	A	3134	1/1	0.72	0.15	67,67,67,67	0
57	MG	a	3484	1/1	0.72	0.20	67,67,67,67	0
57	MG	A	3330	1/1	0.72	0.22	55,55,55,55	0
60	PHE	w	107	11/12	0.72	0.29	56,72,80,81	0
57	MG	A	3614	1/1	0.73	0.10	75,75,75,75	0
57	MG	A	3629	1/1	0.73	0.20	70,70,70,70	0
57	MG	A	3291	1/1	0.74	0.17	60,60,60,60	0
57	MG	A	3451	1/1	0.74	0.11	82,82,82,82	0
57	MG	A	3253	1/1	0.74	0.18	66,66,66,66	0
57	MG	A	3056	1/1	0.75	0.14	68,68,68,68	0
57	MG	a	3410	1/1	0.75	0.14	45,45,45,45	0
57	MG	A	3087	1/1	0.75	0.15	58,58,58,58	0
57	MG	a	3330	1/1	0.75	0.20	63,63,63,63	0
57	MG	a	3340	1/1	0.75	0.12	81,81,81,81	0
57	MG	A	3273	1/1	0.75	0.26	77,77,77,77	0
57	MG	A	3578	1/1	0.75	0.17	64,64,64,64	0
57	MG	X	101	1/1	0.76	0.14	72,72,72,72	0
57	MG	a	3390	1/1	0.76	0.18	45,45,45,45	0
57	MG	A	3586	1/1	0.76	0.20	55,55,55,55	0
57	MG	a	3400	1/1	0.76	0.30	61,61,61,61	0
57	MG	A	3135	1/1	0.76	0.23	54,54,54,54	0
57	MG	A	3461	1/1	0.76	0.17	59,59,59,59	0
57	MG	a	3436	1/1	0.76	0.12	66,66,66,66	0
57	MG	A	3328	1/1	0.76	0.17	62,62,62,62	0
57	MG	A	3577	1/1	0.76	0.22	72,72,72,72	0
57	MG	A	3213	1/1	0.76	0.18	67,67,67,67	0
57	MG	a	3370	1/1	0.76	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	a	3328	1/1	0.77	0.21	60,60,60,60	0
57	MG	A	3602	1/1	0.77	0.14	73,73,73,73	0
57	MG	A	3029	1/1	0.77	0.18	52,52,52,52	0
57	MG	a	3350	1/1	0.77	0.23	73,73,73,73	0
57	MG	a	3358	1/1	0.77	0.26	70,70,70,70	0
57	MG	A	3153	1/1	0.77	0.22	82,82,82,82	0
57	MG	0	102	1/1	0.77	0.07	61,61,61,61	0
57	MG	A	3491	1/1	0.77	0.17	72,72,72,72	0
57	MG	y	702	1/1	0.77	0.19	75,75,75,75	0
57	MG	A	3293	1/1	0.77	0.22	51,51,51,51	0
57	MG	A	3101	1/1	0.78	0.20	74,74,74,74	0
57	MG	A	3108	1/1	0.78	0.12	54,54,54,54	0
57	MG	A	3267	1/1	0.78	0.16	59,59,59,59	0
57	MG	a	3391	1/1	0.78	0.19	72,72,72,72	0
57	MG	A	3124	1/1	0.78	0.12	54,54,54,54	0
57	MG	A	3555	1/1	0.78	0.17	69,69,69,69	0
57	MG	A	3360	1/1	0.78	0.10	60,60,60,60	0
57	MG	A	3209	1/1	0.78	0.14	71,71,71,71	0
57	MG	A	3062	1/1	0.78	0.16	42,42,42,42	0
57	MG	A	3068	1/1	0.78	0.24	56,56,56,56	0
57	MG	a	3472	1/1	0.78	0.10	61,61,61,61	0
57	MG	A	3231	1/1	0.78	0.14	48,48,48,48	0
57	MG	A	3004	1/1	0.78	0.21	55,55,55,55	0
57	MG	A	3326	1/1	0.78	0.24	69,69,69,69	0
57	MG	B	208	1/1	0.78	0.12	74,74,74,74	0
57	MG	A	3272	1/1	0.79	0.10	62,62,62,62	0
57	MG	D	302	1/1	0.79	0.18	74,74,74,74	0
57	MG	F	301	1/1	0.79	0.12	71,71,71,71	0
57	MG	A	3355	1/1	0.79	0.11	84,84,84,84	0
57	MG	A	3287	1/1	0.79	0.12	54,54,54,54	0
57	MG	A	3060	1/1	0.79	0.25	81,81,81,81	0
57	MG	A	3075	1/1	0.79	0.14	67,67,67,67	0
57	MG	a	3361	1/1	0.79	0.21	73,73,73,73	0
57	MG	a	3332	1/1	0.80	0.09	45,45,45,45	0
57	MG	A	3084	1/1	0.80	0.09	57,57,57,57	0
57	MG	A	3045	1/1	0.80	0.22	68,68,68,68	0
57	MG	A	3617	1/1	0.80	0.11	65,65,65,65	0
57	MG	A	3137	1/1	0.80	0.13	59,59,59,59	0
57	MG	A	3627	1/1	0.80	0.18	91,91,91,91	0
57	MG	A	3284	1/1	0.80	0.20	67,67,67,67	0
57	MG	A	3054	1/1	0.80	0.19	71,71,71,71	0
57	MG	A	3366	1/1	0.80	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3104	1/1	0.80	0.16	64,64,64,64	0
57	MG	A	3433	1/1	0.80	0.19	64,64,64,64	0
57	MG	A	3008	1/1	0.80	0.18	80,80,80,80	0
57	MG	A	3315	1/1	0.80	0.15	56,56,56,56	0
57	MG	A	3259	1/1	0.80	0.19	74,74,74,74	0
57	MG	A	3160	1/1	0.80	0.27	61,61,61,61	0
57	MG	A	3482	1/1	0.80	0.11	67,67,67,67	0
57	MG	A	3489	1/1	0.80	0.18	55,55,55,55	0
57	MG	a	3480	1/1	0.80	0.17	77,77,77,77	0
57	MG	A	3165	1/1	0.80	0.34	60,60,60,60	0
57	MG	a	3323	1/1	0.80	0.15	69,69,69,69	0
57	MG	A	3502	1/1	0.80	0.18	56,56,56,56	0
57	MG	A	3081	1/1	0.80	0.17	61,61,61,61	0
57	MG	A	3404	1/1	0.81	0.14	57,57,57,57	0
57	MG	A	3405	1/1	0.81	0.17	61,61,61,61	0
57	MG	A	3276	1/1	0.81	0.12	73,73,73,73	0
57	MG	a	3407	1/1	0.81	0.11	82,82,82,82	0
57	MG	E	304	1/1	0.81	0.18	55,55,55,55	0
57	MG	a	3334	1/1	0.81	0.20	43,43,43,43	0
57	MG	A	3498	1/1	0.81	0.18	76,76,76,76	0
57	MG	A	3260	1/1	0.81	0.12	68,68,68,68	0
57	MG	A	3032	1/1	0.81	0.19	50,50,50,50	0
57	MG	A	3436	1/1	0.81	0.17	87,87,87,87	0
57	MG	A	3245	1/1	0.81	0.22	56,56,56,56	0
57	MG	5	101	1/1	0.81	0.35	69,69,69,69	0
57	MG	A	3129	1/1	0.81	0.13	48,48,48,48	0
57	MG	A	3113	1/1	0.81	0.20	63,63,63,63	0
57	MG	A	3309	1/1	0.82	0.13	52,52,52,52	0
57	MG	A	3246	1/1	0.82	0.20	49,49,49,49	0
57	MG	A	3093	1/1	0.82	0.22	81,81,81,81	0
57	MG	A	3156	1/1	0.82	0.17	86,86,86,86	0
57	MG	a	3393	1/1	0.82	0.31	69,69,69,69	0
57	MG	B	209	1/1	0.82	0.10	70,70,70,70	0
57	MG	a	3327	1/1	0.82	0.14	62,62,62,62	0
57	MG	B	210	1/1	0.82	0.11	68,68,68,68	0
57	MG	A	3563	1/1	0.82	0.15	73,73,73,73	0
57	MG	A	3177	1/1	0.82	0.14	65,65,65,65	0
57	MG	A	3262	1/1	0.82	0.11	63,63,63,63	0
57	MG	A	3126	1/1	0.82	0.17	60,60,60,60	0
57	MG	P	202	1/1	0.82	0.21	86,86,86,86	0
57	MG	A	3244	1/1	0.82	0.18	59,59,59,59	0
57	MG	W	201	1/1	0.82	0.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	v	101	1/1	0.82	0.25	89,89,89,89	0
57	MG	A	3531	1/1	0.82	0.16	91,91,91,91	0
57	MG	A	3150	1/1	0.82	0.16	74,74,74,74	0
57	MG	a	3362	1/1	0.83	0.11	73,73,73,73	0
57	MG	A	3226	1/1	0.83	0.30	68,68,68,68	0
57	MG	A	3334	1/1	0.83	0.17	84,84,84,84	0
57	MG	A	3573	1/1	0.83	0.10	70,70,70,70	0
57	MG	a	3372	1/1	0.83	0.17	47,47,47,47	0
57	MG	A	3003	1/1	0.83	0.13	59,59,59,59	0
57	MG	B	206	1/1	0.83	0.16	75,75,75,75	0
57	MG	7	102	1/1	0.83	0.15	66,66,66,66	0
57	MG	A	3302	1/1	0.83	0.16	59,59,59,59	0
57	MG	A	3065	1/1	0.83	0.26	74,74,74,74	0
57	MG	a	3314	1/1	0.83	0.18	60,60,60,60	0
57	MG	A	3542	1/1	0.83	0.24	60,60,60,60	0
57	MG	A	3439	1/1	0.83	0.14	58,58,58,58	0
57	MG	A	3148	1/1	0.83	0.19	60,60,60,60	0
57	MG	B	215	1/1	0.83	0.11	114,114,114,114	0
57	MG	a	3463	1/1	0.83	0.12	45,45,45,45	0
57	MG	A	3444	1/1	0.83	0.24	48,48,48,48	0
57	MG	A	3263	1/1	0.83	0.17	55,55,55,55	0
57	MG	A	3031	1/1	0.83	0.21	70,70,70,70	0
57	MG	P	201	1/1	0.83	0.25	54,54,54,54	0
57	MG	w	101	1/1	0.83	0.19	60,60,60,60	0
57	MG	a	3354	1/1	0.83	0.19	51,51,51,51	0
57	MG	A	3376	1/1	0.83	0.13	67,67,67,67	0
57	MG	A	3121	1/1	0.83	0.20	62,62,62,62	0
57	MG	A	3243	1/1	0.84	0.18	58,58,58,58	0
57	MG	A	3173	1/1	0.84	0.15	57,57,57,57	0
57	MG	A	3133	1/1	0.84	0.18	44,44,44,44	0
57	MG	A	3092	1/1	0.84	0.24	67,67,67,67	0
57	MG	B	211	1/1	0.84	0.29	61,61,61,61	0
57	MG	B	213	1/1	0.84	0.11	81,81,81,81	0
57	MG	A	3570	1/1	0.84	0.12	57,57,57,57	0
57	MG	A	3061	1/1	0.84	0.20	54,54,54,54	0
57	MG	A	3258	1/1	0.84	0.12	43,43,43,43	0
57	MG	A	3005	1/1	0.84	0.24	40,40,40,40	0
57	MG	a	3380	1/1	0.84	0.20	57,57,57,57	0
57	MG	A	3574	1/1	0.84	0.18	57,57,57,57	0
57	MG	A	3465	1/1	0.84	0.13	68,68,68,68	0
57	MG	A	3466	1/1	0.84	0.16	67,67,67,67	0
57	MG	A	3474	1/1	0.84	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3478	1/1	0.84	0.09	65,65,65,65	0
57	MG	A	3215	1/1	0.84	0.26	66,66,66,66	0
57	MG	A	3365	1/1	0.84	0.13	51,51,51,51	0
57	MG	A	3299	1/1	0.84	0.16	64,64,64,64	0
57	MG	A	3604	1/1	0.84	0.19	64,64,64,64	0
57	MG	A	3138	1/1	0.84	0.30	77,77,77,77	0
57	MG	A	3402	1/1	0.84	0.08	50,50,50,50	0
57	MG	A	3142	1/1	0.84	0.08	84,84,84,84	0
57	MG	A	3161	1/1	0.84	0.10	67,67,67,67	0
57	MG	A	3239	1/1	0.84	0.24	56,56,56,56	0
57	MG	A	3543	1/1	0.84	0.10	71,71,71,71	0
57	MG	A	3423	1/1	0.84	0.17	59,59,59,59	0
57	MG	A	3431	1/1	0.84	0.14	69,69,69,69	0
57	MG	B	204	1/1	0.84	0.16	85,85,85,85	0
57	MG	A	3119	1/1	0.84	0.20	50,50,50,50	0
57	MG	A	3023	1/1	0.85	0.10	48,48,48,48	0
57	MG	A	3218	1/1	0.85	0.23	32,32,32,32	0
57	MG	A	3114	1/1	0.85	0.34	57,57,57,57	0
57	MG	B	218	1/1	0.85	0.15	74,74,74,74	0
57	MG	A	3261	1/1	0.85	0.15	61,61,61,61	0
57	MG	A	3393	1/1	0.85	0.24	57,57,57,57	0
57	MG	A	3152	1/1	0.85	0.26	68,68,68,68	0
57	MG	A	3102	1/1	0.85	0.12	59,59,59,59	0
57	MG	A	3182	1/1	0.85	0.10	53,53,53,53	0
57	MG	A	3505	1/1	0.85	0.21	68,68,68,68	0
57	MG	A	3266	1/1	0.85	0.20	61,61,61,61	0
57	MG	A	3242	1/1	0.85	0.12	63,63,63,63	0
57	MG	A	3269	1/1	0.85	0.14	54,54,54,54	0
57	MG	A	3120	1/1	0.85	0.25	52,52,52,52	0
57	MG	a	3403	1/1	0.85	0.10	61,61,61,61	0
57	MG	a	3405	1/1	0.85	0.18	70,70,70,70	0
57	MG	A	3203	1/1	0.85	0.16	53,53,53,53	0
57	MG	a	3409	1/1	0.85	0.13	74,74,74,74	0
57	MG	6	101	1/1	0.85	0.20	64,64,64,64	0
57	MG	A	3044	1/1	0.85	0.20	72,72,72,72	0
57	MG	a	3430	1/1	0.85	0.12	65,65,65,65	0
57	MG	a	3434	1/1	0.85	0.16	54,54,54,54	0
57	MG	A	3343	1/1	0.85	0.10	69,69,69,69	0
57	MG	a	3455	1/1	0.85	0.11	67,67,67,67	0
57	MG	A	3557	1/1	0.85	0.17	60,60,60,60	0
57	MG	A	3628	1/1	0.85	0.13	87,87,87,87	0
57	MG	a	3468	1/1	0.85	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3352	1/1	0.85	0.13	47,47,47,47	0
57	MG	A	3278	1/1	0.85	0.34	64,64,64,64	0
57	MG	A	3449	1/1	0.85	0.17	51,51,51,51	0
57	MG	e	201	1/1	0.85	0.16	69,69,69,69	0
57	MG	A	3565	1/1	0.85	0.08	67,67,67,67	0
57	MG	l	201	1/1	0.85	0.12	61,61,61,61	0
57	MG	A	3450	1/1	0.85	0.09	57,57,57,57	0
57	MG	A	3279	1/1	0.85	0.11	55,55,55,55	0
57	MG	A	3095	1/1	0.85	0.27	63,63,63,63	0
57	MG	A	3112	1/1	0.85	0.25	66,66,66,66	0
57	MG	a	3388	1/1	0.86	0.11	59,59,59,59	0
57	MG	A	3250	1/1	0.86	0.24	58,58,58,58	0
57	MG	A	3171	1/1	0.86	0.08	37,37,37,37	0
57	MG	A	3096	1/1	0.86	0.20	58,58,58,58	0
57	MG	A	3219	1/1	0.86	0.21	61,61,61,61	0
57	MG	a	3310	1/1	0.86	0.09	52,52,52,52	0
57	MG	A	3117	1/1	0.86	0.34	50,50,50,50	0
57	MG	A	3477	1/1	0.86	0.14	65,65,65,65	0
57	MG	a	3325	1/1	0.86	0.35	55,55,55,55	0
57	MG	A	3180	1/1	0.86	0.26	44,44,44,44	0
57	MG	A	3481	1/1	0.86	0.12	65,65,65,65	0
57	MG	a	3329	1/1	0.86	0.17	46,46,46,46	0
57	MG	A	3066	1/1	0.86	0.13	56,56,56,56	0
57	MG	A	3086	1/1	0.86	0.20	50,50,50,50	0
57	MG	A	3197	1/1	0.86	0.20	40,40,40,40	0
57	MG	A	3624	1/1	0.86	0.10	52,52,52,52	0
57	MG	F	302	1/1	0.86	0.37	52,52,52,52	0
57	MG	A	3039	1/1	0.86	0.23	59,59,59,59	0
57	MG	a	3467	1/1	0.86	0.12	62,62,62,62	0
57	MG	A	3064	1/1	0.86	0.22	50,50,50,50	0
57	MG	a	3360	1/1	0.86	0.27	40,40,40,40	0
57	MG	a	3475	1/1	0.86	0.22	38,38,38,38	0
57	MG	A	3076	1/1	0.86	0.10	41,41,41,41	0
57	MG	V	202	1/1	0.86	0.23	51,51,51,51	0
57	MG	A	3034	1/1	0.86	0.16	71,71,71,71	0
57	MG	A	3632	1/1	0.86	0.12	63,63,63,63	0
57	MG	A	3635	1/1	0.86	0.14	69,69,69,69	0
57	MG	A	3248	1/1	0.86	0.31	57,57,57,57	0
57	MG	a	3378	1/1	0.86	0.20	39,39,39,39	0
57	MG	A	3383	1/1	0.86	0.15	55,55,55,55	0
57	MG	a	3383	1/1	0.86	0.16	56,56,56,56	0
57	MG	A	3425	1/1	0.87	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	G	202	1/1	0.87	0.20	67,67,67,67	0
57	MG	A	3506	1/1	0.87	0.11	49,49,49,49	0
57	MG	A	3511	1/1	0.87	0.11	99,99,99,99	0
57	MG	R	201	1/1	0.87	0.12	67,67,67,67	0
57	MG	A	3236	1/1	0.87	0.36	67,67,67,67	0
57	MG	V	201	1/1	0.87	0.08	53,53,53,53	0
57	MG	A	3346	1/1	0.87	0.17	68,68,68,68	0
57	MG	A	3125	1/1	0.87	0.20	31,31,31,31	0
57	MG	A	3353	1/1	0.87	0.24	79,79,79,79	0
57	MG	A	3036	1/1	0.87	0.17	74,74,74,74	0
57	MG	A	3615	1/1	0.87	0.12	50,50,50,50	0
57	MG	A	3551	1/1	0.87	0.12	63,63,63,63	0
57	MG	A	3147	1/1	0.87	0.16	64,64,64,64	0
57	MG	A	3288	1/1	0.87	0.18	60,60,60,60	0
57	MG	A	3162	1/1	0.87	0.13	71,71,71,71	0
57	MG	x	3002	1/1	0.87	0.19	101,101,101,101	0
57	MG	A	3212	1/1	0.87	0.10	55,55,55,55	0
57	MG	a	3418	1/1	0.87	0.13	67,67,67,67	0
57	MG	A	3103	1/1	0.87	0.21	56,56,56,56	0
57	MG	A	3166	1/1	0.87	0.21	57,57,57,57	0
57	MG	A	3271	1/1	0.87	0.22	57,57,57,57	0
57	MG	a	3324	1/1	0.87	0.29	40,40,40,40	0
57	MG	a	3440	1/1	0.87	0.12	69,69,69,69	0
57	MG	a	3445	1/1	0.87	0.20	66,66,66,66	0
57	MG	a	3446	1/1	0.87	0.12	68,68,68,68	0
57	MG	A	3132	1/1	0.87	0.30	48,48,48,48	0
57	MG	A	3384	1/1	0.87	0.23	51,51,51,51	0
57	MG	A	3046	1/1	0.87	0.14	55,55,55,55	0
57	MG	A	3398	1/1	0.87	0.14	43,43,43,43	0
57	MG	A	3275	1/1	0.87	0.19	63,63,63,63	0
57	MG	A	3052	1/1	0.87	0.19	59,59,59,59	0
57	MG	A	3020	1/1	0.87	0.16	50,50,50,50	0
57	MG	A	3088	1/1	0.87	0.16	63,63,63,63	0
57	MG	a	3481	1/1	0.87	0.21	46,46,46,46	0
57	MG	a	3348	1/1	0.87	0.14	53,53,53,53	0
57	MG	A	3419	1/1	0.87	0.15	74,74,74,74	0
57	MG	A	3342	1/1	0.87	0.09	61,61,61,61	0
57	MG	a	3356	1/1	0.87	0.20	49,49,49,49	0
57	MG	A	3589	1/1	0.87	0.13	46,46,46,46	0
57	MG	A	3593	1/1	0.87	0.18	41,41,41,41	0
57	MG	A	3595	1/1	0.87	0.16	63,63,63,63	0
57	MG	A	3596	1/1	0.87	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3515	1/1	0.88	0.14	48,48,48,48	0
57	MG	A	3434	1/1	0.88	0.11	56,56,56,56	0
57	MG	Q	204	1/1	0.88	0.18	56,56,56,56	0
57	MG	Q	205	1/1	0.88	0.15	55,55,55,55	0
57	MG	A	3107	1/1	0.88	0.32	75,75,75,75	0
57	MG	U	201	1/1	0.88	0.23	72,72,72,72	0
57	MG	A	3053	1/1	0.88	0.30	61,61,61,61	0
57	MG	A	3294	1/1	0.88	0.11	44,44,44,44	0
57	MG	A	3546	1/1	0.88	0.16	53,53,53,53	0
57	MG	A	3297	1/1	0.88	0.23	67,67,67,67	0
57	MG	A	3610	1/1	0.88	0.14	61,61,61,61	0
57	MG	Z	301	1/1	0.88	0.12	66,66,66,66	0
57	MG	A	3550	1/1	0.88	0.14	58,58,58,58	0
57	MG	A	3270	1/1	0.88	0.26	61,61,61,61	0
57	MG	A	3552	1/1	0.88	0.12	64,64,64,64	0
57	MG	A	3620	1/1	0.88	0.18	49,49,49,49	0
57	MG	A	3097	1/1	0.88	0.22	60,60,60,60	0
57	MG	A	3305	1/1	0.88	0.17	70,70,70,70	0
57	MG	A	3370	1/1	0.88	0.14	64,64,64,64	0
57	MG	A	3371	1/1	0.88	0.13	53,53,53,53	0
57	MG	A	3010	1/1	0.88	0.14	41,41,41,41	0
57	MG	A	3631	1/1	0.88	0.11	87,87,87,87	0
57	MG	A	3254	1/1	0.88	0.31	67,67,67,67	0
57	MG	A	3469	1/1	0.88	0.10	54,54,54,54	0
57	MG	A	3471	1/1	0.88	0.19	56,56,56,56	0
57	MG	A	3472	1/1	0.88	0.08	53,53,53,53	0
57	MG	A	3255	1/1	0.88	0.33	57,57,57,57	0
57	MG	A	3185	1/1	0.88	0.34	63,63,63,63	0
57	MG	A	3277	1/1	0.88	0.25	71,71,71,71	0
57	MG	A	3042	1/1	0.88	0.17	92,92,92,92	0
57	MG	A	3116	1/1	0.88	0.23	50,50,50,50	0
57	MG	A	3341	1/1	0.88	0.12	57,57,57,57	0
57	MG	a	3346	1/1	0.88	0.14	50,50,50,50	0
57	MG	A	3130	1/1	0.88	0.21	43,43,43,43	0
57	MG	A	3164	1/1	0.88	0.20	51,51,51,51	0
57	MG	A	3025	1/1	0.88	0.16	60,60,60,60	0
57	MG	A	3592	1/1	0.88	0.15	67,67,67,67	0
57	MG	A	3348	1/1	0.88	0.13	71,71,71,71	0
57	MG	A	3151	1/1	0.88	0.17	43,43,43,43	0
57	MG	A	3073	1/1	0.88	0.21	56,56,56,56	0
57	MG	A	3597	1/1	0.88	0.20	65,65,65,65	0
57	MG	G	203	1/1	0.88	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3426	1/1	0.89	0.17	55,55,55,55	0
57	MG	A	3598	1/1	0.89	0.14	74,74,74,74	0
57	MG	A	3599	1/1	0.89	0.17	57,57,57,57	0
57	MG	A	3476	1/1	0.89	0.14	50,50,50,50	0
57	MG	A	3058	1/1	0.89	0.27	57,57,57,57	0
57	MG	a	3301	1/1	0.89	0.16	49,49,49,49	0
57	MG	A	3222	1/1	0.89	0.20	33,33,33,33	0
57	MG	A	3224	1/1	0.89	0.17	51,51,51,51	0
57	MG	a	3319	1/1	0.89	0.21	39,39,39,39	0
57	MG	a	3320	1/1	0.89	0.11	39,39,39,39	0
57	MG	a	3322	1/1	0.89	0.11	50,50,50,50	0
57	MG	A	3331	1/1	0.89	0.19	54,54,54,54	0
57	MG	A	3006	1/1	0.89	0.16	57,57,57,57	0
57	MG	A	3490	1/1	0.89	0.12	47,47,47,47	0
57	MG	A	3194	1/1	0.89	0.17	34,34,34,34	0
57	MG	a	3422	1/1	0.89	0.09	50,50,50,50	0
57	MG	a	3425	1/1	0.89	0.19	47,47,47,47	0
57	MG	a	3428	1/1	0.89	0.18	46,46,46,46	0
57	MG	A	3085	1/1	0.89	0.24	52,52,52,52	0
57	MG	A	3167	1/1	0.89	0.14	65,65,65,65	0
57	MG	a	3435	1/1	0.89	0.12	57,57,57,57	0
57	MG	A	3030	1/1	0.89	0.16	64,64,64,64	0
57	MG	A	3347	1/1	0.89	0.12	75,75,75,75	0
57	MG	Q	203	1/1	0.89	0.10	45,45,45,45	0
57	MG	a	3337	1/1	0.89	0.21	50,50,50,50	0
57	MG	A	3621	1/1	0.89	0.17	59,59,59,59	0
57	MG	a	3342	1/1	0.89	0.19	50,50,50,50	0
57	MG	A	3510	1/1	0.89	0.15	60,60,60,60	0
57	MG	A	3301	1/1	0.89	0.22	57,57,57,57	0
57	MG	R	202	1/1	0.89	0.17	53,53,53,53	0
57	MG	a	3470	1/1	0.89	0.10	56,56,56,56	0
57	MG	A	3455	1/1	0.89	0.20	73,73,73,73	0
57	MG	A	3525	1/1	0.89	0.10	54,54,54,54	0
57	MG	a	3477	1/1	0.89	0.12	68,68,68,68	0
57	MG	A	3159	1/1	0.89	0.13	78,78,78,78	0
57	MG	A	3175	1/1	0.89	0.15	46,46,46,46	0
57	MG	A	3535	1/1	0.89	0.15	49,49,49,49	0
57	MG	A	3541	1/1	0.89	0.16	56,56,56,56	0
57	MG	A	3001	1/1	0.89	0.24	70,70,70,70	0
57	MG	A	3312	1/1	0.89	0.19	59,59,59,59	0
57	MG	A	3019	1/1	0.89	0.10	49,49,49,49	0
57	MG	0	103	1/1	0.89	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	a	3377	1/1	0.89	0.08	85,85,85,85	0
57	MG	A	3050	1/1	0.89	0.16	39,39,39,39	0
57	MG	A	3591	1/1	0.90	0.10	66,66,66,66	0
57	MG	A	3452	1/1	0.90	0.16	53,53,53,53	0
57	MG	A	3410	1/1	0.90	0.12	51,51,51,51	0
57	MG	A	3192	1/1	0.90	0.23	39,39,39,39	0
57	MG	A	3024	1/1	0.90	0.11	63,63,63,63	0
57	MG	A	3558	1/1	0.90	0.12	73,73,73,73	0
57	MG	A	3367	1/1	0.90	0.20	51,51,51,51	0
57	MG	A	3562	1/1	0.90	0.09	59,59,59,59	0
57	MG	a	3423	1/1	0.90	0.20	66,66,66,66	0
57	MG	a	3341	1/1	0.90	0.14	60,60,60,60	0
57	MG	A	3223	1/1	0.90	0.24	61,61,61,61	0
57	MG	A	3106	1/1	0.90	0.15	57,57,57,57	0
57	MG	A	3174	1/1	0.90	0.16	59,59,59,59	0
57	MG	A	3568	1/1	0.90	0.10	83,83,83,83	0
57	MG	A	3528	1/1	0.90	0.07	51,51,51,51	0
57	MG	A	3027	1/1	0.90	0.09	44,44,44,44	0
57	MG	A	3286	1/1	0.90	0.12	62,62,62,62	0
57	MG	a	3359	1/1	0.90	0.12	65,65,65,65	0
57	MG	A	3028	1/1	0.90	0.24	66,66,66,66	0
57	MG	a	3458	1/1	0.90	0.14	62,62,62,62	0
57	MG	9	101	1/1	0.90	0.12	57,57,57,57	0
57	MG	A	3237	1/1	0.90	0.23	51,51,51,51	0
57	MG	a	3368	1/1	0.90	0.21	44,44,44,44	0
57	MG	E	301	1/1	0.90	0.33	56,56,56,56	0
57	MG	a	3469	1/1	0.90	0.18	42,42,42,42	0
57	MG	A	3118	1/1	0.90	0.41	52,52,52,52	0
57	MG	a	3471	1/1	0.90	0.15	49,49,49,49	0
57	MG	A	3616	1/1	0.90	0.18	59,59,59,59	0
57	MG	a	3302	1/1	0.90	0.09	58,58,58,58	0
57	MG	a	3375	1/1	0.90	0.21	41,41,41,41	0
57	MG	a	3309	1/1	0.90	0.33	37,37,37,37	0
57	MG	A	3111	1/1	0.90	0.13	61,61,61,61	0
57	MG	A	3619	1/1	0.90	0.20	78,78,78,78	0
57	MG	a	3316	1/1	0.90	0.15	54,54,54,54	0
57	MG	A	3143	1/1	0.90	0.18	60,60,60,60	0
57	MG	A	3406	1/1	0.90	0.10	56,56,56,56	0
57	MG	A	3583	1/1	0.90	0.15	55,55,55,55	0
57	MG	w	102	1/1	0.90	0.17	49,49,49,49	0
57	MG	Q	202	1/1	0.90	0.20	51,51,51,51	0
57	MG	A	3091	1/1	0.90	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3497	1/1	0.90	0.13	50,50,50,50	0
57	MG	A	3140	1/1	0.91	0.15	57,57,57,57	0
57	MG	a	3373	1/1	0.91	0.16	63,63,63,63	0
57	MG	A	3241	1/1	0.91	0.08	42,42,42,42	0
57	MG	A	3333	1/1	0.91	0.10	62,62,62,62	0
57	MG	A	3264	1/1	0.91	0.30	65,65,65,65	0
57	MG	A	3339	1/1	0.91	0.11	68,68,68,68	0
57	MG	a	3382	1/1	0.91	0.14	31,31,31,31	0
57	MG	A	3141	1/1	0.91	0.17	55,55,55,55	0
57	MG	A	3290	1/1	0.91	0.18	49,49,49,49	0
57	MG	A	3072	1/1	0.91	0.18	43,43,43,43	0
57	MG	A	3041	1/1	0.91	0.17	42,42,42,42	0
57	MG	A	3488	1/1	0.91	0.16	50,50,50,50	0
57	MG	A	3418	1/1	0.91	0.22	32,32,32,32	0
57	MG	a	3396	1/1	0.91	0.15	42,42,42,42	0
57	MG	A	3633	1/1	0.91	0.18	64,64,64,64	0
57	MG	A	3217	1/1	0.91	0.30	50,50,50,50	0
57	MG	A	3144	1/1	0.91	0.15	38,38,38,38	0
57	MG	B	205	1/1	0.91	0.15	81,81,81,81	0
57	MG	A	3493	1/1	0.91	0.20	33,33,33,33	0
57	MG	A	3007	1/1	0.91	0.12	46,46,46,46	0
57	MG	a	3416	1/1	0.91	0.16	61,61,61,61	0
57	MG	a	3311	1/1	0.91	0.14	51,51,51,51	0
57	MG	A	3109	1/1	0.91	0.10	52,52,52,52	0
57	MG	A	3251	1/1	0.91	0.13	35,35,35,35	0
57	MG	A	3015	1/1	0.91	0.12	43,43,43,43	0
57	MG	A	3079	1/1	0.91	0.21	63,63,63,63	0
57	MG	a	3426	1/1	0.91	0.09	69,69,69,69	0
57	MG	a	3427	1/1	0.91	0.24	50,50,50,50	0
57	MG	A	3358	1/1	0.91	0.10	63,63,63,63	0
57	MG	A	3311	1/1	0.91	0.26	52,52,52,52	0
57	MG	A	3512	1/1	0.91	0.10	51,51,51,51	0
57	MG	B	217	1/1	0.91	0.17	67,67,67,67	0
57	MG	A	3123	1/1	0.91	0.10	51,51,51,51	0
57	MG	A	3314	1/1	0.91	0.14	54,54,54,54	0
57	MG	a	3444	1/1	0.91	0.10	53,53,53,53	0
57	MG	D	303	1/1	0.91	0.58	49,49,49,49	0
57	MG	D	305	1/1	0.91	0.06	37,37,37,37	0
57	MG	A	3442	1/1	0.91	0.10	56,56,56,56	0
57	MG	A	3199	1/1	0.91	0.19	42,42,42,42	0
57	MG	a	3335	1/1	0.91	0.21	37,37,37,37	0
57	MG	a	3460	1/1	0.91	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	a	3462	1/1	0.91	0.08	74,74,74,74	0
57	MG	A	3018	1/1	0.91	0.11	49,49,49,49	0
57	MG	a	3338	1/1	0.91	0.13	66,66,66,66	0
57	MG	A	3533	1/1	0.91	0.13	47,47,47,47	0
57	MG	F	305	1/1	0.91	0.20	59,59,59,59	0
57	MG	G	201	1/1	0.91	0.09	71,71,71,71	0
57	MG	A	3368	1/1	0.91	0.09	47,47,47,47	0
57	MG	A	3538	1/1	0.91	0.09	40,40,40,40	0
57	MG	a	3474	1/1	0.91	0.10	64,64,64,64	0
57	MG	A	3322	1/1	0.91	0.12	61,61,61,61	0
57	MG	a	3476	1/1	0.91	0.07	50,50,50,50	0
57	MG	A	3325	1/1	0.91	0.16	52,52,52,52	0
57	MG	A	3373	1/1	0.91	0.06	64,64,64,64	0
57	MG	A	3457	1/1	0.91	0.10	41,41,41,41	0
57	MG	A	3375	1/1	0.91	0.07	55,55,55,55	0
57	MG	a	3485	1/1	0.91	0.13	51,51,51,51	0
57	MG	A	3464	1/1	0.91	0.10	49,49,49,49	0
57	MG	A	3204	1/1	0.91	0.06	43,43,43,43	0
57	MG	A	3612	1/1	0.91	0.11	53,53,53,53	0
57	MG	l	202	1/1	0.91	0.20	61,61,61,61	0
57	MG	a	3364	1/1	0.91	0.26	56,56,56,56	0
57	MG	A	3613	1/1	0.91	0.16	52,52,52,52	0
57	MG	A	3069	1/1	0.91	0.21	46,46,46,46	0
57	MG	A	3553	1/1	0.91	0.06	40,40,40,40	0
57	MG	A	3467	1/1	0.91	0.20	52,52,52,52	0
57	MG	A	3409	1/1	0.92	0.21	60,60,60,60	0
57	MG	A	3043	1/1	0.92	0.08	59,59,59,59	0
57	MG	A	3412	1/1	0.92	0.12	45,45,45,45	0
57	MG	a	3397	1/1	0.92	0.25	27,27,27,27	0
57	MG	A	3414	1/1	0.92	0.16	31,31,31,31	0
57	MG	A	3257	1/1	0.92	0.12	50,50,50,50	0
57	MG	a	3404	1/1	0.92	0.23	38,38,38,38	0
57	MG	B	212	1/1	0.92	0.10	75,75,75,75	0
57	MG	A	3344	1/1	0.92	0.06	53,53,53,53	0
57	MG	A	3183	1/1	0.92	0.17	54,54,54,54	0
57	MG	A	3090	1/1	0.92	0.19	38,38,38,38	0
57	MG	a	3321	1/1	0.92	0.10	48,48,48,48	0
57	MG	B	216	1/1	0.92	0.12	86,86,86,86	0
57	MG	A	3071	1/1	0.92	0.13	41,41,41,41	0
57	MG	a	3421	1/1	0.92	0.09	61,61,61,61	0
57	MG	A	3350	1/1	0.92	0.12	63,63,63,63	0
57	MG	A	3432	1/1	0.92	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3188	1/1	0.92	0.17	44,44,44,44	0
57	MG	A	3295	1/1	0.92	0.15	30,30,30,30	0
57	MG	A	3518	1/1	0.92	0.07	65,65,65,65	0
57	MG	E	302	1/1	0.92	0.07	35,35,35,35	0
57	MG	a	3331	1/1	0.92	0.13	55,55,55,55	0
57	MG	A	3296	1/1	0.92	0.25	52,52,52,52	0
57	MG	A	3051	1/1	0.92	0.17	43,43,43,43	0
57	MG	A	3356	1/1	0.92	0.19	57,57,57,57	0
57	MG	A	3440	1/1	0.92	0.19	74,74,74,74	0
57	MG	A	3228	1/1	0.92	0.18	62,62,62,62	0
57	MG	A	3149	1/1	0.92	0.21	53,53,53,53	0
57	MG	A	3235	1/1	0.92	0.09	48,48,48,48	0
57	MG	A	3196	1/1	0.92	0.22	44,44,44,44	0
57	MG	a	3345	1/1	0.92	0.12	47,47,47,47	0
57	MG	A	3122	1/1	0.92	0.09	35,35,35,35	0
57	MG	A	3310	1/1	0.92	0.08	45,45,45,45	0
57	MG	A	3611	1/1	0.92	0.18	52,52,52,52	0
57	MG	A	3544	1/1	0.92	0.08	55,55,55,55	0
57	MG	A	3268	1/1	0.92	0.10	58,58,58,58	0
57	MG	A	3198	1/1	0.92	0.18	55,55,55,55	0
57	MG	A	3009	1/1	0.92	0.21	50,50,50,50	0
57	MG	R	203	1/1	0.92	0.12	44,44,44,44	0
57	MG	A	3105	1/1	0.92	0.06	35,35,35,35	0
57	MG	U	202	1/1	0.92	0.11	62,62,62,62	0
57	MG	a	3473	1/1	0.92	0.22	43,43,43,43	0
57	MG	A	3462	1/1	0.92	0.10	53,53,53,53	0
57	MG	A	3372	1/1	0.92	0.10	59,59,59,59	0
57	MG	A	3318	1/1	0.92	0.19	60,60,60,60	0
57	MG	A	3139	1/1	0.92	0.16	62,62,62,62	0
57	MG	A	3207	1/1	0.92	0.09	40,40,40,40	0
57	MG	A	3154	1/1	0.92	0.14	60,60,60,60	0
57	MG	A	3210	1/1	0.92	0.20	56,56,56,56	0
57	MG	A	3211	1/1	0.92	0.23	55,55,55,55	0
57	MG	A	3247	1/1	0.92	0.25	66,66,66,66	0
57	MG	A	3155	1/1	0.92	0.20	44,44,44,44	0
57	MG	A	3115	1/1	0.92	0.08	48,48,48,48	0
57	MG	A	3067	1/1	0.92	0.20	70,70,70,70	0
57	MG	A	3063	1/1	0.92	0.12	62,62,62,62	0
57	MG	a	3387	1/1	0.92	0.05	55,55,55,55	0
57	MG	w	106	1/1	0.92	0.20	45,45,45,45	0
57	MG	A	3407	1/1	0.92	0.07	38,38,38,38	0
57	MG	y	701	1/1	0.92	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3487	1/1	0.92	0.16	60,60,60,60	0
57	MG	A	3181	1/1	0.92	0.12	35,35,35,35	0
61	GDP	y	703	28/28	0.92	0.11	91,120,142,146	0
57	MG	A	3509	1/1	0.93	0.19	51,51,51,51	0
57	MG	A	3392	1/1	0.93	0.08	47,47,47,47	0
57	MG	A	3575	1/1	0.93	0.14	70,70,70,70	0
57	MG	a	3304	1/1	0.93	0.13	55,55,55,55	0
57	MG	a	3306	1/1	0.93	0.20	55,55,55,55	0
57	MG	a	3395	1/1	0.93	0.19	32,32,32,32	0
57	MG	A	3214	1/1	0.93	0.21	52,52,52,52	0
57	MG	A	3349	1/1	0.93	0.09	39,39,39,39	0
57	MG	A	3136	1/1	0.93	0.10	49,49,49,49	0
57	MG	a	3313	1/1	0.93	0.11	61,61,61,61	0
57	MG	A	3580	1/1	0.93	0.17	67,67,67,67	0
57	MG	A	3516	1/1	0.93	0.15	55,55,55,55	0
57	MG	A	3517	1/1	0.93	0.14	51,51,51,51	0
57	MG	A	3169	1/1	0.93	0.22	57,57,57,57	0
57	MG	A	3590	1/1	0.93	0.13	59,59,59,59	0
57	MG	a	3413	1/1	0.93	0.06	54,54,54,54	0
57	MG	A	3047	1/1	0.93	0.14	39,39,39,39	0
57	MG	A	3200	1/1	0.93	0.12	44,44,44,44	0
57	MG	A	3463	1/1	0.93	0.14	46,46,46,46	0
57	MG	a	3420	1/1	0.93	0.10	62,62,62,62	0
57	MG	A	3201	1/1	0.93	0.14	63,63,63,63	0
57	MG	a	3326	1/1	0.93	0.16	48,48,48,48	0
57	MG	A	3172	1/1	0.93	0.24	31,31,31,31	0
57	MG	A	3131	1/1	0.93	0.10	53,53,53,53	0
57	MG	E	303	1/1	0.93	0.12	41,41,41,41	0
57	MG	A	3536	1/1	0.93	0.12	39,39,39,39	0
57	MG	A	3206	1/1	0.93	0.07	65,65,65,65	0
57	MG	A	3082	1/1	0.93	0.42	53,53,53,53	0
57	MG	F	304	1/1	0.93	0.17	60,60,60,60	0
57	MG	A	3190	1/1	0.93	0.19	38,38,38,38	0
57	MG	a	3336	1/1	0.93	0.24	62,62,62,62	0
57	MG	A	3230	1/1	0.93	0.18	46,46,46,46	0
57	MG	A	3252	1/1	0.93	0.21	58,58,58,58	0
57	MG	A	3545	1/1	0.93	0.19	64,64,64,64	0
57	MG	N	201	1/1	0.93	0.12	57,57,57,57	0
57	MG	a	3447	1/1	0.93	0.20	36,36,36,36	0
57	MG	a	3454	1/1	0.93	0.18	39,39,39,39	0
57	MG	A	3422	1/1	0.93	0.10	52,52,52,52	0
57	MG	A	3547	1/1	0.93	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3298	1/1	0.93	0.09	58,58,58,58	0
57	MG	A	3335	1/1	0.93	0.07	56,56,56,56	0
57	MG	a	3461	1/1	0.93	0.08	44,44,44,44	0
57	MG	a	3349	1/1	0.93	0.23	47,47,47,47	0
57	MG	A	3479	1/1	0.93	0.14	43,43,43,43	0
57	MG	a	3352	1/1	0.93	0.18	59,59,59,59	0
57	MG	A	3098	1/1	0.93	0.10	48,48,48,48	0
57	MG	A	3232	1/1	0.93	0.17	36,36,36,36	0
57	MG	A	3483	1/1	0.93	0.12	55,55,55,55	0
57	MG	A	3099	1/1	0.93	0.13	34,34,34,34	0
57	MG	A	3556	1/1	0.93	0.09	55,55,55,55	0
57	MG	A	3195	1/1	0.93	0.15	41,41,41,41	0
57	MG	A	3374	1/1	0.93	0.10	58,58,58,58	0
57	MG	A	3559	1/1	0.93	0.08	46,46,46,46	0
57	MG	A	3308	1/1	0.93	0.09	56,56,56,56	0
57	MG	A	3561	1/1	0.93	0.08	54,54,54,54	0
57	MG	A	3345	1/1	0.93	0.11	44,44,44,44	0
57	MG	A	3379	1/1	0.93	0.16	50,50,50,50	0
57	MG	A	3037	1/1	0.93	0.12	61,61,61,61	0
57	MG	A	3238	1/1	0.93	0.17	45,45,45,45	0
57	MG	a	3487	1/1	0.93	0.15	35,35,35,35	0
57	MG	A	3567	1/1	0.93	0.11	47,47,47,47	0
57	MG	a	3376	1/1	0.93	0.13	46,46,46,46	0
57	MG	A	3499	1/1	0.93	0.07	60,60,60,60	0
57	MG	A	3385	1/1	0.93	0.12	57,57,57,57	0
57	MG	a	3379	1/1	0.93	0.14	30,30,30,30	0
57	MG	B	203	1/1	0.93	0.09	56,56,56,56	0
57	MG	w	105	1/1	0.93	0.22	29,29,29,29	0
57	MG	A	3387	1/1	0.93	0.08	53,53,53,53	0
57	MG	A	3390	1/1	0.93	0.15	46,46,46,46	0
57	MG	a	3384	1/1	0.93	0.12	49,49,49,49	0
57	MG	a	3385	1/1	0.93	0.10	33,33,33,33	0
57	MG	a	3386	1/1	0.93	0.27	41,41,41,41	0
57	MG	A	3507	1/1	0.93	0.10	46,46,46,46	0
57	MG	D	304	1/1	0.94	0.09	74,74,74,74	0
57	MG	A	3189	1/1	0.94	0.24	37,37,37,37	0
57	MG	A	3016	1/1	0.94	0.08	49,49,49,49	0
57	MG	A	3520	1/1	0.94	0.14	80,80,80,80	0
57	MG	A	3523	1/1	0.94	0.16	36,36,36,36	0
57	MG	A	3427	1/1	0.94	0.12	62,62,62,62	0
57	MG	A	3176	1/1	0.94	0.08	35,35,35,35	0
57	MG	A	3193	1/1	0.94	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	F	303	1/1	0.94	0.10	36,36,36,36	0
57	MG	a	3441	1/1	0.94	0.10	62,62,62,62	0
57	MG	A	3021	1/1	0.94	0.14	34,34,34,34	0
57	MG	a	3315	1/1	0.94	0.20	60,60,60,60	0
57	MG	A	3168	1/1	0.94	0.30	48,48,48,48	0
57	MG	A	3534	1/1	0.94	0.19	45,45,45,45	0
57	MG	a	3448	1/1	0.94	0.07	42,42,42,42	0
57	MG	a	3452	1/1	0.94	0.07	52,52,52,52	0
57	MG	A	3306	1/1	0.94	0.08	50,50,50,50	0
57	MG	A	3077	1/1	0.94	0.13	48,48,48,48	0
57	MG	a	3457	1/1	0.94	0.21	41,41,41,41	0
57	MG	A	3437	1/1	0.94	0.12	28,28,28,28	0
57	MG	A	3336	1/1	0.94	0.10	36,36,36,36	0
57	MG	A	3400	1/1	0.94	0.08	35,35,35,35	0
57	MG	Q	201	1/1	0.94	0.18	51,51,51,51	0
57	MG	A	3362	1/1	0.94	0.11	50,50,50,50	0
57	MG	A	3584	1/1	0.94	0.11	62,62,62,62	0
57	MG	a	3465	1/1	0.94	0.06	57,57,57,57	0
57	MG	A	3363	1/1	0.94	0.09	30,30,30,30	0
57	MG	A	3587	1/1	0.94	0.17	48,48,48,48	0
57	MG	B	201	1/1	0.94	0.07	51,51,51,51	0
57	MG	B	202	1/1	0.94	0.13	66,66,66,66	0
57	MG	A	3170	1/1	0.94	0.11	43,43,43,43	0
57	MG	A	3447	1/1	0.94	0.11	67,67,67,67	0
57	MG	A	3448	1/1	0.94	0.30	48,48,48,48	0
57	MG	A	3100	1/1	0.94	0.12	45,45,45,45	0
57	MG	A	3494	1/1	0.94	0.10	42,42,42,42	0
57	MG	A	3184	1/1	0.94	0.23	40,40,40,40	0
57	MG	A	3022	1/1	0.94	0.15	33,33,33,33	0
57	MG	A	3369	1/1	0.94	0.10	54,54,54,54	0
57	MG	A	3454	1/1	0.94	0.13	51,51,51,51	0
57	MG	a	3344	1/1	0.94	0.09	51,51,51,51	0
57	MG	A	3313	1/1	0.94	0.13	44,44,44,44	0
57	MG	a	3486	1/1	0.94	0.14	38,38,38,38	0
57	MG	a	3408	1/1	0.94	0.07	55,55,55,55	0
57	MG	A	3456	1/1	0.94	0.14	47,47,47,47	0
57	MG	A	3080	1/1	0.94	0.18	54,54,54,54	0
57	MG	a	3411	1/1	0.94	0.10	53,53,53,53	0
57	MG	a	3412	1/1	0.94	0.16	48,48,48,48	0
57	MG	m	201	1/1	0.94	0.07	35,35,35,35	0
57	MG	A	3187	1/1	0.94	0.24	47,47,47,47	0
57	MG	a	3414	1/1	0.94	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3415	1/1	0.94	0.17	42,42,42,42	0
57	MG	A	3221	1/1	0.94	0.19	58,58,58,58	0
57	MG	a	3353	1/1	0.94	0.20	48,48,48,48	0
57	MG	A	3274	1/1	0.94	0.11	45,45,45,45	0
57	MG	A	3026	1/1	0.94	0.07	55,55,55,55	0
57	MG	a	3357	1/1	0.94	0.13	48,48,48,48	0
57	MG	A	3324	1/1	0.94	0.15	43,43,43,43	0
57	MG	A	3220	1/1	0.95	0.09	49,49,49,49	0
57	MG	A	3280	1/1	0.95	0.17	32,32,32,32	0
57	MG	A	3443	1/1	0.95	0.14	39,39,39,39	0
57	MG	A	3208	1/1	0.95	0.18	40,40,40,40	0
57	MG	A	3485	1/1	0.95	0.14	38,38,38,38	0
57	MG	A	3626	1/1	0.95	0.13	51,51,51,51	0
57	MG	A	3446	1/1	0.95	0.15	39,39,39,39	0
57	MG	A	3300	1/1	0.95	0.14	60,60,60,60	0
57	MG	A	3539	1/1	0.95	0.07	52,52,52,52	0
57	MG	A	3581	1/1	0.95	0.09	55,55,55,55	0
57	MG	A	3033	1/1	0.95	0.11	39,39,39,39	0
57	MG	a	3451	1/1	0.95	0.10	49,49,49,49	0
57	MG	a	3381	1/1	0.95	0.14	55,55,55,55	0
57	MG	A	3283	1/1	0.95	0.07	55,55,55,55	0
57	MG	A	3413	1/1	0.95	0.10	51,51,51,51	0
57	MG	A	3127	1/1	0.95	0.11	73,73,73,73	0
57	MG	A	3588	1/1	0.95	0.08	40,40,40,40	0
57	MG	A	3146	1/1	0.95	0.13	56,56,56,56	0
57	MG	A	3453	1/1	0.95	0.12	44,44,44,44	0
57	MG	A	3382	1/1	0.95	0.12	36,36,36,36	0
57	MG	A	3307	1/1	0.95	0.09	45,45,45,45	0
57	MG	A	3500	1/1	0.95	0.12	40,40,40,40	0
57	MG	A	3074	1/1	0.95	0.16	42,42,42,42	0
57	MG	A	3503	1/1	0.95	0.15	41,41,41,41	0
57	MG	A	3504	1/1	0.95	0.19	38,38,38,38	0
57	MG	a	3339	1/1	0.95	0.15	50,50,50,50	0
57	MG	A	3012	1/1	0.95	0.07	37,37,37,37	0
57	MG	a	3399	1/1	0.95	0.16	36,36,36,36	0
57	MG	A	3424	1/1	0.95	0.13	57,57,57,57	0
57	MG	a	3401	1/1	0.95	0.30	44,44,44,44	0
57	MG	A	3386	1/1	0.95	0.16	59,59,59,59	0
57	MG	A	3601	1/1	0.95	0.12	45,45,45,45	0
57	MG	A	3289	1/1	0.95	0.07	43,43,43,43	0
57	MG	A	3388	1/1	0.95	0.06	47,47,47,47	0
57	MG	a	3479	1/1	0.95	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	a	3347	1/1	0.95	0.15	41,41,41,41	0
57	MG	A	3429	1/1	0.95	0.12	30,30,30,30	0
57	MG	A	3389	1/1	0.95	0.13	30,30,30,30	0
57	MG	7	103	1/1	0.95	0.08	57,57,57,57	0
57	MG	D	301	1/1	0.95	0.19	41,41,41,41	0
57	MG	A	3070	1/1	0.95	0.08	57,57,57,57	0
57	MG	A	3178	1/1	0.95	0.17	31,31,31,31	0
57	MG	a	3415	1/1	0.95	0.14	62,62,62,62	0
57	MG	A	3364	1/1	0.95	0.07	61,61,61,61	0
57	MG	A	3292	1/1	0.95	0.23	54,54,54,54	0
57	MG	A	3179	1/1	0.95	0.16	43,43,43,43	0
57	MG	a	3303	1/1	0.95	0.13	58,58,58,58	0
57	MG	A	3521	1/1	0.95	0.07	60,60,60,60	0
57	MG	w	104	1/1	0.95	0.11	38,38,38,38	0
57	MG	A	3048	1/1	0.95	0.14	43,43,43,43	0
57	MG	A	3078	1/1	0.95	0.13	47,47,47,47	0
57	MG	a	3363	1/1	0.95	0.23	43,43,43,43	0
57	MG	A	3527	1/1	0.95	0.20	63,63,63,63	0
57	MG	a	3365	1/1	0.95	0.21	45,45,45,45	0
57	MG	A	3035	1/1	0.95	0.07	47,47,47,47	0
57	MG	a	3429	1/1	0.95	0.16	49,49,49,49	0
57	MG	a	3367	1/1	0.96	0.21	30,30,30,30	0
57	MG	A	3438	1/1	0.96	0.08	53,53,53,53	0
57	MG	a	3432	1/1	0.96	0.07	46,46,46,46	0
57	MG	A	3303	1/1	0.96	0.06	55,55,55,55	0
57	MG	A	3519	1/1	0.96	0.14	30,30,30,30	0
57	MG	A	3304	1/1	0.96	0.10	39,39,39,39	0
57	MG	a	3439	1/1	0.96	0.10	48,48,48,48	0
57	MG	A	3089	1/1	0.96	0.10	47,47,47,47	0
57	MG	A	3351	1/1	0.96	0.10	38,38,38,38	0
57	MG	a	3317	1/1	0.96	0.15	26,26,26,26	0
57	MG	a	3318	1/1	0.96	0.12	41,41,41,41	0
57	MG	A	3524	1/1	0.96	0.10	53,53,53,53	0
57	MG	A	3327	1/1	0.96	0.06	49,49,49,49	0
57	MG	A	3526	1/1	0.96	0.05	41,41,41,41	0
57	MG	a	3450	1/1	0.96	0.06	55,55,55,55	0
57	MG	A	3145	1/1	0.96	0.11	48,48,48,48	0
57	MG	A	3445	1/1	0.96	0.07	51,51,51,51	0
57	MG	A	3622	1/1	0.96	0.15	49,49,49,49	0
57	MG	A	3529	1/1	0.96	0.15	56,56,56,56	0
57	MG	A	3484	1/1	0.96	0.08	50,50,50,50	0
57	MG	A	3411	1/1	0.96	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3486	1/1	0.96	0.11	40,40,40,40	0
57	MG	A	3083	1/1	0.96	0.08	37,37,37,37	0
57	MG	A	3579	1/1	0.96	0.10	53,53,53,53	0
57	MG	A	3630	1/1	0.96	0.13	43,43,43,43	0
57	MG	A	3380	1/1	0.96	0.12	52,52,52,52	0
57	MG	A	3202	1/1	0.96	0.30	50,50,50,50	0
57	MG	a	3466	1/1	0.96	0.15	60,60,60,60	0
57	MG	A	3128	1/1	0.96	0.08	45,45,45,45	0
57	MG	a	3394	1/1	0.96	0.12	32,32,32,32	0
57	MG	A	3055	1/1	0.96	0.10	45,45,45,45	0
57	MG	A	3585	1/1	0.96	0.06	47,47,47,47	0
57	MG	A	3225	1/1	0.96	0.16	36,36,36,36	0
57	MG	U	204	1/1	0.96	0.05	37,37,37,37	0
57	MG	A	3205	1/1	0.96	0.06	43,43,43,43	0
57	MG	A	3337	1/1	0.96	0.12	44,44,44,44	0
57	MG	A	3338	1/1	0.96	0.13	30,30,30,30	0
57	MG	A	3227	1/1	0.96	0.17	43,43,43,43	0
57	MG	A	3163	1/1	0.96	0.09	34,34,34,34	0
57	MG	a	3478	1/1	0.96	0.10	48,48,48,48	0
57	MG	A	3460	1/1	0.96	0.12	44,44,44,44	0
57	MG	A	3548	1/1	0.96	0.14	40,40,40,40	0
57	MG	A	3594	1/1	0.96	0.07	37,37,37,37	0
57	MG	a	3482	1/1	0.96	0.11	37,37,37,37	0
57	MG	A	3391	1/1	0.96	0.11	30,30,30,30	0
57	MG	A	3285	1/1	0.96	0.08	50,50,50,50	0
57	MG	a	3351	1/1	0.96	0.14	36,36,36,36	0
57	MG	A	3430	1/1	0.96	0.07	44,44,44,44	0
57	MG	A	3316	1/1	0.96	0.06	47,47,47,47	0
57	MG	8	101	1/1	0.96	0.13	66,66,66,66	0
57	MG	A	3396	1/1	0.96	0.13	38,38,38,38	0
57	MG	a	3417	1/1	0.96	0.12	37,37,37,37	0
57	MG	A	3508	1/1	0.96	0.05	46,46,46,46	0
57	MG	A	3229	1/1	0.96	0.12	46,46,46,46	0
57	MG	A	3399	1/1	0.96	0.17	29,29,29,29	0
57	MG	A	3014	1/1	0.96	0.07	39,39,39,39	0
57	MG	A	3321	1/1	0.96	0.08	41,41,41,41	0
57	MG	A	3513	1/1	0.96	0.13	41,41,41,41	0
57	MG	a	3424	1/1	0.96	0.06	43,43,43,43	0
57	MG	A	3606	1/1	0.96	0.07	55,55,55,55	0
57	MG	A	3110	1/1	0.96	0.06	42,42,42,42	0
57	MG	A	3473	1/1	0.96	0.09	46,46,46,46	0
57	MG	a	3366	1/1	0.96	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3049	1/1	0.97	0.08	41,41,41,41	0
57	MG	A	3420	1/1	0.97	0.12	31,31,31,31	0
57	MG	A	3403	1/1	0.97	0.06	40,40,40,40	0
57	MG	A	3332	1/1	0.97	0.09	39,39,39,39	0
57	MG	A	3094	1/1	0.97	0.13	31,31,31,31	0
57	MG	A	3256	1/1	0.97	0.10	55,55,55,55	0
57	MG	A	3582	1/1	0.97	0.07	63,63,63,63	0
57	MG	A	3359	1/1	0.97	0.05	45,45,45,45	0
57	MG	A	3249	1/1	0.97	0.04	31,31,31,31	0
57	MG	A	3191	1/1	0.97	0.24	33,33,33,33	0
57	MG	A	3013	1/1	0.97	0.09	52,52,52,52	0
57	MG	a	3355	1/1	0.97	0.13	39,39,39,39	0
57	MG	A	3233	1/1	0.97	0.10	53,53,53,53	0
57	MG	A	3468	1/1	0.97	0.10	48,48,48,48	0
57	MG	A	3377	1/1	0.97	0.15	44,44,44,44	0
57	MG	7	101	1/1	0.97	0.19	48,48,48,48	0
57	MG	A	3470	1/1	0.97	0.08	43,43,43,43	0
57	MG	a	3437	1/1	0.97	0.08	54,54,54,54	0
57	MG	A	3566	1/1	0.97	0.09	40,40,40,40	0
57	MG	O	201	1/1	0.97	0.05	38,38,38,38	0
57	MG	A	3317	1/1	0.97	0.10	31,31,31,31	0
57	MG	A	3340	1/1	0.97	0.07	65,65,65,65	0
57	MG	A	3495	1/1	0.97	0.12	40,40,40,40	0
57	MG	A	3329	1/1	0.97	0.10	40,40,40,40	0
57	MG	a	3333	1/1	0.97	0.23	51,51,51,51	0
57	MG	a	3406	1/1	0.97	0.13	52,52,52,52	0
57	MG	a	3449	1/1	0.97	0.11	50,50,50,50	0
57	MG	A	3623	1/1	0.97	0.07	52,52,52,52	0
57	MG	n	101	1/1	0.97	0.12	42,42,42,42	0
57	MG	A	3416	1/1	0.97	0.07	41,41,41,41	0
57	MG	A	3522	1/1	0.97	0.07	51,51,51,51	0
57	MG	w	103	1/1	0.97	0.15	38,38,38,38	0
57	MG	A	3475	1/1	0.97	0.09	55,55,55,55	0
57	MG	a	3305	1/1	0.97	0.12	46,46,46,46	0
57	MG	A	3234	1/1	0.97	0.24	48,48,48,48	0
57	MG	a	3374	1/1	0.97	0.21	30,30,30,30	0
57	MG	a	3307	1/1	0.97	0.05	35,35,35,35	0
57	MG	a	3308	1/1	0.97	0.06	41,41,41,41	0
57	MG	A	3501	1/1	0.97	0.14	46,46,46,46	0
57	MG	a	3343	1/1	0.97	0.14	29,29,29,29	0
57	MG	A	3395	1/1	0.98	0.07	31,31,31,31	0
57	MG	a	3453	1/1	0.98	0.03	41,41,41,41	0

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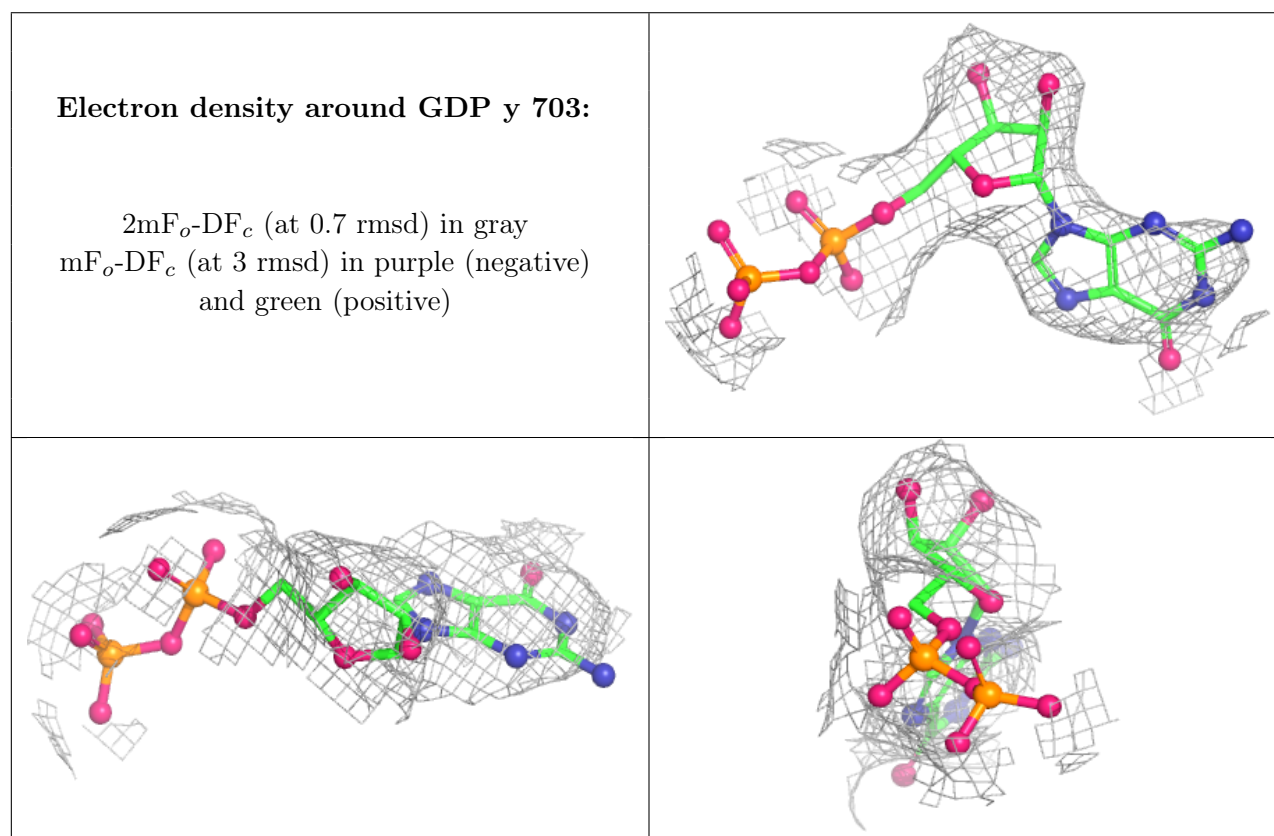
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	A	3537	1/1	0.98	0.07	32,32,32,32	0
57	MG	A	3428	1/1	0.98	0.06	36,36,36,36	0
57	MG	a	3456	1/1	0.98	0.06	59,59,59,59	0
57	MG	A	3496	1/1	0.98	0.08	47,47,47,47	0
57	MG	A	3540	1/1	0.98	0.11	55,55,55,55	0
57	MG	A	3609	1/1	0.98	0.07	39,39,39,39	0
57	MG	A	3401	1/1	0.98	0.08	37,37,37,37	0
57	MG	a	3433	1/1	0.98	0.06	32,32,32,32	0
57	MG	A	3038	1/1	0.98	0.14	55,55,55,55	0
57	MG	A	3397	1/1	0.98	0.07	36,36,36,36	0
57	MG	a	3464	1/1	0.98	0.04	44,44,44,44	0
57	MG	a	3389	1/1	0.98	0.06	38,38,38,38	0
57	MG	A	3323	1/1	0.98	0.06	42,42,42,42	0
57	MG	A	3514	1/1	0.98	0.04	34,34,34,34	0
57	MG	A	3634	1/1	0.98	0.05	56,56,56,56	0
57	MG	A	3417	1/1	0.98	0.09	30,30,30,30	0
57	MG	A	3530	1/1	0.98	0.11	38,38,38,38	0
57	MG	A	3458	1/1	0.98	0.12	27,27,27,27	0
57	MG	A	3618	1/1	0.98	0.09	45,45,45,45	0
57	MG	A	3459	1/1	0.98	0.06	36,36,36,36	0
57	MG	a	3398	1/1	0.98	0.24	27,27,27,27	0
57	MG	A	3480	1/1	0.98	0.06	35,35,35,35	0
58	ZN	4	501	1/1	0.98	0.03	117,117,117,117	0
57	MG	A	3492	1/1	0.98	0.08	62,62,62,62	0
57	MG	A	3381	1/1	0.98	0.13	43,43,43,43	0
57	MG	a	3443	1/1	0.99	0.03	46,46,46,46	0
57	MG	A	3378	1/1	0.99	0.10	31,31,31,31	0
57	MG	A	3394	1/1	0.99	0.12	30,30,30,30	0
57	MG	A	3320	1/1	0.99	0.06	49,49,49,49	0
57	MG	A	3017	1/1	0.99	0.08	63,63,63,63	0
57	MG	a	3438	1/1	0.99	0.08	34,34,34,34	0
57	MG	a	3402	1/1	0.99	0.07	43,43,43,43	0
57	MG	a	3312	1/1	0.99	0.04	26,26,26,26	0
58	ZN	Y	501	1/1	0.99	0.03	92,92,92,92	0
57	MG	A	3421	1/1	0.99	0.07	40,40,40,40	0
58	ZN	5	102	1/1	0.99	0.02	70,70,70,70	0
58	ZN	9	102	1/1	0.99	0.03	72,72,72,72	0
59	SF4	d	501	8/8	0.99	0.05	48,60,64,65	0
57	MG	a	3442	1/1	0.99	0.03	45,45,45,45	0
57	MG	a	3483	1/1	0.99	0.11	39,39,39,39	0
58	ZN	6	102	1/1	1.00	0.02	70,70,70,70	0
57	MG	a	3431	1/1	1.00	0.03	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	n	102	1/1	1.00	0.01	61,61,61,61	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.