



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:14 PM EDT

PDB ID : 5J8B / pdb_00005j8b
Title : Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with
GDP-CP bound to the Thermus thermophilus 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : 2016-04-07
Resolution : 2.60 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:

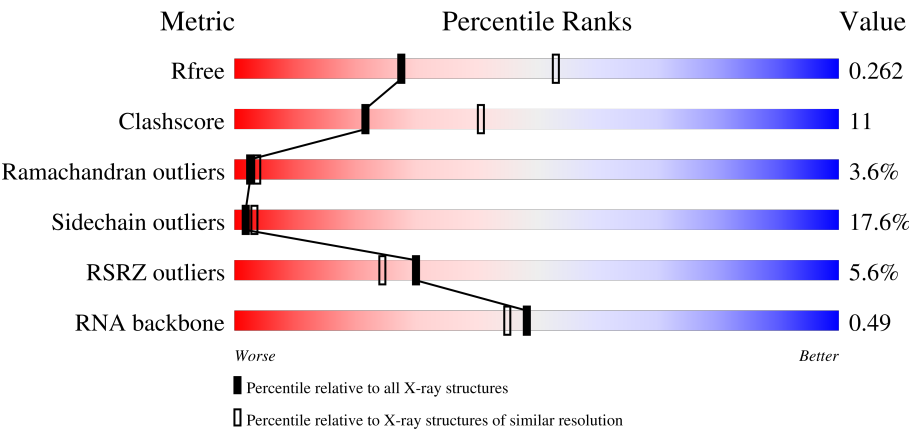
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	4% 59%31%8%
2	B	121	% 60%35%
3	C	228	26%22%29%9%40%
4	D	276	% 66%25%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	J	173	
10	K	147	
11	N	140	
12	O	122	
13	P	150	
14	Q	141	
15	R	118	
16	S	112	
17	T	146	
18	U	118	
19	V	101	
20	W	113	
21	X	96	
22	Y	110	
23	Z	206	
24	0	85	
25	1	98	
26	2	72	
27	3	60	
28	4	71	
29	5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	6	54	
31	7	49	
32	8	65	
33	9	37	
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	
54	u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	v	24	
56	w	76	
57	x	77	
58	y	76	
59	z	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
62	SF4	d	302	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155465 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	2874	Total	C	N	O	P	11	0	0
			61902	27550	11582	19897	2873			

- 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	136	Total	C	N	O	S	1	0	0
			1024	644	190	189	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L10.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	107	Total	C	N	O	S	1	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	94	Total	C	N	O	S	0	0	0
			784	499	150	134	1			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1498	Total	C	N	O	P	4	0	0
			32207	14334	5973	10402	1498			

- 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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	w	74	Total	C	N	O	P	S	1	0	0
			1586	713	285	513	73	2			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	x	77	Total	C	N	O	P	S	3	0	0
			1645	734	297	536	77	1			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	y	74	Total	C	N	O	P	S	0	0	0
			1580	706	285	515	73	1			

- Molecule 59 is a protein called GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	z	671	Total	C	N	O	S	0	0	0
			5200	3333	897	961	9			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	A	644	Total	Mg	0	0
			644	644		
60	B	18	Total	Mg	0	0
			18	18		
60	D	6	Total	Mg	0	0
			6	6		
60	E	5	Total	Mg	0	0
			5	5		
60	F	6	Total	Mg	0	0
			6	6		
60	G	2	Total	Mg	0	0
			2	2		
60	H	1	Total	Mg	0	0
			1	1		
60	N	1	Total	Mg	0	0
			1	1		
60	O	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	P	3	Total 3	Mg 3	0	0
60	Q	2	Total 2	Mg 2	0	0
60	R	2	Total 2	Mg 2	0	0
60	U	1	Total 1	Mg 1	0	0
60	V	2	Total 2	Mg 2	0	0
60	W	1	Total 1	Mg 1	0	0
60	X	1	Total 1	Mg 1	0	0
60	Z	1	Total 1	Mg 1	0	0
60	0	4	Total 4	Mg 4	0	0
60	5	2	Total 2	Mg 2	0	0
60	6	2	Total 2	Mg 2	0	0
60	7	1	Total 1	Mg 1	0	0
60	8	1	Total 1	Mg 1	0	0
60	9	1	Total 1	Mg 1	0	0
60	a	188	Total 188	Mg 188	0	0
60	d	1	Total 1	Mg 1	0	0
60	e	1	Total 1	Mg 1	0	0
60	f	1	Total 1	Mg 1	0	0
60	l	1	Total 1	Mg 1	0	0
60	m	2	Total 2	Mg 2	0	0
60	n	3	Total 3	Mg 3	0	0

Continued on next page...

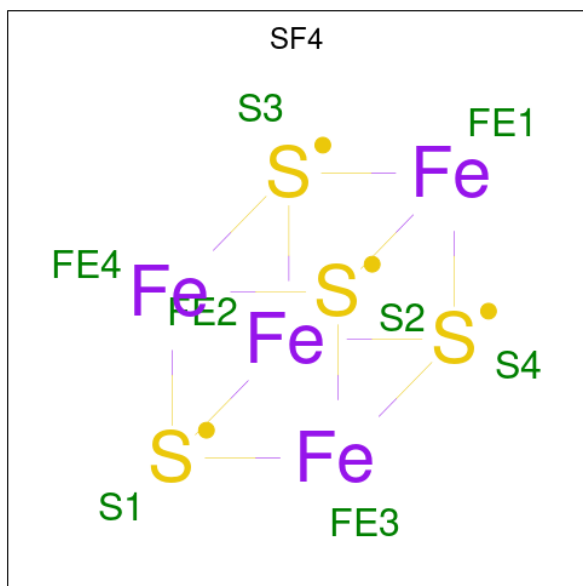
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	v	2	Total	Mg	0	0
			2	2		
60	x	9	Total	Mg	0	0
			9	9		
60	z	2	Total	Mg	0	0
			2	2		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

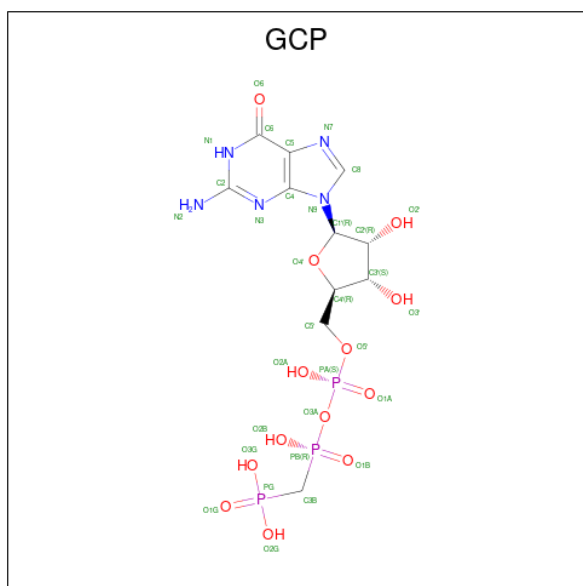
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	Y	1	Total	Zn	0	0
			1	1		
61	4	1	Total	Zn	0	0
			1	1		
61	5	1	Total	Zn	0	0
			1	1		
61	6	1	Total	Zn	0	0
			1	1		
61	9	1	Total	Zn	0	0
			1	1		
61	n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	A	715	Total	O	0	0
			715	715		
64	B	32	Total	O	0	0
			32	32		
64	D	4	Total	O	0	0
			4	4		
64	E	6	Total	O	0	0
			6	6		
64	F	5	Total	O	0	0
			5	5		
64	H	1	Total	O	0	0
			1	1		
64	N	1	Total	O	0	0
			1	1		

Continued on next page...

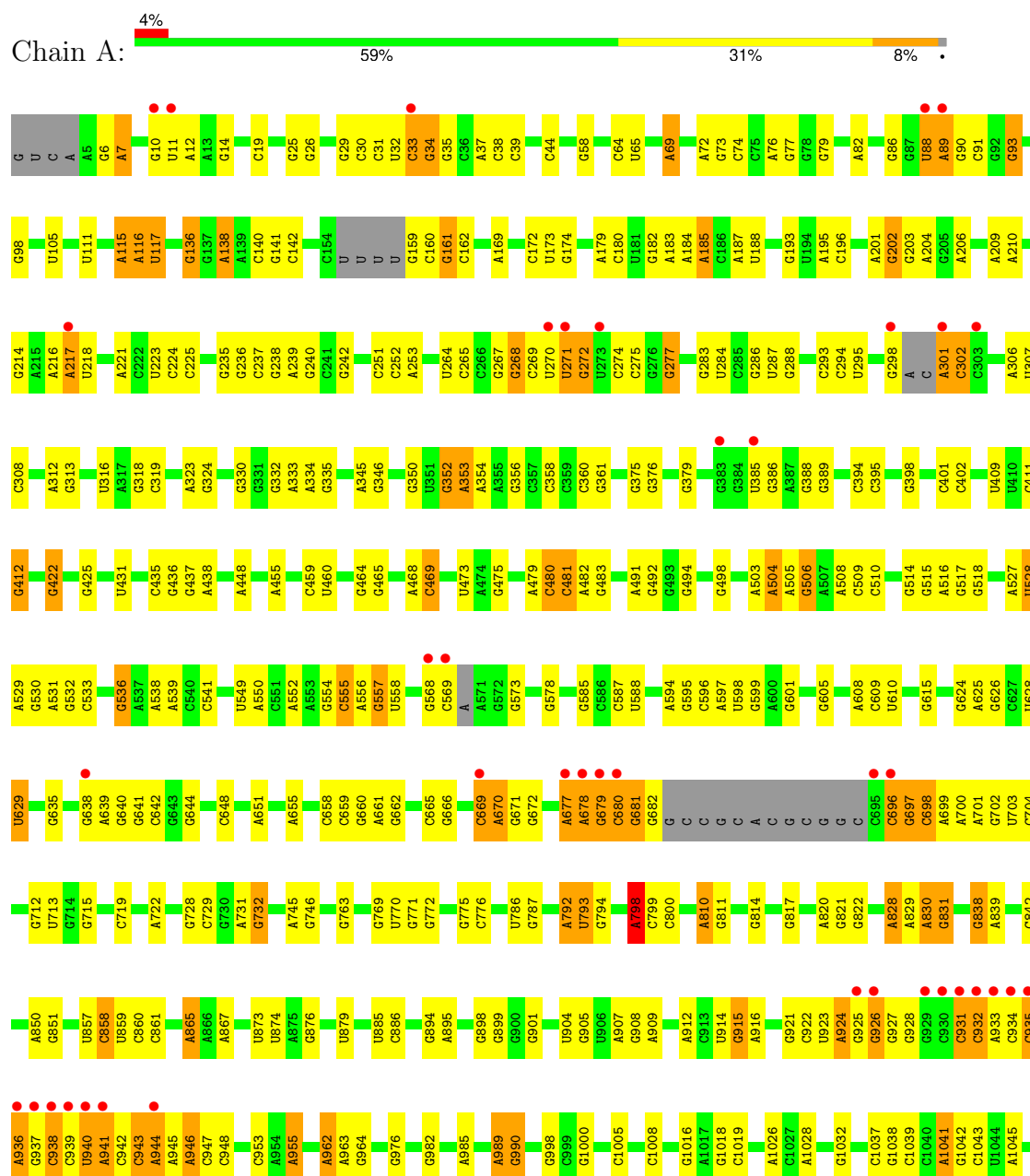
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	O	3	Total 3	O 3	0	0
64	P	8	Total 8	O 8	0	0
64	Q	3	Total 3	O 3	0	0
64	T	2	Total 2	O 2	0	0
64	U	3	Total 3	O 3	0	0
64	V	1	Total 1	O 1	0	0
64	0	3	Total 3	O 3	0	0
64	1	1	Total 1	O 1	0	0
64	3	1	Total 1	O 1	0	0
64	7	1	Total 1	O 1	0	0
64	8	4	Total 4	O 4	0	0
64	a	165	Total 165	O 165	0	0
64	l	1	Total 1	O 1	0	0
64	p	1	Total 1	O 1	0	0
64	v	3	Total 3	O 3	0	0
64	w	1	Total 1	O 1	0	0
64	z	1	Total 1	O 1	0	0

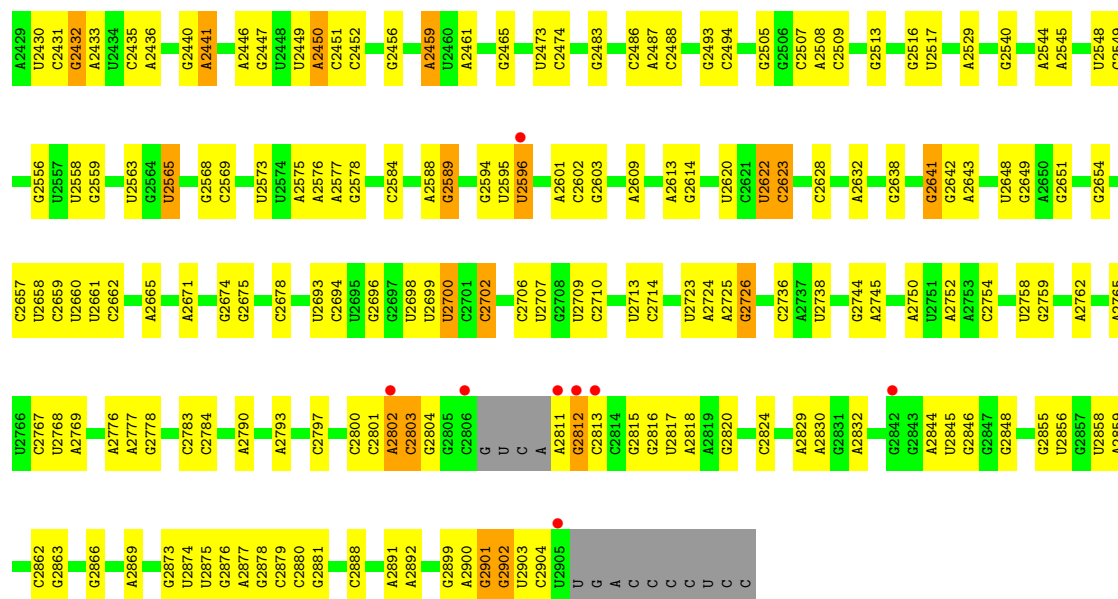
3 Residue-property plots

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.

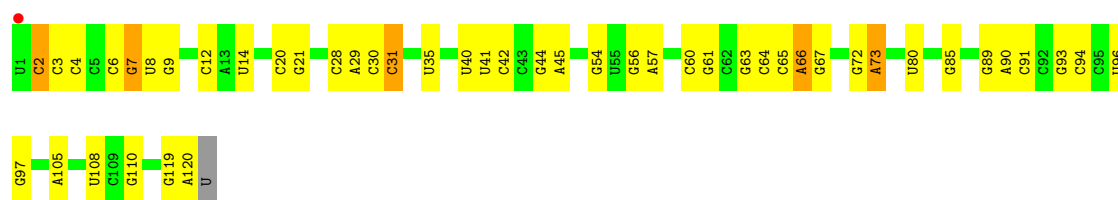
• Molecule 1: 23S Ribosomal RNA



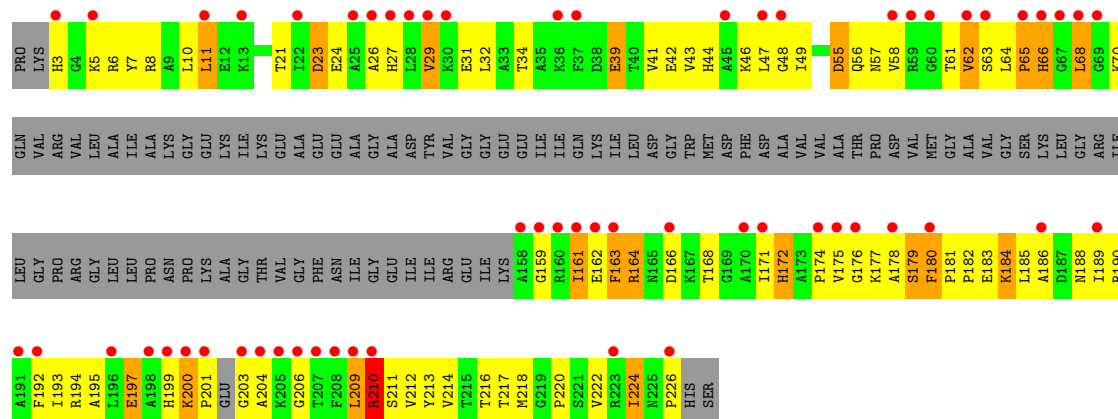
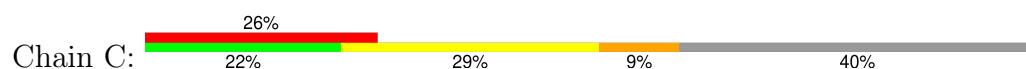




• Molecule 2: 5S Ribosomal RNA

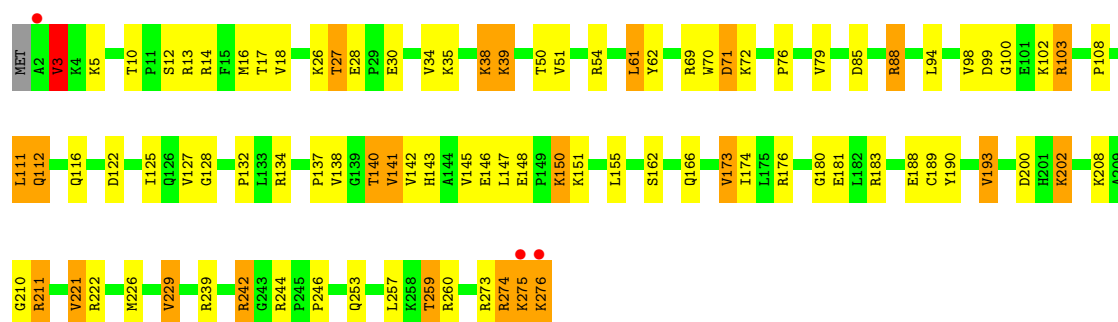


• Molecule 3: 50S ribosomal protein L1

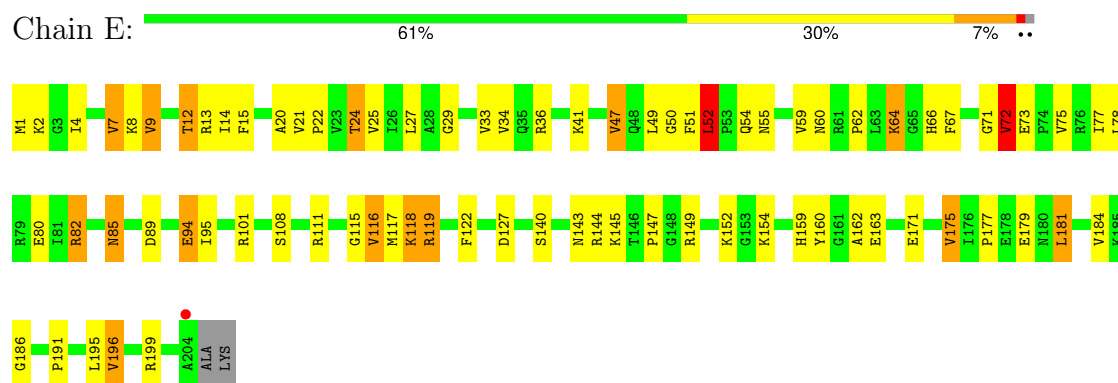


• Molecule 4: 50S ribosomal protein L2

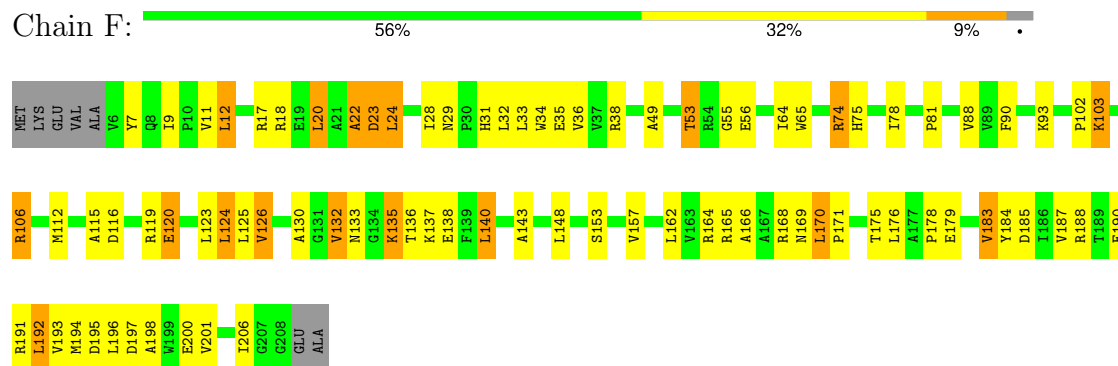




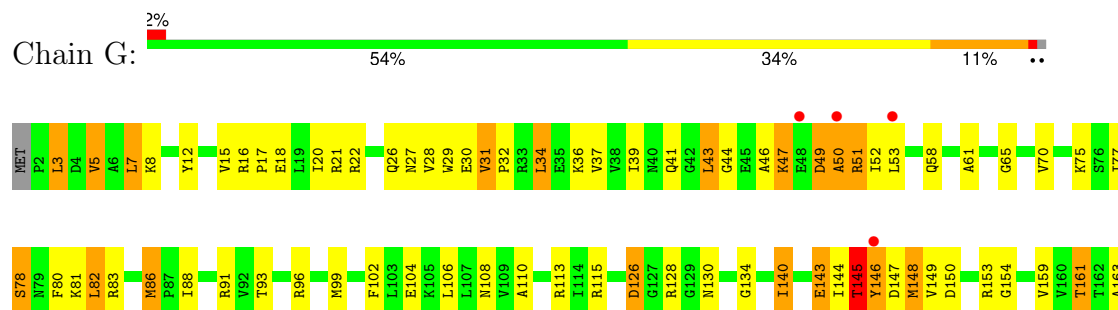
• Molecule 5: 50S ribosomal protein L3



• Molecule 6: 50S ribosomal protein L4

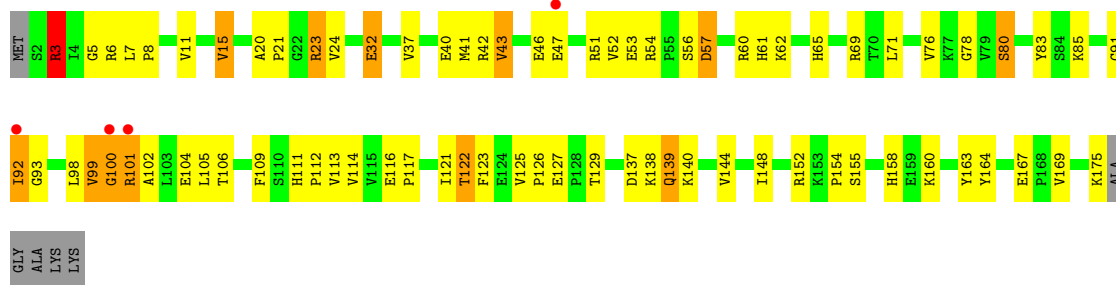


• Molecule 7: 50S ribosomal protein L5

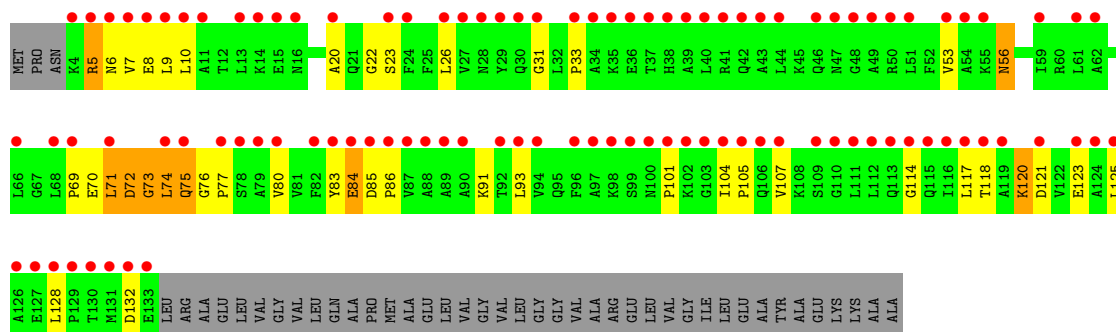




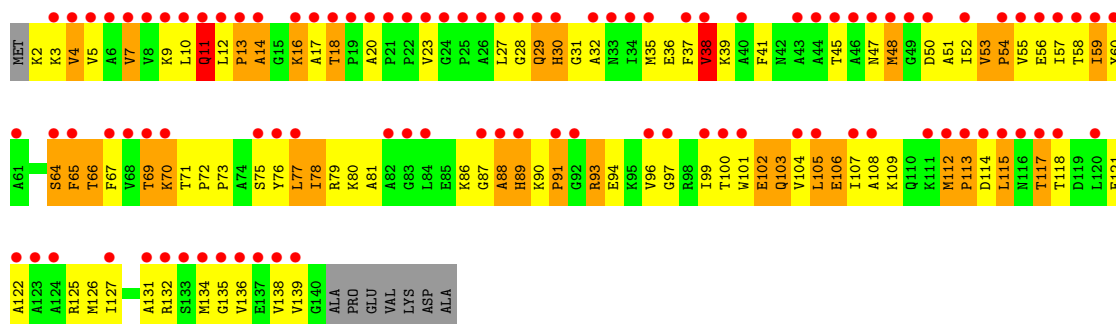
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10

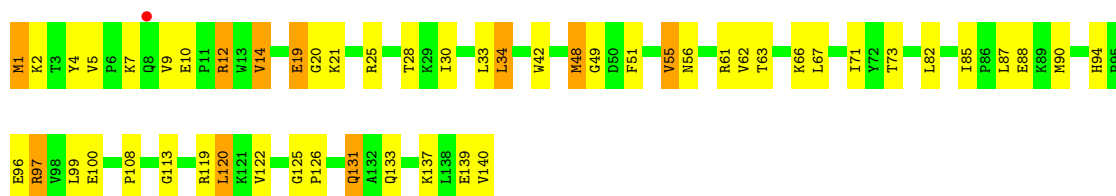


• Molecule 10: 50S ribosomal protein L11



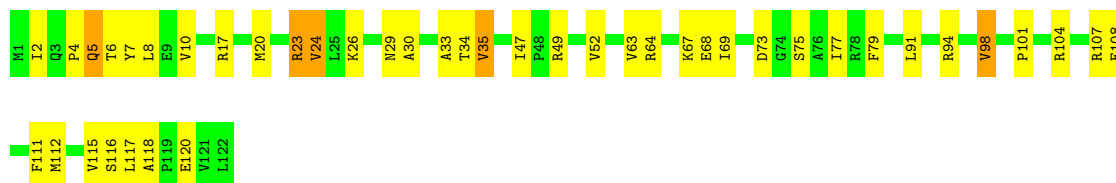
• Molecule 11: 50S ribosomal protein L13





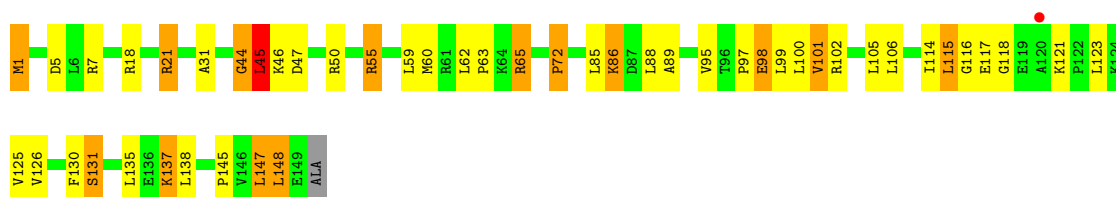
• Molecule 12: 50S ribosomal protein L14

Chain O: 65% 31% .



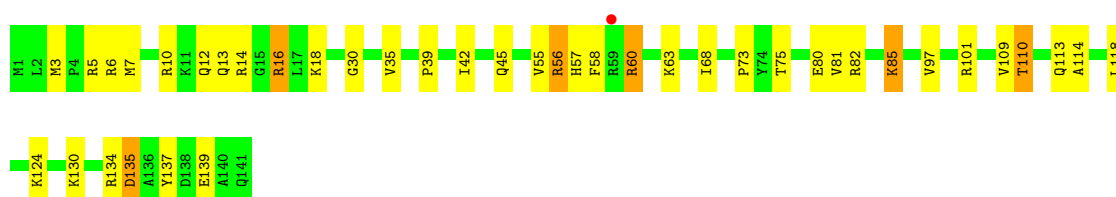
• Molecule 13: 50S ribosomal protein L15

Chain P: 67% 22% 9% ..



• Molecule 14: 50S ribosomal protein L16

Chain Q: 71% 25% .



• Molecule 15: 50S ribosomal protein L17

Chain R: 75% 20% 5%



• Molecule 16: 50S ribosomal protein L18

Chain S: 71% 19% 7% ..



- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21



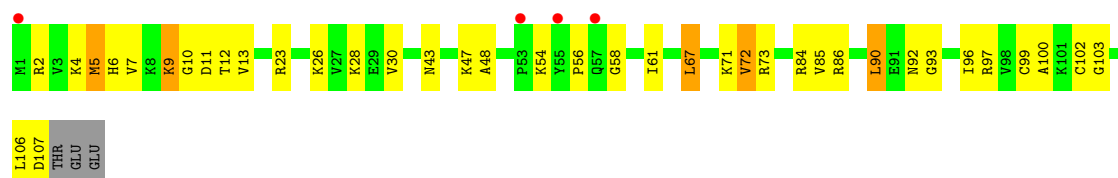
- Molecule 20: 50S ribosomal protein L22



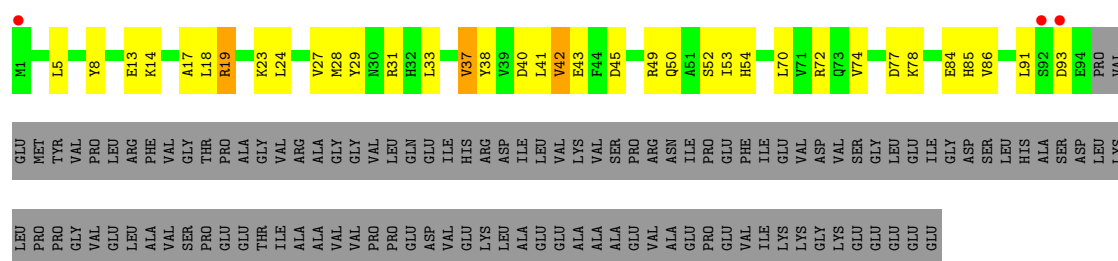
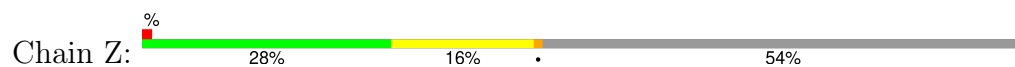
- Molecule 21: 50S ribosomal protein L23



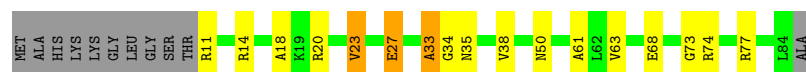
- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L25



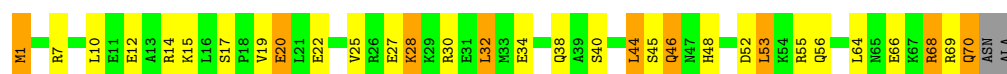
- Molecule 24: 50S ribosomal protein L27



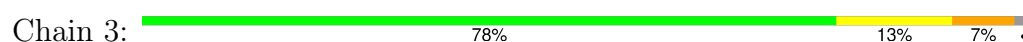
- Molecule 25: 50S ribosomal protein L28

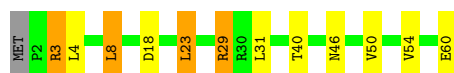


- Molecule 26: 50S ribosomal protein L29

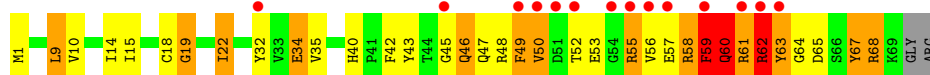


- Molecule 27: 50S ribosomal protein L30





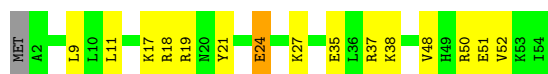
- Molecule 28: 50S ribosomal protein L31



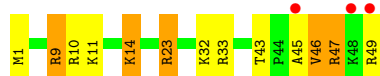
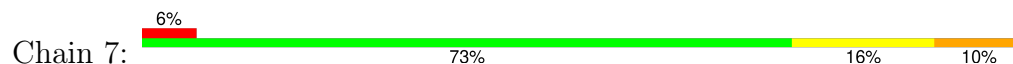
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



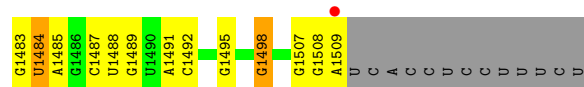
- Molecule 33: 50S ribosomal protein L36



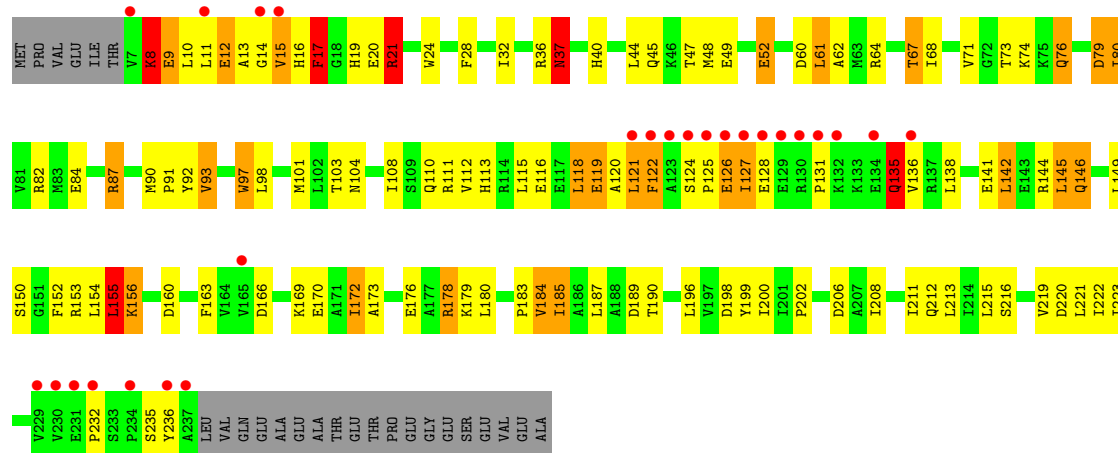
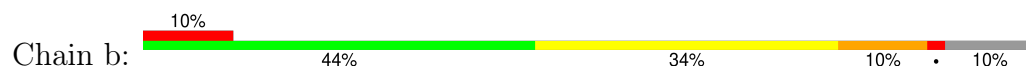
- Molecule 34: 16S Ribosomal RNA



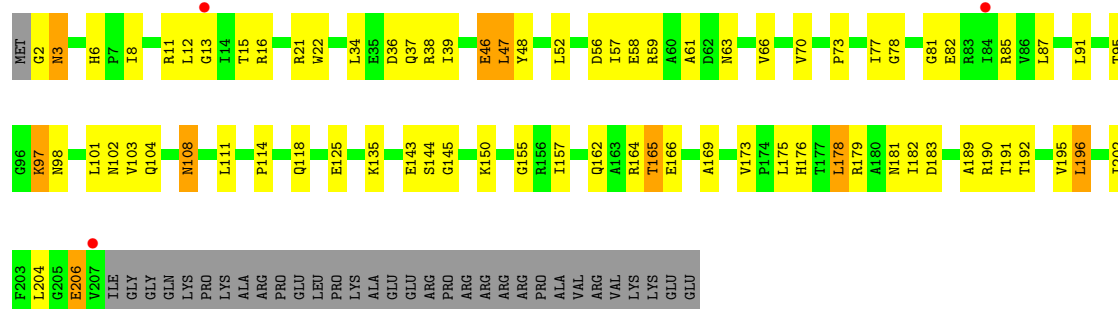




• Molecule 35: 30S ribosomal protein S2



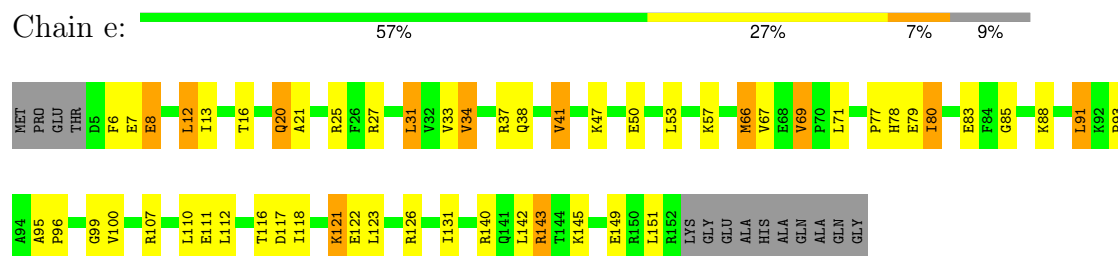
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4



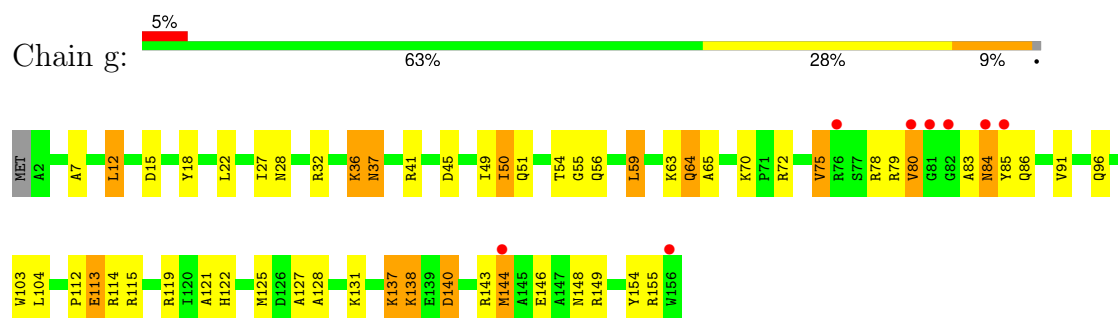
- Molecule 38: 30S ribosomal protein S5



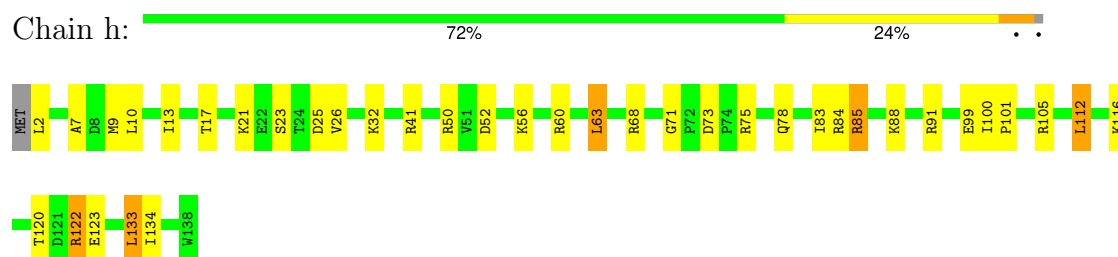
- Molecule 39: 30S ribosomal protein S6



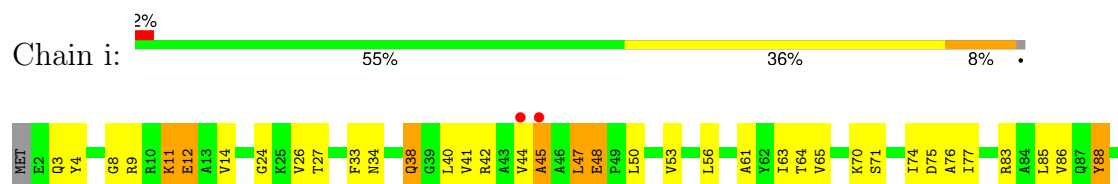
- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8

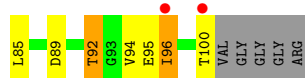


- Molecule 42: 30S ribosomal protein S9





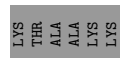
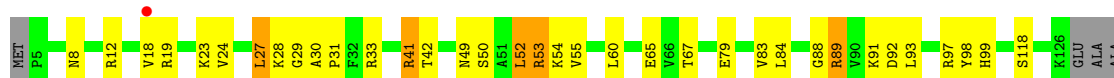
• Molecule 43: 30S ribosomal protein S10



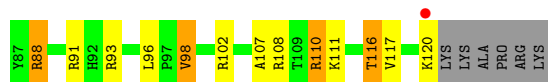
• Molecule 44: 30S ribosomal protein S11



• Molecule 45: 30S ribosomal protein S12



• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14 type Z

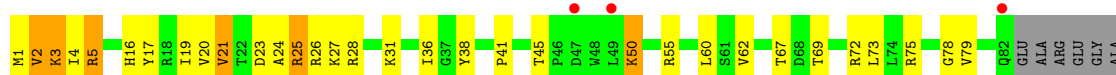




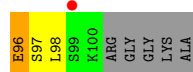
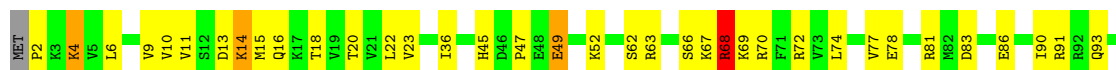
- Molecule 48: 30S ribosomal protein S15



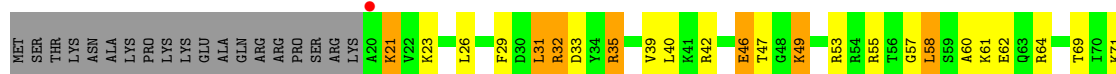
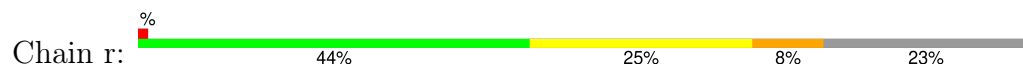
- Molecule 49: 30S ribosomal protein S16



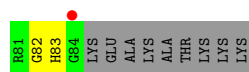
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



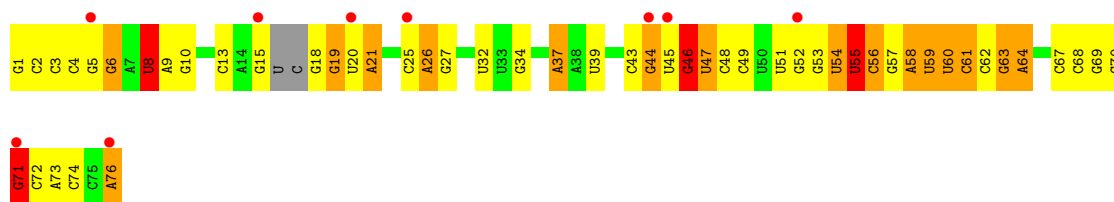
- Molecule 54: 30S ribosomal protein Thx



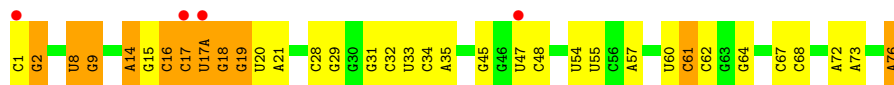
- Molecule 55: mRNA



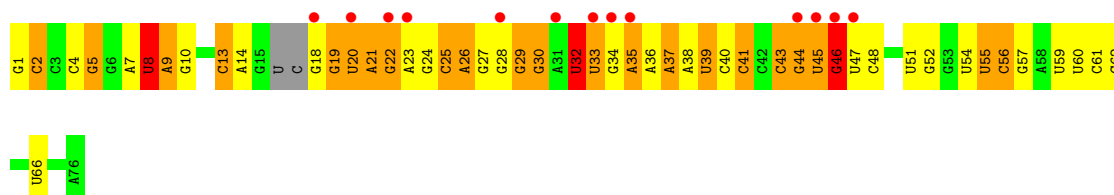
- Molecule 56: A-site tRNA



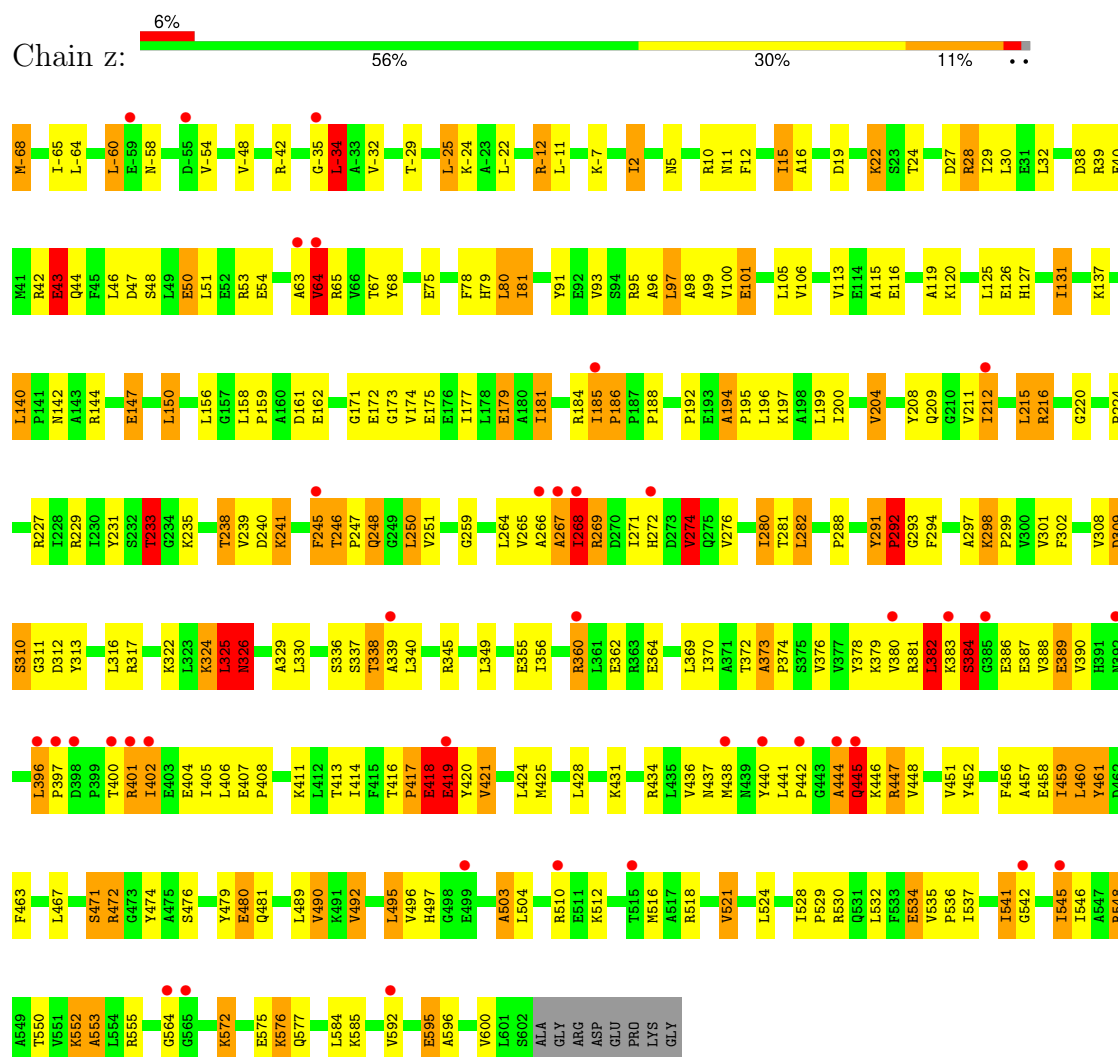
- Molecule 57: P-site tRNA



- Molecule 58: E-site tRNA



- Molecule 59: GDCP fused to the N-terminus of the ribosomal protein L9, Elongation factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.12Å 271.72Å 436.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.60 49.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.52-2.60) 99.4 (49.52-2.60)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.192 , 0.261 0.195 , 0.262	Depositor DCC
R_{free} test set	38580 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	155465	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: 4SU, 5MC, 7MG, GCP, SF4, 5MU, PSU, MIA, MG, ZN

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	0.39	0/69327	0.61	8/108217 (0.0%)
2	B	0.29	0/2878	0.49	0/4490
3	C	0.35	0/1044	0.75	2/1413 (0.1%)
4	D	0.43	0/2186	0.72	2/2944 (0.1%)
5	E	0.40	0/1592	0.69	2/2149 (0.1%)
6	F	0.40	0/1619	0.67	0/2193
7	G	0.33	0/1450	0.63	0/1959
8	H	0.36	0/1356	0.65	0/1834
9	J	0.37	0/640	0.67	1/889 (0.1%)
10	K	0.41	0/1044	0.75	1/1416 (0.1%)
11	N	0.36	0/1144	0.62	0/1543
12	O	0.43	0/943	0.64	0/1269
13	P	0.42	0/1152	0.76	2/1533 (0.1%)
14	Q	0.38	0/1143	0.60	0/1527
15	R	0.35	0/982	0.61	0/1312
16	S	0.33	0/887	0.61	0/1180
17	T	0.39	0/1105	0.62	0/1477
18	U	0.40	0/977	0.68	0/1301
19	V	0.40	0/782	0.64	0/1049
20	W	0.40	0/897	0.63	0/1205
21	X	0.35	0/764	0.61	0/1025
22	Y	0.35	0/819	0.69	0/1095
23	Z	0.30	0/801	0.52	0/1079
24	0	0.36	0/599	0.64	0/798
25	1	0.47	0/762	0.72	0/1014
26	2	0.35	0/590	0.57	0/781
27	3	0.34	0/474	0.62	0/635
28	4	0.34	0/570	0.82	1/768 (0.1%)
29	5	0.39	0/473	0.63	0/639
30	6	0.40	0/460	0.62	0/613
31	7	0.44	0/438	0.71	0/575
32	8	0.43	0/519	0.67	0/684

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.44	0/310	0.73	0/407
34	a	0.35	0/36053	0.57	1/56270 (0.0%)
35	b	0.32	0/1885	0.64	2/2547 (0.1%)
36	c	0.35	1/1574 (0.1%)	0.60	0/2127
37	d	0.33	0/1685	0.56	0/2262
38	e	0.38	0/1145	0.63	0/1543
39	f	0.31	0/819	0.57	0/1111
40	g	0.31	0/1246	0.55	0/1674
41	h	0.34	0/1108	0.53	0/1494
42	i	0.34	0/1002	0.62	0/1346
43	j	0.33	0/711	0.60	0/968
44	k	0.32	0/844	0.55	0/1145
45	l	0.43	0/946	0.73	0/1274
46	m	0.36	0/934	0.70	0/1256
47	n	0.39	0/501	0.67	0/664
48	o	0.34	0/739	0.60	0/985
49	p	0.33	0/697	0.62	0/939
50	q	0.36	0/836	0.69	0/1117
51	r	0.33	0/560	0.56	0/746
52	s	0.35	0/665	0.74	2/897 (0.2%)
53	t	0.37	0/726	0.71	0/961
54	u	0.44	0/203	0.61	0/266
55	v	0.37	0/310	0.59	0/480
56	w	0.34	1/1602 (0.1%)	0.59	2/2493 (0.1%)
57	x	0.40	0/1747	0.63	0/2723
58	y	0.35	1/1628 (0.1%)	0.62	2/2534 (0.1%)
59	z	0.34	0/5296	0.68	11/7179 (0.2%)
All	All	0.37	3/166189 (0.0%)	0.61	39/248014 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	K	0	1
19	V	0	1
26	2	0	1
28	4	0	1
37	d	0	1
39	f	0	1
42	i	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
52	s	0	2
53	t	0	1
59	z	0	6
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	173	VAL	C-N	-5.48	1.21	1.33
58	y	8	4SU	O3'-P	5.07	1.61	1.56
56	w	8	4SU	O3'-P	5.07	1.61	1.56

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	44	GLY	CA-C-N	8.48	136.96	121.70
13	P	44	GLY	C-N-CA	8.48	136.96	121.70
1	A	2013	G	C2'-C3'-O3'	8.13	121.70	109.50
4	D	274	ARG	CA-C-N	7.77	135.69	121.70
4	D	274	ARG	C-N-CA	7.77	135.69	121.70
28	4	59	PHE	N-CA-C	7.21	118.92	110.41
59	z	373	ALA	CA-C-N	7.03	143.87	127.00
59	z	373	ALA	C-N-CA	7.03	143.87	127.00
59	z	552	LYS	CA-C-N	6.75	133.85	121.70
59	z	552	LYS	C-N-CA	6.75	133.85	121.70
3	C	62	VAL	CB-CA-C	6.60	122.12	111.29
9	J	9	LEU	N-CA-C	-6.41	105.17	112.87
56	w	71	G	N1-C2-N2	-6.35	97.16	116.20
59	z	373	ALA	C-N-CD	-6.29	106.76	120.60
5	E	72	VAL	CA-C-N	6.19	132.84	121.70
5	E	72	VAL	C-N-CA	6.19	132.84	121.70
59	z	291	TYR	CA-C-N	6.19	127.57	119.84
59	z	291	TYR	C-N-CA	6.19	127.57	119.84
35	b	155	LEU	CA-C-N	6.09	132.66	121.70
35	b	155	LEU	C-N-CA	6.09	132.66	121.70
1	A	2013	G	P-O3'-C3'	6.06	129.29	120.20
1	A	536	G	O4'-C1'-N9	6.03	117.24	108.20
1	A	677	A	C2'-C3'-O3'	5.82	118.23	109.50
1	A	798	A	C2'-C3'-O3'	5.74	118.11	109.50
59	z	445	GLN	N-CA-C	-5.73	94.95	111.00
1	A	1699	G	C2'-C3'-O3'	5.59	117.88	109.50
3	C	197	GLU	N-CA-C	-5.48	106.67	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	46	G	C4-N9-C1'	5.47	142.92	126.50
52	s	27	GLU	CA-C-N	5.40	131.42	121.70
52	s	27	GLU	C-N-CA	5.40	131.42	121.70
56	w	71	G	N3-C2-N2	5.37	136.02	119.90
10	K	113	PRO	CA-N-CD	-5.27	104.62	112.00
59	z	233	THR	CA-C-N	-5.15	112.97	121.57
59	z	233	THR	C-N-CA	-5.15	112.97	121.57
58	y	46	G	C8-N9-C1'	-5.12	111.66	127.00
34	a	1037	C	O4'-C1'-N1	5.10	116.14	108.50
1	A	2013	G	OP1-P-O3'	-5.06	92.83	108.00
59	z	292	PRO	CA-C-O	-5.03	111.44	120.60
1	A	2297	A	N9-C1'-C2'	5.03	121.54	114.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	2	44	LEU	Peptide
28	4	65	ASP	Peptide
10	K	70	LYS	Peptide
19	V	43	GLU	Peptide
37	d	179	GLU	Peptide
39	f	97	PHE	Peptide
42	i	117	HIS	Peptide
42	i	45	ALA	Peptide
52	s	29	ARG	Peptide
52	s	8	GLY	Peptide
53	t	9	ASN	Peptide
59	z	185	ILE	Peptide
59	z	246	THR	Peptide
59	z	372	THR	Peptide
59	z	396	LEU	Peptide
59	z	419	GLU	Peptide
59	z	480	GLU	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	61902	0	31210	816	1
2	B	2573	0	1306	30	0
3	C	1024	0	1007	84	0
4	D	2136	0	2218	68	0
5	E	1559	0	1618	48	0
6	F	1584	0	1625	53	0
7	G	1425	0	1443	63	0
8	H	1330	0	1407	48	0
9	J	641	0	309	20	0
10	K	1025	0	1066	68	0
11	N	1117	0	1184	27	0
12	O	933	0	996	29	0
13	P	1135	0	1212	40	0
14	Q	1122	0	1179	28	0
15	R	968	0	1033	12	0
16	S	877	0	938	31	0
17	T	1091	0	1151	34	0
18	U	959	0	1019	26	0
19	V	771	0	830	20	0
20	W	886	0	940	24	1
21	X	750	0	814	20	0
22	Y	806	0	881	19	0
23	Z	784	0	796	20	0
24	0	591	0	607	15	0
25	1	755	0	826	22	0
26	2	588	0	643	16	0
27	3	469	0	518	8	0
28	4	557	0	535	34	0
29	5	459	0	476	13	0
30	6	453	0	473	8	0
31	7	430	0	480	9	0
32	8	511	0	571	19	0
33	9	307	0	335	13	0
34	a	32207	0	16255	394	0
35	b	1850	0	1871	72	0
36	c	1550	0	1539	47	0
37	d	1655	0	1673	61	0
38	e	1129	0	1185	28	0
39	f	806	0	793	25	0
40	g	1227	0	1232	34	0
41	h	1088	0	1126	19	0
42	i	983	0	986	34	0
43	j	698	0	637	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	k	829	0	825	17	0
45	l	930	0	980	19	0
46	m	924	0	960	33	0
47	n	492	0	529	16	0
48	o	728	0	760	21	0
49	p	681	0	697	17	0
50	q	823	0	891	21	0
51	r	555	0	618	20	0
52	s	650	0	655	24	0
53	t	724	0	787	13	0
54	u	199	0	208	5	0
55	v	277	0	140	8	0
56	w	1586	0	819	62	0
57	x	1645	0	839	25	0
58	y	1580	0	801	55	0
59	z	5200	0	5309	192	0
60	0	4	0	0	0	0
60	5	2	0	0	0	0
60	6	2	0	0	0	0
60	7	1	0	0	0	0
60	8	1	0	0	0	0
60	9	1	0	0	0	0
60	A	644	0	0	0	0
60	B	18	0	0	0	0
60	D	6	0	0	0	0
60	E	5	0	0	0	0
60	F	6	0	0	0	0
60	G	2	0	0	0	0
60	H	1	0	0	0	0
60	N	1	0	0	0	0
60	O	2	0	0	0	0
60	P	3	0	0	0	0
60	Q	2	0	0	0	0
60	R	2	0	0	0	0
60	U	1	0	0	0	0
60	V	2	0	0	0	0
60	W	1	0	0	0	0
60	X	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	188	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	f	1	0	0	0	0
60	l	1	0	0	0	0
60	m	2	0	0	0	0
60	n	3	0	0	0	0
60	v	2	0	0	0	0
60	x	9	0	0	0	0
60	z	2	0	0	0	0
61	4	1	0	0	0	0
61	5	1	0	0	0	0
61	6	1	0	0	0	0
61	9	1	0	0	0	0
61	Y	1	0	0	0	0
61	n	1	0	0	0	0
62	d	8	0	0	3	0
63	z	32	0	14	4	0
64	0	3	0	0	0	0
64	1	1	0	0	0	0
64	3	1	0	0	0	0
64	7	1	0	0	0	0
64	8	4	0	0	0	0
64	A	715	0	0	37	0
64	B	32	0	0	0	0
64	D	4	0	0	0	0
64	E	6	0	0	1	0
64	F	5	0	0	0	0
64	H	1	0	0	0	0
64	N	1	0	0	0	0
64	O	3	0	0	0	0
64	P	8	0	0	0	0
64	Q	3	0	0	0	0
64	T	2	0	0	0	0
64	U	3	0	0	0	0
64	V	1	0	0	0	0
64	a	165	0	0	4	0
64	l	1	0	0	0	0
64	p	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	z	1	0	0	0	0
All	All	155465	0	104775	2687	1

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 11.

All (2687) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:PRO:C	3:C:203:GLY:HA2	1.75	1.11
58:y:22:G:N7	58:y:46:G:N2	1.98	1.09
3:C:199:HIS:O	3:C:201:PRO:HD3	1.57	1.03
37:d:12:CYS:SG	37:d:19:LEU:HB2	1.98	1.02
10:K:109:LYS:HA	10:K:112:MET:HE3	1.40	1.02
59:z:555:ARG:HH11	59:z:577:GLN:HE22	1.07	0.96
1:A:1091:A:N1	9:J:6:ASN:N	2.14	0.95
35:b:155:LEU:HA	35:b:156:LYS:HB3	1.47	0.94
42:i:128:ARG:NH2	57:x:33:U:OP2	2.01	0.93
1:A:679:G:O6	1:A:698:C:N4	2.02	0.92
35:b:185:ILE:HG22	35:b:199:TYR:HB2	1.48	0.91
58:y:8:4SU:C2	58:y:14:A:H62	1.83	0.91
3:C:201:PRO:C	3:C:203:GLY:CA	2.44	0.91
34:a:1480:A:H2	34:a:1483:G:H1	1.19	0.90
37:d:31:CYS:SG	62:d:302:SF4:FE4	1.64	0.90
1:A:1649:C:OP2	64:A:3701:HOH:O	1.90	0.89
1:A:1064:U:HO2'	1:A:1066:A:H2	0.92	0.89
1:A:1105:U:H4'	1:A:1106:U:H5'	1.55	0.89
34:a:1018:A:H2'	34:a:1019:G:H8	1.37	0.89
36:c:6:HIS:HD2	36:c:8:ILE:H	1.19	0.88
1:A:1813:A:OP2	64:A:3702:HOH:O	1.91	0.88
44:k:91:ARG:NH2	44:k:110:ASP:OD2	2.06	0.88
58:y:22:G:O6	58:y:46:G:N1	2.06	0.87
1:A:1448:C:H5''	1:A:1517:A:H1'	1.56	0.87
58:y:30:G:H1	58:y:40:C:H42	1.21	0.87
5:E:72:VAL:HA	5:E:73:GLU:HB2	1.53	0.86
8:H:42:ARG:NH1	8:H:53:GLU:OE2	2.09	0.86
1:A:2126:C:H41	1:A:2205:G:H1	1.22	0.85
1:A:1812:C:OP1	64:A:3702:HOH:O	1.94	0.85
56:w:52:G:H1	56:w:62:C:H42	1.25	0.84
58:y:32:PSU:HN3	58:y:38:A:H61	1.25	0.84
1:A:1103:G:N2	10:K:126:MET:SD	2.52	0.83
36:c:46:GLU:O	36:c:48:TYR:N	2.11	0.83
1:A:817:G:OP1	31:7:10:ARG:NH1	2.12	0.82
58:y:8:4SU:C2	58:y:14:A:N6	2.42	0.82
53:t:57:ARG:HH12	53:t:100:ILE:HG13	1.44	0.82
8:H:40:GLU:OE2	8:H:60:ARG:NH1	2.10	0.82
1:A:2330:G:H22	16:S:3:ARG:HB2	1.45	0.81
44:k:99:GLN:HG3	44:k:105:VAL:HG21	1.60	0.81
34:a:648:G:H22	34:a:725:G:H1	1.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:z:64:VAL:HG22	59:z:246:THR:HG23	1.60	0.81
59:z:19:ASP:H	63:z:703:GCP:H3B1	1.46	0.81
27:3:8:LEU:HD13	27:3:31:LEU:HD23	1.63	0.81
1:A:2803:C:O2	1:A:2815:G:N1	2.14	0.80
11:N:20:GLY:HA2	11:N:61:ARG:HD2	1.63	0.80
57:x:1:C:H42	57:x:72:A:H61	1.27	0.80
56:w:18:G:O2'	56:w:57:G:N2	2.12	0.80
37:d:31:CYS:HG	62:d:302:SF4:FE4	0.50	0.80
1:A:324:G:OP2	22:Y:84:ARG:NH2	2.15	0.80
1:A:1038:G:OP1	18:U:50:ARG:NH2	2.14	0.79
4:D:69:ARG:NH2	4:D:128:GLY:O	2.15	0.79
4:D:274:ARG:HA	4:D:275:LYS:HB2	1.64	0.79
1:A:1759:U:N3	1:A:1775:G:O6	2.14	0.79
38:e:122:GLU:O	38:e:126:ARG:NH1	2.14	0.79
34:a:1018:A:H2'	34:a:1019:G:C8	2.17	0.79
1:A:1091:A:OP2	1:A:1091:A:H4'	1.75	0.79
1:A:1828:U:H5'	4:D:259:THR:HG22	1.64	0.79
16:S:58:LEU:HB3	16:S:59:LYS:HB2	1.65	0.79
1:A:1099:A:H62	1:A:1150:U:H3	1.29	0.79
1:A:1758:C:H42	1:A:1776:G:H1	1.31	0.79
1:A:1735:A:H62	1:A:1744:A:H2	1.28	0.78
1:A:2018:G:OP2	64:A:3703:HOH:O	1.99	0.78
10:K:13:PRO:HG2	10:K:16:LYS:HB3	1.65	0.78
25:1:50:ARG:HG2	25:1:59:THR:HG22	1.65	0.78
34:a:392:G:O2'	34:a:394:C:OP1	2.00	0.78
1:A:136:G:N2	21:X:44:GLU:OE1	2.17	0.78
13:P:100:LEU:HD22	13:P:105:LEU:HD12	1.65	0.78
1:A:1248:A:H2	1:A:1286:A:H62	1.30	0.78
59:z:216:ARG:HH21	59:z:259:GLY:HA2	1.49	0.78
8:H:121:ILE:HD11	8:H:140:LYS:HG3	1.66	0.78
34:a:1116:G:N2	34:a:1124:C:O2	2.17	0.78
1:A:786:U:OP2	64:A:3704:HOH:O	2.01	0.78
37:d:12:CYS:SG	37:d:19:LEU:CB	2.72	0.77
59:z:292:PRO:HB2	59:z:293:GLY:HA2	1.65	0.77
59:z:131:ILE:HD11	59:z:158:LEU:HD21	1.65	0.77
1:A:655:A:OP1	13:P:65:ARG:NH1	2.18	0.76
34:a:171:C:OP1	53:t:29:LYS:NZ	2.18	0.76
1:A:908:G:OP2	64:A:3705:HOH:O	2.02	0.76
8:H:54:ARG:HH21	8:H:57:ASP:HB2	1.49	0.76
28:4:53:GLU:HG3	28:4:55:ARG:H	1.51	0.76
58:y:13:C:H2'	58:y:14:A:H8	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2415:C:OP2	64:A:3706:HOH:O	2.03	0.76
34:a:1171:C:OP1	43:j:51:ARG:NH2	2.19	0.76
1:A:1775:G:H3'	1:A:1776:G:C8	2.21	0.76
1:A:1760:G:H1	1:A:1774:C:N4	1.84	0.76
35:b:19:HIS:ND1	35:b:189:ASP:OD1	2.17	0.76
42:i:42:ARG:NH2	42:i:75:ASP:OD1	2.16	0.76
59:z:245:PHE:O	59:z:246:THR:OG1	2.02	0.76
1:A:238:G:OP2	32:8:13:ARG:NH2	2.19	0.75
34:a:213:C:O2'	34:a:456:C:N4	2.20	0.75
40:g:75:VAL:HG21	40:g:144:MET:HE3	1.69	0.75
41:h:41:ARG:HH22	41:h:123:GLU:CD	1.94	0.75
3:C:209:LEU:HD13	3:C:209:LEU:H	1.51	0.75
53:t:10:LEU:HB3	53:t:12:ALA:H	1.52	0.75
59:z:10:ARG:HE	59:z:185:ILE:HA	1.50	0.75
59:z:265:VAL:HB	59:z:266:ALA:HB2	1.67	0.75
36:c:58:GLU:HB3	43:j:92:THR:HG21	1.68	0.74
36:c:108:ASN:HD21	36:c:144:SER:HB3	1.53	0.74
1:A:2866:G:N2	1:A:2869:A:OP2	2.20	0.74
12:O:7:TYR:HE1	12:O:20:MET:HE3	1.53	0.74
21:X:31:HIS:HD2	21:X:33:LYS:H	1.33	0.74
37:d:20:TYR:HA	37:d:26:CYS:SG	2.28	0.74
58:y:44:G:H1'	58:y:45:U:C5	2.22	0.74
25:1:76:ARG:HB2	25:1:97:LEU:HD13	1.70	0.73
34:a:557:A:H5'	34:a:557:A:H8	1.50	0.73
3:C:201:PRO:O	3:C:203:GLY:HA2	1.87	0.73
17:T:41:ARG:NH2	34:a:342:G:OP1	2.20	0.73
20:W:68:ARG:HD3	20:W:111:HIS:CD2	2.23	0.73
34:a:1303:C:H3'	34:a:1304:C:H5''	1.70	0.73
1:A:1184:C:O3'	11:N:25:ARG:NH1	2.21	0.73
37:d:20:TYR:HD2	37:d:26:CYS:HB3	1.53	0.73
4:D:180:GLY:HA3	4:D:275:LYS:HG2	1.68	0.73
8:H:137:ASP:HB3	8:H:140:LYS:HG2	1.69	0.73
1:A:679:G:O6	1:A:698:C:N3	2.21	0.73
1:A:2145:G:H5'	3:C:174:PRO:HD3	1.71	0.73
17:T:54:ARG:HA	17:T:59:THR:HB	1.70	0.73
24:O:11:ARG:O	24:O:14:ARG:NH2	2.21	0.73
34:a:1037:C:C4	56:w:34:G:H1'	2.23	0.73
39:f:38:GLU:OE1	39:f:64:GLN:NE2	2.21	0.73
1:A:798:A:H3'	31:7:1:MET:HE1	1.70	0.73
8:H:46:GLU:OE1	8:H:51:ARG:NH2	2.21	0.73
19:V:40:LEU:HB2	19:V:46:VAL:HG12	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:z:250:LEU:HD22	59:z:250:LEU:H	1.54	0.72
1:A:1813:A:OP1	64:A:3704:HOH:O	2.08	0.72
28:4:45:GLY:O	28:4:47:GLN:N	2.20	0.72
7:G:80:PHE:O	7:G:82:LEU:N	2.21	0.72
43:j:16:LEU:HD13	43:j:70:ARG:HG2	1.70	0.72
1:A:1402:U:OP1	31:7:23:ARG:NH1	2.22	0.72
16:S:15:ARG:HH11	16:S:25:ARG:HH21	1.35	0.72
34:a:661:U:H3	34:a:697:G:H22	1.36	0.72
34:a:799:A:OP1	64:a:1801:HOH:O	2.08	0.72
35:b:60:ASP:OD2	35:b:64:ARG:NH2	2.23	0.72
38:e:6:PHE:HB2	38:e:34:VAL:HG22	1.71	0.72
34:a:1141:C:H5	34:a:1163:G:H1	1.34	0.72
39:f:97:PHE:HD1	51:r:31:LEU:HD21	1.54	0.72
20:W:65:LEU:HD12	20:W:68:ARG:HH21	1.54	0.72
37:d:72:GLU:OE1	37:d:207:TYR:OH	2.08	0.72
1:A:1218:A:H4'	1:A:1219:U:OP1	1.90	0.72
1:A:1552:A:O2'	1:A:1553:A:O5'	2.07	0.72
10:K:13:PRO:HB3	10:K:52:ILE:HG12	1.71	0.72
59:z:299:PRO:O	59:z:479:TYR:OH	2.07	0.72
1:A:2330:G:N2	16:S:3:ARG:HB2	2.04	0.72
3:C:21:THR:H	3:C:24:GLU:HB2	1.54	0.72
23:Z:77:ASP:HB2	23:Z:84:GLU:HG3	1.72	0.72
1:A:2461:A:O2'	57:x:76:A:N6	2.23	0.71
1:A:1232:U:H4'	19:V:79:VAL:HG22	1.71	0.71
59:z:-60:LEU:HD21	59:z:-34:LEU:HD23	1.71	0.71
59:z:63:ALA:HA	59:z:81:ILE:HG12	1.72	0.71
35:b:178:ARG:NH1	41:h:71:GLY:O	2.23	0.71
1:A:955:A:H62	14:Q:12:GLN:HA	1.55	0.71
1:A:1311:G:O5'	20:W:15:ARG:NH2	2.23	0.71
7:G:18:GLU:OE1	7:G:22:ARG:NH2	2.23	0.71
59:z:339:ALA:HB1	59:z:340:LEU:HD13	1.71	0.71
6:F:116:ASP:OD1	6:F:119:ARG:NH2	2.24	0.71
34:a:643:U:OP2	48:o:8:LYS:NZ	2.20	0.71
7:G:145:THR:OG1	7:G:146:TYR:N	2.18	0.71
59:z:10:ARG:HG2	59:z:185:ILE:HG13	1.71	0.71
1:A:2648:U:H5''	5:E:82:ARG:HH21	1.55	0.71
1:A:596:C:OP2	64:A:3708:HOH:O	2.09	0.71
44:k:34:ASP:HB3	44:k:40:ILE:HD11	1.73	0.71
34:a:933:U:O2'	52:s:83:HIS:HD2	1.72	0.70
41:h:25:ASP:OD2	41:h:60:ARG:NH2	2.23	0.70
1:A:2197:A:OP1	3:C:7:TYR:OH	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:986:C:H42	34:a:1001:G:H1	1.37	0.70
40:g:103:TRP:CD2	40:g:137:LYS:HG2	2.25	0.70
1:A:2155:A:H1'	1:A:2180:G:H21	1.54	0.70
1:A:88:U:O2'	1:A:89:A:O4'	2.09	0.70
4:D:137:PRO:O	4:D:140:THR:HG23	1.90	0.70
34:a:1480:A:H2	34:a:1483:G:N1	1.89	0.70
56:w:71:G:N2	56:w:72:C:C4	2.59	0.70
34:a:426:A:OP1	37:d:9:CYS:HB2	1.92	0.70
1:A:1109:C:HO2'	10:K:89:HIS:HE2	1.34	0.70
37:d:194:LEU:HD22	37:d:194:LEU:H	1.56	0.70
58:y:9:A:H5'	58:y:46:G:C8	2.27	0.70
2:B:40:U:O4	28:4:1:MET:N	2.24	0.70
37:d:18:LYS:HD3	37:d:33:MET:HB3	1.74	0.70
45:l:53:ARG:HG2	45:l:93:LEU:HD11	1.74	0.70
6:F:185:ASP:HA	6:F:188:ARG:HD3	1.74	0.70
16:S:59:LYS:HE2	16:S:60:GLY:N	2.07	0.69
35:b:87:ARG:NH1	35:b:220:ASP:OD1	2.25	0.69
58:y:10:G:H1	58:y:25:C:H42	1.39	0.69
1:A:2280:A:OP1	64:A:3707:HOH:O	2.09	0.69
3:C:175:VAL:HG22	3:C:176:GLY:H	1.57	0.69
11:N:42:TRP:HA	11:N:48:MET:HE1	1.73	0.69
21:X:31:HIS:CD2	21:X:33:LYS:H	2.09	0.69
1:A:624:G:O2'	1:A:701:A:N6	2.25	0.69
34:a:942:A:OP1	64:a:1802:HOH:O	2.08	0.69
1:A:1784:C:OP1	17:T:96:ARG:NH1	2.25	0.69
15:R:97:VAL:HG22	15:R:114:VAL:HG13	1.73	0.69
59:z:297:ALA:HB1	59:z:349:LEU:HD11	1.75	0.69
1:A:2360:G:OP1	64:A:3709:HOH:O	2.11	0.69
34:a:1037:C:N3	56:w:34:G:H1'	2.07	0.69
47:n:2:ALA:O	47:n:3:ARG:HB2	1.91	0.69
2:B:6:C:H2'	2:B:7:G:H5''	1.75	0.69
3:C:163:PHE:HB2	3:C:171:ILE:HD11	1.75	0.69
17:T:55:ASN:H	17:T:59:THR:HG22	1.58	0.69
59:z:379:LYS:HA	59:z:388:VAL:HA	1.74	0.69
1:A:1220:G:N2	1:A:1222:C:OP2	2.26	0.69
10:K:102:GLU:HA	10:K:105:LEU:HB2	1.74	0.69
16:S:59:LYS:HE2	16:S:60:GLY:H	1.57	0.69
58:y:8:4SU:S4	58:y:14:A:N7	2.65	0.69
8:H:127:GLU:OE2	8:H:129:THR:OG1	2.11	0.69
1:A:1150:U:H2'	1:A:1151:G:C8	2.27	0.69
1:A:1153:U:O2'	1:A:1154:C:O5'	2.09	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1765:G:N2	1:A:1767:U:OP2	2.27	0.68
51:r:46:GLU:H	51:r:46:GLU:CD	2.00	0.68
1:A:2493:G:OP1	64:A:3710:HOH:O	2.11	0.68
3:C:62:VAL:HG13	3:C:63:SER:HA	1.75	0.68
3:C:171:ILE:O	3:C:172:HIS:ND1	2.27	0.68
1:A:555:C:OP2	64:A:3711:HOH:O	2.12	0.68
6:F:29:ASN:H	6:F:112:MET:HE3	1.58	0.68
37:d:65:ARG:HG3	37:d:70:ILE:HG22	1.75	0.68
1:A:1739:U:O2'	4:D:14:ARG:NH2	2.26	0.68
1:A:2622:U:C4	29:5:3:LYS:HG2	2.29	0.68
59:z:65:ARG:O	59:z:246:THR:HG21	1.94	0.68
37:d:20:TYR:CD2	37:d:26:CYS:HB3	2.28	0.68
10:K:69:THR:OG1	10:K:70:LYS:N	2.24	0.68
34:a:825:U:N3	34:a:826:C:O2'	2.26	0.68
58:y:30:G:H1	58:y:40:C:N4	1.90	0.68
1:A:2316:A:H5''	7:G:134:GLY:HA3	1.76	0.68
1:A:679:G:O6	1:A:698:C:C4	2.46	0.68
3:C:179:SER:HA	3:C:180:PHE:O	1.92	0.68
17:T:84:GLN:HG2	17:T:85:LYS:HG2	1.76	0.68
1:A:1898:A:H5'	1:A:1899:G:OP2	1.94	0.67
9:J:26:LEU:HA	9:J:84:GLU:HA	1.74	0.67
40:g:86:GLN:HB2	40:g:148:ASN:ND2	2.09	0.67
1:A:1067:G:N2	1:A:1068:U:O4	2.23	0.67
3:C:182:PRO:C	3:C:184:LYS:H	2.02	0.67
7:G:161:THR:HG22	7:G:163:ALA:H	1.58	0.67
56:w:4:C:N4	56:w:5:G:N7	2.42	0.67
19:V:34:GLU:OE2	19:V:100:ARG:NH2	2.27	0.67
46:m:58:GLU:O	46:m:62:ASN:ND2	2.27	0.67
1:A:1310:A:OP2	64:A:3712:HOH:O	2.12	0.67
59:z:545:ILE:H	59:z:545:ILE:HD13	1.60	0.67
1:A:1637:C:H2'	1:A:1638:G:C8	2.29	0.67
3:C:21:THR:HB	3:C:24:GLU:H	1.59	0.67
38:e:80:ILE:HG22	38:e:91:LEU:HB2	1.77	0.67
59:z:16:ALA:HB3	59:z:22:LYS:HD2	1.74	0.67
56:w:5:G:HO2'	56:w:6:G:H8	1.41	0.67
1:A:926:G:N2	1:A:943:C:N3	2.43	0.67
1:A:1127:U:H3'	1:A:1128:U:H5''	1.76	0.67
7:G:18:GLU:OE2	7:G:21:ARG:NH1	2.27	0.67
34:a:915:A:OP2	64:a:1803:HOH:O	2.11	0.67
1:A:2803:C:H2'	1:A:2804:G:C8	2.30	0.66
14:Q:60:ARG:NH1	56:w:53:G:O2'	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:657:G:H2'	34:a:658:G:C8	2.29	0.66
40:g:78:ARG:HG2	40:g:79:ARG:HD3	1.77	0.66
1:A:1648:A:OP1	64:A:3701:HOH:O	2.12	0.66
6:F:192:LEU:HD13	6:F:194:MET:HE2	1.78	0.66
10:K:41:PHE:HZ	10:K:53:VAL:HB	1.61	0.66
34:a:1095:C:H1'	36:c:179:ARG:HE	1.60	0.66
2:B:8:U:H5''	16:S:15:ARG:HH12	1.61	0.66
34:a:1069:U:H3	34:a:1082:G:H22	1.42	0.66
9:J:73:GLY:O	9:J:75:GLN:N	2.27	0.66
20:W:25:ARG:NH2	20:W:74:ALA:O	2.27	0.66
34:a:50:U:O4	34:a:361:U:H5	1.78	0.66
35:b:127:ILE:HD12	35:b:128:GLU:H	1.60	0.66
37:d:15:GLU:OE2	37:d:66:ARG:NH1	2.28	0.66
59:z:-64:LEU:HD23	59:z:-60:LEU:HD23	1.76	0.66
59:z:51:LEU:HD21	59:z:356:ILE:HG23	1.76	0.66
1:A:448:A:OP2	64:A:3715:HOH:O	2.14	0.66
3:C:194:ARG:NH2	3:C:197:GLU:OE1	2.28	0.66
1:A:1768:G:H3'	1:A:1769:A:H8	1.59	0.66
1:A:1775:G:H3'	1:A:1776:G:H8	1.59	0.66
34:a:1141:C:H5	34:a:1163:G:N1	1.93	0.66
34:a:1260:U:H5''	34:a:1261:A:O4'	1.95	0.66
1:A:931:C:H3'	1:A:932:C:H5''	1.78	0.66
59:z:459:ILE:HG23	59:z:463:PHE:HB3	1.77	0.66
1:A:2824:C:H5'	29:5:29:THR:HG21	1.78	0.66
34:a:953:A:H4'	34:a:954:G:H5''	1.78	0.66
1:A:240:G:P	13:P:50:ARG:HH12	2.19	0.65
1:A:1091:A:N6	9:J:8:GLU:H	1.94	0.65
1:A:1814:A:OP2	64:A:3704:HOH:O	2.14	0.65
34:a:1268:A:H2'	34:a:1269:A:H4'	1.77	0.65
49:p:26:ARG:HD2	49:p:31:LYS:O	1.95	0.65
1:A:2157:C:N4	1:A:2176:G:H1	1.95	0.65
40:g:86:GLN:HB2	40:g:148:ASN:HD22	1.60	0.65
56:w:58:A:O2'	56:w:60:U:OP2	2.14	0.65
1:A:850:A:OP2	64:A:3714:HOH:O	2.14	0.65
1:A:1828:U:OP2	4:D:274:ARG:NH2	2.28	0.65
34:a:402:G:O3'	37:d:3:ARG:NH2	2.30	0.65
42:i:9:ARG:HG2	42:i:14:VAL:HG22	1.77	0.65
1:A:2417:U:C2	13:P:72:PRO:HG2	2.31	0.65
1:A:2568:G:HO2'	56:w:76:A:H8	1.44	0.65
24:0:33:ALA:O	24:0:35:ASN:N	2.29	0.65
37:d:98:GLU:OE2	37:d:103:ASN:ND2	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:g:28:ASN:HD21	40:g:36:LYS:HE3	1.60	0.65
56:w:46:7MG:H3'	56:w:47:U:H4'	1.78	0.65
6:F:157:VAL:HB	6:F:194:MET:HG2	1.77	0.65
29:5:16:ARG:HG2	29:5:16:ARG:HH11	1.62	0.65
34:a:423:U:OP1	37:d:13:ARG:NH2	2.28	0.65
37:d:12:CYS:SG	37:d:19:LEU:N	2.70	0.65
1:A:1423:A:O2'	1:A:1425:G:N7	2.26	0.65
46:m:84:ILE:HG13	46:m:86:CYS:HB2	1.78	0.65
56:w:52:G:H1	56:w:62:C:N4	1.92	0.65
1:A:926:G:H2'	1:A:927:G:C8	2.31	0.64
1:A:1249:U:C2	6:F:171:PRO:HB3	2.32	0.64
1:A:1845:A:OP2	4:D:54:ARG:NH2	2.30	0.64
20:W:79:GLY:HA3	20:W:100:THR:HG22	1.78	0.64
11:N:34:LEU:O	11:N:49:GLY:HA3	1.97	0.64
34:a:432:C:O2'	34:a:433:U:OP2	2.14	0.64
37:d:23:GLY:HA3	37:d:112:VAL:HG22	1.79	0.64
1:A:712:G:H1'	32:8:4:MET:HE3	1.79	0.64
1:A:904:U:OP2	24:0:77:ARG:NH2	2.28	0.64
1:A:1153:U:O2'	1:A:1154:C:H6	1.81	0.64
1:A:2125:G:O6	1:A:2206:C:N4	2.31	0.64
34:a:982:G:N2	34:a:983:A:H1'	2.12	0.64
1:A:1873:C:H5'	4:D:253:GLN:HE22	1.63	0.64
1:A:2762:A:OP2	8:H:62:LYS:NZ	2.28	0.64
34:a:1274:U:P	40:g:41:ARG:HH22	2.20	0.64
39:f:80:ARG:NH1	39:f:88:VAL:O	2.29	0.64
1:A:964:G:N2	1:A:2280:A:OP2	2.31	0.64
1:A:2204:C:H2'	1:A:2205:G:C8	2.33	0.64
34:a:372:G:H5''	49:p:5:ARG:HB2	1.80	0.64
1:A:1124:C:H4'	10:K:132:ARG:CZ	2.28	0.64
1:A:732:G:H5''	31:7:11:LYS:HE2	1.79	0.63
1:A:1092:G:H4'	1:A:1092:G:OP1	1.99	0.63
1:A:1810:A:OP1	64:A:3702:HOH:O	2.15	0.63
1:A:308:C:H42	1:A:379:G:H1	1.46	0.63
37:d:101:LEU:HB2	37:d:138:TYR:HB3	1.80	0.63
1:A:1891:G:H5''	3:C:206:GLY:HA2	1.80	0.63
10:K:23:VAL:HA	10:K:27:LEU:HD13	1.80	0.63
14:Q:16:ARG:HG2	14:Q:18:LYS:HG3	1.81	0.63
23:Z:28:MET:HE3	23:Z:37:VAL:HG21	1.80	0.63
34:a:620:U:H5'	50:q:2:PRO:HG3	1.80	0.63
35:b:116:GLU:HA	35:b:119:GLU:HB2	1.80	0.63
52:s:63:THR:OG1	52:s:65:ASN:ND2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2121:G:H1	1:A:2210:U:H5	1.46	0.63
39:f:82:ARG:HB3	39:f:85:VAL:HG23	1.81	0.63
1:A:237:C:O2	32:8:12:LYS:NZ	2.28	0.63
35:b:60:ASP:OD1	35:b:64:ARG:NH1	2.29	0.63
40:g:85:TYR:HD2	40:g:154:TYR:HE2	1.46	0.63
44:k:84:VAL:HG11	44:k:91:ARG:HE	1.64	0.63
58:y:18:G:O2'	58:y:57:G:N2	2.29	0.63
1:A:33:C:H2'	1:A:34:G:H5'	1.81	0.63
4:D:70:TRP:CE2	4:D:150:LYS:HD2	2.34	0.63
59:z:407:GLU:HG2	59:z:489:LEU:HD11	1.80	0.63
1:A:332:G:N3	1:A:352:G:O2'	2.31	0.63
1:A:2456:G:OP1	6:F:74:ARG:NH2	2.32	0.63
45:l:49:ASN:ND2	45:l:92:ASP:OD2	2.23	0.63
1:A:1735:A:N6	1:A:1744:A:H2	1.97	0.62
35:b:97:TRP:HZ3	35:b:176:GLU:OE2	1.82	0.62
1:A:554:G:N1	64:A:3719:HOH:O	2.18	0.62
1:A:1820:C:H2'	1:A:1821:A:C5	2.34	0.62
25:l:3:LYS:O	25:l:12:PRO:HD3	2.00	0.62
34:a:207:G:O6	34:a:213:C:N4	2.31	0.62
40:g:70:LYS:HD3	40:g:96:GLN:HB3	1.81	0.62
57:x:20:U:O2'	57:x:21:A:H5'	1.99	0.62
1:A:2330:G:N1	16:S:3:ARG:HA	2.15	0.62
15:R:20:LEU:HD21	15:R:40:LYS:HD2	1.81	0.62
37:d:31:CYS:O	37:d:35:ARG:HB2	1.98	0.62
45:l:88:GLY:O	45:l:99:HIS:HD2	1.82	0.62
59:z:379:LYS:HB2	59:z:406:LEU:HD12	1.80	0.62
15:R:28:LEU:HD12	15:R:48:VAL:HG21	1.80	0.62
36:c:114:PRO:O	36:c:118:GLN:HG2	2.00	0.62
59:z:196:LEU:HA	59:z:220:GLY:HA3	1.81	0.62
20:W:83:LYS:O	20:W:84:ARG:HD3	1.98	0.62
59:z:552:LYS:HD3	59:z:553:ALA:HB3	1.81	0.62
1:A:1064:U:O2'	1:A:1066:A:H2	1.73	0.62
1:A:1682:C:OP2	64:A:3718:HOH:O	2.15	0.62
34:a:409:G:N7	37:d:35:ARG:NH1	2.39	0.62
34:a:1259:C:O2'	34:a:1261:A:H8	1.83	0.62
34:a:1300:A:OP1	52:s:3:ARG:NH2	2.32	0.62
38:e:145:LYS:NZ	38:e:149:GLU:OE2	2.23	0.62
40:g:50:ILE:HG23	40:g:121:ALA:HB1	1.81	0.62
50:q:45:HIS:CD2	50:q:47:PRO:HG3	2.35	0.62
1:A:609:C:OP2	13:P:21:ARG:NH2	2.33	0.62
1:A:1000:G:OP2	14:Q:14:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:G:O2'	1:A:2141:G:H5'	1.99	0.62
1:A:926:G:H2'	1:A:927:G:H8	1.64	0.62
10:K:17:ALA:HB1	10:K:38:VAL:HG22	1.80	0.62
19:V:46:VAL:HG13	19:V:52:VAL:HG11	1.80	0.62
41:h:73:ASP:OD1	41:h:75:ARG:HD3	2.00	0.62
59:z:431:LYS:HD2	59:z:458:GLU:HG3	1.80	0.62
1:A:2595:U:H2'	1:A:2596:U:H2'	1.81	0.62
6:F:132:VAL:HA	6:F:138:GLU:HB3	1.82	0.62
34:a:404:A:OP1	37:d:113:SER:OG	2.18	0.61
3:C:179:SER:HA	3:C:180:PHE:C	2.24	0.61
4:D:17:THR:O	4:D:211:ARG:NH2	2.32	0.61
17:T:74:ARG:HH11	17:T:74:ARG:HG2	1.64	0.61
52:s:27:GLU:HB2	52:s:28:LYS:HD2	1.83	0.61
1:A:1070:G:C4	1:A:1179:C:H1'	2.35	0.61
1:A:1210:U:H2'	1:A:1211:C:C6	2.35	0.61
1:A:1632:A:H2'	1:A:1633:C:C6	2.35	0.61
1:A:775:G:OP2	4:D:13:ARG:HD3	2.01	0.61
34:a:349:A:H5'	34:a:349:A:H8	1.65	0.61
1:A:2430:U:O4	64:A:3713:HOH:O	2.14	0.61
6:F:143:ALA:HB1	6:F:148:LEU:HB2	1.82	0.61
10:K:14:ALA:HB2	10:K:53:VAL:HG23	1.82	0.61
18:U:36:ARG:HD2	18:U:40:PHE:CZ	2.35	0.61
34:a:646:G:H2'	34:a:647:A:C8	2.36	0.61
59:z:459:ILE:HG22	59:z:460:LEU:H	1.66	0.61
10:K:108:ALA:O	10:K:112:MET:HG2	2.01	0.61
35:b:80:ILE:HG12	35:b:211:ILE:HG22	1.83	0.61
53:t:13:LEU:H	53:t:13:LEU:HD12	1.64	0.61
58:y:43:C:H3'	58:y:44:G:C8	2.36	0.61
1:A:1150:U:H2'	1:A:1151:G:H8	1.65	0.61
1:A:1288:G:O2'	13:P:7:ARG:NH2	2.33	0.61
1:A:1295:G:N7	13:P:18:ARG:NH2	2.49	0.61
37:d:201:GLN:HE21	37:d:204:ILE:HD12	1.64	0.61
58:y:23:A:H2'	58:y:24:G:H8	1.65	0.61
59:z:194:ALA:HB1	59:z:195:PRO:HA	1.82	0.61
34:a:1037:C:O2'	34:a:1038:A:H5''	1.99	0.61
1:A:2148:G:O6	1:A:2182:C:N4	2.33	0.61
34:a:954:G:OP2	34:a:1340:U:O2'	2.15	0.61
34:a:1113:A:H3'	34:a:1113:A:OP2	2.01	0.61
59:z:267:ALA:C	59:z:268:ILE:HG12	2.25	0.61
1:A:353:A:H2	1:A:1254:A:H2'	1.66	0.60
50:q:67:LYS:O	50:q:69:LYS:N	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:z:324:LYS:HE3	59:z:330:LEU:O	1.99	0.60
14:Q:60:ARG:NH1	56:w:54:5MU:H5''	2.16	0.60
25:1:85:LEU:HB3	25:1:89:GLU:HG3	1.82	0.60
49:p:23:ASP:OD2	49:p:25:ARG:NH1	2.33	0.60
1:A:596:C:N3	5:E:145:LYS:NZ	2.49	0.60
7:G:5:VAL:HG23	7:G:8:LYS:HE2	1.82	0.60
7:G:12:TYR:HA	7:G:16:ARG:HG3	1.81	0.60
28:4:14:ILE:HB	28:4:22:ILE:HG13	1.84	0.60
34:a:944:G:O2'	42:i:127:LYS:O	2.20	0.60
34:a:1210:C:P	46:m:108:ARG:HH22	2.24	0.60
35:b:212:GLN:NE2	35:b:235:SER:OG	2.34	0.60
8:H:106:THR:HG22	8:H:112:PRO:HB3	1.84	0.60
13:P:88:LEU:HD11	13:P:114:ILE:HD12	1.83	0.60
25:1:80:LEU:HG	25:1:81:LYS:H	1.66	0.60
34:a:1374:U:H2'	34:a:1375:G:C8	2.37	0.60
35:b:115:LEU:HD13	35:b:145:LEU:HB3	1.83	0.60
56:w:3:C:C4	56:w:71:G:O6	2.55	0.60
1:A:1643:C:H5'	21:X:36:LYS:HB2	1.83	0.60
1:A:1873:C:H5'	4:D:253:GLN:NE2	2.16	0.60
5:E:117:MET:O	5:E:118:LYS:HB3	2.02	0.60
8:H:98:LEU:HG	8:H:125:VAL:HG23	1.84	0.60
34:a:858:C:OP1	45:l:8:ASN:ND2	2.34	0.60
1:A:235:G:H4'	1:A:412:G:C5	2.36	0.60
1:A:1091:A:N1	9:J:7:VAL:N	2.46	0.60
1:A:1450:U:H2'	1:A:1451:U:C6	2.36	0.60
25:1:23:LYS:HB3	25:1:29:GLY:HA3	1.82	0.60
34:a:1106:A:O2'	43:j:37:PRO:O	2.17	0.60
35:b:84:GLU:HB3	35:b:219:VAL:HG21	1.84	0.60
1:A:1125:C:O2	1:A:1126:U:H6	1.84	0.60
6:F:18:ARG:HH12	6:F:20:LEU:HD23	1.67	0.60
1:A:648:C:O2'	1:A:703:U:OP1	2.17	0.60
1:A:732:G:OP1	31:7:11:LYS:NZ	2.29	0.60
1:A:1603:C:OP2	1:A:1604:A:O2'	2.09	0.60
1:A:1833:A:O2'	4:D:259:THR:HG21	2.02	0.60
17:T:23:ARG:HG3	17:T:120:ARG:NH1	2.17	0.60
20:W:18:ARG:NH1	20:W:76:VAL:O	2.35	0.60
58:y:13:C:H2'	58:y:14:A:C8	2.36	0.60
25:1:72:GLU:OE1	25:1:76:ARG:NH2	2.35	0.59
34:a:77:G:N2	34:a:87:C:H42	2.00	0.59
34:a:734:G:N3	48:o:23:GLY:HA3	2.17	0.59
35:b:12:GLU:C	35:b:14:GLY:H	2.09	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2143:U:O2	3:C:172:HIS:NE2	2.36	0.59
1:A:2298:A:H62	1:A:2355:U:H3	1.50	0.59
19:V:72:VAL:HG13	19:V:85:LYS:HB3	1.83	0.59
57:x:1:C:H2'	57:x:2:G:H8	1.65	0.59
1:A:505:A:OP2	22:Y:47:LYS:NZ	2.34	0.59
1:A:713:U:O2	32:8:2:PRO:HD2	2.02	0.59
1:A:2148:G:O2'	1:A:2149:C:H5'	2.03	0.59
6:F:53:THR:CG2	6:F:55:GLY:H	2.16	0.59
10:K:76:TYR:HB2	10:K:79:ARG:HH21	1.67	0.59
17:T:122:ASP:OD1	17:T:125:ARG:NH2	2.34	0.59
34:a:1328:A:OP1	42:i:120:ARG:NH1	2.27	0.59
35:b:80:ILE:HD13	35:b:212:GLN:HA	1.84	0.59
1:A:1125:C:O2	1:A:1125:C:H2'	2.00	0.59
8:H:76:VAL:O	8:H:80:SER:HB2	2.02	0.59
1:A:69:A:N7	21:X:31:HIS:HE1	2.00	0.59
1:A:938:C:H2'	1:A:939:C:C6	2.37	0.59
10:K:51:ALA:HB3	10:K:72:PRO:HB3	1.84	0.59
34:a:855:C:H5''	41:h:88:LYS:HD3	1.84	0.59
34:a:1107:G:N2	34:a:1110:G:H21	2.00	0.59
1:A:2548:U:H2'	1:A:2549:C:C6	2.38	0.59
50:q:13:ASP:O	50:q:15:MET:N	2.33	0.59
52:s:80:TYR:CZ	52:s:82:GLY:HA2	2.37	0.59
20:W:18:ARG:HG3	20:W:76:VAL:HB	1.83	0.59
21:X:41:ASN:O	21:X:45:THR:HG23	2.03	0.59
34:a:904:G:HO2'	55:v:13:A:H8	1.49	0.59
1:A:330:G:H22	1:A:333:A:H5''	1.67	0.59
1:A:644:G:N3	1:A:644:G:H5'	2.18	0.59
1:A:931:C:H3'	1:A:932:C:C5'	2.32	0.59
1:A:1091:A:N6	9:J:5:ARG:H	2.01	0.59
1:A:2449:U:O2'	1:A:2451:C:OP1	2.18	0.59
34:a:984:A:OP1	34:a:1003:G:N2	2.36	0.59
34:a:1261:A:O2'	34:a:1263:U:OP2	2.15	0.59
13:P:118:GLY:O	13:P:137:LYS:NZ	2.36	0.59
34:a:400:U:H5'	37:d:122:ARG:HD3	1.85	0.59
59:z:188:PRO:HB3	59:z:216:ARG:HH22	1.67	0.59
20:W:46:PHE:O	20:W:50:VAL:HG23	2.03	0.59
28:4:46:GLN:C	28:4:48:ARG:H	2.10	0.59
36:c:22:TRP:NE1	36:c:36:ASP:OD2	2.36	0.59
42:i:118:LYS:O	42:i:120:ARG:N	2.36	0.59
1:A:1099:A:N6	1:A:1150:U:H3	1.97	0.58
2:B:66:A:H61	2:B:108:U:H2'	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:135:ASP:HB3	14:Q:137:TYR:H	1.66	0.58
24:O:33:ALA:O	24:O:61:ALA:HB3	2.02	0.58
35:b:82:ARG:NH1	35:b:92:TYR:OH	2.35	0.58
1:A:696:C:H2'	1:A:697:G:C8	2.39	0.58
1:A:1992:A:OP2	4:D:242:ARG:NH2	2.34	0.58
3:C:171:ILE:HG23	3:C:172:HIS:H	1.66	0.58
6:F:184:TYR:CE2	6:F:188:ARG:HD2	2.37	0.58
8:H:20:ALA:HB1	8:H:21:PRO:HD2	1.84	0.58
9:J:56:ASN:HA	9:J:83:TYR:HA	1.85	0.58
34:a:1262:A:H5''	43:j:40:LEU:HD22	1.85	0.58
1:A:1221:A:H3'	1:A:1222:C:C6	2.38	0.58
3:C:212:VAL:HG21	3:C:226:PRO:HG3	1.84	0.58
12:O:2:ILE:HD12	12:O:6:THR:HG21	1.85	0.58
34:a:979:A:H61	34:a:1023:U:H3	1.50	0.58
38:e:83:GLU:HG2	38:e:88:LYS:HG3	1.84	0.58
40:g:65:ALA:HB1	40:g:127:ALA:HB3	1.84	0.58
48:o:39:LEU:HD13	48:o:56:LEU:HB2	1.84	0.58
1:A:794:G:OP1	20:W:88:ARG:NH2	2.27	0.58
1:A:2135:A:H2'	1:A:2136:G:O4'	2.04	0.58
1:A:2157:C:H42	1:A:2176:G:H1	1.51	0.58
1:A:2431:C:H2'	1:A:2432:G:H5''	1.85	0.58
1:A:2623:C:OP2	29:5:2:ALA:N	2.36	0.58
1:A:2858:U:H4'	1:A:2877:A:C2	2.39	0.58
2:B:8:U:H5''	16:S:15:ARG:NH1	2.18	0.58
6:F:53:THR:HG22	6:F:55:GLY:H	1.68	0.58
34:a:557:A:H5'	34:a:557:A:C8	2.36	0.58
35:b:74:LYS:NZ	35:b:166:ASP:OD2	2.36	0.58
36:c:12:LEU:HD11	47:n:51:GLY:HA2	1.84	0.58
40:g:59:LEU:HD13	40:g:63:LYS:HD2	1.84	0.58
59:z:78:PHE:CE1	59:z:181:ILE:HD11	2.38	0.58
4:D:127:VAL:HA	4:D:193:VAL:HG22	1.84	0.58
34:a:503:C:OP2	45:l:50:SER:OG	2.13	0.58
1:A:2568:G:O2'	56:w:76:A:C8	2.54	0.58
6:F:140:LEU:HD21	6:F:170:LEU:HD11	1.85	0.58
10:K:30:HIS:HA	10:K:59:ILE:HD12	1.85	0.58
34:a:1149:G:N2	34:a:1152:A:OP2	2.33	0.58
43:j:57:LYS:HE2	43:j:60:ARG:NH2	2.18	0.58
1:A:678:A:H3'	1:A:678:A:N3	2.18	0.58
1:A:1538:C:C4	1:A:2226:G:H1'	2.39	0.58
1:A:2417:U:C6	1:A:2417:U:H5'	2.39	0.58
3:C:62:VAL:HG22	3:C:63:SER:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:PRO:HG2	3:C:184:LYS:HB2	1.84	0.58
5:E:24:THR:HG23	5:E:184:VAL:HG23	1.85	0.58
10:K:10:LEU:O	10:K:11:GLN:NE2	2.36	0.58
59:z:245:PHE:HB3	59:z:250:LEU:HD13	1.84	0.58
5:E:36:ARG:HH11	5:E:85:ASN:ND2	2.01	0.58
35:b:79:ASP:OD2	35:b:79:ASP:N	2.37	0.58
58:y:25:C:H2'	58:y:26:A:H5'	1.85	0.58
5:E:2:LYS:HB2	5:E:95:ILE:HD12	1.86	0.58
8:H:3:ARG:HG3	8:H:6:ARG:NH2	2.19	0.58
34:a:113:A:H5''	34:a:114:A:H5'	1.84	0.58
35:b:20:GLU:HA	35:b:21:ARG:NH2	2.19	0.58
41:h:112:LEU:HA	41:h:134:ILE:HG12	1.85	0.58
1:A:138:A:H8	1:A:1453:C:HO2'	1.52	0.58
3:C:164:ARG:HB2	3:C:164:ARG:HH21	1.67	0.58
13:P:86:LYS:HB3	13:P:118:GLY:HA3	1.84	0.58
34:a:954:G:H5'	34:a:1340:U:O2'	2.03	0.58
58:y:8:4SU:H2'	58:y:46:G:O6	2.03	0.58
59:z:291:TYR:CG	59:z:292:PRO:HD2	2.39	0.58
1:A:681:G:H2'	1:A:682:G:C8	2.39	0.57
29:5:35:GLU:HG3	29:5:51:TYR:CG	2.39	0.57
59:z:247:PRO:HD2	59:z:248:GLN:NE2	2.19	0.57
1:A:1091:A:C6	9:J:7:VAL:N	2.62	0.57
59:z:381:ARG:HB2	59:z:386:GLU:HG2	1.86	0.57
1:A:1734:U:O2	1:A:1746:A:H5'	2.04	0.57
39:f:74:ASP:N	39:f:74:ASP:OD2	2.37	0.57
42:i:8:GLY:O	42:i:76:ALA:HB1	2.04	0.57
1:A:172:C:H2'	1:A:173:U:C6	2.38	0.57
1:A:982:G:H5''	1:A:982:G:H8	1.68	0.57
1:A:1897:A:OP2	1:A:1897:A:H8	1.87	0.57
1:A:2339:A:H2'	1:A:2340:G:C8	2.40	0.57
5:E:71:GLY:HA2	5:E:72:VAL:O	2.04	0.57
34:a:1488:U:H2'	34:a:1489:G:C8	2.39	0.57
46:m:88:ARG:HG3	46:m:98:VAL:HG13	1.86	0.57
1:A:629:U:OP1	6:F:102:PRO:HA	2.04	0.57
34:a:1113:A:O2'	42:i:3:GLN:NE2	2.37	0.57
41:h:122:ARG:NH1	41:h:122:ARG:O	2.36	0.57
59:z:360:ARG:NH1	59:z:364:GLU:OE2	2.38	0.57
59:z:382:LEU:H	59:z:382:LEU:HD22	1.70	0.57
5:E:116:VAL:HG13	5:E:122:PHE:HB2	1.85	0.57
19:V:95:LEU:HD13	19:V:97:LYS:HD3	1.86	0.57
46:m:11:ARG:HA	46:m:45:VAL:HB	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:87:ILE:O	48:o:89:GLY:N	2.37	0.57
5:E:4:ILE:HD11	5:E:29:GLY:HA2	1.86	0.57
8:H:100:GLY:HA3	8:H:102:ALA:N	2.19	0.57
34:a:637:A:O5'	41:h:56:LYS:NZ	2.38	0.57
36:c:21:ARG:HH12	36:c:56:ASP:HB3	1.69	0.57
1:A:605:G:OP2	18:U:10:ARG:HD2	2.05	0.57
13:P:65:ARG:HG3	32:8:25:MET:HG3	1.87	0.57
32:8:29:LYS:HE2	32:8:45:GLY:HA2	1.87	0.57
34:a:1200:C:H2'	34:a:1201:U:C6	2.40	0.57
47:n:33:VAL:HA	47:n:40:CYS:HA	1.87	0.57
1:A:1424:A:H8	1:A:1424:A:O5'	1.87	0.57
40:g:28:ASN:ND2	40:g:36:LYS:HE3	2.18	0.57
1:A:353:A:H2	1:A:1254:A:HO2'	1.52	0.57
1:A:922:C:H2'	1:A:923:U:O4'	2.05	0.57
16:S:35:ILE:C	16:S:36:TYR:HD1	2.12	0.57
1:A:1699:G:H3'	15:R:2:ARG:HD3	1.86	0.56
34:a:155:A:H1'	34:a:340:A:C5	2.39	0.56
34:a:1128:C:O2'	34:a:1129:A:OP2	2.17	0.56
56:w:8:4SU:O2'	56:w:21:A:N1	2.32	0.56
17:T:65:LYS:HE3	17:T:67:SER:HB2	1.86	0.56
59:z:27:ASP:OD2	59:z:44:GLN:HA	2.05	0.56
1:A:658:C:H2'	1:A:659:C:C6	2.41	0.56
1:A:2033:G:OP1	20:W:11:ARG:NH2	2.36	0.56
1:A:2043:U:O2'	1:A:2628:C:H5'	2.05	0.56
34:a:1178:U:H3	36:c:162:GLN:HE22	1.52	0.56
34:a:1236:C:H41	43:j:43:ARG:HH12	1.53	0.56
38:e:7:GLU:CD	38:e:37:ARG:HH21	2.14	0.56
51:r:31:LEU:HD11	51:r:62:GLU:HG2	1.86	0.56
59:z:24:THR:OG1	63:z:703:GCP:O2A	2.17	0.56
1:A:679:G:C6	1:A:698:C:N3	2.73	0.56
6:F:183:VAL:O	6:F:187:VAL:HG23	2.05	0.56
10:K:73:PRO:O	10:K:76:TYR:N	2.31	0.56
34:a:1446:A:H2'	34:a:1447:G:O4'	2.05	0.56
38:e:8:GLU:HB2	38:e:34:VAL:HG23	1.88	0.56
40:g:50:ILE:HG22	40:g:125:MET:SD	2.45	0.56
41:h:10:LEU:HD12	41:h:85:ARG:HG2	1.87	0.56
1:A:353:A:H2	1:A:1254:A:C2'	2.18	0.56
34:a:1395:C:H2'	34:a:1396:A:C8	2.39	0.56
49:p:17:TYR:HE2	49:p:41:PRO:HG3	1.69	0.56
57:x:16:C:O2'	57:x:60:U:O3'	2.23	0.56
1:A:2171:U:H2'	1:A:2172:G:C8	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:3:LYS:HD3	10:K:29:GLN:HA	1.88	0.56
14:Q:7:MET:HE1	14:Q:73:PRO:HG3	1.88	0.56
59:z:298:LYS:NZ	59:z:479:TYR:O	2.35	0.56
1:A:2657:C:OP2	1:A:2744:G:O2'	2.23	0.56
4:D:202:LYS:NZ	34:a:758:G:OP1	2.39	0.56
35:b:155:LEU:HA	35:b:156:LYS:CB	2.30	0.56
59:z:418:GLU:OE2	59:z:419:GLU:N	2.39	0.56
1:A:1126:U:O2	10:K:117:THR:N	2.38	0.56
1:A:2226:G:H5'	1:A:2227:G:N7	2.21	0.56
1:A:2370:C:H2'	1:A:2371:A:O4'	2.06	0.56
8:H:41:MET:HE2	8:H:65:HIS:HA	1.87	0.56
13:P:65:ARG:HG3	32:8:25:MET:CG	2.36	0.56
58:y:19:G:H3'	58:y:20:U:C2	2.40	0.56
58:y:33:U:H4'	58:y:33:U:OP1	2.04	0.56
1:A:1313:A:C2	1:A:2034:A:C4	2.94	0.56
34:a:953:A:H5'	34:a:953:A:H8	1.70	0.56
34:a:1171:C:O2	64:a:1804:HOH:O	2.18	0.56
59:z:42:ARG:HH12	59:z:48:SER:HA	1.71	0.56
1:A:678:A:H5''	1:A:679:G:OP2	2.06	0.56
7:G:44:GLY:O	7:G:47:LYS:HB2	2.06	0.56
13:P:1:MET:HE2	13:P:5:ASP:HB3	1.88	0.56
34:a:886:A:H2'	34:a:887:A:C8	2.41	0.56
34:a:1112:C:H4'	34:a:1113:A:OP2	2.04	0.56
34:a:1226:C:H2'	34:a:1227:A:C8	2.40	0.56
36:c:11:ARG:HB3	36:c:15:THR:HG22	1.88	0.56
57:x:8:4SU:H6	57:x:8:4SU:O5'	2.06	0.56
1:A:11:U:H2'	1:A:11:U:O2	2.06	0.55
7:G:83:ARG:O	7:G:86:MET:HB2	2.06	0.55
34:a:985:C:H2'	34:a:986:C:C6	2.40	0.55
56:w:5:G:O6	56:w:68:C:N3	2.39	0.55
59:z:16:ALA:HB2	59:z:106:VAL:HB	1.88	0.55
59:z:247:PRO:HD2	59:z:248:GLN:HE22	1.71	0.55
1:A:90:G:H2'	1:A:91:C:C6	2.41	0.55
4:D:242:ARG:HD3	4:D:242:ARG:N	2.20	0.55
35:b:21:ARG:HD2	35:b:21:ARG:H	1.70	0.55
59:z:47:ASP:O	59:z:53:ARG:NH1	2.39	0.55
12:O:107:ARG:HG3	12:O:112:MET:SD	2.46	0.55
34:a:87:C:H2'	34:a:88:C:C6	2.42	0.55
34:a:715:G:H5'	34:a:750:A:H4'	1.88	0.55
35:b:8:LYS:O	35:b:9:GLU:HB3	2.05	0.55
39:f:9:VAL:HG13	39:f:87:ARG:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:5:G:O2'	56:w:6:G:H8	1.89	0.55
59:z:271:ILE:HG21	59:z:325:LEU:HB3	1.88	0.55
1:A:2217:C:OP2	64:A:3720:HOH:O	2.18	0.55
34:a:150:C:H2'	34:a:151:G:H8	1.70	0.55
38:e:140:ARG:O	38:e:143:ARG:NH2	2.40	0.55
1:A:468:A:H1'	1:A:1245:C:O4'	2.06	0.55
1:A:794:G:P	20:W:88:ARG:HH21	2.29	0.55
1:A:1758:C:N4	1:A:1776:G:H1	2.03	0.55
2:B:2:C:H42	2:B:119:G:H1	1.54	0.55
15:R:44:LEU:HD22	15:R:48:VAL:HG23	1.87	0.55
57:x:1:C:H2'	57:x:2:G:C8	2.41	0.55
59:z:144:ARG:HB3	59:z:147:GLU:HG2	1.87	0.55
1:A:2678:C:H1'	8:H:109:PHE:CD2	2.41	0.55
3:C:10:LEU:HD22	3:C:32:LEU:HA	1.89	0.55
37:d:112:VAL:HG12	37:d:116:GLN:OE1	2.06	0.55
1:A:1113:G:O6	1:A:1114:A:N6	2.39	0.55
1:A:2575:A:C2	1:A:2658:U:H4'	2.41	0.55
22:Y:67:LEU:HD22	22:Y:71:LYS:HD3	1.88	0.55
34:a:798:A:H2'	34:a:800:A:H5''	1.89	0.55
34:a:1418:G:H2'	34:a:1419:U:C6	2.42	0.55
35:b:47:THR:HA	35:b:202:PRO:HG2	1.89	0.55
35:b:120:ALA:O	35:b:121:LEU:HB3	2.06	0.55
41:h:17:THR:HG22	41:h:63:LEU:HG	1.88	0.55
59:z:267:ALA:O	59:z:269:ARG:HD2	2.07	0.55
1:A:1108:G:O2'	10:K:87:GLY:N	2.40	0.55
1:A:2428:C:OP1	13:P:65:ARG:NH2	2.40	0.55
7:G:179:PRO:HB2	28:4:42:PHE:HE2	1.70	0.55
10:K:103:GLN:HG2	10:K:106:GLU:OE2	2.07	0.55
14:Q:56:ARG:HB2	14:Q:56:ARG:NH1	2.22	0.55
40:g:113:GLU:OE1	40:g:122:HIS:ND1	2.40	0.55
45:l:97:ARG:HB2	45:l:98:TYR:CE2	2.41	0.55
50:q:81:ARG:NH2	50:q:83:ASP:OD2	2.33	0.55
1:A:2197:A:H2'	1:A:2198:C:C6	2.41	0.55
10:K:115:LEU:HD22	10:K:126:MET:HE3	1.88	0.55
11:N:120:LEU:HD22	11:N:122:VAL:HG23	1.89	0.55
28:4:15:ILE:HD12	28:4:32:TYR:HE1	1.72	0.55
35:b:110:GLN:HA	35:b:113:HIS:CD2	2.42	0.55
48:o:29:VAL:HG21	48:o:67:LEU:HD13	1.88	0.55
1:A:1067:G:N7	11:N:66:LYS:HE2	2.21	0.55
11:N:108:PRO:O	11:N:113:GLY:HA3	2.06	0.55
39:f:50:TYR:CE2	51:r:77:GLY:HA2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:A:C8	1:A:1066:A:H3'	2.42	0.54
1:A:1856:G:H4'	4:D:242:ARG:CZ	2.37	0.54
1:A:2873:G:OP1	17:T:119:LYS:HD2	2.07	0.54
23:Z:27:VAL:HG12	23:Z:85:HIS:CE1	2.42	0.54
28:4:46:GLN:CD	28:4:48:ARG:HE	2.15	0.54
39:f:100:ASN:HD21	51:r:23:LYS:HG2	1.72	0.54
3:C:39:GLU:HG2	3:C:217:THR:HB	1.89	0.54
9:J:23:SER:HA	9:J:117:LEU:O	2.07	0.54
12:O:49:ARG:NH2	34:a:1406:G:OP1	2.34	0.54
34:a:349:A:H5'	34:a:349:A:C8	2.41	0.54
34:a:446:A:N6	34:a:465:U:H2'	2.22	0.54
34:a:982:G:C2	34:a:983:A:H1'	2.41	0.54
1:A:142:C:O2'	21:X:2:LYS:NZ	2.40	0.54
1:A:1039:C:O2'	1:A:1041:A:OP1	2.16	0.54
4:D:275:LYS:HG3	4:D:276:LYS:H	1.72	0.54
1:A:527:A:H4'	1:A:528:U:H5''	1.88	0.54
1:A:2131:G:OP1	1:A:2139:U:N3	2.40	0.54
1:A:2226:G:H5'	1:A:2227:G:C5	2.42	0.54
34:a:262:G:H5''	34:a:263:C:C5	2.43	0.54
34:a:982:G:N2	34:a:983:A:N3	2.55	0.54
35:b:91:PRO:HB3	35:b:154:LEU:HB2	1.89	0.54
52:s:43:GLU:OE1	52:s:43:GLU:N	2.33	0.54
56:w:51:U:H3	56:w:63:G:H1	1.55	0.54
58:y:10:G:H1	58:y:25:C:N4	2.06	0.54
58:y:28:G:H3'	58:y:29:G:H5''	1.90	0.54
59:z:63:ALA:O	59:z:81:ILE:N	2.28	0.54
1:A:552:A:C2	1:A:2064:C:H4'	2.42	0.54
1:A:703:U:H2'	1:A:704:C:C6	2.42	0.54
1:A:859:U:H2'	1:A:860:C:C6	2.42	0.54
7:G:32:PRO:HB3	7:G:163:ALA:HB2	1.89	0.54
9:J:74:LEU:O	9:J:76:GLY:N	2.33	0.54
34:a:920:G:H21	42:i:124:GLN:NE2	2.05	0.54
36:c:6:HIS:CD2	36:c:8:ILE:H	2.12	0.54
37:d:8:VAL:HB	37:d:21:LEU:HD23	1.89	0.54
56:w:44:G:OP1	56:w:44:G:H4'	2.07	0.54
59:z:93:VAL:HG11	59:z:120:LYS:HD2	1.88	0.54
1:A:1774:C:H3'	1:A:1775:G:O4'	2.07	0.54
1:A:2202:G:O2'	1:A:2203:G:OP1	2.24	0.54
1:A:2750:A:OP2	64:A:3721:HOH:O	2.19	0.54
3:C:6:ARG:NH1	3:C:218:MET:O	2.40	0.54
13:P:62:LEU:O	32:8:13:ARG:HD3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:57:U:H2'	34:a:58:G:C8	2.43	0.54
34:a:596:C:O2	34:a:613:G:N2	2.40	0.54
46:m:50:GLU:O	46:m:54:VAL:HG13	2.08	0.54
56:w:2:C:N3	56:w:71:G:O6	2.40	0.54
1:A:1051:C:C2	1:A:1182:G:N2	2.75	0.54
8:H:3:ARG:HH12	8:H:5:GLY:N	2.05	0.54
10:K:76:TYR:O	10:K:78:ILE:N	2.41	0.54
14:Q:60:ARG:HH12	56:w:54:5MU:H5''	1.71	0.54
34:a:661:U:H3	34:a:697:G:N2	2.05	0.54
35:b:178:ARG:HH11	35:b:178:ARG:HG3	1.71	0.54
35:b:178:ARG:NH2	41:h:68:ARG:HH22	2.06	0.54
59:z:530:ARG:HD3	59:z:552:LYS:HB2	1.89	0.54
1:A:1231:G:H5''	19:V:81:TYR:CE2	2.43	0.54
1:A:1772:C:H42	1:A:1773:C:N4	2.05	0.54
1:A:2226:G:H5'	1:A:2227:G:C6	2.43	0.54
8:H:21:PRO:O	8:H:23:ARG:NH1	2.41	0.54
23:Z:27:VAL:HG22	23:Z:29:TYR:HD2	1.72	0.54
34:a:924:A:H2'	34:a:925:G:C8	2.43	0.54
34:a:1057:G:O2'	34:a:1084:A:N1	2.39	0.54
40:g:45:ASP:O	40:g:49:ILE:HG13	2.07	0.54
51:r:53:ARG:HH21	51:r:60:ALA:N	2.05	0.54
1:A:2450:A:H5'	1:A:2450:A:C8	2.43	0.54
1:A:2797:C:O2'	5:E:66:HIS:ND1	2.38	0.54
4:D:27:THR:OG1	4:D:28:GLU:N	2.41	0.54
34:a:1284:U:C5	46:m:17:VAL:HG21	2.43	0.54
38:e:100:VAL:O	38:e:107:ARG:NH2	2.41	0.54
1:A:541:C:OP1	29:5:16:ARG:NH2	2.41	0.54
1:A:1064:U:H3	1:A:1187:A:H62	1.56	0.54
4:D:166:GLN:HE22	4:D:176:ARG:HH12	1.56	0.54
33:9:7:VAL:HG23	33:9:25:VAL:HG23	1.90	0.54
35:b:80:ILE:HD11	35:b:215:LEU:HB2	1.90	0.54
59:z:231:TYR:O	59:z:233:THR:N	2.40	0.54
1:A:679:G:N1	1:A:698:C:N3	2.55	0.53
1:A:2638:G:O2'	1:A:2793:A:N1	2.36	0.53
5:E:111:ARG:HG3	5:E:160:TYR:CD1	2.43	0.53
13:P:138:LEU:HD23	13:P:145:PRO:HG3	1.90	0.53
34:a:46:U:H2'	34:a:47:G:C8	2.43	0.53
37:d:177:ASP:OD2	37:d:180:GLY:HA3	2.08	0.53
1:A:2318:G:H4'	1:A:2319:G:O5'	2.09	0.53
1:A:2812:G:H2'	1:A:2813:C:O4'	2.08	0.53
3:C:57:ASN:H	3:C:201:PRO:HG2	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:104:ARG:HH22	17:T:43:GLN:HE22	1.56	0.53
15:R:33:ARG:NH1	15:R:115:GLU:OE2	2.38	0.53
34:a:1131:U:O3'	42:i:14:VAL:HG11	2.08	0.53
1:A:425:G:OP2	64:A:3722:HOH:O	2.19	0.53
3:C:177:LYS:HB2	3:C:180:PHE:CD1	2.43	0.53
11:N:49:GLY:O	11:N:119:ARG:NH1	2.42	0.53
42:i:50:LEU:HD23	42:i:85:LEU:HD11	1.91	0.53
48:o:33:THR:HG21	48:o:85:LEU:HD22	1.91	0.53
56:w:67:C:H2'	56:w:68:C:C6	2.44	0.53
59:z:337:SER:OG	59:z:339:ALA:O	2.25	0.53
1:A:792:A:H2'	1:A:2623:C:H5''	1.90	0.53
1:A:1593:C:H2'	1:A:1594:C:C6	2.44	0.53
1:A:2622:U:H5'	1:A:2622:U:H6	1.73	0.53
57:x:1:C:N4	59:z:575:GLU:OE2	2.41	0.53
59:z:78:PHE:CD1	59:z:181:ILE:HD11	2.43	0.53
1:A:238:G:P	32:8:13:ARG:HH22	2.32	0.53
1:A:1521:G:H2'	1:A:1522:C:C6	2.44	0.53
34:a:636:U:O4	34:a:736:G:O2'	2.22	0.53
40:g:37:ASN:O	40:g:41:ARG:HG3	2.08	0.53
54:u:15:ARG:HG2	54:u:15:ARG:HH11	1.73	0.53
1:A:879:U:O2	13:P:55:ARG:NH2	2.41	0.53
1:A:1126:U:H1'	10:K:117:THR:HB	1.89	0.53
1:A:2388:A:H2'	1:A:2389:A:C8	2.44	0.53
34:a:504:A:OP1	45:l:52:LEU:HB2	2.09	0.53
34:a:904:G:O2'	55:v:13:A:H1'	2.08	0.53
34:a:1132:C:O2'	34:a:1262:A:N1	2.40	0.53
36:c:36:ASP:OD1	36:c:57:ILE:HG21	2.09	0.53
56:w:63:G:H5'	56:w:63:G:H8	1.74	0.53
58:y:9:A:N1	58:y:46:G:N2	2.57	0.53
59:z:495:LEU:HD12	59:z:495:LEU:H	1.73	0.53
1:A:1355:G:OP2	31:7:9:ARG:HD2	2.09	0.53
3:C:41:VAL:HB	3:C:176:GLY:HA3	1.90	0.53
7:G:161:THR:CG2	7:G:163:ALA:H	2.21	0.53
10:K:7:VAL:HG22	10:K:9:LYS:HE2	1.90	0.53
10:K:60:TYR:HD2	10:K:64:SER:HB2	1.73	0.53
41:h:120:THR:OG1	41:h:123:GLU:HG3	2.08	0.53
1:A:271:U:O2'	1:A:272:G:OP1	2.20	0.53
16:S:28:VAL:HG21	16:S:98:VAL:HG13	1.90	0.53
34:a:139:G:H2'	34:a:140:G:H8	1.72	0.53
34:a:176:G:N2	34:a:177:U:O4	2.36	0.53
34:a:931:G:H5'	34:a:943:A:H61	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:3:ASN:N	36:c:3:ASN:OD1	2.41	0.53
59:z:490:VAL:HG11	59:z:510:ARG:HD3	1.90	0.53
1:A:1514:C:H2'	1:A:1515:A:C8	2.44	0.53
1:A:2601:A:H5''	4:D:239:ARG:HE	1.74	0.53
4:D:134:ARG:NH1	4:D:188:GLU:OE2	2.40	0.53
5:E:1:MET:HE1	5:E:199:ARG:HD3	1.91	0.53
8:H:52:VAL:HG23	8:H:65:HIS:CD2	2.43	0.53
13:P:47:ASP:OD2	13:P:50:ARG:NH2	2.40	0.53
22:Y:102:CYS:SG	22:Y:103:GLY:N	2.82	0.53
28:4:15:ILE:HD12	28:4:32:TYR:CE1	2.44	0.53
28:4:58:ARG:HG3	28:4:58:ARG:O	2.08	0.53
33:9:23:VAL:H	33:9:36:GLN:NE2	2.07	0.53
33:9:32:HIS:O	33:9:34:GLN:HG3	2.09	0.53
34:a:704:C:O2	51:r:71:LYS:NZ	2.41	0.53
59:z:2:ILE:HG12	59:z:192:PRO:HG2	1.91	0.53
1:A:1839:A:H2'	1:A:1840:A:C8	2.45	0.53
6:F:136:THR:HA	6:F:166:ALA:O	2.09	0.53
7:G:82:LEU:HD23	7:G:88:ILE:HG21	1.91	0.53
17:T:51:ARG:HG3	17:T:98:LYS:HD2	1.90	0.53
34:a:218:U:H2'	34:a:219:U:C6	2.44	0.53
35:b:98:LEU:HG	35:b:101:MET:HE3	1.91	0.53
35:b:110:GLN:HA	35:b:113:HIS:HD2	1.73	0.53
42:i:45:ALA:HB1	42:i:47:LEU:H	1.74	0.53
59:z:68:TYR:OH	59:z:179:GLU:OE2	2.15	0.53
7:G:17:PRO:HA	7:G:20:ILE:HD12	1.90	0.52
8:H:91:GLY:O	8:H:93:GLY:N	2.42	0.52
9:J:70:GLU:O	9:J:72:ASP:N	2.42	0.52
26:2:17:SER:OG	26:2:20:GLU:OE1	2.25	0.52
34:a:508:G:H2'	34:a:509:C:C6	2.43	0.52
42:i:128:ARG:NH1	57:x:35:A:OP2	2.41	0.52
48:o:17:ARG:HG3	48:o:17:ARG:HH11	1.73	0.52
1:A:206:A:C2	1:A:223:U:H4'	2.45	0.52
1:A:483:G:O2'	1:A:494:G:O6	2.25	0.52
1:A:573:G:O2'	1:A:1264:A:N3	2.37	0.52
4:D:71:ASP:CB	4:D:103:ARG:HH22	2.21	0.52
13:P:101:VAL:HG23	13:P:106:LEU:HD12	1.90	0.52
35:b:212:GLN:O	35:b:216:SER:OG	2.19	0.52
37:d:177:ASP:OD2	37:d:182:LYS:HE2	2.09	0.52
57:x:1:C:O2'	57:x:2:G:OP1	2.23	0.52
58:y:23:A:H2'	58:y:24:G:C8	2.44	0.52
1:A:79:G:HO2'	1:A:318:G:HO2'	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:G:OP1	31:7:33:ARG:NH1	2.42	0.52
1:A:2196:C:H1'	3:C:217:THR:O	2.09	0.52
17:T:35:LYS:HD3	17:T:36:GLU:N	2.24	0.52
17:T:74:ARG:HG2	17:T:74:ARG:NH1	2.24	0.52
24:0:23:VAL:HB	24:0:38:VAL:HG22	1.90	0.52
34:a:453:C:H2'	34:a:454:G:O4'	2.09	0.52
53:t:92:LEU:O	53:t:96:GLY:N	2.40	0.52
1:A:1105:U:C4'	1:A:1106:U:H5'	2.35	0.52
3:C:192:PHE:HD2	3:C:193:ILE:HD12	1.74	0.52
6:F:9:ILE:HD13	6:F:123:LEU:HD23	1.92	0.52
7:G:18:GLU:HG2	7:G:175:LEU:HD21	1.90	0.52
15:R:104:ARG:HD2	15:R:109:ALA:HB3	1.90	0.52
22:Y:97:ARG:HD3	22:Y:107:ASP:O	2.09	0.52
28:4:40:HIS:HB3	28:4:43:TYR:HD2	1.74	0.52
34:a:475:G:OP2	37:d:132:ARG:NH2	2.42	0.52
34:a:509:C:OP1	45:l:89:ARG:NH1	2.42	0.52
34:a:979:A:C6	34:a:980:G:C6	2.96	0.52
34:a:1003:G:C8	34:a:1003:G:OP2	2.63	0.52
36:c:87:LEU:O	36:c:91:LEU:HB2	2.10	0.52
40:g:146:GLU:OE1	40:g:149:ARG:NE	2.43	0.52
51:r:32:ARG:HA	51:r:69:THR:HG21	1.90	0.52
1:A:1906:A:H2'	1:A:1907:C:O4'	2.10	0.52
1:A:2614:G:OP1	59:z:572:LYS:NZ	2.42	0.52
1:A:2801:C:H1'	1:A:2900:A:C2	2.44	0.52
6:F:103:LYS:HA	6:F:106:ARG:HG3	1.90	0.52
34:a:386:C:O3'	49:p:28:ARG:NH2	2.41	0.52
34:a:980:G:N2	34:a:1023:U:O2	2.42	0.52
35:b:172:ILE:HD12	35:b:173:ALA:N	2.23	0.52
56:w:62:C:H3'	56:w:63:G:H5''	1.92	0.52
59:z:267:ALA:O	59:z:268:ILE:HG12	2.10	0.52
1:A:1091:A:C6	9:J:5:ARG:N	2.71	0.52
1:A:1153:U:HO2'	1:A:1154:C:C5'	2.21	0.52
1:A:1474:G:H2'	1:A:1475:C:C6	2.45	0.52
1:A:1512:G:H2'	1:A:1593:C:H41	1.75	0.52
1:A:2338:A:H2'	1:A:2339:A:C8	2.43	0.52
3:C:182:PRO:O	3:C:184:LYS:N	2.43	0.52
10:K:27:LEU:HD12	10:K:27:LEU:H	1.74	0.52
34:a:741:U:H2'	34:a:742:G:O4'	2.09	0.52
52:s:50:ALA:HA	52:s:59:PRO:HA	1.92	0.52
7:G:18:GLU:HA	7:G:21:ARG:HH11	1.75	0.52
10:K:101:TRP:NE1	10:K:139:VAL:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:A:H2'	1:A:820:A:N3	2.25	0.52
1:A:1097:C:H42	1:A:1152:G:H1	1.58	0.52
1:A:1220:G:H1'	1:A:1221:A:O5'	2.10	0.52
1:A:1775:G:H5'	1:A:1776:G:OP2	2.10	0.52
48:o:17:ARG:HD3	48:o:26:GLU:HG3	1.90	0.52
59:z:171:GLY:O	59:z:172:GLU:HB3	2.09	0.52
1:A:116:A:H4'	1:A:117:U:OP1	2.09	0.52
1:A:2483:G:H2'	1:A:2486:C:H42	1.74	0.52
1:A:2568:G:H1'	56:w:76:A:H8	1.73	0.52
1:A:2859:A:OP2	1:A:2875:U:H5	1.91	0.52
6:F:11:VAL:HB	6:F:18:ARG:HB3	1.92	0.52
34:a:430:U:H2'	34:a:431:C:C6	2.45	0.52
34:a:442:G:O6	34:a:470:G:O2'	2.27	0.52
34:a:721:A:H2'	34:a:722:C:C6	2.44	0.52
34:a:1004:U:H2'	34:a:1005:G:C8	2.44	0.52
38:e:77:PRO:HD2	38:e:142:LEU:HD22	1.91	0.52
47:n:23:ARG:HD2	47:n:28:GLY:O	2.10	0.52
59:z:131:ILE:HG12	59:z:158:LEU:HD11	1.91	0.52
1:A:504:A:N3	1:A:506:G:H5''	2.25	0.52
1:A:1711:A:H4'	12:O:67:LYS:HB2	1.91	0.52
1:A:1894:U:OP1	1:A:2421:G:O2'	2.20	0.52
4:D:38:LYS:HE3	4:D:39:LYS:O	2.10	0.52
29:5:16:ARG:HG2	29:5:16:ARG:NH1	2.25	0.52
39:f:50:TYR:OH	39:f:87:ARG:NH2	2.43	0.52
57:x:17(A):U:O2'	57:x:18:G:H5''	2.10	0.52
1:A:2045:G:H2'	1:A:2046:C:H6	1.75	0.51
1:A:2494:C:N3	14:Q:124:LYS:NZ	2.58	0.51
1:A:2671:A:OP1	59:z:472:ARG:HA	2.10	0.51
6:F:29:ASN:H	6:F:112:MET:CE	2.23	0.51
42:i:11:LYS:O	42:i:12:GLU:HB2	2.10	0.51
42:i:63:ILE:HG21	42:i:77:ILE:HG12	1.92	0.51
1:A:19:C:OP1	18:U:22:LYS:NZ	2.29	0.51
1:A:963:A:N3	2:B:80:U:O2'	2.39	0.51
1:A:2181:G:N2	1:A:2182:C:O2	2.43	0.51
1:A:2609:A:OP1	64:A:3723:HOH:O	2.19	0.51
5:E:72:VAL:CA	5:E:73:GLU:HB2	2.35	0.51
19:V:28:GLU:O	19:V:61:VAL:HG21	2.10	0.51
32:8:32:LEU:O	32:8:36:LYS:HE3	2.10	0.51
34:a:676:U:O2'	34:a:678:A:N7	2.33	0.51
35:b:61:LEU:HD12	35:b:68:ILE:HD11	1.92	0.51
39:f:2:ARG:NE	39:f:69:GLU:HG2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:3:LYS:O	49:p:21:VAL:HA	2.10	0.51
1:A:1214:G:H2'	1:A:1215:G:O4'	2.10	0.51
4:D:108:PRO:HB3	4:D:143:HIS:CE1	2.45	0.51
8:H:56:SER:HB3	8:H:61:HIS:ND1	2.26	0.51
10:K:100:THR:O	10:K:104:VAL:HG12	2.10	0.51
16:S:25:ARG:HD3	16:S:42:ASP:OD1	2.10	0.51
17:T:27:THR:HB	17:T:89:VAL:HG22	1.93	0.51
34:a:964:A:H2'	34:a:965:G:C8	2.46	0.51
34:a:1127:G:N2	34:a:1129:A:H62	2.08	0.51
59:z:-60:LEU:HD11	59:z:-34:LEU:HD21	1.93	0.51
59:z:338:THR:HB	59:z:503:ALA:HA	1.93	0.51
1:A:214:G:H21	1:A:216:A:H62	1.57	0.51
1:A:293:C:H2'	1:A:294:C:H6	1.76	0.51
1:A:558:U:H5'	18:U:42:ALA:HB1	1.93	0.51
1:A:678:A:N3	1:A:678:A:C2'	2.73	0.51
1:A:1218:A:H1'	1:A:1219:U:H5''	1.91	0.51
3:C:189:ILE:HD11	3:C:214:VAL:HG21	1.92	0.51
9:J:71:LEU:O	9:J:73:GLY:N	2.43	0.51
11:N:73:THR:OG1	11:N:82:LEU:HD11	2.11	0.51
33:9:23:VAL:H	33:9:36:GLN:HE21	1.56	0.51
34:a:1008:C:H2'	34:a:1010:G:C8	2.45	0.51
34:a:1162:A:OP1	42:i:103:THR:OG1	2.24	0.51
43:j:26:ALA:O	43:j:84:GLN:NE2	2.43	0.51
53:t:10:LEU:HB3	53:t:12:ALA:N	2.24	0.51
56:w:63:G:H4'	56:w:63:G:OP1	2.11	0.51
56:w:67:C:H5'	59:z:548:ARG:HB3	1.92	0.51
58:y:26:A:H2'	58:y:27:G:O4'	2.10	0.51
58:y:40:C:H2'	58:y:41:C:C6	2.45	0.51
59:z:-68:MET:SD	59:z:-68:MET:N	2.77	0.51
1:A:670:A:H2'	1:A:671:G:O4'	2.10	0.51
1:A:1066:A:H3'	1:A:1066:A:H8	1.75	0.51
1:A:2045:G:H2'	1:A:2046:C:C6	2.45	0.51
37:d:105:VAL:HG13	37:d:110:PHE:HB2	1.91	0.51
44:k:45:GLY:HA2	44:k:48:ILE:HD11	1.93	0.51
56:w:71:G:H21	56:w:72:C:N4	2.09	0.51
59:z:428:LEU:HD13	59:z:452:TYR:CE1	2.46	0.51
1:A:35:G:N3	1:A:475:G:O2'	2.44	0.51
1:A:1616:A:H2'	1:A:1617:A:C8	2.44	0.51
1:A:1775:G:H2'	1:A:1775:G:N3	2.26	0.51
1:A:2157:C:H3'	1:A:2158:C:C6	2.46	0.51
3:C:66:HIS:HE2	3:C:184:LYS:HD2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:m:85:GLY:HA2	46:m:86:CYS:HB3	1.93	0.51
59:z:38:ASP:N	59:z:38:ASP:OD1	2.43	0.51
4:D:148:GLU:HB2	4:D:151:LYS:HD2	1.92	0.51
5:E:9:VAL:HG13	5:E:25:VAL:O	2.11	0.51
8:H:154:PRO:HB3	8:H:163:TYR:CZ	2.46	0.51
10:K:57:ILE:HG12	10:K:67:PHE:HB3	1.93	0.51
22:Y:92:ASN:N	22:Y:93:GLY:HA2	2.25	0.51
28:4:67:TYR:OH	52:s:42:PRO:HD2	2.11	0.51
34:a:1267:A:H4'	34:a:1268:A:H5'	1.92	0.51
35:b:118:LEU:HB3	35:b:142:LEU:HG	1.90	0.51
46:m:39:ILE:HD12	46:m:56:LEU:HG	1.92	0.51
59:z:-65:ILE:HD11	59:z:-25:LEU:HD13	1.92	0.51
5:E:127:ASP:OD2	64:E:401:HOH:O	2.19	0.51
7:G:113:ARG:O	7:G:140:ILE:HD11	2.11	0.51
36:c:181:ASN:ND2	36:c:204:LEU:HB2	2.25	0.51
43:j:16:LEU:HD23	43:j:94:VAL:HG23	1.93	0.51
59:z:384:SER:OG	59:z:401:ARG:NH1	2.43	0.51
1:A:539:A:H2	1:A:1305:G:N3	2.09	0.51
3:C:56:GLN:HA	3:C:201:PRO:CB	2.41	0.51
6:F:124:LEU:HB3	6:F:193:VAL:HG22	1.92	0.51
22:Y:11:ASP:OD1	22:Y:97:ARG:NH2	2.39	0.51
34:a:1161:A:OP2	42:i:97:LYS:NZ	2.29	0.51
39:f:61:LEU:O	39:f:62:TRP:HB2	2.11	0.51
42:i:112:LYS:HA	42:i:119:ALA:H	1.76	0.51
1:A:115:A:C8	1:A:116:A:C8	2.99	0.51
1:A:353:A:H2	1:A:1254:A:O2'	1.92	0.51
1:A:598:U:H2'	1:A:599:G:C8	2.46	0.51
1:A:885:U:H2'	1:A:886:C:C6	2.46	0.51
1:A:901:G:O2'	24:0:27:GLU:OE2	2.29	0.51
1:A:2573:U:O2'	12:O:23:ARG:HD3	2.11	0.51
1:A:2845:U:H2'	1:A:2846:G:C8	2.46	0.51
16:S:15:ARG:O	16:S:19:LYS:HG2	2.11	0.51
34:a:566:U:H5''	48:o:64:ARG:NH1	2.25	0.51
36:c:157:ILE:HD13	36:c:166:GLU:HG2	1.93	0.51
53:t:45:GLN:HA	53:t:91:LEU:HD22	1.93	0.51
56:w:18:G:HO2'	56:w:57:G:H22	1.48	0.51
1:A:216:A:H2'	1:A:218:U:O4'	2.10	0.50
1:A:932:C:H4'	1:A:932:C:OP1	2.10	0.50
5:E:179:GLU:HB3	5:E:181:LEU:HD22	1.93	0.50
8:H:3:ARG:NH1	8:H:6:ARG:H	2.08	0.50
10:K:122:ALA:O	10:K:126:MET:HE2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1097:C:H2'	34:a:1098:C:H6	1.76	0.50
34:a:1447:G:H2'	34:a:1448:G:C8	2.46	0.50
36:c:73:PRO:HB3	36:c:103:VAL:HG11	1.93	0.50
37:d:173:TRP:CD1	37:d:173:TRP:H	2.28	0.50
1:A:506:G:C4	1:A:531:A:C2	3.00	0.50
1:A:1198:C:H2'	1:A:1199:G:O4'	2.10	0.50
1:A:1216:G:N7	1:A:1217:G:C6	2.79	0.50
1:A:2135:A:O2'	1:A:2188:U:O2'	2.07	0.50
3:C:62:VAL:CG1	3:C:63:SER:HA	2.40	0.50
6:F:24:LEU:HB3	6:F:115:ALA:HB2	1.94	0.50
11:N:131:GLN:H	11:N:131:GLN:CD	2.18	0.50
23:Z:19:ARG:NH1	23:Z:84:GLU:O	2.42	0.50
24:0:23:VAL:HA	24:0:38:VAL:HA	1.93	0.50
34:a:1397:U:H3	34:a:1464:G:H1	1.59	0.50
40:g:70:LYS:HB3	40:g:96:GLN:HG2	1.93	0.50
56:w:2:C:C4	56:w:71:G:O6	2.64	0.50
59:z:-12:ARG:HB2	59:z:-12:ARG:HH11	1.77	0.50
1:A:480:C:N3	1:A:498:G:H5'	2.26	0.50
1:A:1635:U:H2'	1:A:1636:G:C8	2.47	0.50
3:C:177:LYS:O	3:C:179:SER:N	2.44	0.50
4:D:274:ARG:CA	4:D:275:LYS:HB2	2.37	0.50
5:E:24:THR:HG22	5:E:186:GLY:O	2.11	0.50
7:G:49:ASP:N	7:G:49:ASP:OD1	2.43	0.50
20:W:37:ARG:HB3	20:W:37:ARG:HH11	1.77	0.50
34:a:1087:G:P	35:b:111:ARG:HD2	2.51	0.50
45:l:24:VAL:HG22	45:l:27:LEU:HD22	1.93	0.50
59:z:417:PRO:HG2	59:z:420:TYR:HD1	1.76	0.50
1:A:745:A:H2'	1:A:746:G:O4'	2.12	0.50
1:A:1416:G:HO2'	1:A:1417:U:H5	1.60	0.50
1:A:2205:G:H8	1:A:2205:G:OP2	1.95	0.50
1:A:2250:G:P	4:D:244:ARG:HH12	2.34	0.50
13:P:97:PRO:HD3	13:P:126:VAL:O	2.11	0.50
26:2:66:GLU:HA	26:2:69:ARG:NH1	2.27	0.50
34:a:1055:G:H2'	34:a:1056:U:C6	2.45	0.50
42:i:8:GLY:HA3	42:i:76:ALA:O	2.12	0.50
59:z:521:VAL:HG22	59:z:537:ILE:HG22	1.93	0.50
1:A:924:A:N1	1:A:944:A:H2	2.09	0.50
1:A:1223:C:H2'	1:A:1224:C:C6	2.47	0.50
1:A:1612:A:OP1	4:D:211:ARG:NH1	2.43	0.50
1:A:1774:C:C5	1:A:1775:G:C8	3.00	0.50
11:N:56:ASN:N	11:N:125:GLY:O	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:88:LEU:HD22	13:P:95:VAL:HG11	1.93	0.50
34:a:1354:G:OP1	42:i:12:GLU:HB2	2.12	0.50
35:b:160:ASP:O	35:b:183:PRO:HD2	2.12	0.50
52:s:22:LEU:HD22	52:s:27:GLU:HA	1.92	0.50
1:A:1824:U:H2'	1:A:1825:C:C6	2.46	0.50
1:A:2820:G:H5'	5:E:60:ASN:HD22	1.76	0.50
3:C:175:VAL:HG22	3:C:176:GLY:N	2.26	0.50
10:K:14:ALA:H	10:K:53:VAL:H	1.59	0.50
10:K:131:ALA:O	10:K:135:GLY:N	2.43	0.50
16:S:61:ASN:O	16:S:65:VAL:HG23	2.12	0.50
22:Y:56:PRO:C	22:Y:58:GLY:H	2.20	0.50
34:a:171:C:H2'	34:a:172:C:C6	2.46	0.50
34:a:1054:C:OP1	38:e:27:ARG:NH2	2.45	0.50
35:b:19:HIS:CE1	35:b:206:ASP:HB2	2.47	0.50
39:f:82:ARG:HB3	39:f:85:VAL:CG2	2.42	0.50
41:h:101:PRO:HG3	41:h:133:LEU:HD11	1.93	0.50
46:m:96:LEU:O	46:m:110:ARG:NH1	2.38	0.50
58:y:45:U:H5''	58:y:46:G:OP2	2.11	0.50
1:A:76:A:H2'	1:A:77:G:H8	1.76	0.50
4:D:173:VAL:C	4:D:174:ILE:HD13	2.37	0.50
12:O:64:ARG:HB3	12:O:79:PHE:CG	2.47	0.50
24:O:50:ASN:HB3	24:O:63:VAL:HG22	1.92	0.50
28:4:55:ARG:C	28:4:57:GLU:H	2.20	0.50
32:8:8:LYS:O	32:8:12:LYS:HG3	2.11	0.50
34:a:843:A:H2'	34:a:844:C:C6	2.47	0.50
4:D:10:THR:OG1	4:D:13:ARG:HG2	2.12	0.50
5:E:119:ARG:HG2	5:E:160:TYR:HB2	1.93	0.50
6:F:17:ARG:NH1	6:F:17:ARG:HB3	2.27	0.50
35:b:112:VAL:HG23	35:b:149:LEU:HD13	1.94	0.50
37:d:173:TRP:CE3	37:d:189:PRO:HG3	2.47	0.50
48:o:65:ARG:HG2	48:o:68:ARG:NH2	2.27	0.50
1:A:31:C:O2'	1:A:32:U:H5'	2.11	0.50
1:A:552:A:C2	1:A:2063:A:H2'	2.46	0.50
1:A:1732:C:H2'	1:A:1733:G:O4'	2.12	0.50
1:A:2166:C:OP2	1:A:2167:C:N4	2.43	0.50
1:A:2888:C:OP2	64:A:3724:HOH:O	2.19	0.50
10:K:37:PHE:O	10:K:41:PHE:HB3	2.12	0.50
34:a:1103:G:H2'	34:a:1104:U:C6	2.47	0.50
34:a:1334:C:H2'	34:a:1335:G:C8	2.47	0.50
36:c:82:GLU:CD	36:c:85:ARG:HH12	2.19	0.50
1:A:271:U:O2'	1:A:272:G:P	2.70	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1633:C:H2'	1:A:1634:C:C6	2.47	0.49
1:A:1667:G:OP2	64:A:3725:HOH:O	2.20	0.49
1:A:2758:U:OP1	8:H:85:LYS:NZ	2.46	0.49
7:G:46:ALA:O	7:G:51:ARG:HG3	2.11	0.49
34:a:187:C:H2'	34:a:188:C:O4'	2.12	0.49
35:b:32:ILE:HD13	35:b:40:HIS:CD2	2.47	0.49
40:g:79:ARG:O	40:g:84:ASN:HA	2.11	0.49
1:A:1545:G:O2'	4:D:100:GLY:O	2.28	0.49
1:A:2189:G:H5''	1:A:2189:G:H8	1.77	0.49
1:A:2696:G:H5'	12:O:68:GLU:OE1	2.12	0.49
10:K:52:ILE:HB	10:K:73:PRO:HG3	1.94	0.49
10:K:88:ALA:O	10:K:90:LYS:N	2.37	0.49
46:m:9:ILE:HG13	46:m:18:ALA:HB1	1.94	0.49
59:z:245:PHE:C	59:z:246:THR:HG1	2.13	0.49
59:z:414:ILE:HD12	59:z:428:LEU:HD11	1.94	0.49
1:A:1115:A:H5'	1:A:1117:C:OP2	2.12	0.49
1:A:1132:G:C6	1:A:1148:A:C2	3.01	0.49
1:A:1824:U:H2'	1:A:1825:C:H6	1.76	0.49
1:A:2811:A:H1'	1:A:2903:U:H1'	1.93	0.49
7:G:7:LEU:HB2	7:G:104:GLU:HB2	1.94	0.49
18:U:58:ARG:HA	18:U:61:TRP:CE3	2.47	0.49
23:Z:45:ASP:O	23:Z:49:ARG:HG3	2.12	0.49
34:a:305:G:H1'	34:a:592:A:C2	2.47	0.49
34:a:458:A:OP1	49:p:75:ARG:NH2	2.42	0.49
37:d:166:LYS:O	37:d:168:ARG:NH1	2.44	0.49
56:w:26:A:H2'	56:w:27:G:O4'	2.12	0.49
58:y:55:PSU:H5''	58:y:56:C:OP2	2.12	0.49
59:z:188:PRO:HB3	59:z:216:ARG:NH2	2.27	0.49
59:z:302:PHE:HB3	59:z:374:PRO:HG2	1.94	0.49
1:A:88:U:O2'	1:A:89:A:C8	2.59	0.49
1:A:264:U:H2'	1:A:265:C:C6	2.47	0.49
1:A:1091:A:C5	9:J:8:GLU:N	2.80	0.49
1:A:1100:G:H2'	1:A:1101:G:O4'	2.13	0.49
1:A:1548:U:H2'	1:A:1549:C:C6	2.48	0.49
1:A:2044:G:H5'	1:A:2628:C:H4'	1.92	0.49
1:A:2155:A:H5''	1:A:2156:A:OP2	2.12	0.49
1:A:2186:G:H2'	1:A:2187:G:C8	2.47	0.49
2:B:63:G:H2'	2:B:64:C:C6	2.48	0.49
3:C:161:ILE:HD12	3:C:174:PRO:O	2.11	0.49
4:D:88:ARG:HB3	4:D:88:ARG:CZ	2.42	0.49
8:H:21:PRO:HG2	8:H:23:ARG:HH12	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:982:G:H21	34:a:983:A:H1'	1.75	0.49
35:b:20:GLU:HB2	35:b:190:THR:OG1	2.13	0.49
36:c:155:GLY:HA3	36:c:196:LEU:HD22	1.95	0.49
39:f:9:VAL:CG1	39:f:87:ARG:HB2	2.43	0.49
44:k:67:ASP:OD2	44:k:71:LYS:HE3	2.12	0.49
52:s:69:HIS:ND1	52:s:73:GLU:OE1	2.41	0.49
59:z:144:ARG:HB3	59:z:147:GLU:CG	2.43	0.49
1:A:2133:G:H1'	58:y:19:G:O2'	2.12	0.49
1:A:2568:G:H2'	1:A:2569:C:C6	2.48	0.49
4:D:76:PRO:O	4:D:98:VAL:HG23	2.11	0.49
9:J:118:THR:O	9:J:120:LYS:N	2.40	0.49
10:K:32:ALA:HB1	10:K:65:PHE:CD1	2.47	0.49
12:O:111:PHE:O	12:O:115:VAL:HG23	2.13	0.49
15:R:37:THR:OG1	15:R:40:LYS:HB2	2.13	0.49
17:T:56:GLY:O	17:T:59:THR:HG23	2.13	0.49
18:U:19:LYS:O	18:U:22:LYS:HG3	2.13	0.49
34:a:8:G:H21	38:e:121:LYS:HG3	1.78	0.49
34:a:1001:G:H2'	34:a:1002:G:H8	1.77	0.49
34:a:1447:G:H2'	34:a:1448:G:H8	1.77	0.49
1:A:98:G:O2'	26:2:7:ARG:NH2	2.46	0.49
7:G:108:ASN:ND2	28:4:22:ILE:HG21	2.27	0.49
34:a:68:C:H2'	34:a:69:G:C8	2.48	0.49
34:a:928:U:H2'	34:a:929:G:C8	2.47	0.49
36:c:150:LYS:HG3	36:c:169:ALA:HB2	1.93	0.49
36:c:189:ALA:HB3	36:c:196:LEU:HB2	1.95	0.49
37:d:158:ILE:HG22	37:d:162:LEU:HD12	1.94	0.49
56:w:8:4SU:O2	56:w:21:A:H2	1.96	0.49
59:z:194:ALA:HA	59:z:220:GLY:HA2	1.95	0.49
1:A:1121:C:H2'	1:A:1122:A:H8	1.78	0.49
10:K:65:PHE:H	10:K:65:PHE:HD2	1.59	0.49
13:P:121:LYS:HB2	13:P:123:LEU:HG	1.94	0.49
23:Z:8:TYR:HB2	23:Z:38:TYR:CE2	2.47	0.49
34:a:1109:U:H2'	34:a:1109:U:O2	2.12	0.49
36:c:34:LEU:O	36:c:38:ARG:HG3	2.13	0.49
36:c:175:LEU:HD23	36:c:182:ILE:HD13	1.95	0.49
58:y:32:PSU:H5''	58:y:33:U:O5'	2.13	0.49
1:A:925:G:H1	1:A:943:C:H42	1.59	0.49
1:A:1101:G:H5''	1:A:1102:A:O4'	2.12	0.49
1:A:1124:C:O3'	10:K:132:ARG:NH2	2.45	0.49
1:A:2817:U:H5''	1:A:2899:G:O6	2.13	0.49
6:F:17:ARG:HB3	6:F:17:ARG:CZ	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:10:LEU:HB3	26:2:14:ARG:NH1	2.28	0.49
34:a:162:G:C6	34:a:163:G:C5	3.01	0.49
40:g:75:VAL:HG21	40:g:144:MET:HB3	1.95	0.49
51:r:53:ARG:HH21	51:r:60:ALA:H	1.61	0.49
59:z:156:LEU:HB3	59:z:158:LEU:HD23	1.94	0.49
1:A:76:A:H2'	1:A:77:G:C8	2.48	0.49
1:A:173:U:H4'	1:A:206:A:H4'	1.94	0.49
1:A:1228:G:H5'	27:3:29:ARG:NH1	2.27	0.49
1:A:2698:U:H2'	1:A:2699:U:O4'	2.13	0.49
3:C:56:GLN:HA	3:C:201:PRO:HB2	1.95	0.49
14:Q:56:ARG:HB2	14:Q:56:ARG:HH11	1.76	0.49
35:b:17:PHE:N	35:b:17:PHE:CD1	2.79	0.49
35:b:172:ILE:HD12	35:b:173:ALA:H	1.77	0.49
56:w:59:U:H3'	56:w:60:U:O2	2.13	0.49
57:x:61:C:H2'	57:x:62:C:H6	1.78	0.49
1:A:678:A:N3	1:A:678:A:H2'	2.28	0.49
1:A:1643:C:O3'	21:X:35:THR:HG22	2.13	0.49
1:A:2212:G:O2'	1:A:2213:G:H8	1.96	0.49
10:K:18:THR:HA	10:K:35:MET:HE1	1.93	0.49
25:1:62:VAL:HG22	25:1:63:ALA:O	2.13	0.49
34:a:568:G:H2'	34:a:569:G:C8	2.47	0.49
34:a:1464:G:H2'	34:a:1465:G:O4'	2.13	0.49
1:A:64:C:H2'	1:A:65:U:C6	2.48	0.48
1:A:1826:U:H2'	1:A:1827:C:C6	2.48	0.48
1:A:2412:U:OP1	30:6:18:ARG:NH2	2.42	0.48
2:B:12:C:H2'	24:0:73:GLY:HA3	1.95	0.48
3:C:21:THR:HG22	3:C:23:ASP:H	1.78	0.48
12:O:104:ARG:HH22	17:T:43:GLN:NE2	2.11	0.48
34:a:753:G:H4'	34:a:1491:A:H4'	1.94	0.48
34:a:1245:C:H2'	34:a:1246:C:C6	2.48	0.48
38:e:79:GLU:HG3	38:e:93:PRO:HD2	1.95	0.48
51:r:26:LEU:HD23	51:r:29:PHE:CE2	2.48	0.48
59:z:64:VAL:HG12	59:z:80:LEU:HB2	1.94	0.48
59:z:339:ALA:HA	59:z:340:LEU:HA	1.66	0.48
1:A:1116:G:O2'	1:A:1134:G:OP2	2.27	0.48
1:A:1121:C:H2'	1:A:1122:A:C8	2.48	0.48
1:A:1138:G:H21	1:A:1143:A:H62	1.61	0.48
1:A:1268:G:N2	1:A:1271:A:OP2	2.38	0.48
9:J:71:LEU:C	9:J:73:GLY:H	2.21	0.48
27:3:3:ARG:HH11	27:3:60:GLU:HB3	1.77	0.48
34:a:698:G:H2'	34:a:699:A:C8	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:28:LYS:HB2	52:s:29:ARG:CB	2.43	0.48
59:z:65:ARG:H	59:z:246:THR:CG2	2.26	0.48
34:a:886:A:H2'	34:a:887:A:H8	1.78	0.48
46:m:40:ASN:ND2	46:m:43:THR:HG23	2.28	0.48
59:z:204:VAL:HG23	59:z:326:ASN:HD21	1.76	0.48
1:A:346:G:C8	6:F:171:PRO:HG3	2.48	0.48
1:A:947:C:H2'	1:A:948:C:H6	1.79	0.48
1:A:2172:G:H2'	1:A:2173:G:H8	1.78	0.48
1:A:2297:A:H4'	1:A:2298:A:O4'	2.13	0.48
3:C:48:GLY:HA2	3:C:210:ARG:HH11	1.79	0.48
5:E:12:THR:HG22	5:E:13:ARG:H	1.78	0.48
34:a:904:G:O2'	55:v:13:A:H8	1.96	0.48
34:a:1019:G:H3'	34:a:1020:C:C6	2.48	0.48
34:a:1019:G:H3'	34:a:1020:C:H6	1.76	0.48
34:a:1097:C:H2'	34:a:1098:C:C6	2.48	0.48
1:A:1404:A:H61	1:A:1417:U:H3	1.62	0.48
1:A:1896:C:H2'	1:A:1897:A:O4'	2.13	0.48
3:C:47:LEU:HD11	3:C:171:ILE:HB	1.95	0.48
7:G:15:VAL:HG22	7:G:175:LEU:HB3	1.94	0.48
8:H:41:MET:CE	8:H:54:ARG:HB3	2.44	0.48
14:Q:110:THR:HG23	14:Q:113:GLN:OE1	2.14	0.48
17:T:26:ASP:OD1	17:T:91:ARG:HA	2.12	0.48
34:a:511:G:O2'	34:a:519:A:N1	2.35	0.48
34:a:564:U:H2'	34:a:565:G:O4'	2.14	0.48
34:a:604:C:H2'	34:a:605:A:O4'	2.14	0.48
42:i:45:ALA:HB3	42:i:48:GLU:OE1	2.14	0.48
59:z:101:GLU:HG3	59:z:186:PRO:O	2.13	0.48
59:z:378:TYR:O	59:z:389:GLU:N	2.46	0.48
59:z:408:PRO:HG2	59:z:456:PHE:HB3	1.95	0.48
1:A:941:A:H4'	1:A:941:A:OP1	2.14	0.48
1:A:1920:G:N3	1:A:1920:G:H2'	2.29	0.48
1:A:2659:C:H2'	1:A:2660:U:C6	2.49	0.48
1:A:2802:A:H2'	1:A:2802:A:N3	2.28	0.48
10:K:35:MET:HA	10:K:38:VAL:HG23	1.95	0.48
10:K:131:ALA:HB1	10:K:136:VAL:O	2.14	0.48
13:P:63:PRO:HG2	32:8:25:MET:HB2	1.96	0.48
16:S:36:TYR:N	16:S:36:TYR:CD1	2.82	0.48
28:4:18:CYS:SG	28:4:19:GLY:N	2.86	0.48
28:4:63:TYR:N	28:4:63:TYR:CD1	2.80	0.48
34:a:271:G:H5'	50:q:14:LYS:HD2	1.95	0.48
34:a:526:G:H5'	37:d:41:GLY:HA3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1140:A:H4'	34:a:1141:C:O5'	2.13	0.48
37:d:31:CYS:SG	62:d:302:SF4:S2	3.11	0.48
58:y:43:C:H3'	58:y:44:G:H8	1.78	0.48
59:z:224:PRO:HA	59:z:239:VAL:HG23	1.95	0.48
1:A:179:A:H2'	1:A:180:C:C6	2.49	0.48
1:A:594:A:OP2	19:V:78:LYS:NZ	2.37	0.48
1:A:1106:U:O2	10:K:11:GLN:HG2	2.14	0.48
1:A:1200:A:OP1	18:U:55:ARG:HD3	2.13	0.48
1:A:1887:G:C6	1:A:1888:G:C6	3.02	0.48
13:P:89:ALA:HA	13:P:121:LYS:HD2	1.95	0.48
34:a:154:G:H5'	34:a:155:A:OP2	2.14	0.48
34:a:868:G:O2'	34:a:884:G:O6	2.29	0.48
37:d:19:LEU:HD22	37:d:67:ILE:HG13	1.95	0.48
39:f:2:ARG:CZ	39:f:69:GLU:HG2	2.44	0.48
1:A:39:C:N1	1:A:39:C:C5	2.78	0.48
1:A:160:C:H2'	1:A:161:G:H8	1.78	0.48
1:A:1300:U:O5'	1:A:1301:G:H5''	2.13	0.48
1:A:2661:U:H2'	1:A:2662:C:C6	2.49	0.48
3:C:43:VAL:O	3:C:172:HIS:HA	2.14	0.48
10:K:14:ALA:HB2	10:K:41:PHE:CZ	2.48	0.48
25:1:80:LEU:HG	25:1:81:LYS:N	2.29	0.48
27:3:46:ASN:O	27:3:50:VAL:HG22	2.14	0.48
36:c:108:ASN:ND2	36:c:144:SER:HB3	2.24	0.48
40:g:64:GLN:HG2	40:g:128:ALA:HB1	1.96	0.48
45:l:28:LYS:N	45:l:29:GLY:HA2	2.29	0.48
1:A:323:A:H3'	22:Y:84:ARG:NH2	2.28	0.48
1:A:946:A:H2'	1:A:947:C:O4'	2.14	0.48
1:A:1265:C:H2'	1:A:1266:C:C6	2.49	0.48
1:A:1766:A:O2'	1:A:1767:U:H2'	2.13	0.48
1:A:1953:A:H2'	1:A:1954:G:O4'	2.14	0.48
1:A:2702:C:O3'	1:A:2880:C:H4'	2.14	0.48
3:C:164:ARG:HH21	3:C:164:ARG:CB	2.26	0.48
7:G:37:VAL:HG23	7:G:99:MET:HE3	1.96	0.48
7:G:96:ARG:O	7:G:99:MET:HB3	2.13	0.48
7:G:150:ASP:CG	7:G:153:ARG:HH12	2.21	0.48
16:S:34:HIS:CB	16:S:36:TYR:HE1	2.27	0.48
18:U:85:LYS:HE2	18:U:85:LYS:HB3	1.60	0.48
28:4:59:PHE:N	28:4:60:GLN:HB3	2.29	0.48
34:a:204:A:C6	34:a:217:C:H4'	2.49	0.48
41:h:10:LEU:HD22	41:h:83:ILE:HD11	1.95	0.48
42:i:34:ASN:O	42:i:38:GLN:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:m:37:THR:O	46:m:55:ARG:NH1	2.34	0.48
53:t:57:ARG:HH22	53:t:100:ILE:HD12	1.79	0.48
56:w:4:C:C3'	56:w:5:G:H5''	2.44	0.48
1:A:312:A:H2'	1:A:313:G:O4'	2.13	0.48
1:A:1127:U:H3'	1:A:1128:U:C5'	2.41	0.48
1:A:2658:U:H2'	1:A:2659:C:C6	2.49	0.48
7:G:179:PRO:HG3	28:4:43:TYR:OH	2.13	0.48
13:P:59:LEU:HD12	13:P:60:MET:HE2	1.95	0.48
26:2:70:GLN:HE21	26:2:70:GLN:C	2.22	0.48
35:b:62:ALA:HB2	35:b:222:ILE:HD13	1.96	0.48
59:z:528:ILE:HG23	59:z:529:PRO:HD2	1.96	0.48
1:A:183:A:H5''	13:P:46:LYS:HZ1	1.77	0.47
6:F:197:ASP:O	6:F:200:GLU:HB2	2.14	0.47
7:G:143:GLU:CD	7:G:143:GLU:H	2.22	0.47
25:1:3:LYS:HD2	25:1:61:ARG:HH12	1.78	0.47
27:3:23:LEU:HD13	27:3:50:VAL:HG11	1.95	0.47
34:a:71:G:H1	34:a:93:U:H3	1.62	0.47
34:a:1112:C:O5'	34:a:1113:A:H5'	2.13	0.47
34:a:1221:A:H62	34:a:1281:A:N6	2.12	0.47
38:e:110:LEU:HD13	38:e:118:ILE:HG21	1.95	0.47
42:i:44:VAL:HA	42:i:45:ALA:HA	1.50	0.47
45:l:41:ARG:HD3	45:l:42:THR:O	2.14	0.47
46:m:15:VAL:HG11	46:m:48:LEU:HD11	1.95	0.47
52:s:48:THR:HG22	52:s:61:TYR:HD1	1.79	0.47
1:A:29:G:H2'	1:A:30:C:C6	2.49	0.47
1:A:1073:A:H61	1:A:1170:G:H2'	1.79	0.47
3:C:182:PRO:C	3:C:184:LYS:N	2.69	0.47
5:E:47:VAL:O	5:E:80:GLU:HA	2.15	0.47
12:O:98:VAL:HG22	12:O:118:ALA:HA	1.96	0.47
34:a:179:G:H2'	34:a:180:A:C8	2.49	0.47
34:a:296:A:O2'	34:a:548:C:N3	2.36	0.47
34:a:951:G:N3	43:j:54:PHE:HE1	2.11	0.47
35:b:146:GLN:O	35:b:150:SER:HB3	2.14	0.47
47:n:26:ARG:HD3	47:n:43:CYS:HB3	1.96	0.47
58:y:21:A:H2'	58:y:22:G:C8	2.50	0.47
58:y:24:G:H2'	58:y:25:C:O4'	2.13	0.47
1:A:216:A:H3'	1:A:217:A:C5'	2.43	0.47
1:A:1109:C:H2'	1:A:1110:U:O4'	2.14	0.47
1:A:1153:U:O2'	1:A:1154:C:C6	2.66	0.47
1:A:2157:C:H3'	1:A:2158:C:C5	2.49	0.47
1:A:2754:C:OP1	33:9:35:ARG:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:34:LYS:HA	18:U:34:LYS:HD2	1.52	0.47
23:Z:40:ASP:HB3	23:Z:43:GLU:HB2	1.95	0.47
34:a:214:C:H5'	34:a:456:C:N4	2.29	0.47
34:a:953:A:H5'	34:a:953:A:C8	2.48	0.47
34:a:982:G:C2	34:a:983:A:N3	2.83	0.47
56:w:68:C:H5'	59:z:545:ILE:HG13	1.95	0.47
56:w:72:C:N4	56:w:73:A:C5	2.82	0.47
59:z:-68:MET:N	59:z:-48:VAL:O	2.38	0.47
59:z:140:LEU:HD12	59:z:140:LEU:HA	1.77	0.47
59:z:281:THR:OG1	59:z:282:LEU:N	2.43	0.47
59:z:324:LYS:C	59:z:326:ASN:H	2.20	0.47
59:z:555:ARG:HH11	59:z:577:GLN:NE2	1.91	0.47
1:A:515:G:H2'	1:A:516:A:C8	2.50	0.47
1:A:1073:A:N6	1:A:1170:G:H2'	2.28	0.47
1:A:1335:C:H2'	1:A:1336:C:H6	1.79	0.47
1:A:1659:A:C2	20:W:93:ALA:HB2	2.50	0.47
17:T:39:ARG:NH2	34:a:341:C:OP2	2.39	0.47
29:5:8:LYS:O	29:5:9:LYS:HD2	2.14	0.47
30:6:9:LEU:HD13	30:6:51:GLU:HG3	1.97	0.47
35:b:28:PHE:CD1	35:b:190:THR:HA	2.50	0.47
35:b:125:PRO:O	35:b:126:GLU:HG2	2.14	0.47
47:n:14:PRO:HG3	47:n:20:ALA:HB2	1.95	0.47
1:A:1265:C:H2'	1:A:1266:C:H6	1.79	0.47
1:A:1319:A:N1	1:A:1690:C:O2'	2.42	0.47
1:A:2129:C:O2'	1:A:2130:U:H5'	2.14	0.47
1:A:2294:C:C2	1:A:2400:G:C2	3.02	0.47
6:F:34:TRP:CE3	6:F:35:GLU:HG2	2.49	0.47
8:H:3:ARG:HH22	8:H:5:GLY:H	1.63	0.47
10:K:99:ILE:HG23	10:K:103:GLN:HB3	1.96	0.47
34:a:1146:C:H2'	34:a:1147:G:O4'	2.14	0.47
34:a:1258:G:H2'	34:a:1259:C:O4'	2.15	0.47
40:g:149:ARG:HD2	44:k:59:TYR:CZ	2.49	0.47
46:m:30:ALA:O	46:m:34:LEU:HD22	2.15	0.47
59:z:204:VAL:HG13	59:z:212:ILE:HG23	1.96	0.47
1:A:839:A:OP2	1:A:2093:G:H5'	2.15	0.47
1:A:1042:G:OP1	18:U:92:ARG:HG2	2.15	0.47
1:A:1333:U:O2'	1:A:1372:C:O2	2.25	0.47
1:A:1431:C:H2'	1:A:1432:C:C6	2.49	0.47
1:A:2134:U:H6	1:A:2134:U:O5'	1.98	0.47
1:A:2249:G:H2'	1:A:2249:G:N3	2.28	0.47
3:C:186:ALA:HA	3:C:189:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:VAL:HB	17:T:3:ARG:HG2	1.96	0.47
10:K:76:TYR:HB2	10:K:79:ARG:NH2	2.27	0.47
11:N:4:TYR:CD2	18:U:100:VAL:HG11	2.50	0.47
25:1:54:ALA:HB1	25:1:83:GLU:HG3	1.96	0.47
28:4:48:ARG:HA	28:4:48:ARG:CZ	2.44	0.47
34:a:179:G:H2'	34:a:180:A:H8	1.79	0.47
34:a:735:U:H4'	48:o:24:SER:HB2	1.96	0.47
34:a:850:A:C8	34:a:852:G:C8	3.02	0.47
35:b:184:VAL:HG13	35:b:198:ASP:H	1.80	0.47
59:z:115:ALA:HA	59:z:474:TYR:CE1	2.49	0.47
59:z:576:LYS:HE2	59:z:576:LYS:HB2	1.60	0.47
1:A:722:A:H2	1:A:2090:G:N3	2.13	0.47
1:A:786:U:H2'	1:A:787:G:C8	2.49	0.47
1:A:860:C:H2'	1:A:861:C:H6	1.79	0.47
1:A:982:G:H5''	1:A:982:G:C8	2.50	0.47
1:A:1217:G:H2'	1:A:1217:G:OP2	2.15	0.47
1:A:1344:G:H5'	1:A:1346:A:O4'	2.14	0.47
1:A:2801:C:H1'	1:A:2900:A:H2	1.79	0.47
3:C:26:ALA:HB1	3:C:182:PRO:HA	1.96	0.47
7:G:16:ARG:NH1	7:G:31:VAL:HG22	2.30	0.47
9:J:118:THR:N	9:J:121:ASP:O	2.45	0.47
12:O:26:LYS:O	12:O:30:ALA:HB2	2.14	0.47
13:P:44:GLY:CA	13:P:45:LEU:HB2	2.45	0.47
17:T:29:ARG:HD3	17:T:44:ASP:OD1	2.15	0.47
18:U:28:ARG:NH1	18:U:38:THR:OG1	2.46	0.47
34:a:485:C:H2'	34:a:486:G:H8	1.80	0.47
34:a:503:C:H2'	34:a:504:A:O4'	2.15	0.47
34:a:983:A:N7	34:a:1019:G:C6	2.83	0.47
34:a:984:A:H4'	34:a:1020:C:O2'	2.14	0.47
34:a:1226:C:H2'	34:a:1227:A:H8	1.80	0.47
35:b:189:ASP:OD2	35:b:190:THR:N	2.45	0.47
37:d:61:LYS:HD2	37:d:207:TYR:OH	2.15	0.47
38:e:107:ARG:O	38:e:111:GLU:HG3	2.15	0.47
43:j:78:ASN:O	43:j:80:LYS:N	2.48	0.47
46:m:49:THR:OG1	46:m:52:GLU:HG3	2.14	0.47
47:n:21:TYR:OH	47:n:23:ARG:NH2	2.45	0.47
48:o:16:ALA:HB1	48:o:21:ASP:HB3	1.97	0.47
50:q:62:SER:OG	50:q:72:ARG:HD3	2.14	0.47
53:t:87:LYS:O	53:t:91:LEU:HD12	2.15	0.47
59:z:246:THR:HG22	59:z:247:PRO:CD	2.45	0.47
1:A:64:C:H2'	1:A:65:U:H6	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:A:O4'	22:Y:48:ALA:HB1	2.15	0.47
1:A:1128:U:H2'	1:A:1130:A:OP2	2.14	0.47
1:A:1402:U:H2'	1:A:1403:G:O4'	2.15	0.47
10:K:97:GLY:C	10:K:136:VAL:HG23	2.40	0.47
11:N:19:GLU:H	11:N:21:LYS:HG2	1.79	0.47
16:S:11:LYS:HD3	16:S:15:ARG:NH2	2.30	0.47
21:X:50:LYS:O	21:X:84:ALA:N	2.48	0.47
21:X:53:LYS:HB3	21:X:82:GLN:HB3	1.95	0.47
33:9:7:VAL:HG13	33:9:36:GLN:HG3	1.97	0.47
40:g:78:ARG:HD3	40:g:79:ARG:HB2	1.97	0.47
45:l:79:GLU:H	45:l:79:GLU:CD	2.23	0.47
56:w:59:U:H2'	56:w:60:U:H5'	1.96	0.47
56:w:72:C:N4	56:w:73:A:C6	2.83	0.47
59:z:241:LYS:H	59:z:265:VAL:HG23	1.79	0.47
59:z:380:VAL:HG21	59:z:397:PRO:HG2	1.97	0.47
1:A:173:U:H2'	1:A:174:G:C8	2.50	0.47
1:A:235:G:H4'	1:A:412:G:C6	2.49	0.47
1:A:719:C:H5''	6:F:81:PRO:HD2	1.97	0.47
1:A:1039:C:OP1	18:U:53:ARG:NH2	2.48	0.47
1:A:2290:G:O6	24:0:14:ARG:HD2	2.15	0.47
1:A:2376:G:O6	32:8:39:LYS:HE3	2.14	0.47
2:B:31:C:H4'	7:G:29:TRP:CZ2	2.50	0.47
10:K:121:GLU:HB3	10:K:125:ARG:HH21	1.80	0.47
14:Q:137:TYR:OH	23:Z:45:ASP:OD2	2.31	0.47
18:U:104:GLN:H	18:U:104:GLN:HG3	1.36	0.47
25:1:57:GLU:H	25:1:57:GLU:CD	2.22	0.47
34:a:825:U:H3'	34:a:826:C:O4'	2.14	0.47
34:a:1382:C:C2	34:a:1480:A:N6	2.83	0.47
50:q:62:SER:CB	50:q:72:ARG:HD3	2.45	0.47
52:s:45:VAL:HA	52:s:62:ILE:HG22	1.96	0.47
59:z:266:ALA:HA	59:z:268:ILE:HD11	1.97	0.47
1:A:696:C:H2'	1:A:697:G:H8	1.80	0.47
1:A:1126:U:H2'	1:A:1127:U:H5'	1.97	0.47
1:A:1416:G:O2'	1:A:1417:U:H5	1.98	0.47
1:A:2282:G:OP1	24:0:18:ALA:HB1	2.16	0.47
1:A:2803:C:H5	1:A:2901:G:O2'	1.98	0.47
2:B:60:C:H2'	2:B:61:G:H8	1.80	0.47
4:D:132:PRO:HG3	4:D:190:TYR:CE1	2.50	0.47
7:G:49:ASP:O	7:G:51:ARG:N	2.47	0.47
12:O:4:PRO:O	12:O:5:GLN:HB2	2.15	0.47
18:U:108:GLU:O	18:U:112:ARG:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:90:LEU:HD21	22:Y:96:ILE:HG12	1.97	0.47
25:1:8:SER:HB3	25:1:66:HIS:CD2	2.50	0.47
34:a:198:G:H2'	34:a:199:U:C6	2.50	0.47
34:a:859:G:P	45:l:12:ARG:HH22	2.38	0.47
49:p:23:ASP:OD1	49:p:25:ARG:HG3	2.14	0.47
1:A:172:C:H2'	1:A:173:U:H6	1.80	0.46
1:A:201:A:H2'	1:A:202:G:O4'	2.15	0.46
1:A:1295:G:OP2	13:P:21:ARG:NH1	2.45	0.46
1:A:1594:C:H2'	1:A:1595:C:H6	1.80	0.46
1:A:1638:G:H2'	1:A:1639:G:C8	2.50	0.46
1:A:2143:U:H1'	3:C:166:ASP:HB3	1.96	0.46
1:A:2709:U:H2'	1:A:2710:C:C6	2.50	0.46
1:A:2900:A:H3'	1:A:2901:G:C8	2.50	0.46
2:B:3:C:H2'	2:B:4:C:C6	2.50	0.46
3:C:29:VAL:C	3:C:31:GLU:H	2.23	0.46
3:C:55:ASP:OD1	3:C:55:ASP:N	2.28	0.46
3:C:201:PRO:C	3:C:203:GLY:C	2.83	0.46
4:D:112:GLN:OE1	4:D:112:GLN:HA	2.15	0.46
5:E:143:ASN:HD22	5:E:147:PRO:HD2	1.80	0.46
21:X:34:ALA:O	21:X:77:LYS:NZ	2.46	0.46
34:a:38:U:O2'	34:a:484:G:H4'	2.14	0.46
34:a:1485:A:OP2	55:v:13:A:N1	2.48	0.46
51:r:33:ASP:O	51:r:40:LEU:HD11	2.14	0.46
59:z:15:ILE:HD12	59:z:97:LEU:HD21	1.98	0.46
1:A:301:A:H2'	1:A:302:C:C6	2.51	0.46
1:A:554:G:C5	1:A:2043:U:H5''	2.51	0.46
1:A:680:C:N3	1:A:697:G:O6	2.48	0.46
1:A:1127:U:H5''	1:A:1128:U:OP2	2.15	0.46
1:A:1223:C:H2'	1:A:1224:C:H6	1.80	0.46
1:A:1828:U:OP2	4:D:273:ARG:NH2	2.47	0.46
1:A:1863:U:O2'	1:A:1990:A:N1	2.41	0.46
1:A:2723:U:OP1	1:A:2726:G:H4'	2.15	0.46
2:B:30:C:O2'	2:B:57:A:N1	2.39	0.46
20:W:29:LEU:O	20:W:33:ARG:HG3	2.16	0.46
34:a:815:U:H2'	34:a:816:C:C6	2.50	0.46
34:a:1087:G:O5'	35:b:111:ARG:HD2	2.15	0.46
34:a:1100:G:H5''	42:i:104:ARG:NH2	2.31	0.46
34:a:1109:U:O2	34:a:1110:G:C2	2.67	0.46
34:a:1275:G:H2'	34:a:1276:G:H8	1.80	0.46
56:w:4:C:H2'	56:w:5:G:H5''	1.97	0.46
1:A:1446:G:H2'	1:A:1447:C:O4'	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1659:A:N1	20:W:93:ALA:HB2	2.30	0.46
1:A:2800:C:O2'	1:A:2818:A:N3	2.39	0.46
7:G:140:ILE:HD12	7:G:140:ILE:HA	1.75	0.46
10:K:36:GLU:HG3	10:K:67:PHE:HZ	1.80	0.46
23:Z:13:GLU:OE1	23:Z:13:GLU:N	2.31	0.46
23:Z:23:LYS:HB3	23:Z:38:TYR:HD1	1.78	0.46
28:4:61:ARG:HG3	28:4:62:ARG:H	1.79	0.46
34:a:141:G:H2'	34:a:142:G:H8	1.80	0.46
34:a:403:G:P	37:d:3:ARG:HH22	2.37	0.46
34:a:1342:A:H8	34:a:1342:A:OP1	1.99	0.46
35:b:73:THR:OG1	35:b:170:GLU:OE1	2.33	0.46
41:h:9:MET:SD	41:h:32:LYS:HB3	2.56	0.46
59:z:137:LYS:HG2	63:z:703:GCP:C6	2.45	0.46
1:A:1093:A:OP2	1:A:1155:G:N2	2.47	0.46
1:A:1628:C:O2'	1:A:1631:A:N3	2.42	0.46
1:A:1652:C:H4'	1:A:1653:A:O5'	2.15	0.46
1:A:2323:U:H5'	7:G:88:ILE:HD11	1.97	0.46
4:D:79:VAL:HG21	4:D:111:LEU:HD21	1.97	0.46
4:D:146:GLU:HB2	4:D:189:CYS:HB3	1.97	0.46
11:N:94:HIS:HB3	11:N:97:ARG:HD3	1.98	0.46
14:Q:55:VAL:O	14:Q:58:PHE:N	2.45	0.46
24:0:27:GLU:CG	24:0:68:GLU:HA	2.45	0.46
34:a:341:C:H5'	34:a:342:G:C8	2.50	0.46
34:a:705:G:H4'	34:a:706:A:O4'	2.15	0.46
35:b:152:PHE:O	35:b:155:LEU:HD12	2.16	0.46
37:d:58:LEU:HD23	37:d:206:PHE:CE2	2.51	0.46
56:w:55:PSU:H5''	56:w:56:C:OP2	2.15	0.46
59:z:-29:THR:O	59:z:-25:LEU:HB2	2.16	0.46
1:A:138:A:C8	1:A:1453:C:O2'	2.69	0.46
1:A:517:G:H2'	1:A:518:G:O4'	2.15	0.46
1:A:926:G:OP2	1:A:926:G:H8	1.99	0.46
1:A:1228:G:H5'	27:3:29:ARG:HH11	1.80	0.46
1:A:2190:A:H1'	58:y:56:C:O4'	2.15	0.46
1:A:2244:U:H2'	1:A:2245:G:C8	2.50	0.46
1:A:2651:G:OP1	11:N:97:ARG:NH2	2.49	0.46
8:H:83:TYR:CE2	8:H:138:LYS:HB2	2.51	0.46
12:O:34:THR:OG1	12:O:35:VAL:N	2.44	0.46
24:0:33:ALA:C	24:0:35:ASN:H	2.23	0.46
35:b:163:PHE:CD2	35:b:185:ILE:HG13	2.50	0.46
42:i:95:LYS:O	42:i:98:PRO:HD2	2.14	0.46
46:m:67:GLU:OE2	46:m:71:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:o:28:GLN:NE2	48:o:66:LEU:HD21	2.31	0.46
1:A:932:C:OP2	46:m:93:ARG:HG2	2.16	0.46
1:A:1633:C:H2'	1:A:1634:C:H6	1.80	0.46
1:A:2428:C:P	13:P:65:ARG:HH21	2.39	0.46
2:B:63:G:H2'	2:B:64:C:H6	1.80	0.46
3:C:193:ILE:O	3:C:197:GLU:HB2	2.15	0.46
8:H:155:SER:HB3	8:H:158:HIS:O	2.16	0.46
28:4:63:TYR:N	28:4:64:GLY:HA2	2.30	0.46
34:a:8:G:H5'	34:a:294:A:O4'	2.16	0.46
34:a:456:C:H6	34:a:456:C:H2'	1.42	0.46
39:f:12:PRO:HG3	39:f:57:GLN:O	2.15	0.46
47:n:24:CYS:HB3	47:n:29:ARG:H	1.81	0.46
1:A:277:G:OP1	25:1:76:ARG:HB3	2.16	0.46
1:A:307:U:H2'	1:A:308:C:C6	2.49	0.46
1:A:2247:C:H2'	1:A:2248:G:O4'	2.15	0.46
1:A:2297:A:N1	30:6:24:GLU:O	2.49	0.46
6:F:179:GLU:CD	6:F:179:GLU:H	2.23	0.46
7:G:126:ASP:HB3	7:G:128:ARG:H	1.79	0.46
16:S:15:ARG:HH11	16:S:25:ARG:NH2	2.09	0.46
29:5:16:ARG:HD2	29:5:20:ARG:NH1	2.31	0.46
33:9:14:CYS:HA	33:9:27:CYS:HB2	1.97	0.46
34:a:150:C:H2'	34:a:151:G:C8	2.50	0.46
34:a:1161:A:H2'	34:a:1162:A:O4'	2.15	0.46
36:c:22:TRP:HB3	36:c:59:ARG:HB2	1.97	0.46
52:s:5:LEU:HD12	52:s:5:LEU:HA	1.79	0.46
1:A:138:A:H8	1:A:1453:C:O2'	1.97	0.46
1:A:267:G:C2'	1:A:268:G:H5'	2.45	0.46
1:A:549:U:H5'	1:A:578:G:OP1	2.16	0.46
1:A:894:G:H2'	1:A:895:A:C8	2.51	0.46
1:A:1399:A:H2'	1:A:1400:G:O4'	2.16	0.46
1:A:2874:U:C4	1:A:2875:U:C4	3.03	0.46
4:D:102:LYS:C	4:D:103:ARG:HG2	2.40	0.46
7:G:148:MET:C	7:G:148:MET:HE3	2.41	0.46
14:Q:12:GLN:HG2	14:Q:73:PRO:HD2	1.98	0.46
19:V:50:PRO:HG2	19:V:51:VAL:HG12	1.97	0.46
25:1:86:SER:OG	25:1:89:GLU:HG2	2.16	0.46
34:a:720:C:H2'	34:a:721:A:C8	2.51	0.46
37:d:8:VAL:O	37:d:11:LEU:HB2	2.16	0.46
50:q:4:LYS:HA	50:q:4:LYS:HD3	1.81	0.46
51:r:58:LEU:HD13	51:r:62:GLU:HB3	1.96	0.46
58:y:4:C:H2'	58:y:5:G:H5''	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:z:99:ALA:O	59:z:216:ARG:HG3	2.15	0.46
59:z:211:VAL:HG11	59:z:274:VAL:HG21	1.98	0.46
59:z:311:GLY:C	59:z:313:TYR:N	2.73	0.46
59:z:329:ALA:CB	59:z:349:LEU:HD12	2.46	0.46
1:A:1461:G:N2	1:A:1628:C:O2	2.48	0.46
1:A:1524:G:N2	1:A:1561:U:C2	2.84	0.46
1:A:1758:C:N3	1:A:1776:G:N2	2.53	0.46
1:A:1774:C:H5'	1:A:1775:G:OP2	2.16	0.46
1:A:2221:C:C6	1:A:2221:C:H5''	2.50	0.46
2:B:91:C:OP2	14:Q:16:ARG:NH1	2.47	0.46
7:G:126:ASP:HB2	7:G:130:ASN:H	1.81	0.46
10:K:89:HIS:C	10:K:91:PRO:HD3	2.40	0.46
20:W:51:LEU:HD23	20:W:105:VAL:HG11	1.98	0.46
22:Y:5:MET:HE2	22:Y:30:VAL:HG13	1.97	0.46
30:6:37:ARG:O	30:6:38:LYS:HD2	2.16	0.46
34:a:993:A:H2'	34:a:994:A:C8	2.50	0.46
34:a:1487:C:H2'	34:a:1488:U:O4'	2.16	0.46
59:z:116:GLU:OE1	59:z:120:LYS:NZ	2.48	0.46
59:z:199:LEU:O	59:z:215:LEU:HA	2.16	0.46
1:A:105:U:OP1	1:A:316:U:O2'	2.34	0.46
1:A:159:G:C2	1:A:160:C:C2	3.04	0.46
1:A:550:A:OP1	64:A:3726:HOH:O	2.21	0.46
1:A:1829:G:O2'	4:D:181:GLU:OE2	2.28	0.46
1:A:1857:C:OP2	4:D:222:ARG:NH1	2.48	0.46
1:A:2220:A:H5'	25:1:50:ARG:HH21	1.81	0.46
1:A:2713:U:H4'	1:A:2714:C:OP1	2.16	0.46
4:D:16:MET:HE1	4:D:208:LYS:HD3	1.98	0.46
12:O:17:ARG:HH21	12:O:47:ILE:HD13	1.81	0.46
25:1:19:GLN:HB2	25:1:35:THR:HG22	1.98	0.46
34:a:1268:A:C8	34:a:1269:A:H4'	2.51	0.46
43:j:64:GLU:HB3	47:n:59:ALA:HB2	1.98	0.46
44:k:46:GLY:HA2	44:k:50:TYR:O	2.15	0.46
59:z:231:TYR:C	59:z:233:THR:H	2.24	0.46
1:A:865:A:C4	1:A:1233:A:C2	3.05	0.45
1:A:2832:A:OP1	5:E:159:HIS:NE2	2.48	0.45
6:F:135:LYS:HB2	6:F:138:GLU:CD	2.40	0.45
8:H:163:TYR:CE2	8:H:169:VAL:HG22	2.51	0.45
10:K:57:ILE:HA	10:K:66:THR:O	2.15	0.45
11:N:34:LEU:HD12	11:N:34:LEU:HA	1.75	0.45
34:a:401:U:O4	37:d:2:GLY:N	2.49	0.45
34:a:485:C:H2'	34:a:486:G:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:24:TRP:H	35:b:24:TRP:CD1	2.34	0.45
58:y:33:U:H1'	58:y:34:G:C8	2.50	0.45
59:z:-65:ILE:HD11	59:z:-25:LEU:CD1	2.46	0.45
1:A:25:G:H1'	1:A:538:A:N6	2.32	0.45
1:A:1096:G:H5''	1:A:1097:C:OP2	2.16	0.45
10:K:28:GLY:O	10:K:30:HIS:N	2.49	0.45
21:X:60:ARG:NH1	31:7:47:ARG:HH22	2.13	0.45
32:8:29:LYS:HE2	32:8:45:GLY:CA	2.45	0.45
34:a:76:G:H2'	34:a:77:G:H5'	1.99	0.45
34:a:218:U:H2'	34:a:219:U:H6	1.80	0.45
34:a:433:U:H5''	37:d:155:LEU:HD11	1.99	0.45
35:b:32:ILE:HG21	35:b:40:HIS:HD2	1.81	0.45
40:g:80:VAL:HG21	40:g:85:TYR:CD2	2.51	0.45
59:z:42:ARG:NH1	59:z:48:SER:HA	2.30	0.45
59:z:159:PRO:HB2	59:z:162:GLU:HG3	1.98	0.45
59:z:446:LYS:O	59:z:448:VAL:HG23	2.16	0.45
59:z:497:HIS:HB2	59:z:535:VAL:HG13	1.98	0.45
1:A:610:U:H1'	6:F:90:PHE:CG	2.52	0.45
1:A:1602:C:H2'	1:A:1603:C:C6	2.51	0.45
1:A:2172:G:H2'	1:A:2173:G:C8	2.50	0.45
1:A:2186:G:O5'	1:A:2186:G:H8	1.98	0.45
1:A:2235:G:H4'	1:A:2237:C:C2	2.51	0.45
1:A:2375:C:H2'	1:A:2376:G:O4'	2.17	0.45
3:C:43:VAL:HG21	3:C:189:ILE:HG13	1.97	0.45
3:C:209:LEU:H	3:C:209:LEU:CD1	2.25	0.45
5:E:15:PHE:CE1	5:E:20:ALA:HB2	2.51	0.45
8:H:24:VAL:HG13	8:H:37:VAL:HG21	1.97	0.45
16:S:3:ARG:HG2	16:S:3:ARG:HH11	1.80	0.45
19:V:25:LEU:HD12	19:V:25:LEU:HA	1.84	0.45
27:3:3:ARG:NH1	27:3:60:GLU:OE2	2.48	0.45
34:a:1467:G:H2'	34:a:1468:C:O4'	2.17	0.45
35:b:67:THR:HA	35:b:90:MET:HE1	1.97	0.45
36:c:95:THR:O	36:c:97:LYS:HG2	2.15	0.45
46:m:107:ALA:O	46:m:111:LYS:HG3	2.16	0.45
59:z:65:ARG:HB2	59:z:79:HIS:HD2	1.81	0.45
59:z:534:GLU:HG2	59:z:585:LYS:NZ	2.31	0.45
1:A:37:A:H2'	1:A:38:C:C6	2.52	0.45
1:A:238:G:C6	1:A:239:A:C6	3.04	0.45
1:A:1835:U:O2	4:D:50:THR:HB	2.16	0.45
3:C:68:LEU:HD23	3:C:161:ILE:HG22	1.97	0.45
17:T:78:LEU:O	17:T:78:LEU:HD13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:15:LYS:HB2	26:2:15:LYS:HE3	1.64	0.45
34:a:448:A:O4'	49:p:72:ARG:HD3	2.16	0.45
34:a:1021:C:H2'	34:a:1022:C:C6	2.51	0.45
34:a:1477:A:H1'	34:a:1498:G:H5'	1.99	0.45
38:e:20:GLN:HG2	38:e:25:ARG:NE	2.31	0.45
40:g:70:LYS:O	40:g:138:LYS:HE2	2.16	0.45
43:j:53:PRO:O	47:n:41:ARG:NH2	2.49	0.45
59:z:43:GLU:O	59:z:53:ARG:NH2	2.50	0.45
59:z:91:TYR:O	59:z:95:ARG:HG3	2.16	0.45
59:z:147:GLU:CD	59:z:147:GLU:H	2.25	0.45
1:A:904:U:P	24:0:77:ARG:HH22	2.40	0.45
1:A:1076:G:H21	33:9:36:GLN:HE22	1.65	0.45
1:A:1091:A:H61	9:J:5:ARG:C	2.25	0.45
1:A:1216:G:H5'	1:A:1217:G:OP2	2.16	0.45
1:A:1232:U:C4'	19:V:79:VAL:HG22	2.44	0.45
1:A:1531:A:H2'	1:A:1532:G:C8	2.52	0.45
1:A:2198:C:H5''	3:C:213:TYR:CD2	2.51	0.45
3:C:186:ALA:O	3:C:189:ILE:HG22	2.16	0.45
5:E:7:VAL:HG12	5:E:51:PHE:CE1	2.52	0.45
5:E:175:VAL:HG22	5:E:177:PRO:HD3	1.98	0.45
15:R:55:ALA:HB2	15:R:79:LEU:HD13	1.98	0.45
23:Z:40:ASP:OD1	23:Z:42:VAL:HG13	2.15	0.45
34:a:121:G:HO2'	50:q:2:PRO:N	2.14	0.45
34:a:1123:C:H2'	34:a:1124:C:H6	1.80	0.45
40:g:112:PRO:HD2	40:g:113:GLU:OE2	2.17	0.45
59:z:224:PRO:HB3	59:z:240:ASP:O	2.17	0.45
59:z:382:LEU:HA	59:z:402:ILE:HA	1.97	0.45
1:A:1120:C:H5'	1:A:1121:C:OP2	2.17	0.45
1:A:2054:A:O2'	1:A:2056:G:OP2	2.28	0.45
1:A:2765:A:O2'	33:9:15:LYS:HE3	2.16	0.45
3:C:200:LYS:HD3	3:C:204:ALA:H	1.81	0.45
8:H:3:ARG:HH12	8:H:6:ARG:H	1.65	0.45
34:a:407:A:OP2	37:d:25:ARG:NH2	2.48	0.45
37:d:76:ARG:O	37:d:80:GLU:HG2	2.17	0.45
38:e:20:GLN:NE2	38:e:21:ALA:O	2.50	0.45
39:f:4:TYR:CZ	39:f:72:VAL:HG11	2.51	0.45
56:w:3:C:C2	56:w:71:G:N7	2.85	0.45
56:w:4:C:H3'	56:w:5:G:H5''	1.98	0.45
59:z:19:ASP:N	63:z:703:GCP:H3B1	2.23	0.45
59:z:116:GLU:O	59:z:120:LYS:HG2	2.16	0.45
1:A:1066:A:H62	1:A:1185:U:H3	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1763:G:C6	1:A:1764:U:C5	3.05	0.45
1:A:2039:G:OP1	29:5:9:LYS:HE3	2.16	0.45
1:A:2114:G:C6	1:A:2236:A:C8	3.05	0.45
1:A:2226:G:O2'	1:A:2227:G:OP1	2.34	0.45
2:B:66:A:N6	2:B:108:U:H2'	2.30	0.45
3:C:62:VAL:HG22	3:C:63:SER:O	2.17	0.45
7:G:27:ASN:O	7:G:30:GLU:HG2	2.17	0.45
20:W:79:GLY:CA	20:W:100:THR:HG22	2.47	0.45
34:a:427:A:H2'	34:a:428:A:O4'	2.16	0.45
34:a:495:C:C2	34:a:496:U:C5	3.04	0.45
34:a:609:G:H4'	49:p:16:HIS:CD2	2.52	0.45
49:p:55:ARG:HA	49:p:55:ARG:HD2	1.88	0.45
1:A:926:G:N2	1:A:943:C:C4	2.85	0.45
1:A:935:C:H1'	1:A:936:A:H1'	1.99	0.45
1:A:940:U:O2	1:A:940:U:H2'	2.15	0.45
1:A:1202:G:O2'	27:3:31:LEU:HD12	2.16	0.45
1:A:1444:C:OP1	21:X:25:LYS:NZ	2.49	0.45
1:A:2077:G:OP2	64:A:3729:HOH:O	2.21	0.45
4:D:166:GLN:HE22	4:D:176:ARG:NH1	2.14	0.45
6:F:65:TRP:CZ2	6:F:75:HIS:HD2	2.34	0.45
7:G:146:TYR:C	7:G:148:MET:H	2.25	0.45
12:O:98:VAL:CG2	12:O:118:ALA:HA	2.47	0.45
23:Z:45:ASP:OD1	23:Z:49:ARG:NH1	2.47	0.45
34:a:228:G:H1'	34:a:258:A:N1	2.32	0.45
34:a:296:A:H2'	34:a:297:G:O4'	2.17	0.45
34:a:513:G:O6	45:l:49:ASN:HA	2.17	0.45
34:a:928:U:H2'	34:a:929:G:H8	1.82	0.45
34:a:1007:C:O2	34:a:1007:C:H2'	2.17	0.45
39:f:36:ARG:NH1	39:f:66:GLU:OE2	2.41	0.45
58:y:39:PSU:H2'	58:y:40:C:H6	1.82	0.45
59:z:11:ASN:O	59:z:100:VAL:HB	2.16	0.45
1:A:159:G:H2'	1:A:160:C:C6	2.51	0.45
1:A:867:A:H2'	1:A:990:G:H5''	1.98	0.45
1:A:1337:U:H2'	1:A:1338:C:C6	2.51	0.45
1:A:1614:G:H5''	4:D:61:LEU:HD22	1.98	0.45
5:E:143:ASN:HD22	5:E:147:PRO:CD	2.30	0.45
7:G:3:LEU:H	7:G:3:LEU:HD12	1.82	0.45
7:G:47:LYS:HB3	7:G:49:ASP:OD1	2.16	0.45
19:V:29:PRO:HA	19:V:61:VAL:HG23	1.99	0.45
23:Z:74:VAL:HG13	23:Z:86:VAL:HG22	1.97	0.45
28:4:50:VAL:HG11	46:m:65:LYS:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1040:G:H2'	34:a:1041:G:O4'	2.16	0.45
34:a:1359:U:H2'	34:a:1360:A:C8	2.51	0.45
54:u:6:ARG:NH2	54:u:15:ARG:HH21	2.15	0.45
56:w:63:G:H8	56:w:63:G:C5'	2.30	0.45
58:y:39:PSU:H2'	58:y:40:C:C6	2.51	0.45
1:A:6:G:H2'	1:A:7:A:C8	2.52	0.45
1:A:679:G:H2'	1:A:679:G:N3	2.32	0.45
1:A:1463:G:O2'	1:A:1626:A:N6	2.48	0.45
1:A:2824:C:O2	29:5:43:HIS:HE1	1.99	0.45
3:C:62:VAL:CG2	3:C:63:SER:HA	2.47	0.45
7:G:18:GLU:HA	7:G:21:ARG:HD3	1.99	0.45
7:G:78:SER:OG	57:x:19:G:N2	2.50	0.45
12:O:24:VAL:HB	12:O:33:ALA:HB2	1.99	0.45
16:S:65:VAL:O	16:S:69:VAL:HG12	2.16	0.45
23:Z:52:SER:OG	23:Z:53:ILE:N	2.49	0.45
34:a:949:G:N1	34:a:1346:A:OP2	2.44	0.45
35:b:76:GLN:H	35:b:76:GLN:CD	2.24	0.45
44:k:93:GLN:HE21	44:k:93:GLN:HA	1.82	0.45
46:m:91:ARG:HA	46:m:91:ARG:HD2	1.81	0.45
59:z:65:ARG:HB2	59:z:79:HIS:CD2	2.52	0.45
1:A:1070:G:H3'	1:A:1071:U:H5'	1.99	0.44
1:A:1097:C:C2'	1:A:1098:C:H5'	2.48	0.44
1:A:1594:C:H2'	1:A:1595:C:C6	2.51	0.44
4:D:16:MET:HB2	4:D:16:MET:HE3	1.38	0.44
7:G:144:ILE:CG2	7:G:148:MET:HE1	2.46	0.44
8:H:11:VAL:HG13	8:H:15:VAL:HG22	1.98	0.44
10:K:53:VAL:HG11	10:K:70:LYS:C	2.42	0.44
28:4:46:GLN:C	28:4:48:ARG:N	2.74	0.44
28:4:68:ARG:C	28:4:68:ARG:HH21	2.25	0.44
34:a:501:G:H5'	34:a:503:C:C2	2.52	0.44
47:n:2:ALA:HB3	47:n:6:LEU:HD22	1.98	0.44
53:t:33:ILE:HG12	53:t:62:LEU:HB3	2.00	0.44
58:y:19:G:H1'	58:y:20:U:OP1	2.17	0.44
1:A:916:A:C2	1:A:953:C:C2	3.06	0.44
1:A:2026:A:H5''	64:A:3771:HOH:O	2.17	0.44
1:A:2544:A:H2'	1:A:2545:A:O4'	2.18	0.44
8:H:3:ARG:HB3	8:H:3:ARG:HH11	1.81	0.44
8:H:7:LEU:HD12	8:H:8:PRO:HD2	1.99	0.44
16:S:59:LYS:HB3	16:S:60:GLY:H	1.67	0.44
30:6:19:ARG:N	30:6:19:ARG:HD2	2.32	0.44
34:a:18:U:H1'	34:a:1063:A:N3	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:225:U:H2'	34:a:226:G:O4'	2.17	0.44
34:a:986:C:N4	34:a:1001:G:H1	2.10	0.44
34:a:1031:G:OP1	47:n:3:ARG:HB3	2.18	0.44
39:f:2:ARG:HD3	39:f:92:LYS:NZ	2.33	0.44
44:k:87:THR:HG22	44:k:91:ARG:NH1	2.33	0.44
59:z:200:ILE:HG22	59:z:276:VAL:HG12	2.00	0.44
59:z:552:LYS:HA	59:z:553:ALA:HB3	1.98	0.44
1:A:703:U:H2'	1:A:704:C:H6	1.81	0.44
1:A:1143:A:H2'	1:A:1144:G:H5'	1.99	0.44
1:A:2155:A:O2'	1:A:2181:G:H1'	2.18	0.44
1:A:2208:G:H2'	1:A:2209:C:O4'	2.16	0.44
1:A:2261:G:OP1	14:Q:85:LYS:NZ	2.51	0.44
1:A:2855:G:H2'	1:A:2856:U:C6	2.52	0.44
5:E:181:LEU:HD12	5:E:181:LEU:HA	1.81	0.44
7:G:16:ARG:HB2	7:G:17:PRO:HD3	2.00	0.44
11:N:48:MET:HB2	11:N:48:MET:HE3	1.61	0.44
24:0:27:GLU:HG2	24:0:68:GLU:HA	1.99	0.44
34:a:17:A:O2'	38:e:16:THR:HB	2.18	0.44
34:a:1409:C:H2'	34:a:1410:U:H6	1.81	0.44
44:k:84:VAL:HG21	44:k:95:ILE:HD11	1.97	0.44
59:z:421:VAL:O	59:z:425:MET:HG3	2.16	0.44
1:A:469:C:H4'	6:F:49:ALA:HB2	2.00	0.44
1:A:928:G:H1	1:A:939:C:H42	1.65	0.44
1:A:1832:A:N1	1:A:1852:G:H1'	2.33	0.44
1:A:2783:C:H2'	1:A:2784:C:C6	2.52	0.44
3:C:24:GLU:O	3:C:27:HIS:HB2	2.18	0.44
3:C:62:VAL:HG13	3:C:63:SER:CA	2.44	0.44
7:G:145:THR:HG23	7:G:148:MET:SD	2.57	0.44
11:N:55:VAL:HG13	11:N:126:PRO:HA	1.98	0.44
30:6:35:GLU:CD	30:6:50:ARG:HE	2.26	0.44
34:a:168:U:H5''	34:a:204:A:O4'	2.17	0.44
34:a:215:C:H2'	34:a:216:G:O4'	2.17	0.44
34:a:514:G:H4'	34:a:515:U:OP2	2.17	0.44
34:a:981:G:H3'	34:a:982:G:C8	2.52	0.44
34:a:988:G:H2'	34:a:988:G:N3	2.33	0.44
34:a:1091:G:H5'	36:c:176:HIS:CD2	2.53	0.44
36:c:125:GLU:OE1	36:c:190:ARG:HG2	2.18	0.44
40:g:140:ASP:OD1	40:g:143:ARG:NH2	2.50	0.44
50:q:93:GLN:O	50:q:96:GLU:HG2	2.18	0.44
58:y:1:G:O2'	58:y:2:C:OP1	2.33	0.44
59:z:227:ARG:HE	59:z:238:THR:CG2	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:G:OP1	4:D:12:SER:HB2	2.18	0.44
1:A:810:A:H5'	4:D:210:GLY:CA	2.48	0.44
1:A:1940:A:N1	34:a:1473:U:O2'	2.44	0.44
1:A:1964:U:H5'	59:z:532:LEU:HD11	1.99	0.44
1:A:2166:C:H3'	1:A:2167:C:N1	2.33	0.44
1:A:2862:C:H2'	1:A:2863:G:C8	2.53	0.44
3:C:201:PRO:O	3:C:203:GLY:CA	2.59	0.44
6:F:184:TYR:CD2	6:F:188:ARG:HD2	2.52	0.44
34:a:207:G:H2'	34:a:208:C:O4'	2.17	0.44
34:a:1011:C:H2'	34:a:1012:G:C8	2.52	0.44
34:a:1125:G:H2'	34:a:1126:G:O4'	2.18	0.44
34:a:1325:G:H4'	42:i:122:ALA:HB3	1.99	0.44
34:a:1491:A:H2'	34:a:1492:C:C6	2.52	0.44
38:e:95:ALA:HB1	38:e:96:PRO:HD2	2.00	0.44
43:j:95:GLU:HG2	43:j:96:ILE:H	1.82	0.44
1:A:459:C:C4	1:A:460:U:O4	2.70	0.44
1:A:682:G:H8	1:A:682:G:O5'	2.00	0.44
1:A:907:A:C2	1:A:962:A:C4	3.05	0.44
1:A:1097:C:H2'	1:A:1098:C:H5'	2.00	0.44
1:A:1404:A:N1	1:A:1417:U:O4	2.50	0.44
1:A:1501:G:O2'	1:A:2862:C:OP1	2.26	0.44
3:C:64:LEU:HA	3:C:65:PRO:O	2.17	0.44
5:E:7:VAL:HG12	5:E:51:PHE:HE1	1.82	0.44
6:F:120:GLU:H	6:F:120:GLU:HG3	1.67	0.44
17:T:106:SER:O	17:T:110:ILE:HG13	2.17	0.44
26:2:66:GLU:HA	26:2:69:ARG:HH11	1.82	0.44
35:b:172:ILE:O	35:b:176:GLU:HG3	2.17	0.44
38:e:122:GLU:HG2	38:e:131:ILE:HD12	1.99	0.44
50:q:96:GLU:HG3	50:q:97:SER:N	2.33	0.44
56:w:5:G:N1	56:w:68:C:O2	2.50	0.44
59:z:291:TYR:CD1	59:z:292:PRO:HD2	2.53	0.44
1:A:671:G:H2'	1:A:672:G:O4'	2.18	0.44
1:A:2141:G:O2'	1:A:2142:G:H5'	2.17	0.44
1:A:2752:A:C6	1:A:2776:A:C8	3.06	0.44
3:C:192:PHE:CD2	3:C:193:ILE:HD12	2.53	0.44
8:H:152:ARG:HD3	8:H:152:ARG:HA	1.75	0.44
14:Q:56:ARG:NH2	56:w:64:A:OP1	2.50	0.44
34:a:629:C:H2'	34:a:630:U:C6	2.53	0.44
34:a:925:G:H2'	34:a:926:C:O4'	2.18	0.44
36:c:22:TRP:CE2	47:n:54:PRO:HG3	2.52	0.44
37:d:173:TRP:CD1	37:d:173:TRP:N	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:s:10:PHE:HE2	52:s:37:ARG:HD3	1.83	0.44
52:s:14:HIS:C	52:s:14:HIS:CD2	2.95	0.44
57:x:61:C:H2'	57:x:62:C:C6	2.52	0.44
59:z:97:LEU:O	59:z:127:HIS:CE1	2.71	0.44
1:A:715:G:H5'	64:A:3870:HOH:O	2.17	0.44
1:A:1302:C:H2'	1:A:1303:C:C6	2.53	0.44
1:A:1803:A:C5	1:A:1859:A:H1'	2.53	0.44
1:A:2346:A:C8	1:A:2348:G:C5	3.05	0.44
1:A:2783:C:H2'	1:A:2784:C:H6	1.82	0.44
3:C:44:HIS:HA	3:C:172:HIS:HB3	2.00	0.44
10:K:103:GLN:HA	10:K:106:GLU:OE1	2.18	0.44
17:T:41:ARG:CZ	34:a:341:C:H3'	2.48	0.44
18:U:94:ASN:HB3	19:V:4:ILE:HD13	2.00	0.44
22:Y:13:VAL:HB	22:Y:72:VAL:HG13	2.00	0.44
34:a:493:A:H5''	37:d:55:ALA:HB2	1.98	0.44
34:a:980:G:C2	34:a:981:G:C5	3.06	0.44
34:a:1043:C:C5	36:c:2:GLY:HA3	2.52	0.44
36:c:101:LEU:HD12	36:c:102:ASN:H	1.83	0.44
37:d:155:LEU:HD23	37:d:157:LEU:H	1.82	0.44
40:g:54:THR:O	40:g:56:GLN:N	2.50	0.44
56:w:10:G:O6	56:w:25:C:N3	2.51	0.44
56:w:43:C:H2'	56:w:44:G:H5''	1.99	0.44
59:z:245:PHE:HB3	59:z:250:LEU:CD1	2.47	0.44
59:z:545:ILE:H	59:z:545:ILE:CD1	2.29	0.44
1:A:7:A:H5'	11:N:51:PHE:CE2	2.53	0.44
1:A:989:A:C4	1:A:2459:A:C2	3.06	0.44
1:A:1132:G:N2	1:A:1148:A:H1'	2.32	0.44
1:A:1844:G:H4'	4:D:51:VAL:HG21	1.99	0.44
1:A:1910:A:N1	1:A:2245:G:H1'	2.33	0.44
1:A:1991:A:OP2	64:A:3727:HOH:O	2.21	0.44
1:A:2155:A:H1'	1:A:2180:G:N2	2.29	0.44
2:B:20:C:H2'	2:B:21:G:O4'	2.18	0.44
3:C:62:VAL:CB	3:C:63:SER:HA	2.48	0.44
5:E:54:GLN:OE1	5:E:55:ASN:N	2.51	0.44
5:E:117:MET:O	5:E:118:LYS:CB	2.65	0.44
6:F:12:LEU:HA	6:F:12:LEU:HD12	1.71	0.44
7:G:61:ALA:O	7:G:65:GLY:N	2.41	0.44
7:G:144:ILE:HG23	7:G:148:MET:HE1	1.98	0.44
32:8:16:ILE:HD12	32:8:59:LYS:HG2	1.99	0.44
33:9:11:CYS:O	33:9:14:CYS:HB2	2.18	0.44
34:a:246:A:H4'	34:a:247:G:O5'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:822:G:N2	34:a:824:C:H5'	2.33	0.44
34:a:1218:A:H2'	34:a:1219:C:C6	2.53	0.44
34:a:1482:G:OP1	34:a:1485:A:H4'	2.18	0.44
35:b:103:THR:HA	35:b:180:LEU:HD11	2.00	0.44
36:c:73:PRO:O	36:c:77:ILE:HG12	2.17	0.44
42:i:105:ASP:OD1	42:i:107:ARG:NH2	2.31	0.44
1:A:185:A:N6	1:A:2441:A:H2'	2.32	0.43
1:A:2181:G:H5'	1:A:2182:C:OP2	2.18	0.43
4:D:71:ASP:HB3	4:D:103:ARG:HH22	1.83	0.43
7:G:173:LEU:HB3	7:G:178:PHE:CG	2.53	0.43
12:O:7:TYR:CE1	12:O:20:MET:HB2	2.53	0.43
19:V:52:VAL:HG23	19:V:52:VAL:O	2.18	0.43
26:2:38:GLN:HB3	26:2:44:LEU:HB2	2.00	0.43
34:a:276:C:OP1	50:q:91:ARG:NH1	2.51	0.43
34:a:510:C:OP2	45:l:91:LYS:HE3	2.18	0.43
34:a:1152:A:H2'	34:a:1153:G:O4'	2.18	0.43
38:e:110:LEU:HD13	38:e:118:ILE:HD13	2.00	0.43
43:j:11:PHE:HE1	43:j:67:THR:HG22	1.82	0.43
46:m:39:ILE:O	46:m:40:ASN:HB3	2.17	0.43
49:p:4:ILE:HG23	49:p:36:ILE:HD11	2.00	0.43
50:q:66:SER:OG	50:q:69:LYS:HB3	2.18	0.43
59:z:173:GLY:O	59:z:177:ILE:HG13	2.18	0.43
59:z:381:ARG:NH1	59:z:404:GLU:OE2	2.51	0.43
59:z:411:LYS:O	59:z:479:TYR:HA	2.17	0.43
1:A:699:A:H2'	1:A:700:A:O4'	2.18	0.43
1:A:989:A:H2	64:A:4351:HOH:O	2.01	0.43
1:A:1043:C:P	18:U:92:ARG:HH22	2.41	0.43
1:A:1210:U:H2'	1:A:1211:C:H6	1.81	0.43
1:A:1446:G:H4'	1:A:1569:G:H4'	2.00	0.43
1:A:1884:A:H2'	1:A:1885:G:O4'	2.18	0.43
1:A:2113:U:H4'	1:A:2114:G:O5'	2.19	0.43
1:A:2189:G:H3'	1:A:2190:A:H5''	2.00	0.43
4:D:5:LYS:HE3	4:D:17:THR:HG22	1.99	0.43
4:D:242:ARG:HG2	4:D:246:PRO:HG3	2.00	0.43
12:O:73:ASP:OD1	12:O:75:SER:OG	2.35	0.43
14:Q:10:ARG:NH2	57:x:64:G:O2'	2.38	0.43
34:a:321:A:H2'	34:a:322:G:O4'	2.18	0.43
34:a:448:A:C6	34:a:449:C:C4	3.06	0.43
34:a:812:A:H2'	34:a:813:G:O4'	2.18	0.43
34:a:826:C:H2'	34:a:827:C:H6	1.83	0.43
34:a:1274:U:H2'	34:a:1275:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:c:16:ARG:NH1	36:c:183:ASP:OD1	2.46	0.43
48:o:6:GLU:H	48:o:6:GLU:CD	2.26	0.43
1:A:224:C:H2'	1:A:225:C:H6	1.83	0.43
1:A:681:G:C6	1:A:682:G:C6	3.06	0.43
1:A:1092:G:N2	1:A:1156:A:N6	2.65	0.43
1:A:1760:G:H2'	1:A:1761:G:O4'	2.18	0.43
1:A:2046:C:H2'	1:A:2047:C:C6	2.53	0.43
1:A:2153:U:C4	3:C:5:LYS:HG3	2.53	0.43
1:A:2588:A:H5''	1:A:2589:G:H5'	2.00	0.43
1:A:2693:U:O2	5:E:22:PRO:HB3	2.18	0.43
5:E:52:LEU:HD12	5:E:52:LEU:HA	1.85	0.43
6:F:126:VAL:O	6:F:196:LEU:N	2.51	0.43
7:G:36:LYS:C	7:G:99:MET:HE3	2.44	0.43
8:H:117:PRO:HB3	8:H:123:PHE:CE2	2.54	0.43
8:H:164:TYR:HB2	8:H:167:GLU:HB2	1.99	0.43
18:U:97:ASP:OD2	18:U:101:ARG:HD2	2.18	0.43
28:4:34:GLU:HB3	46:m:57:ARG:NH2	2.32	0.43
34:a:36:G:O2'	45:l:118:SER:O	2.20	0.43
34:a:251:G:H2'	34:a:252:U:C6	2.54	0.43
34:a:366:C:C2	34:a:388:G:N2	2.86	0.43
37:d:70:ILE:HG23	37:d:75:PHE:HB2	2.00	0.43
38:e:50:GLU:HB2	38:e:53:LEU:HD13	1.99	0.43
44:k:62:GLN:O	44:k:66:LEU:HG	2.18	0.43
44:k:73:MET:HE1	44:k:102:GLY:HA3	2.00	0.43
53:t:49:ALA:HB2	53:t:92:LEU:HD22	2.00	0.43
1:A:269:C:O2'	1:A:271:U:OP2	2.37	0.43
1:A:293:C:H2'	1:A:294:C:C6	2.54	0.43
1:A:509:C:H2'	1:A:510:C:C6	2.53	0.43
1:A:666:G:H21	1:A:670:A:H2	1.62	0.43
1:A:1209:G:H2'	1:A:1210:U:C6	2.52	0.43
1:A:2678:C:H1'	8:H:109:PHE:HD2	1.81	0.43
7:G:16:ARG:HH22	7:G:28:VAL:HB	1.82	0.43
16:S:80:LEU:HD12	16:S:80:LEU:HA	1.78	0.43
26:2:45:SER:O	26:2:46:GLN:HB2	2.17	0.43
31:7:10:ARG:HG2	31:7:14:LYS:HD3	2.00	0.43
34:a:640:C:O2'	48:o:28:GLN:NE2	2.38	0.43
45:l:30:ALA:HB1	45:l:31:PRO:HD2	2.01	0.43
59:z:492:VAL:HG13	59:z:541:ILE:HD13	2.00	0.43
59:z:595:GLU:H	59:z:595:GLU:HG2	1.49	0.43
1:A:358:C:H4'	22:Y:73:ARG:HD3	2.00	0.43
1:A:793:U:O2	1:A:2035:A:H1'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:G:H8	1:A:1016:G:O5'	2.02	0.43
1:A:1404:A:C6	1:A:1417:U:O4	2.72	0.43
1:A:1768:G:H3'	1:A:1769:A:C8	2.46	0.43
1:A:1778:G:N2	1:A:1779:A:C4	2.86	0.43
1:A:2226:G:H5'	1:A:2227:G:O6	2.19	0.43
1:A:2507:C:O2'	1:A:2508:A:H5'	2.18	0.43
4:D:3:VAL:HG13	4:D:17:THR:HB	2.00	0.43
4:D:26:LYS:NZ	4:D:30:GLU:OE1	2.51	0.43
6:F:31:HIS:NE2	6:F:35:GLU:OE2	2.52	0.43
6:F:153:SER:OG	6:F:190:GLU:HG3	2.18	0.43
6:F:184:TYR:O	6:F:188:ARG:HG3	2.19	0.43
12:O:29:ASN:N	12:O:29:ASN:OD1	2.50	0.43
28:4:62:ARG:HB3	28:4:63:TYR:H	1.60	0.43
34:a:55:C:N4	34:a:349:A:OP2	2.42	0.43
34:a:68:C:H2'	34:a:69:G:H8	1.83	0.43
34:a:136:A:H2'	34:a:137:G:O4'	2.18	0.43
34:a:703:C:H1'	51:r:49:LYS:HG3	2.01	0.43
36:c:164:ARG:HG2	36:c:165:THR:N	2.33	0.43
36:c:179:ARG:NH1	36:c:206:GLU:OE1	2.52	0.43
40:g:144:MET:SD	58:y:40:C:H1'	2.59	0.43
48:o:9:GLN:O	48:o:13:GLN:HG3	2.18	0.43
52:s:11:VAL:HG12	52:s:12:ASP:H	1.83	0.43
59:z:116:GLU:HA	59:z:119:ALA:HB3	1.99	0.43
1:A:251:C:O2'	1:A:455:A:N3	2.49	0.43
1:A:810:A:H5'	4:D:210:GLY:HA2	1.99	0.43
1:A:1026:A:OP1	64:A:3730:HOH:O	2.22	0.43
1:A:1468:G:OP1	1:A:1537:G:O2'	2.36	0.43
1:A:1587:G:OP2	1:A:1588:A:O2'	2.28	0.43
1:A:1593:C:H2'	1:A:1594:C:H6	1.84	0.43
1:A:1934:A:C8	34:a:1472:G:H4'	2.54	0.43
2:B:29:A:H2'	2:B:30:C:C6	2.54	0.43
6:F:64:ILE:HG21	6:F:78:ILE:HG23	2.00	0.43
7:G:32:PRO:HB2	7:G:172:LEU:HD22	2.00	0.43
10:K:127:ILE:H	10:K:127:ILE:HG12	1.67	0.43
12:O:77:ILE:HG13	17:T:74:ARG:HG3	2.00	0.43
19:V:1:MET:HB3	19:V:99:ILE:HD12	2.00	0.43
34:a:480:A:H4'	34:a:481:A:OP1	2.18	0.43
34:a:942:A:N3	34:a:947:A:O2'	2.44	0.43
34:a:1238:A:H5''	34:a:1240:G:N3	2.33	0.43
35:b:115:LEU:O	35:b:119:GLU:N	2.51	0.43
36:c:77:ILE:HG13	36:c:78:GLY:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:12:LEU:HD22	38:e:13:ILE:N	2.34	0.43
40:g:113:GLU:CG	40:g:119:ARG:HG2	2.48	0.43
48:o:54:ARG:O	48:o:58:MET:HG3	2.19	0.43
49:p:75:ARG:O	49:p:78:GLY:N	2.41	0.43
50:q:22:LEU:HD12	50:q:23:VAL:N	2.33	0.43
56:w:4:C:N4	56:w:5:G:C5	2.86	0.43
59:z:10:ARG:NE	59:z:185:ILE:HA	2.27	0.43
1:A:283:G:C2	1:A:284:U:O4	2.70	0.43
1:A:503:A:C6	1:A:505:A:C6	3.07	0.43
1:A:771:G:C6	1:A:772:G:N1	2.86	0.43
1:A:908:G:H2'	1:A:909:A:O4'	2.18	0.43
1:A:1218:A:H1'	1:A:1219:U:C5'	2.48	0.43
1:A:2602:C:H2'	1:A:2603:G:C8	2.53	0.43
2:B:3:C:H2'	2:B:4:C:H6	1.83	0.43
2:B:96:U:H2'	2:B:97:G:C8	2.54	0.43
7:G:150:ASP:OD2	7:G:153:ARG:NH1	2.51	0.43
11:N:12:ARG:HD3	11:N:14:VAL:HG23	2.00	0.43
13:P:115:LEU:HA	13:P:131:SER:HB3	2.01	0.43
18:U:27:LEU:HB3	18:U:31:SER:HB3	2.01	0.43
19:V:61:VAL:HG23	19:V:61:VAL:O	2.18	0.43
28:4:59:PHE:H	28:4:59:PHE:HD1	1.67	0.43
34:a:898:U:H2'	34:a:899:U:C6	2.54	0.43
34:a:952:A:OP1	47:n:29:ARG:NH2	2.52	0.43
37:d:152:SER:HB2	37:d:155:LEU:HD12	2.01	0.43
38:e:78:HIS:HA	41:h:105:ARG:HG3	2.00	0.43
49:p:5:ARG:NH2	49:p:24:ALA:O	2.49	0.43
55:v:19:U:C4	56:w:37:MIA:H113	2.53	0.43
56:w:60:U:O2'	56:w:61:C:H5'	2.18	0.43
56:w:70:G:N1	56:w:71:G:N7	2.67	0.43
59:z:436:VAL:HG23	59:z:437:ASN:HB2	1.99	0.43
59:z:496:VAL:HG23	59:z:537:ILE:HG12	2.00	0.43
1:A:31:C:C2'	1:A:32:U:H5'	2.48	0.43
1:A:224:C:H2'	1:A:225:C:C6	2.53	0.43
1:A:928:G:H22	1:A:939:C:N4	2.17	0.43
1:A:1066:A:C8	1:A:1066:A:C3'	3.02	0.43
1:A:1144:G:O2'	1:A:1145:C:H5'	2.19	0.43
1:A:1283:G:O2'	1:A:1284:G:H5'	2.19	0.43
1:A:1765:G:H5'	1:A:1766:A:H5''	2.01	0.43
6:F:32:LEU:O	6:F:36:VAL:HG23	2.19	0.43
8:H:111:HIS:H	8:H:111:HIS:CD2	2.36	0.43
10:K:18:THR:O	10:K:20:ALA:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:23:ARG:NH1	16:S:85:VAL:O	2.47	0.43
16:S:59:LYS:HB3	16:S:65:VAL:HG22	2.00	0.43
28:4:59:PHE:N	28:4:59:PHE:CD1	2.87	0.43
34:a:343:G:H2'	34:a:344:G:O4'	2.19	0.43
59:z:471:SER:O	59:z:471:SER:OG	2.32	0.43
1:A:140:C:H2'	1:A:141:G:O4'	2.19	0.43
1:A:641:G:H2'	1:A:642:C:O4'	2.19	0.43
1:A:800:C:O2'	1:A:1317:A:N1	2.47	0.43
1:A:955:A:C5	14:Q:13:GLN:HG3	2.54	0.43
1:A:1092:G:H2'	1:A:1155:G:N2	2.33	0.43
1:A:1335:C:H2'	1:A:1336:C:C6	2.54	0.43
1:A:2700:U:O2	1:A:2700:U:H2'	2.17	0.43
1:A:2736:C:OP1	5:E:118:LYS:NZ	2.51	0.43
4:D:72:LYS:NZ	4:D:99:ASP:OD1	2.40	0.43
5:E:67:PHE:CE1	5:E:75:VAL:HG22	2.54	0.43
10:K:77:LEU:O	10:K:78:ILE:HB	2.18	0.43
19:V:31:ALA:O	19:V:61:VAL:HG22	2.19	0.43
19:V:52:VAL:HG23	19:V:55:ALA:HB3	2.01	0.43
28:4:58:ARG:HD2	52:s:65:ASN:HA	1.99	0.43
34:a:138:A:N3	34:a:138:A:H2'	2.34	0.43
34:a:295:G:H2'	34:a:296:A:C8	2.54	0.43
34:a:1008:C:H6	34:a:1010:G:N7	2.17	0.43
34:a:1369:G:H2'	34:a:1370:G:H8	1.83	0.43
35:b:141:GLU:O	35:b:145:LEU:HB2	2.19	0.43
39:f:22:GLU:OE2	39:f:82:ARG:HD3	2.18	0.43
43:j:32:ALA:HA	43:j:33:GLN:HA	1.90	0.43
52:s:22:LEU:HD12	52:s:31:ILE:HD11	2.01	0.43
59:z:418:GLU:HA	59:z:446:LYS:HA	2.01	0.43
1:A:12:A:N1	1:A:549:U:H2'	2.34	0.43
1:A:353:A:HO2'	1:A:354:A:H8	1.61	0.43
1:A:360:C:H2'	1:A:361:G:O4'	2.19	0.43
1:A:1216:G:H3'	1:A:1217:G:C8	2.54	0.43
1:A:1404:A:N6	1:A:1417:U:H3	2.16	0.43
1:A:2107:U:H2'	1:A:2108:G:C8	2.53	0.43
1:A:2256:U:H5''	1:A:2257:G:H5'	2.01	0.43
1:A:2330:G:H1	16:S:3:ARG:HA	1.83	0.43
1:A:2558:U:H2'	1:A:2559:G:C8	2.53	0.43
4:D:34:VAL:HA	4:D:62:TYR:O	2.19	0.43
4:D:145:VAL:HB	4:D:155:LEU:HB2	1.99	0.43
7:G:39:ILE:HD11	7:G:102:PHE:CZ	2.54	0.43
8:H:24:VAL:HG11	8:H:43:VAL:HG11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:78:GLY:C	8:H:80:SER:H	2.26	0.43
10:K:9:LYS:HE3	10:K:9:LYS:HB2	1.78	0.43
34:a:825:U:C5	34:a:826:C:H1'	2.53	0.43
34:a:1132:C:H2'	34:a:1133:U:C6	2.53	0.43
34:a:1218:A:OP1	54:u:2:GLY:HA3	2.18	0.43
35:b:21:ARG:H	35:b:21:ARG:CD	2.29	0.43
37:d:70:ILE:HG21	37:d:75:PHE:HD1	1.83	0.43
59:z:431:LYS:HA	59:z:458:GLU:HG2	2.01	0.43
1:A:173:U:H2'	1:A:174:G:H8	1.82	0.42
1:A:830:A:C6	4:D:229:VAL:HG11	2.53	0.42
1:A:1113:G:C6	1:A:1114:A:C6	3.07	0.42
1:A:1635:U:H2'	1:A:1636:G:H8	1.82	0.42
1:A:1711:A:H2'	1:A:1712:G:O4'	2.19	0.42
1:A:2085:C:H2'	1:A:2086:C:C6	2.54	0.42
1:A:2190:A:C8	1:A:2190:A:OP1	2.72	0.42
6:F:136:THR:HG22	6:F:140:LEU:HD23	2.00	0.42
8:H:32:GLU:OE1	8:H:32:GLU:N	2.52	0.42
10:K:125:ARG:H	10:K:125:ARG:HG3	1.62	0.42
25:1:82:LEU:HA	25:1:85:LEU:CD2	2.49	0.42
28:4:9:LEU:HD12	28:4:9:LEU:HA	1.88	0.42
34:a:556:A:H5'	34:a:557:A:OP2	2.19	0.42
34:a:604:C:C2	37:d:135:LEU:HG	2.54	0.42
34:a:1008:C:H2'	34:a:1008:C:H6	1.54	0.42
34:a:1355:U:H5''	42:i:71:SER:HB3	2.01	0.42
34:a:1396:A:H2	34:a:1465:G:H22	1.67	0.42
40:g:12:LEU:H	40:g:12:LEU:HD12	1.84	0.42
41:h:13:ILE:O	41:h:17:THR:HG23	2.19	0.42
45:l:52:LEU:O	45:l:54:LYS:NZ	2.46	0.42
46:m:108:ARG:HA	46:m:108:ARG:HD3	1.62	0.42
57:x:19:G:C4	57:x:57:A:C2	3.07	0.42
57:x:73:A:N7	59:z:572:LYS:HG3	2.34	0.42
58:y:45:U:OP2	58:y:46:G:H5''	2.19	0.42
1:A:669:C:H3'	1:A:669:C:H6	1.84	0.42
1:A:1761:G:O6	1:A:1773:C:N3	2.52	0.42
1:A:2126:C:H2'	1:A:2127:G:H5''	2.00	0.42
1:A:2903:U:H2'	1:A:2904:C:C6	2.54	0.42
7:G:106:LEU:HA	7:G:110:ALA:HB3	2.02	0.42
12:O:120:GLU:OE2	17:T:67:SER:OG	2.30	0.42
14:Q:39:PRO:HA	14:Q:97:VAL:O	2.19	0.42
21:X:12:VAL:HG22	21:X:29:TRP:CE2	2.55	0.42
22:Y:9:LYS:HA	22:Y:10:GLY:HA2	1.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:86:ARG:NH1	22:Y:100:ALA:HA	2.35	0.42
34:a:565:G:O2'	34:a:566:U:H5'	2.19	0.42
34:a:643:U:OP1	48:o:9:GLN:NE2	2.52	0.42
34:a:904:G:C6	34:a:1483:G:C6	3.07	0.42
34:a:1147:G:C6	34:a:1148:C:C4	3.08	0.42
34:a:1239:U:O2	34:a:1239:U:H2'	2.19	0.42
35:b:71:VAL:HA	35:b:93:VAL:HG23	2.00	0.42
39:f:97:PHE:CZ	51:r:61:LYS:HE2	2.54	0.42
56:w:19:G:N2	56:w:57:G:H1'	2.34	0.42
58:y:9:A:H5'	58:y:46:G:H8	1.78	0.42
59:z:39:ARG:HD3	59:z:39:ARG:HA	1.83	0.42
59:z:497:HIS:HA	59:z:536:PRO:HG2	2.00	0.42
1:A:242:G:O6	32:8:5:LYS:HD3	2.19	0.42
1:A:828:A:H5'	1:A:829:A:N7	2.34	0.42
1:A:1093:A:OP2	1:A:1154:C:N4	2.53	0.42
1:A:1185:U:OP1	11:N:25:ARG:NH1	2.53	0.42
2:B:41:U:H5	7:G:70:VAL:O	2.02	0.42
17:T:50:ILE:HB	17:T:99:LEU:HB2	2.01	0.42
21:X:43:VAL:HG13	21:X:47:PHE:HD1	1.83	0.42
37:d:100:ARG:NH1	37:d:137:SER:HB3	2.33	0.42
49:p:69:THR:O	49:p:73:LEU:HG	2.19	0.42
50:q:86:GLU:O	50:q:90:ILE:HG12	2.19	0.42
53:t:60:GLU:HG3	53:t:81:LYS:HD2	2.01	0.42
57:x:14:A:H2'	57:x:15:G:H5'	2.01	0.42
58:y:61:C:H2'	58:y:62:C:C6	2.54	0.42
1:A:240:G:OP2	13:P:50:ARG:NH1	2.52	0.42
1:A:1251:C:H2'	1:A:1252:C:H6	1.85	0.42
1:A:1424:A:H4'	1:A:1425:G:OP2	2.19	0.42
1:A:2143:U:O2	3:C:172:HIS:CE1	2.73	0.42
3:C:68:LEU:HD12	3:C:70:LYS:HB3	2.02	0.42
5:E:101:ARG:CZ	5:E:171:GLU:HB2	2.50	0.42
10:K:45:THR:HA	10:K:48:MET:HE1	2.02	0.42
20:W:37:ARG:HB3	20:W:37:ARG:NH1	2.34	0.42
21:X:34:ALA:HA	21:X:38:GLU:OE1	2.18	0.42
26:2:1:MET:HB2	26:2:52:ASP:OD1	2.19	0.42
34:a:152:G:H1	34:a:159:U:H3	1.67	0.42
34:a:152:G:H2'	34:a:153:G:C8	2.54	0.42
34:a:251:G:H2'	34:a:252:U:H6	1.84	0.42
34:a:378:A:H2'	34:a:379:A:C8	2.53	0.42
34:a:993:A:C2	34:a:1201:U:H1'	2.54	0.42
34:a:1160:G:P	42:i:97:LYS:HE3	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1484:U:H5''	55:v:13:A:N1	2.34	0.42
36:c:13:GLY:HA3	47:n:57:ARG:NH1	2.34	0.42
38:e:99:GLY:O	38:e:117:ASP:HA	2.19	0.42
1:A:935:C:H1'	1:A:936:A:C1'	2.50	0.42
1:A:1524:G:O2'	1:A:1604:A:C2	2.71	0.42
1:A:2488:C:O2	33:9:4:ARG:NH2	2.47	0.42
3:C:190:ARG:O	3:C:194:ARG:HG2	2.19	0.42
7:G:173:LEU:HD13	7:G:178:PHE:CE2	2.54	0.42
9:J:8:GLU:C	9:J:10:LEU:N	2.76	0.42
11:N:131:GLN:OE1	11:N:131:GLN:N	2.52	0.42
12:O:101:PRO:HG3	17:T:67:SER:HB3	2.01	0.42
16:S:34:HIS:HB2	16:S:36:TYR:HE1	1.83	0.42
30:6:11:LEU:HB2	30:6:21:TYR:HB2	2.01	0.42
34:a:505:G:N7	45:l:53:ARG:NH2	2.67	0.42
34:a:964:A:H2'	34:a:965:G:O4'	2.18	0.42
34:a:1005:G:N3	34:a:1005:G:H2'	2.35	0.42
36:c:11:ARG:HD3	36:c:15:THR:CG2	2.50	0.42
50:q:18:THR:HG23	50:q:69:LYS:HE3	2.00	0.42
58:y:22:G:O6	58:y:46:G:C6	2.70	0.42
59:z:28:ARG:HB3	59:z:174:VAL:HG11	2.02	0.42
59:z:444:ALA:HA	59:z:445:GLN:HB2	2.02	0.42
1:A:398:G:P	25:1:69:LYS:HZ1	2.43	0.42
1:A:1054:A:O4'	18:U:59:ARG:HG2	2.20	0.42
1:A:1344:G:H5''	1:A:1345:U:OP1	2.20	0.42
1:A:1670:C:H2'	1:A:1671:G:O4'	2.20	0.42
1:A:1883:A:H2'	1:A:1884:A:C8	2.54	0.42
2:B:93:G:H2'	2:B:94:C:C6	2.54	0.42
7:G:77:ILE:HD12	7:G:82:LEU:HD11	2.02	0.42
17:T:45:PHE:HE2	17:T:63:VAL:HB	1.85	0.42
28:4:61:ARG:HG3	28:4:62:ARG:N	2.35	0.42
30:6:21:TYR:CD2	30:6:38:LYS:HG2	2.54	0.42
34:a:99:G:H2'	34:a:100:C:C6	2.55	0.42
34:a:980:G:H2'	34:a:981:G:H8	1.84	0.42
34:a:1470:A:O2'	34:a:1471:A:O5'	2.37	0.42
43:j:82:ILE:HA	43:j:85:LEU:HD12	2.01	0.42
53:t:43:LEU:HD12	53:t:43:LEU:HA	1.91	0.42
59:z:396:LEU:HB3	59:z:397:PRO:O	2.19	0.42
1:A:769:G:H2'	1:A:770:U:O4'	2.18	0.42
1:A:914:U:C4	1:A:915:G:N7	2.88	0.42
1:A:1032:G:O2'	1:A:1045:A:N3	2.47	0.42
1:A:1091:A:C6	9:J:6:ASN:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2132:C:OP2	1:A:2166:C:N4	2.48	0.42
1:A:2505:G:O2'	14:Q:80:GLU:HA	2.19	0.42
5:E:59:VAL:CG1	5:E:64:LYS:HG3	2.50	0.42
6:F:133:ASN:N	6:F:138:GLU:OE1	2.44	0.42
7:G:41:GLN:HG2	7:G:154:GLY:O	2.20	0.42
10:K:76:TYR:CE2	10:K:77:LEU:HD23	2.55	0.42
16:S:51:ALA:HB3	16:S:73:LEU:HB2	2.00	0.42
34:a:529:C:O2'	34:a:533:C:OP1	2.29	0.42
35:b:49:GLU:O	35:b:52:GLU:HB3	2.19	0.42
35:b:104:ASN:O	35:b:108:ILE:HG12	2.20	0.42
44:k:83:ILE:H	44:k:83:ILE:HG12	1.71	0.42
59:z:16:ALA:HB3	59:z:22:LYS:CD	2.44	0.42
59:z:50:GLU:OE2	59:z:51:LEU:N	2.53	0.42
59:z:292:PRO:HB2	59:z:293:GLY:CA	2.44	0.42
1:A:557:G:H5'	18:U:24:TYR:CE2	2.55	0.42
1:A:1185:U:H4'	1:A:1187:A:O4'	2.20	0.42
1:A:1185:U:P	11:N:25:ARG:HH12	2.42	0.42
1:A:2049:U:H2'	1:A:2050:G:O4'	2.19	0.42
1:A:2129:C:C2'	1:A:2130:U:H5'	2.49	0.42
1:A:2137:G:H2'	1:A:2138:A:N7	2.35	0.42
1:A:2254:U:H2'	1:A:2255:U:C6	2.55	0.42
1:A:2432:G:C5'	1:A:2432:G:H8	2.33	0.42
1:A:2641:G:O4'	1:A:2902:G:H1'	2.19	0.42
7:G:49:ASP:O	7:G:50:ALA:C	2.62	0.42
34:a:45:G:C6	34:a:46:U:C2	3.08	0.42
34:a:156:A:H2'	34:a:157:A:O4'	2.20	0.42
37:d:88:VAL:O	37:d:92:VAL:HG23	2.19	0.42
46:m:57:ARG:HG2	46:m:61:GLU:OE2	2.20	0.42
56:w:67:C:H2'	56:w:68:C:H6	1.84	0.42
58:y:9:A:C2	58:y:45:U:C4	3.07	0.42
58:y:19:G:H4'	58:y:20:U:OP2	2.20	0.42
58:y:24:G:C2	58:y:25:C:H1'	2.54	0.42
58:y:33:U:HO2'	58:y:34:G:H8	1.67	0.42
1:A:504:A:H4'	1:A:505:A:OP1	2.20	0.42
1:A:660:G:H4'	1:A:662:G:O3'	2.20	0.42
1:A:1185:U:H6	11:N:63:THR:OG1	2.03	0.42
1:A:1358:U:H2'	1:A:1655:A:C2	2.54	0.42
1:A:1820:C:H5''	1:A:1821:A:OP1	2.20	0.42
1:A:1850:U:C2	4:D:202:LYS:HD2	2.54	0.42
1:A:2622:U:H3'	1:A:2622:U:OP2	2.20	0.42
2:B:28:C:OP1	16:S:36:TYR:OH	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:144:VAL:O	8:H:148:ILE:HG12	2.19	0.42
15:R:33:ARG:NH2	29:5:57:VAL:O	2.42	0.42
17:T:51:ARG:HG3	17:T:98:LYS:CD	2.50	0.42
23:Z:14:LYS:HE2	23:Z:14:LYS:HB2	1.88	0.42
26:2:28:LYS:HG3	26:2:53:LEU:HD21	2.01	0.42
29:5:16:ARG:NH1	29:5:17:ASP:OD1	2.52	0.42
34:a:45:G:H2'	34:a:46:U:O4'	2.20	0.42
34:a:150:C:C2	34:a:151:G:C8	3.08	0.42
34:a:1107:G:H21	34:a:1110:G:H21	1.65	0.42
42:i:53:VAL:HB	42:i:92:TYR:CE1	2.55	0.42
48:o:87:ILE:HG22	48:o:88:ARG:N	2.35	0.42
58:y:43:C:H4'	58:y:44:G:OP1	2.20	0.42
59:z:125:LEU:C	59:z:127:HIS:H	2.28	0.42
1:A:93:G:O2'	26:2:48:HIS:ND1	2.41	0.42
1:A:333:A:O2'	1:A:335:G:N7	2.32	0.42
1:A:1162:G:H2'	1:A:1163:C:C6	2.54	0.42
1:A:2494:C:OP1	56:w:1:G:O2'	2.29	0.42
6:F:29:ASN:N	6:F:112:MET:HE3	2.32	0.42
14:Q:139:GLU:OE2	23:Z:54:HIS:HE1	2.03	0.42
20:W:32:ALA:CB	20:W:51:LEU:HD11	2.49	0.42
21:X:21:PHE:C	21:X:23:GLU:H	2.27	0.42
33:9:4:ARG:O	33:9:36:GLN:HA	2.20	0.42
34:a:137:G:H3'	34:a:138:A:H8	1.84	0.42
34:a:397:C:H1'	34:a:606:A:H1'	2.02	0.42
34:a:843:A:H5'	34:a:1061:U:O4	2.20	0.42
34:a:944:G:C2	57:x:34:C:H5'	2.55	0.42
34:a:1382:C:C2	34:a:1384:G:C5	3.08	0.42
37:d:49:ARG:O	37:d:50:ARG:C	2.62	0.42
37:d:107:ARG:HD3	37:d:173:TRP:HH2	1.85	0.42
41:h:122:ARG:HD2	41:h:122:ARG:HA	1.31	0.42
42:i:26:VAL:HG13	42:i:61:ALA:HB3	2.02	0.42
44:k:50:TYR:CD1	44:k:54:ARG:HB3	2.55	0.42
49:p:38:TYR:CZ	49:p:50:LYS:HB2	2.55	0.42
52:s:39:THR:HG22	52:s:40:ILE:O	2.20	0.42
57:x:1:C:HO2'	57:x:2:G:P	2.42	0.42
59:z:10:ARG:HH21	59:z:185:ILE:HA	1.84	0.42
59:z:459:ILE:HG22	59:z:460:LEU:N	2.34	0.42
1:A:435:C:O2'	1:A:436:G:H5'	2.20	0.41
1:A:480:C:H3'	1:A:481:C:H5''	2.02	0.41
1:A:955:A:N1	1:A:2288:G:H1'	2.35	0.41
1:A:998:G:H5''	14:Q:13:GLN:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1685:U:O2'	1:A:1686:C:H5'	2.19	0.41
1:A:2118:C:H2'	1:A:2119:U:O4'	2.19	0.41
1:A:2333:A:H2'	1:A:2334:G:O4'	2.20	0.41
1:A:2878:G:H2'	1:A:2879:C:O4'	2.20	0.41
6:F:9:ILE:HD12	6:F:22:ALA:HB2	2.02	0.41
10:K:71:THR:HA	10:K:72:PRO:HD2	1.90	0.41
21:X:54:VAL:HG22	21:X:81:VAL:HG12	2.02	0.41
22:Y:9:LYS:HD2	22:Y:28:LYS:O	2.20	0.41
25:1:10:LYS:NZ	25:1:65:SER:OG	2.51	0.41
34:a:39:G:C2	34:a:393:A:C2	3.08	0.41
34:a:568:G:H2'	34:a:569:G:H8	1.85	0.41
34:a:1001:G:H2'	34:a:1002:G:C8	2.54	0.41
34:a:1240:G:O2'	34:a:1241:C:H5'	2.20	0.41
34:a:1456:C:H2'	34:a:1457:C:C6	2.55	0.41
58:y:21:A:C2	58:y:46:G:C6	3.08	0.41
1:A:89:A:H2'	1:A:90:G:O4'	2.19	0.41
1:A:195:A:H2'	1:A:196:C:O4'	2.19	0.41
1:A:394:C:H2'	1:A:395:C:O4'	2.20	0.41
1:A:770:U:H2'	1:A:771:G:O4'	2.19	0.41
1:A:829:A:O2'	1:A:831:G:OP1	2.34	0.41
1:A:1090:A:H5''	1:A:1091:A:O5'	2.20	0.41
3:C:163:PHE:N	3:C:163:PHE:CD1	2.88	0.41
4:D:221:VAL:HG22	4:D:226:MET:HE3	2.02	0.41
5:E:50:GLY:HA2	5:E:77:ILE:O	2.19	0.41
12:O:98:VAL:HG13	12:O:117:LEU:HB3	2.02	0.41
34:a:551:G:H2'	34:a:552:G:O4'	2.20	0.41
34:a:1208:C:O4'	52:s:83:HIS:HE1	2.02	0.41
34:a:1211:A:OP1	46:m:116:THR:HB	2.20	0.41
34:a:1221:A:H62	34:a:1281:A:H62	1.67	0.41
35:b:153:ARG:HG3	35:b:154:LEU:HD22	2.00	0.41
40:g:91:VAL:HB	40:g:96:GLN:HE21	1.85	0.41
48:o:26:GLU:H	48:o:26:GLU:HG2	1.53	0.41
59:z:440:TYR:O	59:z:442:PRO:HD3	2.20	0.41
59:z:504:LEU:HD13	59:z:524:LEU:HD11	2.01	0.41
1:A:74:C:OP1	26:2:55:ARG:HD3	2.20	0.41
1:A:814:G:O2'	1:A:1424:A:N1	2.51	0.41
1:A:947:C:H2'	1:A:948:C:C6	2.55	0.41
1:A:1774:C:H6	1:A:1774:C:H5''	1.84	0.41
1:A:2148:G:C6	1:A:2183:G:C2	3.08	0.41
1:A:2556:G:O2'	1:A:2576:A:N1	2.48	0.41
3:C:10:LEU:HD21	3:C:34:THR:OG1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:SER:O	5:E:162:ALA:HA	2.19	0.41
12:O:91:LEU:HB3	12:O:111:PHE:CE1	2.55	0.41
13:P:98:GLU:HA	13:P:101:VAL:HB	2.01	0.41
13:P:148:LEU:HD23	13:P:148:LEU:N	2.34	0.41
26:2:64:LEU:HD11	26:2:68:ARG:NH2	2.35	0.41
34:a:75:C:H2'	34:a:76:G:H8	1.85	0.41
34:a:648:G:P	51:r:64:ARG:HH21	2.43	0.41
34:a:1006:C:O2	34:a:1006:C:H2'	2.20	0.41
35:b:163:PHE:HA	35:b:185:ILE:HG12	2.01	0.41
36:c:77:ILE:HG13	36:c:78:GLY:N	2.35	0.41
42:i:33:PHE:CD1	42:i:33:PHE:C	2.98	0.41
44:k:48:ILE:HD12	44:k:63:LEU:HB2	2.03	0.41
46:m:3:ARG:HB3	46:m:7:VAL:O	2.19	0.41
50:q:22:LEU:HD12	50:q:23:VAL:H	1.86	0.41
56:w:2:C:H6	56:w:2:C:H3'	1.85	0.41
59:z:65:ARG:N	59:z:246:THR:HG21	2.34	0.41
1:A:88:U:O2'	1:A:89:A:H8	2.02	0.41
1:A:319:C:OP2	22:Y:4:LYS:NZ	2.46	0.41
1:A:628:U:H4'	1:A:704:C:H4'	2.03	0.41
1:A:1217:G:O2'	1:A:1218:A:O5'	2.36	0.41
1:A:1381:A:H2'	1:A:1382:G:C8	2.55	0.41
1:A:1525:G:H5'	1:A:1604:A:C2	2.55	0.41
1:A:1786:G:H4'	1:A:1788:G:O4'	2.20	0.41
1:A:2152:G:OP1	1:A:2153:U:O2'	2.30	0.41
1:A:2198:C:H2'	1:A:2199:C:O4'	2.20	0.41
1:A:2594:G:H2'	1:A:2595:U:O4'	2.21	0.41
3:C:189:ILE:HD11	3:C:214:VAL:CG2	2.50	0.41
12:O:23:ARG:HG3	12:O:24:VAL:N	2.34	0.41
26:2:52:ASP:O	26:2:56:GLN:HG3	2.21	0.41
34:a:136:A:H1'	34:a:177:U:O2	2.21	0.41
34:a:251:G:H1'	50:q:16:GLN:NE2	2.35	0.41
36:c:11:ARG:HD3	36:c:15:THR:HG21	2.03	0.41
37:d:100:ARG:HH12	37:d:137:SER:HB3	1.84	0.41
40:g:18:TYR:CD2	40:g:59:LEU:HG	2.54	0.41
46:m:8:GLU:CB	46:m:9:ILE:HG22	2.49	0.41
51:r:21:LYS:HG2	51:r:57:GLY:HA3	2.02	0.41
56:w:68:C:OP1	59:z:548:ARG:NE	2.47	0.41
59:z:309:ASP:O	59:z:310:SER:HB3	2.19	0.41
1:A:728:G:N2	1:A:842:C:C2	2.88	0.41
1:A:998:G:N3	1:A:2285:A:C2	2.89	0.41
1:A:1552:A:O2'	1:A:1553:A:H8	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1945:C:H2'	1:A:1946:C:O4'	2.21	0.41
1:A:2198:C:H5''	3:C:213:TYR:CG	2.55	0.41
1:A:2859:A:N7	1:A:2877:A:O2'	2.53	0.41
2:B:9:G:OP1	16:S:19:LYS:NZ	2.52	0.41
2:B:14:U:O2	2:B:108:U:H4'	2.20	0.41
3:C:8:ARG:HA	3:C:11:LEU:HB3	2.02	0.41
3:C:68:LEU:O	3:C:175:VAL:HG21	2.20	0.41
3:C:201:PRO:O	3:C:203:GLY:C	2.64	0.41
6:F:74:ARG:H	6:F:74:ARG:HG3	1.48	0.41
13:P:130:PHE:HB3	13:P:135:LEU:HG	2.03	0.41
17:T:37:GLY:HA2	17:T:38:ASN:HA	1.63	0.41
18:U:90:VAL:CG1	18:U:95:LEU:HD13	2.51	0.41
34:a:60:A:H3'	34:a:327:G:H22	1.86	0.41
34:a:146:A:H2'	34:a:147:A:O4'	2.20	0.41
34:a:933:U:OP1	46:m:120:LYS:HG3	2.20	0.41
34:a:966:G:C2	34:a:967:C:H1'	2.55	0.41
39:f:30:LEU:HD23	39:f:30:LEU:HA	1.88	0.41
50:q:67:LYS:O	50:q:68:ARG:C	2.62	0.41
56:w:58:A:O2'	56:w:59:U:H5''	2.19	0.41
59:z:27:ASP:HA	59:z:30:LEU:HD12	2.01	0.41
1:A:388:G:H2'	1:A:389:G:O4'	2.19	0.41
1:A:552:A:N1	1:A:2063:A:H2'	2.35	0.41
1:A:857:U:H2'	13:P:21:ARG:HA	2.01	0.41
1:A:1126:U:C6	10:K:126:MET:HE1	2.55	0.41
1:A:1389:G:H4'	1:A:1429:A:C5	2.56	0.41
1:A:1531:A:H2'	1:A:1532:G:H8	1.85	0.41
1:A:1621:C:H2'	1:A:1622:U:C6	2.55	0.41
1:A:1904:G:H8	1:A:1904:G:O5'	2.03	0.41
1:A:2166:C:H3'	1:A:2167:C:C6	2.55	0.41
1:A:2373:G:OP1	32:8:44:LYS:NZ	2.54	0.41
1:A:2558:U:O2	12:O:23:ARG:NH2	2.53	0.41
1:A:2563:U:C2	1:A:2565:U:H5'	2.55	0.41
1:A:2759:G:O6	1:A:2767:C:H5''	2.20	0.41
1:A:2901:G:H8	1:A:2901:G:O5'	2.04	0.41
4:D:85:ASP:OD2	4:D:88:ARG:HD2	2.21	0.41
8:H:98:LEU:HD23	8:H:98:LEU:HA	1.86	0.41
10:K:12:LEU:H	10:K:54:PRO:HA	1.86	0.41
15:R:70:LEU:O	15:R:72:ASP:N	2.49	0.41
20:W:24:ILE:HA	20:W:27:LYS:HG3	2.01	0.41
34:a:762:G:O2'	44:k:119:CYS:HB3	2.21	0.41
34:a:798:A:N7	34:a:800:A:C4	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1054:C:H2'	34:a:1055:G:H8	1.86	0.41
43:j:69:ASN:O	43:j:70:ARG:HD3	2.20	0.41
46:m:54:VAL:HA	46:m:57:ARG:NH1	2.35	0.41
46:m:73:GLU:OE2	46:m:77:ASN:ND2	2.53	0.41
51:r:47:THR:OG1	51:r:83:GLU:O	2.36	0.41
59:z:311:GLY:C	59:z:313:TYR:H	2.29	0.41
1:A:601:G:C2	1:A:1307:A:C4	3.08	0.41
1:A:1113:G:N2	1:A:1140:A:O2'	2.53	0.41
1:A:1457:A:H61	1:A:1635:U:H3	1.68	0.41
1:A:1467:G:H1'	1:A:1541:A:N1	2.34	0.41
1:A:2120:U:O2	1:A:2120:U:H2'	2.20	0.41
1:A:2152:G:H5''	1:A:2154:G:O4'	2.20	0.41
1:A:2473:U:H2'	1:A:2474:C:C6	2.56	0.41
1:A:2649:G:P	5:E:82:ARG:HH22	2.44	0.41
5:E:195:LEU:HD12	5:E:196:VAL:N	2.36	0.41
20:W:29:LEU:HD21	20:W:33:ARG:NH2	2.35	0.41
34:a:157:A:C5	34:a:158:C:H1'	2.55	0.41
34:a:379:A:C5	34:a:380:G:H1'	2.55	0.41
35:b:128:GLU:HA	35:b:135:GLN:OE1	2.21	0.41
36:c:22:TRP:CZ2	47:n:54:PRO:HG3	2.56	0.41
37:d:20:TYR:HD2	37:d:26:CYS:CB	2.27	0.41
39:f:99:ALA:HB2	51:r:31:LEU:HD13	2.03	0.41
57:x:67:C:H2'	57:x:68:C:C6	2.55	0.41
59:z:12:PHE:O	59:z:100:VAL:HG11	2.20	0.41
59:z:194:ALA:HB1	59:z:195:PRO:CA	2.50	0.41
59:z:584:LEU:HD23	59:z:584:LEU:HA	1.79	0.41
1:A:33:C:H2'	1:A:34:G:C5'	2.49	0.41
1:A:464:G:H2'	1:A:465:G:H8	1.86	0.41
1:A:1217:G:H1'	1:A:1218:A:H5'	2.03	0.41
1:A:1489:G:H2'	1:A:1491:C:C5	2.56	0.41
1:A:1631:A:H8	1:A:1631:A:OP2	2.04	0.41
1:A:2039:G:O2'	18:U:34:LYS:HE3	2.21	0.41
1:A:2159:C:N4	1:A:2174:G:N2	2.69	0.41
11:N:1:MET:HE3	11:N:1:MET:HB2	1.89	0.41
14:Q:12:GLN:HE21	14:Q:12:GLN:HB2	1.53	0.41
23:Z:70:LEU:HA	23:Z:70:LEU:HD23	1.75	0.41
34:a:370:A:C6	34:a:371:U:C4	3.08	0.41
34:a:528:G:C6	34:a:529:C:C4	3.08	0.41
34:a:725:G:H2'	34:a:726:G:O4'	2.21	0.41
34:a:1054:C:H2'	34:a:1055:G:C8	2.56	0.41
34:a:1107:G:N2	34:a:1110:G:N2	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1259:C:O2'	34:a:1261:A:C8	2.69	0.41
34:a:1382:C:H4'	34:a:1383:C:O5'	2.20	0.41
36:c:111:LEU:HD11	36:c:144:SER:O	2.19	0.41
42:i:4:TYR:CE1	42:i:88:TYR:HD2	2.39	0.41
56:w:5:G:C6	56:w:69:G:C6	3.09	0.41
57:x:17:C:C5	57:x:17(A):U:C4	3.08	0.41
59:z:382:LEU:HB2	59:z:383:LYS:H	1.43	0.41
1:A:271:U:HO2'	1:A:272:G:P	2.38	0.41
1:A:345:A:OP2	6:F:169:ASN:HB2	2.21	0.41
1:A:401:C:H2'	1:A:402:C:C6	2.56	0.41
1:A:422:G:H1'	25:1:42:GLN:HB3	2.02	0.41
1:A:464:G:H2'	1:A:465:G:C8	2.55	0.41
1:A:515:G:H2'	1:A:516:A:H8	1.86	0.41
1:A:609:C:N4	13:P:31:ALA:HB3	2.36	0.41
1:A:1043:C:P	18:U:92:ARG:NH2	2.93	0.41
1:A:1213:G:H2'	1:A:1214:G:O4'	2.21	0.41
1:A:1597:C:H2'	1:A:1598:G:O4'	2.20	0.41
1:A:1784:C:H2'	1:A:1785:A:O4'	2.21	0.41
1:A:2189:G:N1	1:A:2191:A:H3'	2.36	0.41
1:A:2194:A:N1	3:C:218:MET:HE1	2.36	0.41
1:A:2845:U:C4	1:A:2892:A:N6	2.89	0.41
2:B:54:G:H21	7:G:29:TRP:NE1	2.18	0.41
3:C:195:ALA:C	3:C:197:GLU:N	2.78	0.41
5:E:36:ARG:HH11	5:E:85:ASN:HD22	1.68	0.41
6:F:137:LYS:HA	6:F:140:LEU:HB2	2.02	0.41
6:F:178:PRO:HB3	6:F:198:ALA:HB1	2.03	0.41
13:P:147:LEU:C	13:P:148:LEU:HD23	2.46	0.41
14:Q:30:GLY:O	14:Q:134:ARG:HD3	2.21	0.41
15:R:48:VAL:O	15:R:51:LEU:N	2.54	0.41
16:S:78:LEU:HD12	16:S:108:GLY:O	2.20	0.41
17:T:74:ARG:HH11	17:T:74:ARG:CG	2.33	0.41
19:V:30:GLY:H	19:V:61:VAL:HG23	1.86	0.41
20:W:17:VAL:HG13	20:W:76:VAL:HG21	2.02	0.41
26:2:32:LEU:HD23	26:2:32:LEU:HA	1.86	0.41
34:a:103:A:C6	34:a:322:G:C6	3.08	0.41
34:a:143:G:N2	34:a:144:A:C4	2.89	0.41
34:a:774:A:N1	34:a:1475:G:H5''	2.36	0.41
34:a:1009:C:H5	34:a:1015:G:C2	2.39	0.41
34:a:1110:G:H8	34:a:1111:C:C5	2.39	0.41
34:a:1115:C:H2'	34:a:1116:G:H8	1.86	0.41
34:a:1384:G:C2	34:a:1385:C:H1'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1409:C:H2'	34:a:1410:U:C6	2.56	0.41
34:a:1438:A:H2'	34:a:1439:G:O4'	2.21	0.41
35:b:28:PHE:O	35:b:32:ILE:HG13	2.21	0.41
38:e:31:LEU:HD23	38:e:31:LEU:HA	1.91	0.41
39:f:2:ARG:HD3	39:f:92:LYS:HZ3	1.85	0.41
41:h:7:ALA:HB2	41:h:85:ARG:HD2	2.02	0.41
42:i:40:LEU:HD21	42:i:70:LYS:HD3	2.03	0.41
50:q:10:VAL:HA	50:q:20:THR:O	2.20	0.41
59:z:324:LYS:O	59:z:326:ASN:N	2.54	0.41
59:z:418:GLU:HB3	59:z:446:LYS:HG2	2.02	0.41
1:A:491:A:N3	1:A:729:C:H1'	2.36	0.41
1:A:810:A:OP1	4:D:208:LYS:HE3	2.21	0.41
1:A:898:G:H2'	1:A:899:G:C8	2.55	0.41
1:A:1132:G:C6	1:A:1134:G:C2	3.08	0.41
1:A:2648:U:C4	1:A:2649:G:C6	3.09	0.41
2:B:89:G:C6	2:B:90:A:C6	3.09	0.41
5:E:60:ASN:CG	5:E:62:PRO:HD2	2.46	0.41
10:K:14:ALA:CB	10:K:53:VAL:HG23	2.49	0.41
16:S:36:TYR:HD1	16:S:36:TYR:N	2.19	0.41
17:T:16:ARG:HG3	17:T:18:ASP:OD2	2.20	0.41
17:T:119:LYS:O	17:T:123:GLN:HG3	2.21	0.41
28:4:49:PHE:HB3	28:4:50:VAL:H	1.65	0.41
34:a:964:A:H1'	52:s:54:GLY:O	2.21	0.41
34:a:1011:C:H2'	34:a:1012:G:H8	1.86	0.41
34:a:1305:G:H2'	34:a:1306:A:C8	2.56	0.41
34:a:1481:A:C6	55:v:12:A:H8	2.38	0.41
36:c:91:LEU:HA	36:c:91:LEU:HD12	1.78	0.41
46:m:39:ILE:HD13	46:m:52:GLU:HB3	2.03	0.41
54:u:15:ARG:HG2	54:u:15:ARG:NH1	2.36	0.41
59:z:91:TYR:CE1	59:z:95:ARG:HD3	2.55	0.41
59:z:161:ASP:OD2	59:z:161:ASP:N	2.48	0.41
59:z:376:VAL:HG21	59:z:457:ALA:HB2	2.03	0.41
1:A:858:C:H1'	1:A:1295:G:C2	2.56	0.40
1:A:1130:A:H1'	1:A:1150:U:H1'	2.03	0.40
1:A:1847:G:H2'	1:A:1848:U:H5'	2.02	0.40
1:A:2139:U:O4	1:A:2170:G:H1'	2.20	0.40
1:A:2147:A:C6	1:A:2184:C:H4'	2.56	0.40
2:B:73:A:C4	2:B:105:A:C2	3.08	0.40
4:D:147:LEU:HD13	4:D:155:LEU:HD11	2.02	0.40
7:G:34:LEU:HG	7:G:99:MET:HE2	2.03	0.40
10:K:99:ILE:HG12	10:K:136:VAL:CG2	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:65:ARG:NE	32:8:25:MET:HE2	2.36	0.40
13:P:85:LEU:HG	13:P:116:GLY:HA2	2.03	0.40
34:a:89:G:C6	34:a:90:U:C4	3.09	0.40
34:a:300:U:H2'	34:a:301:G:C8	2.56	0.40
34:a:1481:A:N1	55:v:12:A:H8	2.19	0.40
38:e:41:VAL:O	38:e:66:MET:HA	2.21	0.40
49:p:1:MET:HG2	49:p:2:VAL:O	2.21	0.40
56:w:27:G:OP2	56:w:27:G:H8	2.04	0.40
56:w:52:G:N2	56:w:62:C:N3	2.60	0.40
58:y:51:U:H2'	58:y:52:G:C8	2.55	0.40
59:z:418:GLU:HB2	59:z:419:GLU:H	1.59	0.40
59:z:504:LEU:CD1	59:z:524:LEU:HD11	2.51	0.40
1:A:26:G:N2	1:A:536:G:H1'	2.36	0.40
1:A:2052:A:C6	1:A:2509:C:H1'	2.57	0.40
1:A:2053:G:OP2	1:A:2465:G:O2'	2.28	0.40
1:A:2283:U:H5''	1:A:2284:A:OP1	2.21	0.40
1:A:2706:C:H2'	1:A:2707:U:H6	1.85	0.40
1:A:2858:U:N3	1:A:2876:G:O4'	2.52	0.40
2:B:44:G:OP2	28:4:1:MET:N	2.33	0.40
3:C:195:ALA:C	3:C:197:GLU:H	2.29	0.40
6:F:22:ALA:O	6:F:23:ASP:HB3	2.21	0.40
22:Y:12:THR:OG1	22:Y:26:LYS:NZ	2.52	0.40
34:a:1210:C:H4'	46:m:116:THR:HA	2.03	0.40
34:a:1350:C:H5'	43:j:60:ARG:NH1	2.36	0.40
37:d:17:VAL:HG11	37:d:63:LYS:HD2	2.03	0.40
37:d:202:LEU:HD23	37:d:202:LEU:HA	1.85	0.40
38:e:66:MET:HE3	38:e:66:MET:HB3	1.88	0.40
39:f:89:MET:HE1	51:r:72:ARG:HB3	2.03	0.40
58:y:35:A:C2	58:y:36:A:H1'	2.56	0.40
59:z:264:LEU:HD21	59:z:280:ILE:CD1	2.51	0.40
1:A:182:G:H2'	1:A:183:A:O4'	2.21	0.40
1:A:251:C:H2'	1:A:252:C:O4'	2.21	0.40
1:A:274:C:H2'	1:A:275:C:C6	2.56	0.40
1:A:330:G:H21	1:A:353:A:H62	1.68	0.40
1:A:353:A:O2'	1:A:354:A:C8	2.72	0.40
1:A:635:G:O2'	1:A:639:A:N1	2.40	0.40
1:A:830:A:H3'	64:A:4065:HOH:O	2.20	0.40
1:A:839:A:H1'	64:A:4127:HOH:O	2.21	0.40
1:A:2363:A:H8	1:A:2363:A:O5'	2.04	0.40
1:A:2430:U:OP1	32:8:41:ILE:HD12	2.21	0.40
2:B:42:C:O2	7:G:93:THR:N	2.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:LEU:HA	3:C:175:VAL:HG21	2.02	0.40
8:H:101:ARG:H	8:H:101:ARG:HG3	1.41	0.40
10:K:56:GLU:O	10:K:67:PHE:HA	2.22	0.40
18:U:92:ARG:HA	18:U:95:LEU:HB2	2.01	0.40
20:W:68:ARG:HD2	20:W:109:GLU:CD	2.47	0.40
25:1:83:GLU:HA	25:1:84:GLY:HA2	1.55	0.40
34:a:137:G:C4	34:a:138:A:C8	3.10	0.40
34:a:379:A:OP1	34:a:449:C:O2'	2.37	0.40
36:c:143:GLU:C	36:c:145:GLY:H	2.28	0.40
37:d:150:GLU:HA	37:d:153:ARG:CB	2.51	0.40
51:r:35:ARG:HE	51:r:35:ARG:HB2	1.62	0.40
56:w:69:G:C6	56:w:70:G:C5	3.10	0.40
58:y:28:G:C2	58:y:43:C:C2	3.09	0.40
1:A:111:U:O2'	21:X:33:LYS:NZ	2.48	0.40
1:A:409:U:H2'	1:A:411:C:H5	1.86	0.40
1:A:941:A:N3	1:A:941:A:H2'	2.36	0.40
1:A:1463:G:H8	1:A:1463:G:O5'	2.05	0.40
4:D:141:VAL:HG23	4:D:162:SER:HB2	2.03	0.40
5:E:8:LYS:HD3	5:E:191:PRO:O	2.20	0.40
5:E:115:GLY:O	5:E:119:ARG:HB2	2.21	0.40
6:F:56:GLU:OE2	6:F:93:LYS:NZ	2.47	0.40
8:H:54:ARG:NH2	8:H:57:ASP:HB2	2.27	0.40
11:N:96:GLU:O	11:N:100:GLU:HG3	2.21	0.40
14:Q:68:ILE:HG22	14:Q:101:ARG:HE	1.87	0.40
14:Q:114:ALA:O	14:Q:118:LEU:HG	2.22	0.40
23:Z:14:LYS:HB3	23:Z:17:ALA:H	1.86	0.40
23:Z:24:LEU:HD21	23:Z:86:VAL:HG23	2.03	0.40
28:4:14:ILE:HB	28:4:22:ILE:CG1	2.50	0.40
33:9:3:VAL:HA	33:9:35:ARG:O	2.21	0.40
34:a:531:A:H4'	34:a:532:G:O5'	2.21	0.40
34:a:765:A:C4	34:a:786:A:C2	3.09	0.40
34:a:993:A:OP1	52:s:18:LYS:NZ	2.54	0.40
36:c:178:LEU:HD13	36:c:178:LEU:HA	1.98	0.40
39:f:22:GLU:OE1	39:f:84:ASN:HB2	2.21	0.40
48:o:70:LEU:HD12	48:o:70:LEU:HA	1.89	0.40
59:z:329:ALA:HB2	59:z:349:LEU:HD12	2.03	0.40
59:z:596:ALA:O	59:z:600:VAL:HG23	2.21	0.40
1:A:587:C:H2'	1:A:588:U:O4'	2.22	0.40
1:A:830:A:C8	1:A:838:G:C5	3.10	0.40
1:A:1385:U:OP1	21:X:16:LYS:NZ	2.49	0.40
1:A:1958:A:C8	1:A:1960:U:H2'	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2447:G:O2'	1:A:2609:A:N1	2.49	0.40
1:A:2641:G:H2'	1:A:2642:G:C8	2.55	0.40
5:E:94:GLU:H	5:E:94:GLU:HG2	1.59	0.40
7:G:43:LEU:HB3	7:G:44:GLY:H	1.66	0.40
8:H:139:GLN:CD	8:H:139:GLN:C	2.89	0.40
11:N:30:ILE:HG22	11:N:34:LEU:HD22	2.01	0.40
12:O:2:ILE:HB	12:O:33:ALA:HB3	2.04	0.40
13:P:95:VAL:HA	13:P:99:LEU:HD23	2.02	0.40
34:a:514:G:P	34:a:514:G:H3'	2.60	0.40
34:a:855:C:O2'	34:a:856:G:H5'	2.22	0.40
35:b:32:ILE:HG21	35:b:40:HIS:CD2	2.57	0.40
35:b:36:ARG:O	35:b:37:ASN:HB2	2.21	0.40
36:c:63:ASN:ND2	36:c:98:ASN:OD1	2.53	0.40
52:s:22:LEU:HB3	52:s:27:GLU:HG2	2.04	0.40
54:u:3:LYS:HD3	54:u:14:TRP:CD1	2.57	0.40
57:x:9:G:C6	57:x:45:G:C6	3.10	0.40
57:x:28:C:H2'	57:x:29:G:H8	1.87	0.40
58:y:56:C:H2'	58:y:57:G:O4'	2.20	0.40
59:z:29:ILE:HG21	59:z:80:LEU:HD21	2.04	0.40
59:z:81:ILE:HG21	59:z:96:ALA:HB1	2.03	0.40
59:z:150:LEU:HD13	59:z:150:LEU:HA	1.86	0.40
59:z:416:THR:O	59:z:447:ARG:NH1	2.54	0.40
59:z:419:GLU:C	59:z:421:VAL:N	2.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:G:N2	20:W:111:HIS:O[4_557]	2.15	0.05

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	C	130/228 (57%)	94 (72%)	25 (19%)	11 (8%)	0	0
4	D	273/276 (99%)	255 (93%)	15 (6%)	3 (1%)	11	25
5	E	202/206 (98%)	188 (93%)	11 (5%)	3 (2%)	8	18
6	F	201/210 (96%)	184 (92%)	12 (6%)	5 (2%)	4	8
7	G	179/182 (98%)	162 (90%)	10 (6%)	7 (4%)	2	3
8	H	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	2	3
9	J	128/173 (74%)	76 (59%)	22 (17%)	30 (23%)	0	0
10	K	137/147 (93%)	85 (62%)	31 (23%)	21 (15%)	0	0
11	N	138/140 (99%)	129 (94%)	5 (4%)	4 (3%)	3	6
12	O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	34
13	P	147/150 (98%)	129 (88%)	16 (11%)	2 (1%)	9	19
14	Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	38
15	R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
16	S	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	6	13
17	T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	34
18	U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
19	V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	12
20	W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	25
22	Y	105/110 (96%)	89 (85%)	12 (11%)	4 (4%)	2	3
23	Z	92/206 (45%)	84 (91%)	8 (9%)	0	100	100
24	0	72/85 (85%)	67 (93%)	3 (4%)	2 (3%)	4	6
25	1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	3	5
26	2	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	8	18
27	3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	0
29	5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	7	47/49 (96%)	44 (94%)	1 (2%)	2 (4%)	2	2
32	8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	9	35/37 (95%)	35 (100%)	0	0	100	100
35	b	229/256 (90%)	192 (84%)	23 (10%)	14 (6%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/239 (85%)	177 (87%)	20 (10%)	7 (3%)	3	4
37	d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	8	18
38	e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	5	11
39	f	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	3	5
40	g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	3	5
41	h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
42	i	125/128 (98%)	113 (90%)	5 (4%)	7 (6%)	1	1
43	j	94/105 (90%)	79 (84%)	6 (6%)	9 (10%)	0	0
44	k	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	14	30
45	l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	16	34
46	m	117/126 (93%)	102 (87%)	9 (8%)	6 (5%)	1	2
47	n	58/61 (95%)	57 (98%)	0	1 (2%)	7	15
48	o	86/89 (97%)	78 (91%)	5 (6%)	3 (4%)	3	4
49	p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	21
50	q	97/105 (92%)	86 (89%)	8 (8%)	3 (3%)	3	5
51	r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	s	81/93 (87%)	72 (89%)	4 (5%)	5 (6%)	1	1
53	t	94/106 (89%)	84 (89%)	4 (4%)	6 (6%)	1	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
59	z	669/679 (98%)	568 (85%)	62 (9%)	39 (6%)	1	1
All	All	6534/7143 (92%)	5800 (89%)	497 (8%)	237 (4%)	2	4

All (237) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	PRO
3	C	172	HIS
3	C	224	ILE
4	D	275	LYS
6	F	130	ALA
6	F	165	ARG
7	G	47	LYS
7	G	50	ALA
7	G	81	LYS
8	H	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	J	71	LEU
9	J	74	LEU
9	J	77	PRO
9	J	80	VAL
9	J	104	ILE
9	J	105	PRO
9	J	107	VAL
9	J	128	LEU
10	K	13	PRO
10	K	38	VAL
10	K	39	LYS
10	K	78	ILE
10	K	89	HIS
10	K	93	ARG
10	K	96	VAL
13	P	45	LEU
17	T	127	ALA
19	V	100	ARG
21	X	94	GLY
24	0	33	ALA
28	4	49	PHE
28	4	55	ARG
35	b	8	LYS
35	b	37	ASN
35	b	131	PRO
36	c	47	LEU
36	c	61	ALA
39	f	62	TRP
43	j	29	ARG
43	j	55	LYS
43	j	79	ARG
46	m	85	GLY
47	n	3	ARG
48	o	88	ARG
49	p	67	THR
50	q	14	LYS
52	s	14	HIS
52	s	30	LEU
53	t	95	ALA
53	t	99	LEU
53	t	100	ILE
59	z	98	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	z	235	LYS
59	z	373	ALA
59	z	390	VAL
59	z	444	ALA
59	z	459	ILE
3	C	66	HIS
3	C	179	SER
3	C	183	GLU
4	D	125	ILE
5	E	118	LYS
6	F	22	ALA
7	G	52	ILE
7	G	126	ASP
7	G	147	ASP
8	H	47	GLU
8	H	92	ILE
9	J	75	GLN
9	J	91	LYS
9	J	93	LEU
9	J	123	GLU
9	J	125	LEU
9	J	132	ASP
10	K	29	GLN
10	K	77	LEU
10	K	91	PRO
12	O	5	GLN
14	Q	60	ARG
16	S	59	LYS
19	V	42	GLY
22	Y	2	ARG
22	Y	6	HIS
24	0	34	GLY
26	2	46	GLN
28	4	46	GLN
28	4	60	GLN
31	7	45	ALA
31	7	46	VAL
35	b	17	PHE
35	b	122	PHE
35	b	135	GLN
35	b	236	TYR
36	c	46	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	d	5	ILE
37	d	36	ARG
38	e	85	GLY
39	f	38	GLU
40	g	83	ALA
42	i	88	TYR
42	i	118	LYS
43	j	34	VAL
44	k	105	VAL
46	m	7	VAL
46	m	49	THR
50	q	68	ARG
52	s	26	GLY
59	z	-35	GLY
59	z	-34	LEU
59	z	64	VAL
59	z	97	LEU
59	z	268	ILE
59	z	272	HIS
59	z	384	SER
59	z	389	GLU
59	z	400	THR
59	z	417	PRO
59	z	542	GLY
59	z	564	GLY
3	C	178	ALA
4	D	3	VAL
8	H	122	THR
9	J	22	GLY
9	J	33	PRO
9	J	56	ASN
9	J	69	PRO
9	J	84	GLU
9	J	101	PRO
10	K	11	GLN
10	K	14	ALA
10	K	31	GLY
10	K	50	ASP
10	K	54	PRO
10	K	113	PRO
11	N	7	LYS
22	Y	5	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	1	3	LYS
28	4	56	VAL
28	4	62	ARG
35	b	16	HIS
35	b	21	ARG
36	c	81	GLY
36	c	108	ASN
36	c	206	GLU
37	d	166	LYS
39	f	61	LEU
40	g	7	ALA
40	g	84	ASN
42	i	119	ALA
43	j	30	SER
45	l	19	ARG
59	z	288	PRO
59	z	292	PRO
59	z	326	ASN
59	z	382	LEU
59	z	418	GLU
59	z	461	TYR
3	C	159	GLY
3	C	210	ARG
5	E	52	LEU
6	F	23	ASP
8	H	3	ARG
9	J	72	ASP
10	K	16	LYS
10	K	81	ALA
10	K	114	ASP
11	N	88	GLU
16	S	84	GLN
22	Y	54	LYS
25	1	79	GLY
35	b	13	ALA
35	b	15	VAL
35	b	121	LEU
35	b	232	PRO
40	g	55	GLY
40	g	80	VAL
42	i	24	GLY
42	i	105	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	j	32	ALA
46	m	40	ASN
48	o	24	SER
52	s	29	ARG
59	z	43	GLU
59	z	294	PHE
59	z	445	GLN
59	z	460	LEU
59	z	503	ALA
3	C	220	PRO
5	E	72	VAL
6	F	7	TYR
9	J	5	ARG
9	J	31	GLY
9	J	120	LYS
10	K	4	VAL
10	K	88	ALA
11	N	2	LYS
11	N	19	GLU
25	l	83	GLU
35	b	52	GLU
36	c	66	VAL
38	e	8	GLU
38	e	69	VAL
42	i	12	GLU
46	m	86	CYS
50	q	49	GLU
52	s	25	LYS
59	z	194	ALA
59	z	310	SER
59	z	325	LEU
59	z	421	VAL
59	z	472	ARG
59	z	553	ALA
3	C	180	PHE
7	G	145	THR
8	H	99	VAL
9	J	20	ALA
9	J	114	GLY
43	j	77	PRO
43	j	78	ASN
53	t	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	t	97	ALA
59	z	81	ILE
59	z	267	ALA
43	j	75	ILE
46	m	6	GLY
48	o	87	ILE
59	z	274	VAL
53	t	47	GLY
8	H	100	GLY
9	J	53	VAL
9	J	86	PRO
9	J	85	ASP
28	4	19	GLY
42	i	74	ILE
59	z	186	PRO
9	J	73	GLY
13	P	72	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	C	103/180 (57%)	76 (74%)	27 (26%)	0	1
4	D	215/218 (99%)	182 (85%)	33 (15%)	3	5
5	E	164/166 (99%)	134 (82%)	30 (18%)	2	3
6	F	160/166 (96%)	130 (81%)	30 (19%)	1	2
7	G	143/156 (92%)	115 (80%)	28 (20%)	1	2
8	H	144/148 (97%)	123 (85%)	21 (15%)	3	6
10	K	104/111 (94%)	70 (67%)	34 (33%)	0	0
11	N	118/119 (99%)	93 (79%)	25 (21%)	1	2
12	O	100/100 (100%)	88 (88%)	12 (12%)	5	10
13	P	115/116 (99%)	99 (86%)	16 (14%)	3	7
14	Q	111/111 (100%)	93 (84%)	18 (16%)	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	R	101/101 (100%)	83 (82%)	18 (18%)	2	3
16	S	87/88 (99%)	73 (84%)	14 (16%)	2	4
17	T	115/127 (91%)	97 (84%)	18 (16%)	2	4
18	U	93/94 (99%)	80 (86%)	13 (14%)	3	6
19	V	80/82 (98%)	66 (82%)	14 (18%)	2	3
20	W	90/92 (98%)	78 (87%)	12 (13%)	4	8
21	X	77/78 (99%)	66 (86%)	11 (14%)	3	6
22	Y	85/91 (93%)	74 (87%)	11 (13%)	4	8
23	Z	84/179 (47%)	71 (84%)	13 (16%)	2	5
24	0	59/67 (88%)	55 (93%)	4 (7%)	14	32
25	1	80/83 (96%)	64 (80%)	16 (20%)	1	2
26	2	65/67 (97%)	50 (77%)	15 (23%)	1	1
27	3	51/52 (98%)	43 (84%)	8 (16%)	2	4
28	4	60/63 (95%)	45 (75%)	15 (25%)	0	1
29	5	51/52 (98%)	44 (86%)	7 (14%)	3	7
30	6	51/52 (98%)	46 (90%)	5 (10%)	7	17
31	7	42/42 (100%)	34 (81%)	8 (19%)	1	2
32	8	53/55 (96%)	48 (91%)	5 (9%)	8	18
33	9	34/34 (100%)	29 (85%)	5 (15%)	3	6
35	b	193/220 (88%)	145 (75%)	48 (25%)	0	1
36	c	142/188 (76%)	126 (89%)	16 (11%)	5	12
37	d	169/181 (93%)	143 (85%)	26 (15%)	2	5
38	e	113/123 (92%)	92 (81%)	21 (19%)	1	3
39	f	83/90 (92%)	63 (76%)	20 (24%)	1	1
40	g	118/127 (93%)	95 (80%)	23 (20%)	1	2
41	h	114/119 (96%)	97 (85%)	17 (15%)	3	5
42	i	90/99 (91%)	77 (86%)	13 (14%)	3	6
43	j	65/92 (71%)	52 (80%)	13 (20%)	1	2
44	k	82/99 (83%)	73 (89%)	9 (11%)	6	13
45	l	97/109 (89%)	83 (86%)	14 (14%)	3	6
46	m	89/101 (88%)	74 (83%)	15 (17%)	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	n	49/50 (98%)	40 (82%)	9 (18%)	1	3
48	o	78/80 (98%)	69 (88%)	9 (12%)	5	11
49	p	69/74 (93%)	56 (81%)	13 (19%)	1	2
50	q	94/97 (97%)	79 (84%)	15 (16%)	2	4
51	r	59/77 (77%)	47 (80%)	12 (20%)	1	2
52	s	68/80 (85%)	57 (84%)	11 (16%)	2	4
53	t	69/82 (84%)	60 (87%)	9 (13%)	4	8
54	u	18/22 (82%)	16 (89%)	2 (11%)	6	12
59	z	542/560 (97%)	424 (78%)	118 (22%)	1	2
All	All	5236/5760 (91%)	4317 (82%)	919 (18%)	2	3

All (919) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	HIS
3	C	11	LEU
3	C	23	ASP
3	C	29	VAL
3	C	39	GLU
3	C	42	GLU
3	C	46	LYS
3	C	49	ILE
3	C	55	ASP
3	C	58	VAL
3	C	61	THR
3	C	68	LEU
3	C	161	ILE
3	C	162	GLU
3	C	163	PHE
3	C	164	ARG
3	C	168	THR
3	C	184	LYS
3	C	185	LEU
3	C	188	ASN
3	C	200	LYS
3	C	209	LEU
3	C	210	ARG
3	C	211	SER
3	C	216	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	222	VAL
3	C	224	ILE
4	D	3	VAL
4	D	18	VAL
4	D	27	THR
4	D	35	LYS
4	D	38	LYS
4	D	39	LYS
4	D	61	LEU
4	D	71	ASP
4	D	88	ARG
4	D	94	LEU
4	D	103	ARG
4	D	111	LEU
4	D	112	GLN
4	D	116	GLN
4	D	122	ASP
4	D	138	VAL
4	D	140	THR
4	D	141	VAL
4	D	142	VAL
4	D	150	LYS
4	D	173	VAL
4	D	183	ARG
4	D	193	VAL
4	D	200	ASP
4	D	202	LYS
4	D	211	ARG
4	D	221	VAL
4	D	229	VAL
4	D	242	ARG
4	D	257	LEU
4	D	259	THR
4	D	260	ARG
4	D	276	LYS
5	E	7	VAL
5	E	9	VAL
5	E	12	THR
5	E	14	ILE
5	E	21	VAL
5	E	24	THR
5	E	27	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	33	VAL
5	E	34	VAL
5	E	41	LYS
5	E	47	VAL
5	E	49	LEU
5	E	52	LEU
5	E	64	LYS
5	E	78	LEU
5	E	82	ARG
5	E	85	ASN
5	E	89	ASP
5	E	94	GLU
5	E	116	VAL
5	E	119	ARG
5	E	140	SER
5	E	144	ARG
5	E	149	ARG
5	E	152	LYS
5	E	154	LYS
5	E	163	GLU
5	E	175	VAL
5	E	181	LEU
5	E	196	VAL
6	F	12	LEU
6	F	20	LEU
6	F	24	LEU
6	F	28	ILE
6	F	33	LEU
6	F	38	ARG
6	F	53	THR
6	F	74	ARG
6	F	88	VAL
6	F	103	LYS
6	F	106	ARG
6	F	120	GLU
6	F	124	LEU
6	F	125	LEU
6	F	126	VAL
6	F	132	VAL
6	F	135	LYS
6	F	140	LEU
6	F	162	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	164	ARG
6	F	168	ARG
6	F	170	LEU
6	F	175	THR
6	F	176	LEU
6	F	183	VAL
6	F	191	ARG
6	F	192	LEU
6	F	195	ASP
6	F	201	VAL
6	F	206	ILE
7	G	3	LEU
7	G	5	VAL
7	G	7	LEU
7	G	26	GLN
7	G	31	VAL
7	G	34	LEU
7	G	43	LEU
7	G	49	ASP
7	G	51	ARG
7	G	53	LEU
7	G	58	GLN
7	G	75	LYS
7	G	78	SER
7	G	82	LEU
7	G	86	MET
7	G	91	ARG
7	G	115	ARG
7	G	140	ILE
7	G	143	GLU
7	G	145	THR
7	G	146	TYR
7	G	148	MET
7	G	149	VAL
7	G	159	VAL
7	G	161	THR
7	G	164	GLU
7	G	175	LEU
7	G	181	ARG
8	H	3	ARG
8	H	15	VAL
8	H	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	32	GLU
8	H	43	VAL
8	H	57	ASP
8	H	69	ARG
8	H	71	LEU
8	H	80	SER
8	H	92	ILE
8	H	99	VAL
8	H	101	ARG
8	H	104	GLU
8	H	105	LEU
8	H	113	VAL
8	H	114	VAL
8	H	116	GLU
8	H	122	THR
8	H	139	GLN
8	H	160	LYS
8	H	175	LYS
10	K	2	LYS
10	K	4	VAL
10	K	5	VAL
10	K	7	VAL
10	K	11	GLN
10	K	18	THR
10	K	30	HIS
10	K	38	VAL
10	K	47	ASN
10	K	48	MET
10	K	53	VAL
10	K	55	VAL
10	K	58	THR
10	K	59	ILE
10	K	64	SER
10	K	65	PHE
10	K	66	THR
10	K	69	THR
10	K	75	SER
10	K	80	LYS
10	K	86	LYS
10	K	93	ARG
10	K	94	GLU
10	K	102	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	K	103	GLN
10	K	105	LEU
10	K	106	GLU
10	K	107	ILE
10	K	112	MET
10	K	115	LEU
10	K	117	THR
10	K	118	THR
10	K	134	MET
10	K	138	VAL
11	N	1	MET
11	N	5	VAL
11	N	9	VAL
11	N	10	GLU
11	N	12	ARG
11	N	14	VAL
11	N	28	THR
11	N	33	LEU
11	N	34	LEU
11	N	48	MET
11	N	55	VAL
11	N	62	VAL
11	N	67	LEU
11	N	71	ILE
11	N	85	ILE
11	N	87	LEU
11	N	90	MET
11	N	97	ARG
11	N	99	LEU
11	N	120	LEU
11	N	131	GLN
11	N	133	GLN
11	N	137	LYS
11	N	139	GLU
11	N	140	VAL
12	O	8	LEU
12	O	10	VAL
12	O	23	ARG
12	O	24	VAL
12	O	35	VAL
12	O	52	VAL
12	O	63	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	O	69	ILE
12	O	94	ARG
12	O	98	VAL
12	O	108	GLU
12	O	116	SER
13	P	1	MET
13	P	21	ARG
13	P	45	LEU
13	P	55	ARG
13	P	65	ARG
13	P	86	LYS
13	P	98	GLU
13	P	101	VAL
13	P	102	ARG
13	P	115	LEU
13	P	117	GLU
13	P	125	VAL
13	P	131	SER
13	P	137	LYS
13	P	147	LEU
13	P	148	LEU
14	Q	3	MET
14	Q	5	ARG
14	Q	6	ARG
14	Q	16	ARG
14	Q	35	VAL
14	Q	42	ILE
14	Q	45	GLN
14	Q	56	ARG
14	Q	57	HIS
14	Q	63	LYS
14	Q	75	THR
14	Q	81	VAL
14	Q	82	ARG
14	Q	85	LYS
14	Q	109	VAL
14	Q	110	THR
14	Q	130	LYS
14	Q	135	ASP
15	R	6	SER
15	R	18	LEU
15	R	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	R	29	LEU
15	R	33	ARG
15	R	36	THR
15	R	40	LYS
15	R	44	LEU
15	R	54	LEU
15	R	60	LEU
15	R	65	LEU
15	R	75	LEU
15	R	79	LEU
15	R	89	ASP
15	R	91	GLN
15	R	100	LEU
15	R	111	LEU
15	R	114	VAL
16	S	3	ARG
16	S	11	LYS
16	S	15	ARG
16	S	19	LYS
16	S	20	ARG
16	S	36	TYR
16	S	43	GLU
16	S	46	VAL
16	S	48	LEU
16	S	49	VAL
16	S	59	LYS
16	S	69	VAL
16	S	73	LEU
16	S	78	LEU
17	T	6	LEU
17	T	8	LYS
17	T	13	ARG
17	T	16	ARG
17	T	23	ARG
17	T	34	VAL
17	T	39	ARG
17	T	41	ARG
17	T	49	VAL
17	T	50	ILE
17	T	59	THR
17	T	74	ARG
17	T	89	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	T	96	ARG
17	T	108	ARG
17	T	113	LYS
17	T	118	ARG
17	T	125	ARG
18	U	18	LEU
18	U	31	SER
18	U	34	LYS
18	U	59	ARG
18	U	60	LEU
18	U	74	LEU
18	U	83	LEU
18	U	85	LYS
18	U	89	GLU
18	U	95	LEU
18	U	100	VAL
18	U	104	GLN
18	U	108	GLU
19	V	25	LEU
19	V	32	THR
19	V	43	GLU
19	V	46	VAL
19	V	51	VAL
19	V	57	VAL
19	V	58	VAL
19	V	62	LEU
19	V	66	ARG
19	V	71	LEU
19	V	72	VAL
19	V	79	VAL
19	V	80	GLN
19	V	95	LEU
20	W	6	ILE
20	W	11	ARG
20	W	19	LEU
20	W	23	LEU
20	W	30	GLU
20	W	37	ARG
20	W	51	LEU
20	W	63	ASP
20	W	92	ARG
20	W	100	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	W	107	LEU
20	W	111	HIS
21	X	8	ILE
21	X	23	GLU
21	X	35	THR
21	X	51	VAL
21	X	52	VAL
21	X	57	LEU
21	X	65	ARG
21	X	72	LYS
21	X	76	ARG
21	X	80	ILE
21	X	95	LEU
22	Y	7	VAL
22	Y	9	LYS
22	Y	23	ARG
22	Y	43	ASN
22	Y	61	ILE
22	Y	67	LEU
22	Y	72	VAL
22	Y	85	VAL
22	Y	90	LEU
22	Y	99	CYS
22	Y	106	LEU
23	Z	5	LEU
23	Z	18	LEU
23	Z	19	ARG
23	Z	31	ARG
23	Z	33	LEU
23	Z	37	VAL
23	Z	41	LEU
23	Z	42	VAL
23	Z	50	GLN
23	Z	72	ARG
23	Z	78	LYS
23	Z	91	LEU
23	Z	93	ASP
24	0	20	ARG
24	0	23	VAL
24	0	27	GLU
24	0	74	ARG
25	1	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	1	14	VAL
25	1	21	ARG
25	1	30	VAL
25	1	35	THR
25	1	37	ILE
25	1	40	ARG
25	1	51	VAL
25	1	52	ARG
25	1	57	GLU
25	1	58	ILE
25	1	69	LYS
25	1	71	TYR
25	1	80	LEU
25	1	85	LEU
25	1	95	LEU
26	2	1	MET
26	2	12	GLU
26	2	19	VAL
26	2	20	GLU
26	2	22	GLU
26	2	25	VAL
26	2	27	GLU
26	2	28	LYS
26	2	30	ARG
26	2	32	LEU
26	2	34	GLU
26	2	40	SER
26	2	53	LEU
26	2	68	ARG
26	2	70	GLN
27	3	3	ARG
27	3	4	LEU
27	3	8	LEU
27	3	18	ASP
27	3	23	LEU
27	3	29	ARG
27	3	40	THR
27	3	54	VAL
28	4	9	LEU
28	4	10	VAL
28	4	22	ILE
28	4	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	4	35	VAL
28	4	50	VAL
28	4	52	THR
28	4	58	ARG
28	4	59	PHE
28	4	60	GLN
28	4	61	ARG
28	4	62	ARG
28	4	63	TYR
28	4	67	TYR
28	4	68	ARG
29	5	6	VAL
29	5	9	LYS
29	5	16	ARG
29	5	29	THR
29	5	40	LYS
29	5	48	GLU
29	5	56	LYS
30	6	17	LYS
30	6	24	GLU
30	6	27	LYS
30	6	48	VAL
30	6	52	VAL
31	7	9	ARG
31	7	14	LYS
31	7	23	ARG
31	7	32	LYS
31	7	43	THR
31	7	46	VAL
31	7	47	ARG
31	7	49	ARG
32	8	14	VAL
32	8	23	VAL
32	8	26	LYS
32	8	32	LEU
32	8	41	ILE
33	9	7	VAL
33	9	12	ASP
33	9	22	ARG
33	9	35	ARG
33	9	36	GLN
35	b	8	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	b	9	GLU
35	b	10	LEU
35	b	11	LEU
35	b	12	GLU
35	b	15	VAL
35	b	17	PHE
35	b	21	ARG
35	b	37	ASN
35	b	44	LEU
35	b	45	GLN
35	b	48	MET
35	b	61	LEU
35	b	67	THR
35	b	76	GLN
35	b	79	ASP
35	b	80	ILE
35	b	87	ARG
35	b	93	VAL
35	b	97	TRP
35	b	118	LEU
35	b	119	GLU
35	b	122	PHE
35	b	124	SER
35	b	126	GLU
35	b	127	ILE
35	b	135	GLN
35	b	136	VAL
35	b	138	LEU
35	b	142	LEU
35	b	144	ARG
35	b	145	LEU
35	b	146	GLN
35	b	155	LEU
35	b	156	LYS
35	b	169	LYS
35	b	172	ILE
35	b	178	ARG
35	b	179	LYS
35	b	184	VAL
35	b	185	ILE
35	b	187	LEU
35	b	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	b	200	ILE
35	b	208	ILE
35	b	213	LEU
35	b	221	LEU
35	b	223	ILE
36	c	3	ASN
36	c	37	GLN
36	c	39	ILE
36	c	47	LEU
36	c	52	LEU
36	c	70	VAL
36	c	97	LYS
36	c	104	GLN
36	c	135	LYS
36	c	165	THR
36	c	178	LEU
36	c	191	THR
36	c	192	THR
36	c	195	VAL
36	c	196	LEU
36	c	202	ILE
37	d	5	ILE
37	d	9	CYS
37	d	15	GLU
37	d	18	LYS
37	d	21	LEU
37	d	28	SER
37	d	58	LEU
37	d	76	ARG
37	d	107	ARG
37	d	108	LEU
37	d	135	LEU
37	d	137	SER
37	d	141	ARG
37	d	150	GLU
37	d	156	GLU
37	d	158	ILE
37	d	162	LEU
37	d	163	GLU
37	d	168	ARG
37	d	170	VAL
37	d	174	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	d	178	VAL
37	d	186	LEU
37	d	188	LEU
37	d	194	LEU
37	d	201	GLN
38	e	12	LEU
38	e	20	GLN
38	e	31	LEU
38	e	33	VAL
38	e	34	VAL
38	e	38	GLN
38	e	41	VAL
38	e	47	LYS
38	e	57	LYS
38	e	66	MET
38	e	67	VAL
38	e	69	VAL
38	e	71	LEU
38	e	80	ILE
38	e	91	LEU
38	e	112	LEU
38	e	116	THR
38	e	121	LYS
38	e	123	LEU
38	e	143	ARG
38	e	151	LEU
39	f	9	VAL
39	f	10	LEU
39	f	14	LEU
39	f	15	ASP
39	f	21	LEU
39	f	25	ILE
39	f	32	ASN
39	f	40	VAL
39	f	45	LEU
39	f	54	LYS
39	f	61	LEU
39	f	69	GLU
39	f	72	VAL
39	f	73	ASN
39	f	74	ASP
39	f	81	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	f	83	ASP
39	f	87	ARG
39	f	94	GLN
39	f	98	LEU
40	g	12	LEU
40	g	15	ASP
40	g	22	LEU
40	g	27	ILE
40	g	32	ARG
40	g	36	LYS
40	g	37	ASN
40	g	50	ILE
40	g	51	GLN
40	g	59	LEU
40	g	64	GLN
40	g	72	ARG
40	g	75	VAL
40	g	104	LEU
40	g	113	GLU
40	g	114	ARG
40	g	115	ARG
40	g	131	LYS
40	g	137	LYS
40	g	138	LYS
40	g	140	ASP
40	g	144	MET
40	g	155	ARG
41	h	2	LEU
41	h	21	LYS
41	h	23	SER
41	h	26	VAL
41	h	50	ARG
41	h	52	ASP
41	h	63	LEU
41	h	78	GLN
41	h	84	ARG
41	h	85	ARG
41	h	91	ARG
41	h	99	GLU
41	h	100	ILE
41	h	112	LEU
41	h	116	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	h	122	ARG
41	h	133	LEU
42	i	11	LYS
42	i	27	THR
42	i	38	GLN
42	i	41	VAL
42	i	47	LEU
42	i	48	GLU
42	i	56	LEU
42	i	64	THR
42	i	65	VAL
42	i	83	ARG
42	i	86	VAL
42	i	108	VAL
42	i	121	ARG
43	j	15	THR
43	j	16	LEU
43	j	30	SER
43	j	35	SER
43	j	43	ARG
43	j	46	ARG
43	j	70	ARG
43	j	72	VAL
43	j	84	GLN
43	j	89	ASP
43	j	92	THR
43	j	96	ILE
43	j	100	THR
44	k	32	ILE
44	k	48	ILE
44	k	54	ARG
44	k	70	LYS
44	k	83	ILE
44	k	93	GLN
44	k	99	GLN
44	k	104	GLN
44	k	109	VAL
45	l	18	VAL
45	l	23	LYS
45	l	27	LEU
45	l	33	ARG
45	l	41	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	l	52	LEU
45	l	53	ARG
45	l	55	VAL
45	l	60	LEU
45	l	65	GLU
45	l	67	THR
45	l	83	VAL
45	l	84	LEU
45	l	89	ARG
46	m	9	ILE
46	m	11	ARG
46	m	15	VAL
46	m	34	LEU
46	m	40	ASN
46	m	49	THR
46	m	70	LEU
46	m	73	GLU
46	m	79	LYS
46	m	88	ARG
46	m	98	VAL
46	m	102	ARG
46	m	110	ARG
46	m	116	THR
46	m	117	VAL
47	n	3	ARG
47	n	4	LYS
47	n	6	LEU
47	n	7	ILE
47	n	8	GLU
47	n	18	VAL
47	n	33	VAL
47	n	41	ARG
47	n	44	LEU
48	o	24	SER
48	o	26	GLU
48	o	39	LEU
48	o	66	LEU
48	o	67	LEU
48	o	82	ILE
48	o	83	GLU
48	o	84	LYS
48	o	88	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	p	2	VAL
49	p	3	LYS
49	p	5	ARG
49	p	19	ILE
49	p	20	VAL
49	p	21	VAL
49	p	25	ARG
49	p	27	LYS
49	p	45	THR
49	p	50	LYS
49	p	60	LEU
49	p	62	VAL
49	p	79	VAL
50	q	4	LYS
50	q	6	LEU
50	q	9	VAL
50	q	11	VAL
50	q	36	ILE
50	q	49	GLU
50	q	52	LYS
50	q	63	ARG
50	q	68	ARG
50	q	70	ARG
50	q	74	LEU
50	q	77	VAL
50	q	78	GLU
50	q	96	GLU
50	q	98	LEU
51	r	21	LYS
51	r	31	LEU
51	r	32	ARG
51	r	35	ARG
51	r	39	VAL
51	r	42	ARG
51	r	46	GLU
51	r	49	LYS
51	r	55	ARG
51	r	58	LEU
51	r	84	LYS
51	r	87	ARG
52	s	5	LEU
52	s	14	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	s	15	LEU
52	s	27	GLU
52	s	28	LYS
52	s	37	ARG
52	s	45	VAL
52	s	48	THR
52	s	65	ASN
52	s	67	VAL
52	s	71	LEU
53	t	9	ASN
53	t	10	LEU
53	t	24	LEU
53	t	39	LYS
53	t	43	LEU
53	t	51	GLU
53	t	62	LEU
53	t	80	ARG
53	t	84	LEU
54	u	7	ARG
54	u	12	LYS
59	z	-68	MET
59	z	-60	LEU
59	z	-58	ASN
59	z	-54	VAL
59	z	-42	ARG
59	z	-34	LEU
59	z	-32	VAL
59	z	-25	LEU
59	z	-24	LYS
59	z	-22	LEU
59	z	-12	ARG
59	z	-11	LEU
59	z	-7	LYS
59	z	2	ILE
59	z	5	ASN
59	z	15	ILE
59	z	22	LYS
59	z	28	ARG
59	z	32	LEU
59	z	40	GLU
59	z	43	GLU
59	z	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	z	50	GLU
59	z	54	GLU
59	z	64	VAL
59	z	67	THR
59	z	75	GLU
59	z	80	LEU
59	z	101	GLU
59	z	105	LEU
59	z	113	VAL
59	z	126	GLU
59	z	131	ILE
59	z	140	LEU
59	z	142	ASN
59	z	147	GLU
59	z	150	LEU
59	z	175	GLU
59	z	179	GLU
59	z	181	ILE
59	z	184	ARG
59	z	197	LYS
59	z	204	VAL
59	z	208	TYR
59	z	209	GLN
59	z	212	ILE
59	z	215	LEU
59	z	216	ARG
59	z	229	ARG
59	z	233	THR
59	z	238	THR
59	z	241	LYS
59	z	245	PHE
59	z	248	GLN
59	z	250	LEU
59	z	251	VAL
59	z	268	ILE
59	z	269	ARG
59	z	274	VAL
59	z	280	ILE
59	z	282	LEU
59	z	298	LYS
59	z	301	VAL
59	z	308	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	z	309	ASP
59	z	312	ASP
59	z	316	LEU
59	z	317	ARG
59	z	322	LYS
59	z	324	LYS
59	z	325	LEU
59	z	326	ASN
59	z	336	SER
59	z	338	THR
59	z	345	ARG
59	z	355	GLU
59	z	360	ARG
59	z	362	GLU
59	z	369	LEU
59	z	370	ILE
59	z	382	LEU
59	z	384	SER
59	z	387	GLU
59	z	401	ARG
59	z	402	ILE
59	z	405	ILE
59	z	413	THR
59	z	418	GLU
59	z	419	GLU
59	z	424	LEU
59	z	434	ARG
59	z	438	MET
59	z	441	LEU
59	z	447	ARG
59	z	451	VAL
59	z	461	TYR
59	z	467	LEU
59	z	471	SER
59	z	476	SER
59	z	480	GLU
59	z	481	GLN
59	z	490	VAL
59	z	492	VAL
59	z	495	LEU
59	z	512	LYS
59	z	516	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	z	518	ARG
59	z	521	VAL
59	z	534	GLU
59	z	541	ILE
59	z	545	ILE
59	z	546	ILE
59	z	548	ARG
59	z	550	THR
59	z	572	LYS
59	z	576	LYS
59	z	592	VAL
59	z	595	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	115	GLN
4	D	164	GLN
4	D	166	GLN
4	D	253	GLN
5	E	85	ASN
5	E	143	ASN
6	F	69	HIS
6	F	75	HIS
6	F	169	ASN
7	G	26	GLN
7	G	41	GLN
8	H	139	GLN
10	K	11	GLN
10	K	30	HIS
12	O	3	GLN
12	O	90	GLN
14	Q	12	GLN
14	Q	45	GLN
15	R	50	HIS
17	T	43	GLN
17	T	84	GLN
17	T	123	GLN
18	U	72	HIS
19	V	80	GLN
21	X	31	HIS
22	Y	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	Z	50	GLN
23	Z	54	HIS
24	0	17	GLN
24	0	35	ASN
26	2	46	GLN
26	2	70	GLN
28	4	20	ASN
28	4	60	GLN
33	9	20	HIS
33	9	36	GLN
35	b	16	HIS
35	b	113	HIS
35	b	212	GLN
36	c	6	HIS
36	c	37	GLN
36	c	63	ASN
36	c	104	GLN
36	c	108	ASN
36	c	118	GLN
36	c	162	GLN
36	c	176	HIS
36	c	181	ASN
37	d	42	GLN
37	d	77	ASN
37	d	123	HIS
37	d	125	HIS
37	d	199	ASN
37	d	201	GLN
38	e	73	ASN
38	e	141	GLN
39	f	73	ASN
39	f	100	ASN
40	g	28	ASN
40	g	68	ASN
40	g	148	ASN
42	i	89	ASN
42	i	124	GLN
43	j	56	HIS
43	j	68	HIS
43	j	69	ASN
44	k	38	ASN
44	k	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	l	99	HIS
46	m	40	ASN
46	m	92	HIS
48	o	9	GLN
48	o	28	GLN
48	o	62	GLN
50	q	16	GLN
52	s	57	HIS
52	s	65	ASN
52	s	83	HIS
53	t	75	ASN
59	z	-58	ASN
59	z	127	HIS
59	z	183	GLN
59	z	248	GLN
59	z	275	GLN
59	z	326	ASN
59	z	426	GLN
59	z	429	GLN
59	z	439	ASN
59	z	538	GLN
59	z	577	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2868/2915 (98%)	470 (16%)	42 (1%)
2	B	119/121 (98%)	14 (11%)	0
34	a	1496/1521 (98%)	245 (16%)	0
55	v	12/24 (50%)	1 (8%)	0
56	w	72/76 (94%)	26 (36%)	0
57	x	76/77 (98%)	13 (17%)	0
58	y	72/76 (94%)	29 (40%)	0
All	All	4715/4810 (98%)	798 (16%)	42 (0%)

All (798) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	10	G
1	A	14	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	G
1	A	44	C
1	A	58	G
1	A	69	A
1	A	72	A
1	A	73	G
1	A	82	A
1	A	86	G
1	A	88	U
1	A	89	A
1	A	93	G
1	A	115	A
1	A	116	A
1	A	117	U
1	A	136	G
1	A	138	A
1	A	161	G
1	A	162	C
1	A	169	A
1	A	184	A
1	A	185	A
1	A	187	A
1	A	188	U
1	A	193	G
1	A	202	G
1	A	203	G
1	A	204	A
1	A	209	A
1	A	210	A
1	A	217	A
1	A	221	A
1	A	236	G
1	A	253	A
1	A	268	G
1	A	270	U
1	A	271	U
1	A	272	G
1	A	277	G
1	A	286	G
1	A	287	U
1	A	288	G
1	A	295	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	G
1	A	302	C
1	A	306	A
1	A	334	A
1	A	350	G
1	A	352	G
1	A	353	A
1	A	356	G
1	A	375	G
1	A	376	G
1	A	386	G
1	A	412	G
1	A	422	G
1	A	431	U
1	A	437	G
1	A	438	A
1	A	469	C
1	A	473	U
1	A	479	A
1	A	480	C
1	A	481	C
1	A	482	A
1	A	504	A
1	A	506	G
1	A	528	U
1	A	529	A
1	A	530	G
1	A	532	G
1	A	533	C
1	A	555	C
1	A	556	A
1	A	557	G
1	A	568	G
1	A	569	C
1	A	585	G
1	A	595	G
1	A	597	A
1	A	608	A
1	A	615	G
1	A	625	A
1	A	626	G
1	A	629	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	638	G
1	A	640	G
1	A	651	A
1	A	661	A
1	A	665	C
1	A	669	C
1	A	670	A
1	A	677	A
1	A	678	A
1	A	679	G
1	A	680	C
1	A	681	G
1	A	696	C
1	A	697	G
1	A	698	C
1	A	702	G
1	A	732	G
1	A	763	G
1	A	776	C
1	A	792	A
1	A	793	U
1	A	798	A
1	A	799	C
1	A	810	A
1	A	811	G
1	A	821	G
1	A	822	G
1	A	828	A
1	A	830	A
1	A	831	G
1	A	838	G
1	A	851	G
1	A	858	C
1	A	865	A
1	A	873	U
1	A	874	U
1	A	876	G
1	A	905	G
1	A	912	A
1	A	915	G
1	A	921	G
1	A	924	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	926	G
1	A	931	C
1	A	932	C
1	A	933	A
1	A	934	C
1	A	935	C
1	A	936	A
1	A	937	G
1	A	938	C
1	A	940	U
1	A	941	A
1	A	942	C
1	A	943	C
1	A	944	A
1	A	945	A
1	A	946	A
1	A	955	A
1	A	962	A
1	A	976	G
1	A	985	A
1	A	989	A
1	A	990	G
1	A	1005	C
1	A	1018	G
1	A	1019	C
1	A	1028	A
1	A	1041	A
1	A	1050	C
1	A	1057	U
1	A	1058	C
1	A	1060	G
1	A	1067	G
1	A	1078	U
1	A	1084	G
1	A	1090	A
1	A	1091	A
1	A	1092	G
1	A	1093	A
1	A	1096	G
1	A	1097	C
1	A	1098	C
1	A	1099	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1103	G
1	A	1106	U
1	A	1107	G
1	A	1111	U
1	A	1114	A
1	A	1115	A
1	A	1117	C
1	A	1118	A
1	A	1120	C
1	A	1121	C
1	A	1125	C
1	A	1127	U
1	A	1128	U
1	A	1131	A
1	A	1132	G
1	A	1133	A
1	A	1135	U
1	A	1136	G
1	A	1142	U
1	A	1145	C
1	A	1154	C
1	A	1156	A
1	A	1157	G
1	A	1173	A
1	A	1174	A
1	A	1175	U
1	A	1179	C
1	A	1180	G
1	A	1185	U
1	A	1186	U
1	A	1187	A
1	A	1194	G
1	A	1216	G
1	A	1217	G
1	A	1218	A
1	A	1219	U
1	A	1220	G
1	A	1221	A
1	A	1222	C
1	A	1254	A
1	A	1255	U
1	A	1264	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1265	C
1	A	1281	G
1	A	1284	G
1	A	1289	G
1	A	1293	G
1	A	1295	G
1	A	1298	A
1	A	1301	G
1	A	1302	C
1	A	1316	G
1	A	1317	A
1	A	1318	U
1	A	1345	U
1	A	1346	A
1	A	1350	C
1	A	1404	A
1	A	1410	A
1	A	1417	U
1	A	1425	G
1	A	1430	G
1	A	1461	G
1	A	1462	C
1	A	1465	U
1	A	1466	G
1	A	1473	C
1	A	1482	C
1	A	1490	A
1	A	1501	G
1	A	1506	A
1	A	1507	G
1	A	1513	C
1	A	1517	A
1	A	1528	G
1	A	1529	G
1	A	1539	A
1	A	1553	A
1	A	1554	C
1	A	1555	A
1	A	1557	G
1	A	1578	C
1	A	1588	A
1	A	1589	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1600	A
1	A	1604	A
1	A	1606	G
1	A	1612	A
1	A	1615	A
1	A	1624	U
1	A	1626	A
1	A	1627	G
1	A	1630	C
1	A	1631	A
1	A	1653	A
1	A	1654	A
1	A	1655	A
1	A	1662	C
1	A	1694	C
1	A	1700	A
1	A	1720	G
1	A	1742	G
1	A	1746	A
1	A	1761	G
1	A	1765	G
1	A	1766	A
1	A	1767	U
1	A	1768	G
1	A	1769	A
1	A	1770	G
1	A	1773	C
1	A	1774	C
1	A	1775	G
1	A	1776	G
1	A	1777	G
1	A	1778	G
1	A	1788	G
1	A	1793	G
1	A	1794	G
1	A	1799	G
1	A	1803	A
1	A	1821	A
1	A	1830	C
1	A	1831	G
1	A	1846	G
1	A	1869	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1877	A
1	A	1897	A
1	A	1898	A
1	A	1899	G
1	A	1921	A
1	A	1927	G
1	A	1950	G
1	A	1951	G
1	A	1958	A
1	A	1959	A
1	A	1962	C
1	A	1976	U
1	A	1981	A
1	A	1984	U
1	A	1988	C
1	A	1991	A
1	A	1992	A
1	A	1993	A
1	A	2013	G
1	A	2014	U
1	A	2018	G
1	A	2041	A
1	A	2044	G
1	A	2052	A
1	A	2053	G
1	A	2054	A
1	A	2064	C
1	A	2076	C
1	A	2077	G
1	A	2081	A
1	A	2082	G
1	A	2083	A
1	A	2090	G
1	A	2120	U
1	A	2123	U
1	A	2124	C
1	A	2125	G
1	A	2126	C
1	A	2127	G
1	A	2128	C
1	A	2130	U
1	A	2134	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2137	G
1	A	2140	A
1	A	2141	G
1	A	2142	G
1	A	2147	A
1	A	2149	C
1	A	2152	G
1	A	2153	U
1	A	2155	A
1	A	2156	A
1	A	2157	C
1	A	2159	C
1	A	2160	C
1	A	2161	C
1	A	2164	C
1	A	2165	U
1	A	2167	C
1	A	2168	G
1	A	2177	G
1	A	2178	G
1	A	2179	A
1	A	2180	G
1	A	2181	G
1	A	2182	C
1	A	2186	G
1	A	2187	G
1	A	2188	U
1	A	2189	G
1	A	2190	A
1	A	2193	U
1	A	2199	C
1	A	2200	C
1	A	2203	G
1	A	2205	G
1	A	2206	C
1	A	2208	G
1	A	2211	G
1	A	2213	G
1	A	2214	G
1	A	2219	A
1	A	2220	A
1	A	2221	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2226	G
1	A	2227	G
1	A	2228	A
1	A	2230	G
1	A	2236	A
1	A	2249	G
1	A	2250	G
1	A	2284	A
1	A	2286	C
1	A	2294	C
1	A	2298	A
1	A	2316	A
1	A	2318	G
1	A	2319	G
1	A	2330	G
1	A	2331	A
1	A	2332	G
1	A	2333	A
1	A	2336	G
1	A	2338	A
1	A	2345	G
1	A	2347	A
1	A	2354	C
1	A	2358	C
1	A	2365	G
1	A	2372	A
1	A	2394	G
1	A	2396	C
1	A	2399	A
1	A	2404	A
1	A	2417	U
1	A	2418	G
1	A	2425	G
1	A	2432	G
1	A	2433	A
1	A	2435	C
1	A	2436	A
1	A	2440	G
1	A	2441	A
1	A	2446	A
1	A	2450	A
1	A	2452	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2459	A
1	A	2487	A
1	A	2513	G
1	A	2516	G
1	A	2517	U
1	A	2529	A
1	A	2540	G
1	A	2565	U
1	A	2577	A
1	A	2578	G
1	A	2584	C
1	A	2589	G
1	A	2596	U
1	A	2613	A
1	A	2620	U
1	A	2622	U
1	A	2623	C
1	A	2632	A
1	A	2641	G
1	A	2643	A
1	A	2654	G
1	A	2665	A
1	A	2674	G
1	A	2675	G
1	A	2694	C
1	A	2700	U
1	A	2702	C
1	A	2724	A
1	A	2725	A
1	A	2726	G
1	A	2738	U
1	A	2745	A
1	A	2769	A
1	A	2777	A
1	A	2778	G
1	A	2790	A
1	A	2802	A
1	A	2803	C
1	A	2812	G
1	A	2816	G
1	A	2829	A
1	A	2830	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2844	A
1	A	2848	G
1	A	2881	G
1	A	2891	A
1	A	2902	G
2	B	2	C
2	B	7	G
2	B	31	C
2	B	35	U
2	B	45	A
2	B	56	G
2	B	65	C
2	B	66	A
2	B	67	G
2	B	72	G
2	B	73	A
2	B	85	G
2	B	110	G
2	B	120	A
34	a	7	G
34	a	8	G
34	a	10	G
34	a	23	G
34	a	32	G
34	a	33	A
34	a	40	G
34	a	49	C
34	a	52	A
34	a	62	G
34	a	72	C
34	a	73	C
34	a	74	G
34	a	76	G
34	a	78	G
34	a	87	C
34	a	88	C
34	a	89	G
34	a	91	G
34	a	92	G
34	a	93	U
34	a	95	A
34	a	114	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	115	C
34	a	126	C
34	a	137	G
34	a	138	A
34	a	139	G
34	a	152	G
34	a	154	G
34	a	155	A
34	a	158	C
34	a	177	U
34	a	204	A
34	a	209	U
34	a	210	U
34	a	211	U
34	a	212	G
34	a	216	G
34	a	243	G
34	a	247	G
34	a	262	G
34	a	263	C
34	a	282	G
34	a	285	G
34	a	314	G
34	a	317	A
34	a	324	C
34	a	328	G
34	a	338	C
34	a	339	U
34	a	340	A
34	a	341	C
34	a	342	G
34	a	343	G
34	a	348	C
34	a	349	A
34	a	350	G
34	a	352	A
34	a	363	U
34	a	368	C
34	a	380	G
34	a	394	C
34	a	402	G
34	a	407	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	408	A
34	a	409	G
34	a	410	A
34	a	420	G
34	a	425	U
34	a	426	A
34	a	433	U
34	a	441	G
34	a	447	A
34	a	451	C
34	a	455	A
34	a	456	C
34	a	457	G
34	a	470	G
34	a	481	A
34	a	482	U
34	a	489	G
34	a	493	A
34	a	494	A
34	a	495	C
34	a	502	C
34	a	508	G
34	a	511	G
34	a	514	G
34	a	515	U
34	a	516	A
34	a	531	A
34	a	543	A
34	a	545	U
34	a	556	A
34	a	557	A
34	a	558	A
34	a	560	G
34	a	561	G
34	a	591	A
34	a	614	G
34	a	615	G
34	a	616	A
34	a	621	G
34	a	634	G
34	a	637	A
34	a	649	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	650	G
34	a	671	A
34	a	672	G
34	a	679	A
34	a	707	U
34	a	715	G
34	a	718	G
34	a	733	C
34	a	739	G
34	a	761	A
34	a	777	U
34	a	778	A
34	a	799	A
34	a	801	C
34	a	803	A
34	a	812	A
34	a	823	U
34	a	824	C
34	a	825	U
34	a	826	C
34	a	837	A
34	a	852	G
34	a	880	G
34	a	891	A
34	a	892	A
34	a	904	G
34	a	905	G
34	a	912	C
34	a	913	A
34	a	920	G
34	a	938	U
34	a	939	U
34	a	944	G
34	a	946	A
34	a	947	A
34	a	949	G
34	a	953	A
34	a	954	G
34	a	955	A
34	a	971	G
34	a	978	U
34	a	985	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	986	C
34	a	988	G
34	a	989	G
34	a	996	G
34	a	1002	G
34	a	1003	G
34	a	1004	U
34	a	1005	G
34	a	1006	C
34	a	1007	C
34	a	1008	C
34	a	1009	C
34	a	1010	G
34	a	1014	G
34	a	1016	G
34	a	1017	G
34	a	1019	G
34	a	1020	C
34	a	1027	A
34	a	1037	C
34	a	1049	C
34	a	1068	U
34	a	1071	G
34	a	1077	G
34	a	1078	U
34	a	1084	A
34	a	1107	G
34	a	1108	U
34	a	1109	U
34	a	1110	G
34	a	1112	C
34	a	1113	A
34	a	1114	G
34	a	1116	G
34	a	1120	C
34	a	1122	G
34	a	1123	C
34	a	1128	C
34	a	1129	A
34	a	1135	A
34	a	1140	A
34	a	1141	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1142	U
34	a	1143	G
34	a	1164	G
34	a	1178	U
34	a	1179	G
34	a	1195	A
34	a	1209	A
34	a	1218	A
34	a	1220	A
34	a	1222	U
34	a	1239	U
34	a	1240	G
34	a	1252	C
34	a	1260	U
34	a	1262	A
34	a	1267	A
34	a	1268	A
34	a	1269	A
34	a	1272	G
34	a	1281	A
34	a	1282	G
34	a	1283	U
34	a	1284	U
34	a	1287	G
34	a	1301	A
34	a	1302	C
34	a	1304	C
34	a	1320	G
34	a	1328	A
34	a	1329	G
34	a	1347	U
34	a	1353	G
34	a	1360	A
34	a	1377	A
34	a	1380	C
34	a	1381	A
34	a	1402	G
34	a	1423	C
34	a	1425	G
34	a	1431	U
34	a	1432	A
34	a	1433	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1434	G
34	a	1447	G
34	a	1470	A
34	a	1471	A
34	a	1472	G
34	a	1481	A
34	a	1484	U
34	a	1495	G
34	a	1498	G
34	a	1507	G
34	a	1508	G
34	a	1509	A
55	v	24	A
56	w	6	G
56	w	8	4SU
56	w	9	A
56	w	13	C
56	w	15	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	26	A
56	w	44	G
56	w	45	U
56	w	46	7MG
56	w	47	U
56	w	48	C
56	w	49	C
56	w	55	PSU
56	w	56	C
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	63	G
56	w	64	A
56	w	71	G
56	w	74	C
56	w	76	A
57	x	2	G
57	x	9	G
57	x	14	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	x	16	C
57	x	17	C
57	x	17(A)	U
57	x	18	G
57	x	19	G
57	x	31	G
57	x	47	U
57	x	48	C
57	x	61	C
57	x	76	A
58	y	2	C
58	y	5	G
58	y	7	A
58	y	8	4SU
58	y	9	A
58	y	13	C
58	y	19	G
58	y	20	U
58	y	21	A
58	y	22	G
58	y	25	C
58	y	26	A
58	y	29	G
58	y	30	G
58	y	32	PSU
58	y	33	U
58	y	35	A
58	y	37	MIA
58	y	41	C
58	y	43	C
58	y	44	G
58	y	45	U
58	y	46	G
58	y	47	U
58	y	48	C
58	y	56	C
58	y	59	U
58	y	60	U
58	y	66	U

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	33	C
1	A	88	U
1	A	184	A
1	A	270	U
1	A	271	U
1	A	301	A
1	A	385	U
1	A	514	G
1	A	669	C
1	A	677	A
1	A	731	A
1	A	792	A
1	A	798	A
1	A	810	A
1	A	1008	C
1	A	1018	G
1	A	1037	C
1	A	1097	C
1	A	1120	C
1	A	1132	G
1	A	1153	U
1	A	1218	A
1	A	1220	G
1	A	1238	A
1	A	1254	A
1	A	1424	A
1	A	1465	U
1	A	1653	A
1	A	1699	G
1	A	2013	G
1	A	2123	U
1	A	2166	C
1	A	2202	G
1	A	2212	G
1	A	2329	G
1	A	2417	U
1	A	2432	G
1	A	2433	A
1	A	2450	A
1	A	2622	U
1	A	2768	U
1	A	2901	G

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

17 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$
58	PSU	y	32	58	18,21,22	1.43	3 (16%)	21,30,33	1.94	3 (14%)
58	MIA	y	37	34,58	21,24,32	1.71	4 (19%)	30,35,47	2.04	7 (23%)
56	PSU	w	32	56	18,21,22	1.46	2 (11%)	21,30,33	2.02	5 (23%)
56	PSU	w	39	56	18,21,22	1.30	2 (11%)	21,30,33	2.06	5 (23%)
56	5MU	w	54	56	19,22,23	1.40	4 (21%)	27,32,35	1.82	7 (25%)
58	PSU	y	55	58	18,21,22	1.41	2 (11%)	21,30,33	2.04	4 (19%)
56	7MG	w	46	56	23,26,27	1.39	5 (21%)	27,39,42	2.50	6 (22%)
56	PSU	w	55	56	18,21,22	1.36	2 (11%)	21,30,33	1.89	4 (19%)
57	5MU	x	54	60,57	19,22,23	1.29	4 (21%)	27,32,35	2.14	6 (22%)
56	4SU	w	8	56	18,21,22	1.91	5 (27%)	25,30,33	2.00	5 (20%)
58	PSU	y	39	58	18,21,22	1.50	2 (11%)	21,30,33	1.95	6 (28%)
57	PSU	x	55	57	18,21,22	1.43	3 (16%)	21,30,33	1.99	5 (23%)
56	MIA	w	37	56	27,29,32	2.35	7 (25%)	38,41,47	2.91	15 (39%)
57	4SU	x	8	57	18,21,22	2.19	6 (33%)	25,30,33	2.11	5 (20%)
58	5MU	y	54	58	19,22,23	1.44	6 (31%)	27,32,35	2.00	9 (33%)
57	5MC	x	32	57	19,22,23	1.60	3 (15%)	26,32,35	1.15	2 (7%)
58	4SU	y	8	58	18,21,22	4.77	7 (38%)	25,30,33	12.20	8 (32%)

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
58	PSU	y	32	58	-	4/7/25/26	0/2/2/2
58	MIA	y	37	34,58	-	2/7/25/34	0/3/3/3
56	PSU	w	32	56	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	w	39	56	-	0/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
58	PSU	y	55	58	-	0/7/25/26	0/2/2/2
56	7MG	w	46	56	-	3/7/37/38	0/3/3/3
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
57	5MU	x	54	60,57	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
58	PSU	y	39	58	-	0/7/25/26	0/2/2/2
57	PSU	x	55	57	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	6/14/31/34	0/3/3/3
57	4SU	x	8	57	-	0/7/25/26	0/2/2/2
58	5MU	y	54	58	-	0/7/25/26	0/2/2/2
57	5MC	x	32	57	-	0/7/25/26	0/2/2/2
58	4SU	y	8	58	-	2/7/25/26	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	8	4SU	O2-C2	-12.93	1.00	1.23
58	y	8	4SU	C4-N3	11.35	1.49	1.37
56	w	37	MIA	C2-S10	-7.46	1.69	1.75
56	w	37	MIA	C13-C14	6.61	1.52	1.32
57	x	8	4SU	C4-N3	-6.00	1.31	1.37
57	x	32	5MC	C5-C4	5.64	1.48	1.44
58	y	37	MIA	C5-C4	5.35	1.48	1.39
58	y	8	4SU	C5-C4	5.14	1.48	1.42
58	y	8	4SU	C6-C5	5.13	1.47	1.35
58	y	8	4SU	C4-S4	-5.07	1.59	1.68
58	y	8	4SU	C2-N1	4.90	1.46	1.38
56	w	8	4SU	C4-S4	-4.86	1.60	1.68
56	w	37	MIA	C5-C4	4.25	1.46	1.39
58	y	39	PSU	C6-C5	4.25	1.40	1.35
56	w	32	PSU	C6-C5	4.24	1.40	1.35
57	x	8	4SU	C2-N3	-4.10	1.30	1.38
56	w	8	4SU	C4-N3	-3.94	1.33	1.37
58	y	32	PSU	C6-C5	3.73	1.39	1.35
56	w	55	PSU	C6-C5	3.71	1.39	1.35
58	y	55	PSU	C6-C5	3.70	1.39	1.35
56	w	39	PSU	C6-C5	3.56	1.39	1.35
56	w	46	7MG	C5-C4	3.54	1.48	1.37
57	x	55	PSU	C4-N3	-3.29	1.32	1.38
56	w	46	7MG	C4-N9	-3.08	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	x	8	4SU	C4-S4	-2.99	1.63	1.68
56	w	54	5MU	C6-C5	2.96	1.39	1.34
58	y	37	MIA	C5-C6	2.92	1.49	1.41
57	x	8	4SU	C5-C4	-2.85	1.39	1.42
58	y	54	5MU	C2-N1	2.83	1.42	1.38
57	x	54	5MU	C4-N3	-2.80	1.33	1.38
58	y	39	PSU	C4-N3	-2.77	1.33	1.38
56	w	37	MIA	C5-N7	-2.72	1.34	1.39
56	w	8	4SU	C5-C4	-2.71	1.39	1.42
56	w	32	PSU	C4-N3	-2.68	1.33	1.38
57	x	8	4SU	C6-C5	2.66	1.41	1.35
57	x	32	5MC	C6-N1	-2.65	1.33	1.38
58	y	32	PSU	C4-N3	-2.65	1.33	1.38
57	x	54	5MU	C6-C5	2.64	1.38	1.34
58	y	55	PSU	C4-N3	-2.61	1.34	1.38
57	x	8	4SU	O2-C2	2.59	1.27	1.23
56	w	54	5MU	C4-N3	-2.55	1.34	1.38
58	y	54	5MU	C6-C5	2.49	1.38	1.34
56	w	55	PSU	C4-N3	-2.48	1.34	1.38
57	x	32	5MC	C6-C5	2.47	1.38	1.34
57	x	55	PSU	C2-N3	-2.47	1.33	1.37
58	y	54	5MU	C4-C5	2.45	1.48	1.44
56	w	39	PSU	C4-N3	-2.44	1.34	1.38
56	w	54	5MU	C2-N1	2.41	1.42	1.38
56	w	54	5MU	C4-C5	2.39	1.48	1.44
58	y	37	MIA	C8-N7	2.34	1.36	1.31
58	y	8	4SU	C6-N1	2.34	1.43	1.38
58	y	54	5MU	C4-N3	-2.33	1.34	1.38
56	w	8	4SU	C2-N3	-2.32	1.33	1.38
57	x	54	5MU	C6-N1	-2.30	1.34	1.38
57	x	55	PSU	C6-C5	2.27	1.37	1.35
56	w	46	7MG	C8-N9	2.25	1.47	1.45
56	w	8	4SU	C2-N1	2.25	1.42	1.38
56	w	46	7MG	C6-N1	-2.23	1.34	1.38
56	w	37	MIA	C4-N9	-2.18	1.33	1.37
56	w	46	7MG	C5-C6	2.17	1.48	1.43
56	w	37	MIA	C8-N7	2.16	1.35	1.31
56	w	37	MIA	C5-C6	2.16	1.47	1.41
58	y	54	5MU	C2-N3	-2.13	1.34	1.38
58	y	37	MIA	C5-N7	-2.12	1.35	1.39
58	y	32	PSU	C4-C5	2.10	1.50	1.44
57	x	54	5MU	C2-N3	-2.09	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	54	5MU	C6-N1	-2.04	1.34	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	8	4SU	O2-C2-N1	-41.14	69.25	122.80
58	y	8	4SU	O2-C2-N3	-40.19	47.40	121.49
58	y	8	4SU	C6-C5-C4	-12.81	108.86	119.95
58	y	8	4SU	C5-C4-N3	11.16	125.13	114.75
56	w	46	7MG	N9-C4-N3	8.55	137.99	125.46
56	w	37	MIA	C12-C13-C14	-8.53	111.69	127.01
56	w	37	MIA	C5-C4-N3	-7.63	119.14	127.18
58	y	8	4SU	C5-C4-S4	-7.50	115.74	124.31
57	x	8	4SU	C4-N3-C2	6.69	133.73	127.31
56	w	37	MIA	C11-S10-C2	-6.62	97.28	102.25
56	w	32	PSU	N1-C2-N3	6.53	122.06	115.17
57	x	55	PSU	N1-C2-N3	6.38	121.90	115.17
58	y	8	4SU	C4-N3-C2	-6.38	121.20	127.31
56	w	37	MIA	N3-C4-N9	6.31	135.00	126.99
58	y	39	PSU	N1-C2-N3	6.24	121.75	115.17
58	y	32	PSU	N1-C2-N3	6.16	121.67	115.17
58	y	55	PSU	N1-C2-N3	6.15	121.65	115.17
56	w	39	PSU	N1-C2-N3	6.09	121.59	115.17
58	y	37	MIA	C5-C4-N3	-5.83	118.69	126.72
56	w	55	PSU	N1-C2-N3	5.62	121.09	115.17
57	x	54	5MU	N3-C2-N1	5.49	122.04	114.89
56	w	8	4SU	C4-N3-C2	-5.46	122.08	127.31
56	w	8	4SU	C5-C4-N3	5.19	119.57	114.75
56	w	46	7MG	N9-C8-N7	-5.15	96.08	103.37
56	w	46	7MG	C5-C4-N3	-5.12	118.53	128.13
57	x	54	5MU	C4-N3-C2	-5.00	120.78	127.34
58	y	37	MIA	N3-C4-N9	4.93	135.55	127.17
56	w	37	MIA	C16-C14-C13	-4.67	108.65	122.66
56	w	39	PSU	C4-N3-C2	-4.50	120.17	126.37
58	y	54	5MU	C4-N3-C2	-4.46	121.49	127.34
56	w	54	5MU	N3-C2-N1	4.44	120.67	114.89
58	y	55	PSU	C4-N3-C2	-4.35	120.38	126.37
56	w	46	7MG	C2-N3-C4	4.30	119.70	112.30
57	x	54	5MU	O4-C4-C5	-4.26	120.04	124.92
58	y	54	5MU	N3-C2-N1	4.24	120.41	114.89
57	x	8	4SU	C5-C4-S4	4.15	129.05	124.31
57	x	55	PSU	C4-N3-C2	-4.14	120.66	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	55	PSU	C4-N3-C2	-4.10	120.73	126.37
58	y	54	5MU	C5-C4-N3	4.09	118.88	115.32
58	y	54	5MU	O4-C4-C5	-4.02	120.31	124.92
56	w	54	5MU	C4-N3-C2	-4.00	122.09	127.34
57	x	54	5MU	O2-C2-N1	-3.98	117.62	122.80
56	w	32	PSU	C4-N3-C2	-3.89	121.01	126.37
56	w	8	4SU	N3-C2-N1	3.83	119.88	114.89
58	y	39	PSU	C4-N3-C2	-3.77	121.18	126.37
58	y	32	PSU	C4-N3-C2	-3.75	121.20	126.37
57	x	8	4SU	C6-C5-C4	-3.73	116.72	119.95
58	y	37	MIA	C2-N3-C4	3.71	120.89	111.83
58	y	37	MIA	N3-C2-N1	-3.67	123.02	128.58
57	x	54	5MU	C5-C4-N3	3.65	118.50	115.32
56	w	54	5MU	C5-C4-N3	3.59	118.44	115.32
56	w	37	MIA	C15-C14-C13	-3.55	112.01	122.66
57	x	8	4SU	O2-C2-N1	3.49	127.34	122.80
56	w	54	5MU	O4-C4-C5	-3.46	120.96	124.92
58	y	8	4SU	C5-C6-N1	3.45	127.45	121.84
57	x	8	4SU	S4-C4-N3	-3.37	116.68	120.20
57	x	54	5MU	C5-C6-N1	-3.29	119.74	123.31
57	x	32	5MC	C5-C6-N1	-3.26	119.77	123.31
56	w	37	MIA	C2-N3-C4	3.20	120.67	112.29
58	y	54	5MU	C5-C6-N1	-3.19	119.85	123.31
58	y	37	MIA	C4-C5-N7	-3.17	106.96	110.58
58	y	55	PSU	O2-C2-N1	-3.16	119.53	122.79
56	w	8	4SU	C5-C4-S4	-3.03	120.85	124.31
56	w	37	MIA	C4-N9-C8	3.01	108.90	105.74
56	w	37	MIA	C4-C5-N7	-2.99	107.16	110.58
56	w	37	MIA	C6-C5-N7	2.97	135.66	132.43
58	y	32	PSU	O2-C2-N1	-2.89	119.81	122.79
56	w	39	PSU	C5-C6-N1	-2.83	118.22	122.14
57	x	32	5MC	C5-C4-N3	-2.70	118.98	121.75
56	w	39	PSU	O2-C2-N1	-2.70	120.00	122.79
58	y	37	MIA	C4-N9-C8	2.68	108.55	105.74
56	w	32	PSU	O2-C2-N1	-2.67	120.04	122.79
57	x	55	PSU	C5-C6-N1	-2.65	118.47	122.14
58	y	39	PSU	C5-C6-N1	-2.63	118.49	122.14
58	y	55	PSU	C6-C5-C4	-2.52	116.47	118.17
56	w	54	5MU	C5-C6-N1	-2.49	120.61	123.31
58	y	54	5MU	C5M-C5-C4	2.49	121.44	118.78
56	w	8	4SU	C1'-N1-C2	2.45	121.98	117.59
58	y	8	4SU	C1'-N1-C2	2.42	121.95	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	y	39	PSU	O2-C2-N3	-2.41	117.58	121.86
57	x	55	PSU	O2-C2-N3	-2.39	117.61	121.86
56	w	37	MIA	C5-N7-C8	2.38	107.19	103.45
56	w	37	MIA	C2-N1-C6	2.34	121.98	117.54
56	w	46	7MG	C5-C6-N1	2.33	115.05	110.94
56	w	32	PSU	C5-C6-N1	-2.32	118.93	122.14
56	w	55	PSU	O2-C2-N1	-2.31	120.41	122.79
56	w	37	MIA	N3-C2-N1	-2.30	122.81	127.00
58	y	39	PSU	O4'-C1'-C2'	2.26	108.27	105.15
58	y	37	MIA	C5-N7-C8	2.26	107.00	103.45
56	w	37	MIA	N6-C6-N1	2.24	121.33	118.33
57	x	55	PSU	O2-C2-N1	-2.23	120.48	122.79
56	w	46	7MG	C5-C4-N9	-2.23	103.48	106.33
56	w	32	PSU	O2-C2-N3	-2.23	117.91	121.86
56	w	55	PSU	C5-C6-N1	-2.22	119.06	122.14
56	w	37	MIA	N9-C8-N7	-2.15	110.88	113.94
56	w	54	5MU	C5M-C5-C4	2.12	121.04	118.78
56	w	54	5MU	C1'-N1-C2	2.07	121.31	117.59
58	y	39	PSU	O2-C2-N1	-2.06	120.67	122.79
56	w	39	PSU	O4'-C1'-C2'	2.05	107.99	105.15
58	y	54	5MU	C1'-N1-C2	2.04	121.26	117.59
58	y	54	5MU	C5M-C5-C6	-2.04	120.09	122.85
58	y	54	5MU	C1'-N1-C6	-2.02	117.83	121.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
58	y	32	PSU	C2'-C1'-C5-C4
58	y	32	PSU	C2'-C1'-C5-C6
56	w	46	7MG	O4'-C4'-C5'-O5'
58	y	8	4SU	C2'-C1'-N1-C2
56	w	46	7MG	C3'-C4'-C5'-O5'
58	y	8	4SU	C2'-C1'-N1-C6
58	y	37	MIA	C3'-C4'-C5'-O5'
58	y	32	PSU	C4'-C5'-O5'-P
56	w	37	MIA	N1-C6-N6-C12
56	w	37	MIA	N1-C2-S10-C11
58	y	32	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
56	w	37	MIA	N3-C2-S10-C11
56	w	46	7MG	C4'-C5'-O5'-P
58	y	37	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	y	32	PSU	2	0
56	w	54	5MU	2	0
58	y	55	PSU	1	0
56	w	46	7MG	1	0
56	w	55	PSU	1	0
56	w	8	4SU	2	0
58	y	39	PSU	2	0
56	w	37	MIA	1	0
57	x	8	4SU	1	0
58	y	8	4SU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 927 ligands modelled in this entry, 925 are monoatomic - leaving 2 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	$\# Z > 2$
62	SF4	d	302	37	0,12,12	-	-	-		
63	GCP	z	703	60	32,34,34	2.17	11 (34%)	49,54,54	1.97	13 (26%)

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
62	SF4	d	302	37	-	-	0/6/5/5
63	GCP	z	703	60	-	10/19/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	703	GCP	PB-O2B	-6.10	1.41	1.56
63	z	703	GCP	PG-O3G	-4.45	1.45	1.55
63	z	703	GCP	C6-N1	-3.87	1.31	1.38
63	z	703	GCP	C5-N7	-3.30	1.32	1.39
63	z	703	GCP	PB-O1B	2.83	1.58	1.51
63	z	703	GCP	C4-N9	-2.80	1.30	1.38
63	z	703	GCP	PA-O3A	-2.63	1.56	1.59
63	z	703	GCP	C8-N9	-2.60	1.31	1.37
63	z	703	GCP	PG-O1G	2.45	1.55	1.50
63	z	703	GCP	PA-O2A	-2.24	1.44	1.55
63	z	703	GCP	C5-C4	2.08	1.44	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	703	GCP	C5-C4-N3	-6.41	118.19	128.39
63	z	703	GCP	N9-C4-N3	5.30	136.55	125.95
63	z	703	GCP	C2-N3-C4	5.11	121.10	112.30
63	z	703	GCP	O3'-C3'-C2'	-2.81	102.79	111.82
63	z	703	GCP	C6-C5-N7	2.81	135.41	130.29
63	z	703	GCP	O3G-PG-O2G	2.55	115.24	107.96
63	z	703	GCP	C2'-C1'-N9	-2.50	106.29	113.25
63	z	703	GCP	O6-C6-C5	-2.47	120.02	126.53
63	z	703	GCP	O2G-PG-O1G	-2.29	106.47	112.39
63	z	703	GCP	C5-C6-N1	2.26	119.00	113.25
63	z	703	GCP	C4-C5-N7	-2.11	107.32	110.67
63	z	703	GCP	C2-N1-C6	-2.05	121.40	125.11
63	z	703	GCP	O3'-C3'-C4'	-2.01	105.30	111.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

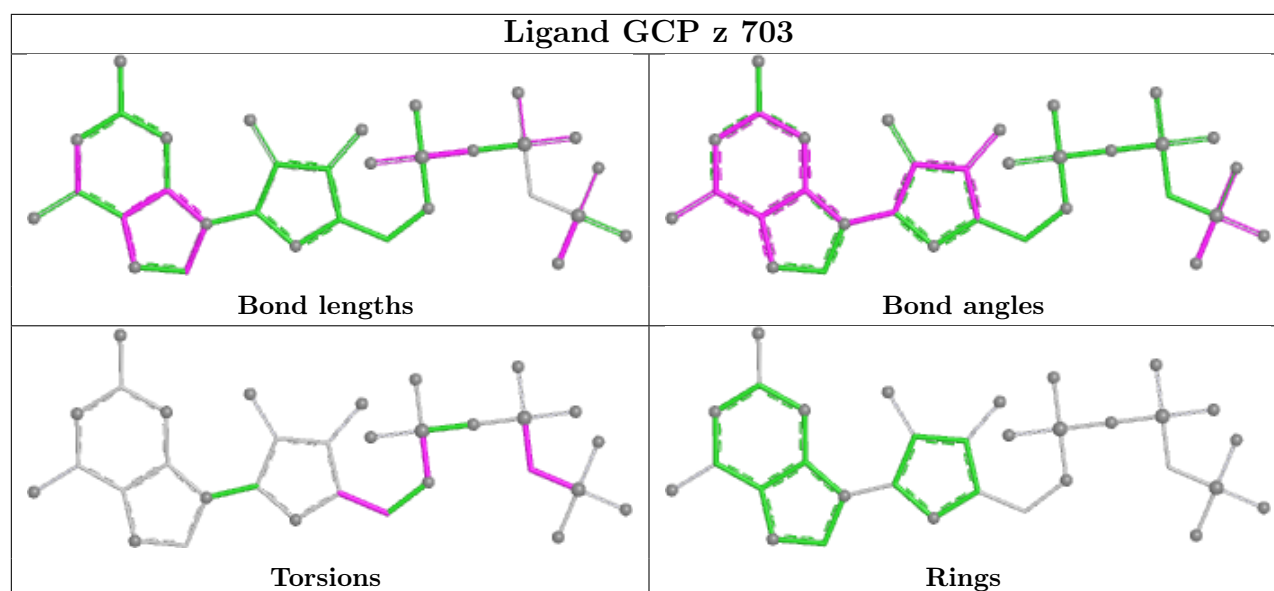
Mol	Chain	Res	Type	Atoms
63	z	703	GCP	PB-C3B-PG-O1G
63	z	703	GCP	PB-C3B-PG-O2G
63	z	703	GCP	PG-C3B-PB-O1B
63	z	703	GCP	C5'-O5'-PA-O2A
63	z	703	GCP	O4'-C4'-C5'-O5'
63	z	703	GCP	C3'-C4'-C5'-O5'
63	z	703	GCP	PB-C3B-PG-O3G
63	z	703	GCP	PG-C3B-PB-O2B
63	z	703	GCP	C5'-O5'-PA-O3A
63	z	703	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	d	302	SF4	3	0
63	z	703	GCP	4	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	2874/2915 (98%)	-0.43	114 (3%) 42 37	20, 37, 80, 93	403 (14%)
2	B	120/121 (99%)	-0.04	1 (0%) 82 80	33, 53, 65, 83	14 (11%)
3	C	136/228 (59%)	2.03	59 (43%) 0 0	35, 74, 85, 96	104 (76%)
4	D	275/276 (99%)	-0.35	3 (1%) 78 74	16, 35, 45, 53	36 (13%)
5	E	204/206 (99%)	-0.17	1 (0%) 87 85	19, 39, 59, 74	35 (17%)
6	F	203/210 (96%)	-0.01	0 100 100	21, 48, 68, 82	30 (14%)
7	G	181/182 (99%)	0.53	4 (2%) 62 57	40, 54, 70, 77	35 (19%)
8	H	174/180 (96%)	0.17	4 (2%) 61 55	34, 51, 63, 69	29 (16%)
9	J	130/173 (75%)	2.81	102 (78%) 0 0	81, 134, 176, 200	9 (6%)
10	K	139/147 (94%)	2.77	99 (71%) 0 0	60, 83, 95, 103	112 (80%)
11	N	140/140 (100%)	-0.12	1 (0%) 84 82	23, 40, 58, 74	21 (15%)
12	O	122/122 (100%)	-0.38	0 100 100	25, 37, 47, 60	6 (4%)
13	P	149/150 (99%)	0.03	1 (0%) 84 82	20, 45, 60, 78	34 (22%)
14	Q	141/141 (100%)	-0.23	1 (0%) 84 82	24, 39, 54, 70	34 (24%)
15	R	118/118 (100%)	-0.18	0 100 100	24, 42, 51, 62	15 (12%)
16	S	110/112 (98%)	0.24	1 (0%) 81 78	39, 49, 59, 70	23 (20%)
17	T	131/146 (89%)	0.02	5 (3%) 44 38	31, 43, 65, 87	19 (14%)
18	U	116/118 (98%)	-0.26	0 100 100	24, 37, 47, 52	21 (18%)
19	V	101/101 (100%)	-0.14	1 (0%) 79 76	26, 45, 55, 65	11 (10%)
20	W	112/113 (99%)	0.01	3 (2%) 56 50	26, 39, 54, 72	21 (18%)
21	X	95/96 (98%)	0.31	2 (2%) 63 58	36, 47, 66, 76	13 (13%)
22	Y	107/110 (97%)	0.45	4 (3%) 45 39	43, 51, 72, 82	19 (17%)
23	Z	94/206 (45%)	0.36	3 (3%) 50 44	40, 56, 69, 85	14 (14%)
24	0	74/85 (87%)	-0.26	0 100 100	25, 38, 48, 64	13 (17%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	1	97/98 (98%)	0.16	6 (6%) 26 21	21, 38, 66, 72	20 (20%)
26	2	70/72 (97%)	0.28	0 100 100	40, 54, 62, 77	12 (17%)
27	3	59/60 (98%)	-0.21	0 100 100	28, 42, 61, 66	9 (15%)
28	4	69/71 (97%)	1.22	14 (20%) 3 2	48, 67, 78, 80	25 (36%)
29	5	59/60 (98%)	-0.19	0 100 100	21, 41, 58, 65	8 (13%)
30	6	53/54 (98%)	-0.22	0 100 100	31, 38, 45, 50	11 (20%)
31	7	49/49 (100%)	-0.28	3 (6%) 27 22	24, 28, 40, 59	9 (18%)
32	8	64/65 (98%)	-0.34	0 100 100	24, 32, 36, 42	7 (10%)
33	9	37/37 (100%)	-0.04	0 100 100	29, 36, 45, 52	9 (24%)
34	a	1498/1521 (98%)	-0.30	46 (3%) 51 45	26, 43, 79, 93	194 (12%)
35	b	231/256 (90%)	0.94	26 (11%) 10 8	44, 66, 80, 92	54 (23%)
36	c	206/239 (86%)	0.28	3 (1%) 72 68	37, 54, 70, 82	16 (7%)
37	d	208/209 (99%)	0.62	9 (4%) 40 34	42, 56, 72, 81	45 (21%)
38	e	148/162 (91%)	-0.07	0 100 100	33, 45, 54, 69	22 (14%)
39	f	100/101 (99%)	0.52	3 (3%) 52 47	47, 62, 72, 82	16 (16%)
40	g	155/156 (99%)	0.43	8 (5%) 33 27	37, 54, 75, 85	38 (24%)
41	h	137/138 (99%)	-0.18	0 100 100	36, 45, 53, 61	13 (9%)
42	i	127/128 (99%)	0.51	3 (2%) 59 54	32, 59, 73, 77	13 (10%)
43	j	96/105 (91%)	0.78	13 (13%) 7 5	30, 61, 82, 86	22 (22%)
44	k	114/129 (88%)	0.15	2 (1%) 67 63	31, 50, 63, 68	16 (14%)
45	l	122/132 (92%)	-0.22	1 (0%) 82 80	26, 38, 52, 61	17 (13%)
46	m	119/126 (94%)	0.48	7 (5%) 28 23	28, 53, 71, 73	22 (18%)
47	n	60/61 (98%)	-0.03	1 (1%) 69 64	31, 42, 52, 57	4 (6%)
48	o	88/89 (98%)	0.08	0 100 100	33, 46, 59, 65	20 (22%)
49	p	82/88 (93%)	0.52	3 (3%) 45 39	38, 53, 64, 70	13 (15%)
50	q	99/105 (94%)	0.03	1 (1%) 79 76	37, 47, 56, 60	17 (17%)
51	r	68/88 (77%)	0.16	1 (1%) 72 68	42, 54, 71, 81	13 (19%)
52	s	83/93 (89%)	0.39	3 (3%) 46 40	34, 51, 68, 76	11 (13%)
53	t	96/106 (90%)	0.39	7 (7%) 21 17	36, 46, 54, 69	15 (15%)
54	u	23/27 (85%)	0.18	0 100 100	32, 43, 47, 47	3 (13%)
55	v	13/24 (54%)	0.33	3 (23%) 2 1	34, 45, 58, 71	4 (30%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	w	67/76 (88%)	1.14	9 (13%) 7 5	41, 75, 83, 86	52 (77%)
57	x	73/77 (94%)	-0.15	4 (5%) 30 25	25, 46, 64, 70	13 (17%)
58	y	68/76 (89%)	0.93	13 (19%) 3 2	27, 75, 91, 94	39 (57%)
59	z	671/679 (98%)	0.68	38 (5%) 29 24	25, 61, 78, 90	154 (22%)
All	All	11355/11953 (94%)	0.06	636 (5%) 30 24	16, 46, 80, 200	2027 (17%)

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	4	56	VAL	7.2
28	4	49	PHE	6.5
40	g	82	GLY	6.4
1	A	932	C	6.3
9	J	37	THR	5.9
10	K	135	GLY	5.9
34	a	91	G	5.6
3	C	67	GLY	5.5
9	J	49	ALA	5.4
10	K	6	ALA	5.3
9	J	6	ASN	5.3
10	K	88	ALA	5.3
10	K	122	ALA	5.3
1	A	934	C	5.3
9	J	94	VAL	5.3
10	K	9	LYS	5.2
10	K	104	VAL	5.2
9	J	43	ALA	5.1
3	C	204	ALA	5.1
35	b	126	GLU	5.1
17	T	131	ALA	5.1
34	a	1109	U	5.0
10	K	52	ILE	5.0
1	A	2178	G	5.0
9	J	55	LYS	5.0
9	J	78	SER	5.0
3	C	205	LYS	4.9
10	K	34	ILE	4.9
1	A	1774	C	4.9
35	b	125	PRO	4.9
1	A	935	C	4.9
10	K	22	PRO	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2158	C	4.8
10	K	116	ASN	4.8
10	K	84	LEU	4.8
1	A	569	C	4.8
3	C	45	ALA	4.7
35	b	127	ILE	4.7
34	a	73	C	4.7
1	A	1777	G	4.7
40	g	80	VAL	4.7
34	a	1432	A	4.6
10	K	8	VAL	4.6
10	K	96	VAL	4.6
20	W	111	HIS	4.5
34	a	1108	U	4.5
40	g	81	GLY	4.4
10	K	7	VAL	4.4
9	J	74	LEU	4.4
9	J	97	ALA	4.4
10	K	77	LEU	4.4
35	b	232	PRO	4.3
28	4	59	PHE	4.3
10	K	59	ILE	4.3
10	K	20	ALA	4.3
9	J	34	ALA	4.3
3	C	207	THR	4.3
1	A	2806	C	4.3
10	K	5	VAL	4.3
3	C	160	ARG	4.2
10	K	124	ALA	4.2
25	1	2	SER	4.2
9	J	54	ALA	4.2
43	j	33	GLN	4.2
3	C	68	LEU	4.2
9	J	14	LYS	4.1
10	K	87	GLY	4.1
28	4	45	GLY	4.1
9	J	99	SER	4.1
10	K	45	THR	4.1
34	a	1010	G	4.1
9	J	38	HIS	4.1
10	K	10	LEU	4.1
34	a	1011	C	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	J	82	PHE	4.1
9	J	42	GLN	4.0
35	b	230	VAL	4.0
9	J	36	GLU	4.0
9	J	39	ALA	4.0
9	J	10	LEU	4.0
10	K	138	VAL	4.0
43	j	100	THR	4.0
1	A	2159	C	4.0
9	J	87	VAL	4.0
10	K	4	VAL	4.0
9	J	111	LEU	4.0
9	J	7	VAL	3.9
10	K	118	THR	3.9
35	b	130	ARG	3.9
1	A	1775	G	3.9
3	C	196	LEU	3.9
10	K	139	VAL	3.9
10	K	82	ALA	3.9
1	A	2812	G	3.9
34	a	1013	A	3.9
3	C	63	SER	3.9
35	b	129	GLU	3.9
21	X	95	LEU	3.9
3	C	198	ALA	3.9
35	b	236	TYR	3.8
1	A	933	A	3.8
10	K	136	VAL	3.8
9	J	47	ASN	3.8
10	K	58	THR	3.8
25	1	80	LEU	3.8
10	K	113	PRO	3.8
59	z	-59	GLU	3.8
34	a	1112	C	3.8
35	b	237	ALA	3.8
3	C	58	VAL	3.8
3	C	175	VAL	3.8
10	K	68	VAL	3.8
10	K	107	ILE	3.7
59	z	185	ILE	3.7
34	a	90	U	3.7
34	a	614	G	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	29	VAL	3.7
1	A	1125	C	3.7
34	a	75	C	3.7
34	a	1007	C	3.7
53	t	9	ASN	3.7
9	J	4	LYS	3.7
28	4	54	GLY	3.7
10	K	25	PRO	3.7
10	K	56	GLU	3.7
34	a	1012	G	3.7
59	z	565	GLY	3.7
45	l	18	VAL	3.7
46	m	8	GLU	3.7
10	K	123	ALA	3.6
9	J	105	PRO	3.6
31	7	49	ARG	3.6
57	x	17	C	3.6
9	J	133	GLU	3.6
10	K	115	LEU	3.6
10	K	97	GLY	3.6
9	J	83	TYR	3.6
1	A	1773	C	3.6
52	s	13	ASP	3.6
1	A	2157	C	3.5
9	J	96	PHE	3.5
9	J	51	LEU	3.5
9	J	117	LEU	3.5
10	K	27	LEU	3.5
34	a	1509	A	3.5
10	K	28	GLY	3.5
43	j	32	ALA	3.5
10	K	19	PRO	3.5
3	C	162	GLU	3.5
3	C	200	LYS	3.5
1	A	1778	G	3.4
3	C	203	GLY	3.4
10	K	17	ALA	3.4
3	C	62	VAL	3.4
3	C	158	ALA	3.4
31	7	45	ALA	3.4
1	A	1126	U	3.4
1	A	2802	A	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	69	GLY	3.4
35	b	134	GLU	3.4
57	x	47	U	3.4
34	a	1003	G	3.4
10	K	43	ALA	3.4
37	d	154	ASN	3.4
35	b	122	PHE	3.4
1	A	931	C	3.3
1	A	2813	C	3.3
35	b	124	SER	3.3
3	C	174	PRO	3.3
9	J	13	LEU	3.3
9	J	125	LEU	3.3
1	A	1091	A	3.3
4	D	276	LYS	3.3
9	J	116	ILE	3.3
9	J	79	ALA	3.3
59	z	268	ILE	3.3
1	A	1217	G	3.3
34	a	78	G	3.3
9	J	106	GLN	3.3
9	J	11	ALA	3.3
10	K	3	LYS	3.3
9	J	132	ASP	3.3
10	K	18	THR	3.3
23	Z	92	SER	3.3
9	J	103	GLY	3.3
10	K	92	GLY	3.3
31	7	48	LYS	3.2
10	K	108	ALA	3.2
34	a	74	G	3.2
56	w	45	U	3.2
1	A	1771	C	3.2
10	K	91	PRO	3.2
3	C	206	GLY	3.2
1	A	2155	A	3.2
1	A	2227	G	3.2
58	y	34	G	3.2
9	J	33	PRO	3.2
10	K	21	PRO	3.2
1	A	930	C	3.2
36	c	207	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	J	35	LYS	3.2
9	J	98	LYS	3.2
9	J	112	LEU	3.2
9	J	69	PRO	3.2
10	K	37	PHE	3.2
9	J	5	ARG	3.1
1	A	1102	A	3.1
35	b	231	GLU	3.1
9	J	30	GLN	3.1
3	C	161	ILE	3.1
9	J	24	PHE	3.1
1	A	1220	G	3.1
34	a	1014	G	3.1
25	l	81	LYS	3.1
46	m	120	LYS	3.1
9	J	44	LEU	3.1
10	K	54	PRO	3.1
1	A	677	A	3.1
56	w	20	U	3.1
9	J	29	TYR	3.1
40	g	84	ASN	3.1
59	z	397	PRO	3.1
9	J	126	ALA	3.1
10	K	46	ALA	3.1
59	z	267	ALA	3.1
9	J	28	ASN	3.1
9	J	85	ASP	3.1
3	C	201	PRO	3.1
22	Y	53	PRO	3.1
1	A	298	G	3.1
1	A	638	G	3.1
10	K	100	THR	3.1
43	j	36	GLY	3.1
10	K	14	ALA	3.1
35	b	229	VAL	3.1
10	K	75	SER	3.1
9	J	40	LEU	3.0
9	J	66	LEU	3.0
10	K	40	ALA	3.0
10	K	61	ALA	3.0
59	z	64	VAL	3.0
9	J	50	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	J	92	THR	3.0
10	K	24	GLY	3.0
9	J	62	ALA	3.0
9	J	8	GLU	3.0
10	K	89	HIS	3.0
1	A	1583	G	3.0
1	A	1761	G	3.0
42	i	91	ASP	3.0
57	x	1	C	3.0
10	K	55	VAL	3.0
7	G	48	GLU	3.0
9	J	115	GLN	3.0
40	g	85	TYR	3.0
28	4	55	ARG	3.0
10	K	131	ALA	3.0
34	a	77	G	3.0
34	a	1005	G	3.0
1	A	2167	C	3.0
10	K	30	HIS	2.9
43	j	78	ASN	2.9
35	b	123	ALA	2.9
1	A	678	A	2.9
1	A	2152	G	2.9
58	y	45	U	2.9
49	p	82	GLN	2.9
28	4	51	ASP	2.9
9	J	48	GLY	2.9
9	J	119	ALA	2.9
9	J	124	ALA	2.9
3	C	208	PHE	2.9
9	J	53	VAL	2.9
3	C	199	HIS	2.9
1	A	217	A	2.9
34	a	615	G	2.9
3	C	60	GLY	2.9
9	J	130	THR	2.9
35	b	136	VAL	2.9
1	A	2165	U	2.9
36	c	13	GLY	2.9
59	z	-35	GLY	2.9
59	z	564	GLY	2.9
9	J	118	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2186	G	2.9
3	C	178	ALA	2.9
39	f	98	LEU	2.9
51	r	20	ALA	2.9
59	z	266	ALA	2.9
2	B	1	U	2.8
1	A	929	G	2.8
21	X	65	ARG	2.8
10	K	11	GLN	2.8
35	b	131	PRO	2.8
34	a	983	A	2.8
10	K	111	LYS	2.8
1	A	2154	G	2.8
58	y	44	G	2.8
3	C	47	LEU	2.8
3	C	209	LEU	2.8
10	K	44	ALA	2.8
3	C	192	PHE	2.8
35	b	128	GLU	2.8
59	z	419	GLU	2.8
34	a	1004	U	2.8
58	y	33	U	2.8
1	A	1156	A	2.8
1	A	2179	A	2.8
3	C	171	ILE	2.8
43	j	75	ILE	2.8
9	J	61	LEU	2.8
20	W	112	GLY	2.8
9	J	15	GLU	2.8
10	K	32	ALA	2.8
28	4	52	THR	2.8
3	C	210	ARG	2.8
43	j	96	ILE	2.7
1	A	270	U	2.7
34	a	1000	G	2.7
9	J	59	ILE	2.7
9	J	16	ASN	2.7
58	y	47	U	2.7
1	A	936	A	2.7
35	b	132	LYS	2.7
34	a	341	C	2.7
28	4	57	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	n	2	ALA	2.7
55	v	24	A	2.7
1	A	33	C	2.7
1	A	1758	C	2.7
9	J	93	LEU	2.7
25	1	26	ARG	2.7
3	C	180	PHE	2.7
1	A	2177	G	2.6
9	J	75	GLN	2.6
1	A	1465	U	2.6
53	t	100	ILE	2.6
10	K	112	MET	2.6
3	C	59	ARG	2.6
3	C	223	ARG	2.6
9	J	80	VAL	2.6
46	m	2	ALA	2.6
9	J	129	PRO	2.6
59	z	400	THR	2.6
59	z	515	THR	2.6
34	a	76	G	2.6
34	a	707	U	2.6
58	y	20	U	2.6
20	W	68	ARG	2.6
59	z	360	ARG	2.6
10	K	16	LYS	2.6
1	A	941	A	2.6
9	J	23	SER	2.6
10	K	13	PRO	2.6
1	A	1117	C	2.6
10	K	99	ILE	2.6
22	Y	1	MET	2.6
25	1	71	TYR	2.6
1	A	88	U	2.6
58	y	22	G	2.6
3	C	163	PHE	2.6
9	J	104	ILE	2.6
59	z	385	GLY	2.6
3	C	26	ALA	2.6
4	D	2	ALA	2.6
9	J	107	VAL	2.6
10	K	26	ALA	2.6
10	K	114	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	a	1114	G	2.5
3	C	11	LEU	2.5
35	b	11	LEU	2.5
53	t	98	PRO	2.5
10	K	134	MET	2.5
34	a	210	U	2.5
10	K	50	ASP	2.5
10	K	127	ILE	2.5
10	K	49	GLY	2.5
52	s	84	GLY	2.5
53	t	103	GLY	2.5
59	z	442	PRO	2.5
35	b	15	VAL	2.5
5	E	204	ALA	2.5
13	P	120	ALA	2.5
17	T	130	ALA	2.5
1	A	695	C	2.5
1	A	939	C	2.5
9	J	100	ASN	2.5
9	J	9	LEU	2.5
3	C	176	GLY	2.5
1	A	10	G	2.5
1	A	2131	G	2.5
35	b	7	VAL	2.5
43	j	74	ILE	2.5
1	A	2132	C	2.5
1	A	1219	U	2.5
9	J	84	GLU	2.5
57	x	17(A)	U	2.5
28	4	63	TYR	2.5
9	J	46	GLN	2.5
10	K	29	GLN	2.5
46	m	7	VAL	2.5
9	J	68	LEU	2.4
59	z	545	ILE	2.4
1	A	1092	G	2.4
1	A	1554	C	2.4
9	J	86	PRO	2.4
23	Z	1	MET	2.4
9	J	113	GLN	2.4
11	N	8	GLN	2.4
3	C	22	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	189	ILE	2.4
10	K	105	LEU	2.4
35	b	121	LEU	2.4
53	t	10	LEU	2.4
59	z	212	ILE	2.4
1	A	944	A	2.4
23	Z	93	ASP	2.4
49	p	47	ASP	2.4
1	A	1103	G	2.4
8	H	100	GLY	2.4
10	K	83	GLY	2.4
34	a	1009	C	2.4
1	A	273	U	2.4
28	4	62	ARG	2.4
10	K	33	ASN	2.4
9	J	121	ASP	2.4
3	C	13	LYS	2.4
9	J	77	PRO	2.4
1	A	925	G	2.4
1	A	1776	G	2.4
10	K	76	TYR	2.4
43	j	79	ARG	2.4
56	w	5	G	2.4
10	K	47	ASN	2.4
9	J	109	SER	2.4
43	j	35	SER	2.4
59	z	383	LYS	2.4
9	J	101	PRO	2.4
28	4	61	ARG	2.4
1	A	2811	A	2.4
3	C	25	ALA	2.4
3	C	191	ALA	2.4
10	K	65	PHE	2.4
37	d	195	ALA	2.4
10	K	12	LEU	2.3
16	S	58	LEU	2.3
1	A	385	U	2.3
1	A	1127	U	2.3
1	A	1763	G	2.3
1	A	2212	G	2.3
9	J	123	GLU	2.3
3	C	166	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	K	23	VAL	2.3
28	4	50	VAL	2.3
3	C	170	ALA	2.3
9	J	89	ALA	2.3
59	z	444	ALA	2.3
1	A	89	A	2.3
1	A	1090	A	2.3
1	A	2140	A	2.3
4	D	275	LYS	2.3
10	K	70	LYS	2.3
59	z	398	ASP	2.3
56	w	44	G	2.3
3	C	48	GLY	2.3
9	J	31	GLY	2.3
9	J	110	GLY	2.3
34	a	456	C	2.3
34	a	987	C	2.3
34	a	1433	C	2.3
7	G	53	LEU	2.3
9	J	71	LEU	2.3
42	i	45	ALA	2.3
3	C	5	LYS	2.3
3	C	30	LYS	2.3
10	K	137	GLU	2.3
17	T	38	ASN	2.3
1	A	1553	A	2.3
59	z	542	GLY	2.3
1	A	940	U	2.3
1	A	1135	U	2.3
35	b	165	VAL	2.3
10	K	67	PHE	2.3
1	A	696	C	2.3
34	a	89	G	2.3
34	a	92	G	2.3
56	w	25	C	2.3
59	z	272	HIS	2.3
28	4	32	TYR	2.3
9	J	41	ARG	2.3
35	b	234	PRO	2.3
1	A	301	A	2.3
1	A	1221	A	2.3
10	K	101	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	b	14	GLY	2.3
9	J	27	VAL	2.3
10	K	120	LEU	2.3
10	K	57	ILE	2.2
37	d	12	CYS	2.2
59	z	402	ILE	2.2
37	d	169	LYS	2.2
46	m	49	THR	2.2
10	K	60	TYR	2.2
59	z	440	TYR	2.2
1	A	1630	C	2.2
1	A	1765	G	2.2
1	A	2213	G	2.2
56	w	15	G	2.2
56	w	52	G	2.2
58	y	18	G	2.2
53	t	47	GLY	2.2
40	g	156	TRP	2.2
59	z	380	VAL	2.2
3	C	36	LYS	2.2
8	H	92	ILE	2.2
9	J	88	ALA	2.2
34	a	340	A	2.2
56	w	76	A	2.2
58	y	35	A	2.2
10	K	48	MET	2.2
1	A	11	U	2.2
34	a	211	U	2.2
10	K	132	ARG	2.2
1	A	680	C	2.2
34	a	1006	C	2.2
59	z	445	GLN	2.2
1	A	2137	G	2.2
9	J	128	LEU	2.2
46	m	48	LEU	2.2
49	p	49	LEU	2.2
56	w	71	G	2.2
3	C	186	ALA	2.2
8	H	47	GLU	2.2
1	A	1764	U	2.2
39	f	100	ASN	2.2
3	C	65	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	226	PRO	2.2
43	j	30	SER	2.2
10	K	35	MET	2.2
1	A	938	C	2.2
3	C	27	HIS	2.2
59	z	339	ALA	2.2
1	A	1762	G	2.2
1	A	2168	G	2.2
34	a	1015	G	2.2
1	A	1218	A	2.2
1	A	1759	U	2.2
17	T	37	GLY	2.2
19	V	101	GLY	2.2
52	s	26	GLY	2.2
10	K	38	VAL	2.2
10	K	133	SER	2.2
3	C	3	HIS	2.2
37	d	170	VAL	2.2
3	C	37	PHE	2.2
59	z	245	PHE	2.2
9	J	90	ALA	2.1
1	A	2185	C	2.1
10	K	69	THR	2.1
1	A	679	G	2.1
1	A	2189	G	2.1
43	j	76	ASN	2.1
7	G	146	TYR	2.1
25	l	82	LEU	2.1
1	A	1131	A	2.1
3	C	159	GLY	2.1
9	J	114	GLY	2.1
1	A	271	U	2.1
1	A	2905	U	2.1
59	z	-55	ASP	2.1
50	q	99	SER	2.1
7	G	50	ALA	2.1
43	j	25	GLU	2.1
1	A	669	C	2.1
53	t	62	LEU	2.1
1	A	568	G	2.1
1	A	937	G	2.1
1	A	2842	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	c	84	ILE	2.1
1	A	1106	U	2.1
9	J	20	ALA	2.1
34	a	825	U	2.1
55	v	14	A	2.1
9	J	127	GLU	2.1
40	g	76	ARG	2.1
9	J	131	MET	2.1
22	Y	57	GLN	2.1
3	C	28	LEU	2.1
1	A	303	C	2.1
42	i	44	VAL	2.1
59	z	510	ARG	2.1
1	A	383	G	2.1
1	A	926	G	2.1
1	A	1215	G	2.1
1	A	2202	G	2.1
1	A	1552	A	2.1
1	A	2191	A	2.1
1	A	2596	U	2.1
10	K	117	THR	2.1
55	v	12	A	2.1
9	J	26	LEU	2.1
39	f	14	LEU	2.1
59	z	396	LEU	2.1
59	z	392	ASN	2.1
44	k	50	TYR	2.1
44	k	75	TYR	2.1
17	T	129	ARG	2.0
37	d	192	GLU	2.0
46	m	51	ALA	2.0
1	A	2128	C	2.0
1	A	2160	C	2.0
9	J	102	LYS	2.0
34	a	1008	C	2.0
34	a	1037	C	2.0
1	A	2138	A	2.0
58	y	23	A	2.0
58	y	28	G	2.0
58	y	31	A	2.0
58	y	46	G	2.0
59	z	592	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
59	z	401	ARG	2.0
37	d	179	GLU	2.0
59	z	499	GLU	2.0
59	z	63	ALA	2.0
10	K	64	SER	2.0
40	g	144	MET	2.0
59	z	438	MET	2.0
34	a	87	C	2.0
37	d	188	LEU	2.0
3	C	66	HIS	2.0
34	a	86	U	2.0
8	H	101	ARG	2.0
14	Q	59	ARG	2.0
34	a	138	A	2.0
37	d	168	ARG	2.0
22	Y	55	TYR	2.0

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

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
56	PSU	w	55	20/21	0.52	0.14	96,105,110,111	13
58	PSU	y	32	20/21	0.71	0.15	92,98,106,108	11
56	7MG	w	46	24/25	0.73	0.14	91,97,102,104	13
58	MIA	y	37	22/30	0.77	0.15	75,84,87,89	8
56	5MU	w	54	21/22	0.78	0.14	94,99,101,104	14
58	PSU	y	39	20/21	0.78	0.13	85,93,96,96	8
58	PSU	y	55	20/21	0.81	0.13	68,75,84,88	11
58	5MU	y	54	21/22	0.84	0.13	67,72,82,83	11
58	4SU	y	8	20/21	0.86	0.12	78,95,101,102	10
56	4SU	w	8	20/21	0.87	0.10	86,92,95,95	12
56	PSU	w	32	20/21	0.91	0.09	54,61,66,72	2
56	PSU	w	39	20/21	0.93	0.10	54,63,69,70	7
56	MIA	w	37	27/30	0.93	0.10	42,47,52,52	8
57	4SU	x	8	20/21	0.95	0.08	41,49,54,54	7
57	5MU	x	54	21/22	0.95	0.09	40,51,55,61	10
57	PSU	x	55	20/21	0.96	0.08	39,51,54,57	7
57	5MC	x	32	21/22	0.97	0.09	33,40,44,46	4

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($\text{\AA}^2$)	Q<0.9
60	MG	B	206	1/1	0.50	0.18	86,86,86,86	0
60	MG	A	3586	1/1	0.60	0.18	75,75,75,75	0
60	MG	A	3255	1/1	0.60	0.15	94,94,94,94	0
60	MG	A	3068	1/1	0.64	0.29	69,69,69,69	0
60	MG	A	3290	1/1	0.68	0.17	56,56,56,56	0
60	MG	A	3394	1/1	0.71	0.11	81,81,81,81	0
60	MG	A	3498	1/1	0.72	0.16	68,68,68,68	0
60	MG	B	211	1/1	0.72	0.30	69,69,69,69	0
60	MG	B	215	1/1	0.72	0.11	75,75,75,75	1
60	MG	a	1614	1/1	0.72	0.14	75,75,75,75	0
60	MG	A	3517	1/1	0.73	0.20	85,85,85,85	0
60	MG	A	3151	1/1	0.73	0.19	72,72,72,72	0
60	MG	A	3514	1/1	0.73	0.16	69,69,69,69	0
60	MG	a	1758	1/1	0.74	0.17	72,72,72,72	0
60	MG	A	3275	1/1	0.75	0.20	55,55,55,55	1
60	MG	A	3155	1/1	0.75	0.14	65,65,65,65	0
60	MG	a	1636	1/1	0.75	0.25	59,59,59,59	0
60	MG	a	1705	1/1	0.75	0.15	72,72,72,72	0
60	MG	A	3130	1/1	0.75	0.10	55,55,55,55	0
60	MG	e	201	1/1	0.75	0.09	78,78,78,78	0
60	MG	x	109	1/1	0.75	0.20	77,77,77,77	0
60	MG	a	1601	1/1	0.76	0.14	68,68,68,68	0
60	MG	a	1603	1/1	0.76	0.21	67,67,67,67	0
60	MG	A	3492	1/1	0.76	0.17	64,64,64,64	1
60	MG	A	3049	1/1	0.76	0.20	68,68,68,68	0
60	MG	A	3209	1/1	0.77	0.28	72,72,72,72	0
60	MG	a	1626	1/1	0.77	0.14	52,52,52,52	0
60	MG	A	3520	1/1	0.77	0.25	55,55,55,55	0
60	MG	a	1690	1/1	0.77	0.20	69,69,69,69	0
60	MG	A	3050	1/1	0.78	0.20	60,60,60,60	0
60	MG	V	202	1/1	0.78	0.22	73,73,73,73	0
60	MG	A	3236	1/1	0.78	0.24	47,47,47,47	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3246	1/1	0.78	0.18	66,66,66,66	0
60	MG	A	3508	1/1	0.79	0.10	68,68,68,68	0
60	MG	a	1641	1/1	0.79	0.17	68,68,68,68	0
60	MG	a	1689	1/1	0.79	0.26	74,74,74,74	0
60	MG	A	3610	1/1	0.79	0.11	62,62,62,62	0
60	MG	A	3144	1/1	0.79	0.17	51,51,51,51	0
60	MG	A	3063	1/1	0.79	0.22	49,49,49,49	0
60	MG	a	1623	1/1	0.79	0.16	46,46,46,46	1
60	MG	A	3253	1/1	0.79	0.13	67,67,67,67	0
60	MG	A	3061	1/1	0.80	0.12	43,43,43,43	0
60	MG	A	3556	1/1	0.80	0.11	35,35,35,35	1
60	MG	A	3423	1/1	0.80	0.14	73,73,73,73	0
60	MG	A	3441	1/1	0.80	0.15	52,52,52,52	0
60	MG	A	3630	1/1	0.80	0.21	34,34,34,34	1
60	MG	A	3252	1/1	0.80	0.15	76,76,76,76	0
60	MG	A	3496	1/1	0.80	0.24	33,33,33,33	1
60	MG	A	3277	1/1	0.80	0.15	47,47,47,47	1
60	MG	A	3282	1/1	0.80	0.20	68,68,68,68	0
60	MG	A	3157	1/1	0.80	0.30	40,40,40,40	1
60	MG	A	3295	1/1	0.80	0.23	58,58,58,58	0
60	MG	A	3551	1/1	0.81	0.15	71,71,71,71	0
60	MG	A	3333	1/1	0.81	0.14	61,61,61,61	1
60	MG	A	3572	1/1	0.81	0.12	58,58,58,58	0
60	MG	a	1662	1/1	0.81	0.13	53,53,53,53	0
60	MG	5	102	1/1	0.81	0.17	58,58,58,58	0
60	MG	A	3358	1/1	0.81	0.15	46,46,46,46	1
60	MG	A	3234	1/1	0.81	0.13	61,61,61,61	0
60	MG	A	3283	1/1	0.81	0.12	41,41,41,41	0
60	MG	a	1759	1/1	0.81	0.15	53,53,53,53	0
60	MG	a	1765	1/1	0.81	0.10	55,55,55,55	0
60	MG	a	1782	1/1	0.81	0.30	62,62,62,62	0
60	MG	a	1615	1/1	0.81	0.18	54,54,54,54	0
60	MG	A	3525	1/1	0.81	0.10	37,37,37,37	0
60	MG	6	101	1/1	0.82	0.20	42,42,42,42	1
60	MG	A	3188	1/1	0.82	0.20	39,39,39,39	0
60	MG	A	3344	1/1	0.82	0.15	70,70,70,70	0
60	MG	A	3011	1/1	0.82	0.25	53,53,53,53	0
60	MG	a	1732	1/1	0.82	0.12	54,54,54,54	0
60	MG	A	3249	1/1	0.82	0.14	72,72,72,72	0
60	MG	A	3554	1/1	0.82	0.14	67,67,67,67	0
60	MG	A	3420	1/1	0.82	0.12	55,55,55,55	0
60	MG	a	1779	1/1	0.82	0.16	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3559	1/1	0.82	0.17	38,38,38,38	1
60	MG	a	1787	1/1	0.82	0.33	40,40,40,40	1
60	MG	A	3179	1/1	0.82	0.22	61,61,61,61	0
60	MG	a	1653	1/1	0.82	0.20	61,61,61,61	0
60	MG	A	3464	1/1	0.83	0.11	56,56,56,56	0
60	MG	a	1664	1/1	0.83	0.24	62,62,62,62	0
60	MG	A	3194	1/1	0.83	0.12	63,63,63,63	0
60	MG	A	3578	1/1	0.83	0.15	60,60,60,60	0
60	MG	a	1701	1/1	0.83	0.10	66,66,66,66	0
60	MG	A	3052	1/1	0.83	0.13	51,51,51,51	1
60	MG	a	1612	1/1	0.83	0.09	57,57,57,57	0
60	MG	A	3531	1/1	0.83	0.10	55,55,55,55	0
60	MG	A	3537	1/1	0.83	0.09	45,45,45,45	0
60	MG	A	3548	1/1	0.83	0.15	65,65,65,65	0
60	MG	A	3154	1/1	0.83	0.14	67,67,67,67	0
60	MG	A	3278	1/1	0.83	0.11	56,56,56,56	0
60	MG	a	1638	1/1	0.83	0.14	53,53,53,53	0
60	MG	F	301	1/1	0.83	0.07	44,44,44,44	0
60	MG	A	3146	1/1	0.83	0.17	72,72,72,72	0
60	MG	A	3054	1/1	0.84	0.12	48,48,48,48	0
60	MG	a	1643	1/1	0.84	0.22	58,58,58,58	0
60	MG	a	1648	1/1	0.84	0.16	58,58,58,58	0
60	MG	R	202	1/1	0.84	0.11	62,62,62,62	0
60	MG	a	1661	1/1	0.84	0.17	69,69,69,69	0
60	MG	V	201	1/1	0.84	0.18	55,55,55,55	0
60	MG	A	3256	1/1	0.84	0.13	62,62,62,62	0
60	MG	Z	301	1/1	0.84	0.13	61,61,61,61	0
60	MG	A	3262	1/1	0.84	0.11	50,50,50,50	1
60	MG	A	3573	1/1	0.84	0.19	34,34,34,34	1
60	MG	A	3169	1/1	0.84	0.16	44,44,44,44	1
60	MG	a	1715	1/1	0.84	0.19	58,58,58,58	0
60	MG	a	1729	1/1	0.84	0.14	50,50,50,50	0
60	MG	A	3580	1/1	0.84	0.10	43,43,43,43	0
60	MG	A	3002	1/1	0.84	0.16	58,58,58,58	0
60	MG	A	3450	1/1	0.84	0.20	58,58,58,58	0
60	MG	A	3335	1/1	0.84	0.14	59,59,59,59	1
60	MG	A	3343	1/1	0.84	0.11	64,64,64,64	0
60	MG	B	207	1/1	0.84	0.09	76,76,76,76	0
60	MG	a	1635	1/1	0.84	0.09	55,55,55,55	0
60	MG	A	3119	1/1	0.84	0.13	68,68,68,68	0
60	MG	A	3356	1/1	0.84	0.10	50,50,50,50	0
60	MG	z	701	1/1	0.84	0.13	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3606	1/1	0.85	0.12	56,56,56,56	0
60	MG	A	3167	1/1	0.85	0.14	51,51,51,51	0
60	MG	A	3618	1/1	0.85	0.12	57,57,57,57	0
60	MG	A	3248	1/1	0.85	0.17	48,48,48,48	1
60	MG	A	3141	1/1	0.85	0.14	42,42,42,42	1
60	MG	A	3081	1/1	0.85	0.23	56,56,56,56	0
60	MG	A	3094	1/1	0.85	0.16	55,55,55,55	0
60	MG	A	3189	1/1	0.85	0.27	50,50,50,50	0
60	MG	A	3107	1/1	0.85	0.19	55,55,55,55	0
60	MG	a	1667	1/1	0.85	0.11	55,55,55,55	0
60	MG	A	3195	1/1	0.85	0.26	55,55,55,55	0
60	MG	A	3364	1/1	0.85	0.10	45,45,45,45	0
60	MG	A	3263	1/1	0.85	0.10	67,67,67,67	0
60	MG	A	3266	1/1	0.85	0.10	67,67,67,67	0
60	MG	5	101	1/1	0.85	0.14	44,44,44,44	1
60	MG	A	3267	1/1	0.85	0.10	64,64,64,64	0
60	MG	A	3108	1/1	0.85	0.22	60,60,60,60	0
60	MG	A	3448	1/1	0.85	0.20	60,60,60,60	0
60	MG	A	3225	1/1	0.85	0.14	54,54,54,54	0
60	MG	A	3576	1/1	0.85	0.09	59,59,59,59	0
60	MG	A	3034	1/1	0.85	0.15	59,59,59,59	0
60	MG	A	3010	1/1	0.85	0.14	32,32,32,32	1
60	MG	a	1620	1/1	0.85	0.18	47,47,47,47	0
60	MG	d	301	1/1	0.85	0.27	59,59,59,59	0
60	MG	A	3240	1/1	0.85	0.10	56,56,56,56	0
60	MG	A	3603	1/1	0.85	0.17	50,50,50,50	0
60	MG	A	3605	1/1	0.85	0.22	50,50,50,50	0
60	MG	A	3604	1/1	0.86	0.17	64,64,64,64	0
60	MG	A	3259	1/1	0.86	0.13	60,60,60,60	0
60	MG	A	3323	1/1	0.86	0.16	72,72,72,72	0
60	MG	A	3029	1/1	0.86	0.12	48,48,48,48	0
60	MG	A	3097	1/1	0.86	0.18	56,56,56,56	0
60	MG	a	1642	1/1	0.86	0.20	70,70,70,70	0
60	MG	A	3265	1/1	0.86	0.23	64,64,64,64	0
60	MG	B	203	1/1	0.86	0.08	56,56,56,56	0
60	MG	B	204	1/1	0.86	0.21	63,63,63,63	0
60	MG	a	1659	1/1	0.86	0.13	55,55,55,55	0
60	MG	a	1660	1/1	0.86	0.11	53,53,53,53	0
60	MG	A	3057	1/1	0.86	0.21	72,72,72,72	0
60	MG	A	3353	1/1	0.86	0.11	60,60,60,60	0
60	MG	a	1663	1/1	0.86	0.18	60,60,60,60	0
60	MG	A	3208	1/1	0.86	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3536	1/1	0.86	0.21	57,57,57,57	0
60	MG	a	1675	1/1	0.86	0.15	61,61,61,61	0
60	MG	a	1676	1/1	0.86	0.12	58,58,58,58	0
60	MG	a	1680	1/1	0.86	0.24	60,60,60,60	0
60	MG	A	3269	1/1	0.86	0.22	64,64,64,64	0
60	MG	A	3271	1/1	0.86	0.22	71,71,71,71	0
60	MG	A	3083	1/1	0.86	0.10	51,51,51,51	0
60	MG	A	3418	1/1	0.86	0.09	48,48,48,48	0
60	MG	A	3276	1/1	0.86	0.08	51,51,51,51	1
60	MG	a	1717	1/1	0.86	0.22	54,54,54,54	0
60	MG	A	3557	1/1	0.86	0.12	70,70,70,70	0
60	MG	A	3250	1/1	0.86	0.23	64,64,64,64	0
60	MG	A	3432	1/1	0.86	0.13	54,54,54,54	0
60	MG	A	3223	1/1	0.86	0.21	52,52,52,52	0
60	MG	a	1761	1/1	0.86	0.11	55,55,55,55	1
60	MG	A	3442	1/1	0.86	0.23	60,60,60,60	0
60	MG	a	1604	1/1	0.86	0.15	64,64,64,64	0
60	MG	a	1611	1/1	0.86	0.11	58,58,58,58	0
60	MG	A	3110	1/1	0.86	0.22	25,25,25,25	1
60	MG	A	3231	1/1	0.86	0.20	68,68,68,68	0
60	MG	A	3284	1/1	0.86	0.10	39,39,39,39	1
60	MG	x	102	1/1	0.86	0.21	77,77,77,77	0
60	MG	x	108	1/1	0.86	0.20	55,55,55,55	0
60	MG	A	3594	1/1	0.86	0.15	85,85,85,85	0
60	MG	A	3085	1/1	0.86	0.17	70,70,70,70	0
60	MG	O	201	1/1	0.87	0.10	55,55,55,55	0
60	MG	P	201	1/1	0.87	0.14	59,59,59,59	0
60	MG	A	3244	1/1	0.87	0.12	53,53,53,53	0
60	MG	A	3088	1/1	0.87	0.12	53,53,53,53	0
60	MG	A	3511	1/1	0.87	0.14	50,50,50,50	0
60	MG	A	3579	1/1	0.87	0.10	50,50,50,50	0
60	MG	0	103	1/1	0.87	0.16	53,53,53,53	0
60	MG	a	1669	1/1	0.87	0.24	60,60,60,60	0
60	MG	A	3072	1/1	0.87	0.09	46,46,46,46	0
60	MG	A	3406	1/1	0.87	0.17	74,74,74,74	0
60	MG	A	3006	1/1	0.87	0.17	52,52,52,52	1
60	MG	A	3600	1/1	0.87	0.09	53,53,53,53	0
60	MG	a	1602	1/1	0.87	0.12	57,57,57,57	0
60	MG	A	3307	1/1	0.87	0.12	60,60,60,60	0
60	MG	a	1703	1/1	0.87	0.13	57,57,57,57	1
60	MG	A	3530	1/1	0.87	0.13	38,38,38,38	1
60	MG	A	3309	1/1	0.87	0.12	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3321	1/1	0.87	0.10	49,49,49,49	0
60	MG	A	3438	1/1	0.87	0.15	77,77,77,77	0
60	MG	A	3612	1/1	0.87	0.09	62,62,62,62	0
60	MG	A	3541	1/1	0.87	0.08	63,63,63,63	0
60	MG	A	3098	1/1	0.87	0.11	61,61,61,61	0
60	MG	A	3636	1/1	0.87	0.19	37,37,37,37	1
60	MG	a	1627	1/1	0.87	0.14	47,47,47,47	0
60	MG	a	1632	1/1	0.87	0.16	42,42,42,42	0
60	MG	A	3233	1/1	0.87	0.10	56,56,56,56	0
60	MG	A	3066	1/1	0.87	0.17	58,58,58,58	0
60	MG	A	3235	1/1	0.87	0.08	43,43,43,43	0
60	MG	A	3205	1/1	0.87	0.10	53,53,53,53	0
60	MG	A	3237	1/1	0.87	0.15	43,43,43,43	1
60	MG	A	3563	1/1	0.87	0.09	46,46,46,46	0
60	MG	A	3022	1/1	0.87	0.17	59,59,59,59	0
60	MG	N	201	1/1	0.87	0.16	42,42,42,42	0
60	MG	A	3184	1/1	0.88	0.24	30,30,30,30	0
60	MG	A	3075	1/1	0.88	0.11	60,60,60,60	1
60	MG	A	3581	1/1	0.88	0.10	63,63,63,63	0
60	MG	a	1686	1/1	0.88	0.15	61,61,61,61	0
60	MG	a	1618	1/1	0.88	0.28	54,54,54,54	0
60	MG	D	305	1/1	0.88	0.20	43,43,43,43	0
60	MG	A	3493	1/1	0.88	0.12	48,48,48,48	1
60	MG	F	303	1/1	0.88	0.11	53,53,53,53	0
60	MG	A	3588	1/1	0.88	0.18	60,60,60,60	0
60	MG	A	3332	1/1	0.88	0.11	53,53,53,53	0
60	MG	A	3058	1/1	0.88	0.09	59,59,59,59	0
60	MG	A	3056	1/1	0.88	0.09	39,39,39,39	0
60	MG	A	3555	1/1	0.88	0.16	63,63,63,63	0
60	MG	a	1755	1/1	0.88	0.08	40,40,40,40	0
60	MG	A	3039	1/1	0.88	0.21	63,63,63,63	0
60	MG	A	3513	1/1	0.88	0.20	58,58,58,58	0
60	MG	A	3257	1/1	0.88	0.10	52,52,52,52	0
60	MG	A	3291	1/1	0.88	0.17	55,55,55,55	0
60	MG	a	1772	1/1	0.88	0.16	62,62,62,62	0
60	MG	a	1778	1/1	0.88	0.09	53,53,53,53	0
60	MG	A	3613	1/1	0.88	0.22	67,67,67,67	0
60	MG	A	3564	1/1	0.88	0.10	52,52,52,52	0
60	MG	a	1786	1/1	0.88	0.17	38,38,38,38	1
60	MG	A	3274	1/1	0.88	0.14	66,66,66,66	0
60	MG	A	3148	1/1	0.88	0.10	47,47,47,47	0
60	MG	A	3449	1/1	0.88	0.09	29,29,29,29	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3577	1/1	0.88	0.16	60,60,60,60	0
60	MG	a	1606	1/1	0.88	0.10	48,48,48,48	0
60	MG	a	1609	1/1	0.88	0.23	51,51,51,51	0
60	MG	A	3126	1/1	0.88	0.09	28,28,28,28	1
60	MG	A	3436	1/1	0.89	0.07	43,43,43,43	0
60	MG	0	101	1/1	0.89	0.12	39,39,39,39	0
60	MG	0	102	1/1	0.89	0.09	47,47,47,47	0
60	MG	A	3016	1/1	0.89	0.20	59,59,59,59	0
60	MG	A	3254	1/1	0.89	0.19	62,62,62,62	0
60	MG	a	1665	1/1	0.89	0.17	47,47,47,47	1
60	MG	A	3545	1/1	0.89	0.08	42,42,42,42	0
60	MG	A	3132	1/1	0.89	0.14	43,43,43,43	1
60	MG	a	1671	1/1	0.89	0.17	48,48,48,48	0
60	MG	7	101	1/1	0.89	0.12	63,63,63,63	0
60	MG	A	3175	1/1	0.89	0.12	62,62,62,62	0
60	MG	A	3207	1/1	0.89	0.21	61,61,61,61	0
60	MG	A	3082	1/1	0.89	0.15	43,43,43,43	1
60	MG	A	3454	1/1	0.89	0.13	44,44,44,44	0
60	MG	A	3099	1/1	0.89	0.10	51,51,51,51	0
60	MG	A	3467	1/1	0.89	0.09	37,37,37,37	0
60	MG	B	201	1/1	0.89	0.08	53,53,53,53	1
60	MG	A	3561	1/1	0.89	0.18	60,60,60,60	0
60	MG	A	3217	1/1	0.89	0.16	56,56,56,56	1
60	MG	A	3289	1/1	0.89	0.12	59,59,59,59	0
60	MG	a	1718	1/1	0.89	0.13	55,55,55,55	1
60	MG	A	3569	1/1	0.89	0.07	41,41,41,41	0
60	MG	A	3220	1/1	0.89	0.15	45,45,45,45	0
60	MG	a	1733	1/1	0.89	0.21	51,51,51,51	0
60	MG	a	1751	1/1	0.89	0.16	59,59,59,59	0
60	MG	A	3362	1/1	0.89	0.15	47,47,47,47	0
60	MG	a	1625	1/1	0.89	0.17	60,60,60,60	0
60	MG	A	3064	1/1	0.89	0.14	58,58,58,58	0
60	MG	A	3374	1/1	0.89	0.21	54,54,54,54	0
60	MG	A	3292	1/1	0.89	0.13	47,47,47,47	0
60	MG	A	3164	1/1	0.89	0.18	31,31,31,31	0
60	MG	A	3301	1/1	0.89	0.14	54,54,54,54	0
60	MG	A	3227	1/1	0.89	0.20	63,63,63,63	0
60	MG	a	1640	1/1	0.89	0.20	68,68,68,68	0
60	MG	a	1785	1/1	0.89	0.25	53,53,53,53	0
60	MG	P	202	1/1	0.89	0.18	59,59,59,59	0
60	MG	P	203	1/1	0.89	0.09	45,45,45,45	1
60	MG	A	3191	1/1	0.89	0.08	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	a	1646	1/1	0.89	0.12	52,52,52,52	0
60	MG	n	101	1/1	0.89	0.32	64,64,64,64	0
60	MG	A	3316	1/1	0.89	0.13	63,63,63,63	0
60	MG	A	3435	1/1	0.89	0.09	51,51,51,51	0
60	MG	a	1657	1/1	0.89	0.10	57,57,57,57	0
60	MG	W	201	1/1	0.89	0.22	59,59,59,59	0
60	MG	A	3535	1/1	0.90	0.12	55,55,55,55	0
60	MG	A	3142	1/1	0.90	0.08	57,57,57,57	0
60	MG	A	3143	1/1	0.90	0.17	55,55,55,55	0
60	MG	A	3228	1/1	0.90	0.15	49,49,49,49	0
60	MG	A	3428	1/1	0.90	0.08	56,56,56,56	0
60	MG	A	3027	1/1	0.90	0.07	62,62,62,62	0
60	MG	A	3550	1/1	0.90	0.31	65,65,65,65	0
60	MG	a	1649	1/1	0.90	0.26	67,67,67,67	0
60	MG	a	1651	1/1	0.90	0.20	64,64,64,64	0
60	MG	B	214	1/1	0.90	0.11	59,59,59,59	0
60	MG	A	3076	1/1	0.90	0.33	33,33,33,33	1
60	MG	A	3553	1/1	0.90	0.10	51,51,51,51	1
60	MG	A	3118	1/1	0.90	0.13	64,64,64,64	0
60	MG	F	302	1/1	0.90	0.16	32,32,32,32	1
60	MG	A	3437	1/1	0.90	0.10	30,30,30,30	1
60	MG	F	306	1/1	0.90	0.12	46,46,46,46	0
60	MG	A	3320	1/1	0.90	0.12	62,62,62,62	0
60	MG	A	3149	1/1	0.90	0.12	54,54,54,54	0
60	MG	a	1666	1/1	0.90	0.29	68,68,68,68	0
60	MG	A	3044	1/1	0.90	0.14	25,25,25,25	1
60	MG	A	3443	1/1	0.90	0.12	41,41,41,41	0
60	MG	a	1670	1/1	0.90	0.08	57,57,57,57	0
60	MG	A	3562	1/1	0.90	0.09	67,67,67,67	0
60	MG	a	1673	1/1	0.90	0.11	60,60,60,60	0
60	MG	A	3270	1/1	0.90	0.10	51,51,51,51	0
60	MG	A	3100	1/1	0.90	0.12	66,66,66,66	0
60	MG	A	3568	1/1	0.90	0.08	61,61,61,61	0
60	MG	A	3196	1/1	0.90	0.14	51,51,51,51	0
60	MG	A	3452	1/1	0.90	0.08	69,69,69,69	0
60	MG	A	3336	1/1	0.90	0.10	52,52,52,52	0
60	MG	a	1700	1/1	0.90	0.16	50,50,50,50	0
60	MG	A	3574	1/1	0.90	0.09	39,39,39,39	0
60	MG	A	3462	1/1	0.90	0.10	58,58,58,58	0
60	MG	A	3342	1/1	0.90	0.20	58,58,58,58	0
60	MG	A	3197	1/1	0.90	0.09	48,48,48,48	1
60	MG	A	3470	1/1	0.90	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3485	1/1	0.90	0.12	59,59,59,59	0
60	MG	9	101	1/1	0.90	0.19	50,50,50,50	0
60	MG	a	1731	1/1	0.90	0.10	49,49,49,49	0
60	MG	A	3199	1/1	0.90	0.13	45,45,45,45	0
60	MG	A	3350	1/1	0.90	0.10	59,59,59,59	0
60	MG	A	3101	1/1	0.90	0.11	47,47,47,47	0
60	MG	a	1753	1/1	0.90	0.23	46,46,46,46	0
60	MG	A	3589	1/1	0.90	0.07	42,42,42,42	0
60	MG	a	1605	1/1	0.90	0.09	54,54,54,54	0
60	MG	A	3591	1/1	0.90	0.12	39,39,39,39	1
60	MG	A	3593	1/1	0.90	0.08	70,70,70,70	0
60	MG	A	3131	1/1	0.90	0.18	57,57,57,57	0
60	MG	A	3597	1/1	0.90	0.17	47,47,47,47	0
60	MG	A	3158	1/1	0.90	0.14	38,38,38,38	1
60	MG	A	3602	1/1	0.90	0.14	48,48,48,48	0
60	MG	A	3160	1/1	0.90	0.32	57,57,57,57	0
60	MG	A	3214	1/1	0.90	0.11	44,44,44,44	1
60	MG	A	3102	1/1	0.90	0.10	55,55,55,55	0
60	MG	A	3382	1/1	0.90	0.14	30,30,30,30	0
60	MG	A	3519	1/1	0.90	0.11	48,48,48,48	0
60	MG	A	3388	1/1	0.90	0.08	31,31,31,31	0
60	MG	a	1629	1/1	0.90	0.09	44,44,44,44	0
60	MG	a	1631	1/1	0.90	0.16	42,42,42,42	0
60	MG	A	3391	1/1	0.90	0.20	56,56,56,56	0
60	MG	A	3135	1/1	0.90	0.17	59,59,59,59	0
60	MG	A	3036	1/1	0.90	0.11	25,25,25,25	1
60	MG	A	3463	1/1	0.91	0.28	48,48,48,48	0
60	MG	A	3607	1/1	0.91	0.11	54,54,54,54	0
60	MG	A	3305	1/1	0.91	0.06	38,38,38,38	0
60	MG	A	3092	1/1	0.91	0.11	58,58,58,58	0
60	MG	A	3468	1/1	0.91	0.09	37,37,37,37	1
60	MG	A	3268	1/1	0.91	0.08	52,52,52,52	0
60	MG	a	1674	1/1	0.91	0.24	50,50,50,50	0
60	MG	A	3624	1/1	0.91	0.31	63,63,63,63	0
60	MG	A	3628	1/1	0.91	0.19	35,35,35,35	0
60	MG	a	1677	1/1	0.91	0.08	63,63,63,63	0
60	MG	a	1679	1/1	0.91	0.13	39,39,39,39	0
60	MG	A	3482	1/1	0.91	0.13	38,38,38,38	0
60	MG	A	3633	1/1	0.91	0.17	30,30,30,30	0
60	MG	A	3242	1/1	0.91	0.23	61,61,61,61	0
60	MG	A	3644	1/1	0.91	0.13	42,42,42,42	0
60	MG	a	1691	1/1	0.91	0.16	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3488	1/1	0.91	0.11	41,41,41,41	0
60	MG	A	3395	1/1	0.91	0.12	51,51,51,51	0
60	MG	A	3147	1/1	0.91	0.19	50,50,50,50	0
60	MG	A	3180	1/1	0.91	0.17	44,44,44,44	0
60	MG	a	1713	1/1	0.91	0.20	43,43,43,43	0
60	MG	A	3215	1/1	0.91	0.18	44,44,44,44	0
60	MG	A	3328	1/1	0.91	0.10	62,62,62,62	0
60	MG	A	3121	1/1	0.91	0.10	38,38,38,38	1
60	MG	A	3008	1/1	0.91	0.10	42,42,42,42	0
60	MG	B	216	1/1	0.91	0.08	53,53,53,53	0
60	MG	A	3221	1/1	0.91	0.23	49,49,49,49	0
60	MG	A	3106	1/1	0.91	0.11	46,46,46,46	1
60	MG	a	1741	1/1	0.91	0.17	63,63,63,63	0
60	MG	A	3280	1/1	0.91	0.21	46,46,46,46	0
60	MG	A	3012	1/1	0.91	0.10	60,60,60,60	0
60	MG	A	3523	1/1	0.91	0.08	31,31,31,31	0
60	MG	G	201	1/1	0.91	0.15	48,48,48,48	0
60	MG	H	201	1/1	0.91	0.10	62,62,62,62	0
60	MG	A	3084	1/1	0.91	0.13	56,56,56,56	0
60	MG	a	1762	1/1	0.91	0.11	52,52,52,52	0
60	MG	A	3528	1/1	0.91	0.10	51,51,51,51	0
60	MG	a	1770	1/1	0.91	0.19	56,56,56,56	0
60	MG	A	3585	1/1	0.91	0.21	46,46,46,46	0
60	MG	A	3133	1/1	0.91	0.09	36,36,36,36	1
60	MG	A	3060	1/1	0.91	0.07	54,54,54,54	0
60	MG	A	3532	1/1	0.91	0.10	41,41,41,41	0
60	MG	A	3111	1/1	0.91	0.09	46,46,46,46	0
60	MG	a	1656	1/1	0.91	0.11	60,60,60,60	0
60	MG	A	3114	1/1	0.91	0.17	42,42,42,42	0
60	MG	A	3203	1/1	0.91	0.22	52,52,52,52	0
60	MG	A	3451	1/1	0.91	0.13	45,45,45,45	0
60	MG	A	3542	1/1	0.91	0.20	63,63,63,63	0
60	MG	A	3543	1/1	0.91	0.08	51,51,51,51	0
60	MG	x	107	1/1	0.91	0.11	69,69,69,69	0
60	MG	A	3117	1/1	0.91	0.11	48,48,48,48	0
60	MG	A	3367	1/1	0.91	0.06	40,40,40,40	0
60	MG	A	3032	1/1	0.91	0.17	50,50,50,50	0
60	MG	a	1678	1/1	0.92	0.15	36,36,36,36	0
60	MG	A	3173	1/1	0.92	0.19	37,37,37,37	0
60	MG	a	1621	1/1	0.92	0.10	64,64,64,64	0
60	MG	a	1681	1/1	0.92	0.15	55,55,55,55	0
60	MG	a	1683	1/1	0.92	0.21	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	E	303	1/1	0.92	0.18	32,32,32,32	1
60	MG	A	3544	1/1	0.92	0.18	53,53,53,53	0
60	MG	A	3297	1/1	0.92	0.10	35,35,35,35	1
60	MG	A	3421	1/1	0.92	0.10	57,57,57,57	0
60	MG	a	1693	1/1	0.92	0.21	39,39,39,39	0
60	MG	A	3422	1/1	0.92	0.15	52,52,52,52	0
60	MG	A	3599	1/1	0.92	0.09	45,45,45,45	0
60	MG	A	3232	1/1	0.92	0.11	35,35,35,35	0
60	MG	a	1704	1/1	0.92	0.14	52,52,52,52	0
60	MG	A	3212	1/1	0.92	0.07	46,46,46,46	0
60	MG	a	1711	1/1	0.92	0.06	48,48,48,48	0
60	MG	A	3355	1/1	0.92	0.14	61,61,61,61	0
60	MG	a	1714	1/1	0.92	0.15	54,54,54,54	0
60	MG	a	1637	1/1	0.92	0.19	54,54,54,54	0
60	MG	A	3434	1/1	0.92	0.07	41,41,41,41	0
60	MG	A	3115	1/1	0.92	0.21	27,27,27,27	1
60	MG	A	3505	1/1	0.92	0.06	41,41,41,41	0
60	MG	a	1730	1/1	0.92	0.19	53,53,53,53	0
60	MG	A	3128	1/1	0.92	0.08	37,37,37,37	0
60	MG	U	201	1/1	0.92	0.21	30,30,30,30	1
60	MG	a	1644	1/1	0.92	0.14	46,46,46,46	0
60	MG	A	3560	1/1	0.92	0.15	58,58,58,58	0
60	MG	a	1748	1/1	0.92	0.07	46,46,46,46	0
60	MG	a	1749	1/1	0.92	0.18	54,54,54,54	0
60	MG	A	3360	1/1	0.92	0.11	54,54,54,54	0
60	MG	A	3361	1/1	0.92	0.12	64,64,64,64	0
60	MG	a	1754	1/1	0.92	0.08	42,42,42,42	0
60	MG	A	3089	1/1	0.92	0.12	58,58,58,58	0
60	MG	A	3622	1/1	0.92	0.28	57,57,57,57	0
60	MG	a	1655	1/1	0.92	0.18	47,47,47,47	0
60	MG	A	3218	1/1	0.92	0.22	52,52,52,52	0
60	MG	A	3182	1/1	0.92	0.23	43,43,43,43	0
60	MG	a	1764	1/1	0.92	0.17	37,37,37,37	0
60	MG	A	3183	1/1	0.92	0.17	21,21,21,21	0
60	MG	a	1767	1/1	0.92	0.09	45,45,45,45	0
60	MG	A	3264	1/1	0.92	0.12	23,23,23,23	1
60	MG	A	3384	1/1	0.92	0.08	39,39,39,39	0
60	MG	A	3637	1/1	0.92	0.25	37,37,37,37	0
60	MG	A	3091	1/1	0.92	0.10	49,49,49,49	0
60	MG	A	3041	1/1	0.92	0.06	38,38,38,38	0
60	MG	a	1783	1/1	0.92	0.30	60,60,60,60	0
60	MG	A	3453	1/1	0.92	0.13	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3055	1/1	0.92	0.08	47,47,47,47	0
60	MG	B	205	1/1	0.92	0.18	52,52,52,52	0
60	MG	A	3190	1/1	0.92	0.24	58,58,58,58	0
60	MG	A	3404	1/1	0.92	0.18	35,35,35,35	0
60	MG	B	209	1/1	0.92	0.13	60,60,60,60	0
60	MG	A	3229	1/1	0.92	0.09	39,39,39,39	0
60	MG	B	213	1/1	0.92	0.11	52,52,52,52	0
60	MG	A	3540	1/1	0.92	0.14	57,57,57,57	0
60	MG	A	3465	1/1	0.92	0.09	59,59,59,59	0
60	MG	A	3408	1/1	0.92	0.10	33,33,33,33	0
60	MG	A	3431	1/1	0.93	0.16	52,52,52,52	0
60	MG	A	3570	1/1	0.93	0.09	54,54,54,54	0
60	MG	a	1616	1/1	0.93	0.14	54,54,54,54	0
60	MG	A	3238	1/1	0.93	0.07	38,38,38,38	0
60	MG	A	3433	1/1	0.93	0.08	27,27,27,27	1
60	MG	a	1692	1/1	0.93	0.17	41,41,41,41	0
60	MG	A	3123	1/1	0.93	0.09	30,30,30,30	1
60	MG	a	1695	1/1	0.93	0.21	40,40,40,40	0
60	MG	a	1696	1/1	0.93	0.27	52,52,52,52	0
60	MG	B	212	1/1	0.93	0.10	52,52,52,52	0
60	MG	A	3357	1/1	0.93	0.17	36,36,36,36	0
60	MG	A	3518	1/1	0.93	0.07	39,39,39,39	0
60	MG	A	3219	1/1	0.93	0.20	50,50,50,50	0
60	MG	a	1628	1/1	0.93	0.12	45,45,45,45	0
60	MG	a	1710	1/1	0.93	0.10	53,53,53,53	1
60	MG	A	3359	1/1	0.93	0.09	63,63,63,63	0
60	MG	a	1712	1/1	0.93	0.10	54,54,54,54	0
60	MG	D	304	1/1	0.93	0.12	36,36,36,36	1
60	MG	A	3124	1/1	0.93	0.10	32,32,32,32	1
60	MG	A	3037	1/1	0.93	0.07	44,44,44,44	0
60	MG	A	3145	1/1	0.93	0.19	61,61,61,61	0
60	MG	A	3127	1/1	0.93	0.09	24,24,24,24	1
60	MG	A	3312	1/1	0.93	0.06	40,40,40,40	0
60	MG	A	3368	1/1	0.93	0.12	36,36,36,36	0
60	MG	A	3534	1/1	0.93	0.12	35,35,35,35	0
60	MG	A	3201	1/1	0.93	0.18	45,45,45,45	0
60	MG	A	3381	1/1	0.93	0.15	56,56,56,56	0
60	MG	A	3319	1/1	0.93	0.09	43,43,43,43	0
60	MG	a	1744	1/1	0.93	0.09	46,46,46,46	0
60	MG	A	3538	1/1	0.93	0.12	39,39,39,39	0
60	MG	A	3251	1/1	0.93	0.08	46,46,46,46	0
60	MG	A	3386	1/1	0.93	0.08	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Q	201	1/1	0.93	0.19	47,47,47,47	0
60	MG	R	201	1/1	0.93	0.15	50,50,50,50	0
60	MG	a	1654	1/1	0.93	0.09	50,50,50,50	0
60	MG	A	3461	1/1	0.93	0.08	40,40,40,40	0
60	MG	A	3024	1/1	0.93	0.10	40,40,40,40	0
60	MG	A	3104	1/1	0.93	0.14	25,25,25,25	0
60	MG	A	3087	1/1	0.93	0.07	41,41,41,41	0
60	MG	A	3014	1/1	0.93	0.08	37,37,37,37	0
60	MG	A	3402	1/1	0.93	0.16	36,36,36,36	0
60	MG	A	3071	1/1	0.93	0.19	61,61,61,61	0
60	MG	a	1768	1/1	0.93	0.18	43,43,43,43	0
60	MG	a	1769	1/1	0.93	0.10	58,58,58,58	0
60	MG	A	3134	1/1	0.93	0.09	25,25,25,25	0
60	MG	a	1771	1/1	0.93	0.07	67,67,67,67	0
60	MG	A	3474	1/1	0.93	0.15	44,44,44,44	0
60	MG	a	1773	1/1	0.93	0.10	58,58,58,58	0
60	MG	a	1777	1/1	0.93	0.09	32,32,32,32	1
60	MG	0	104	1/1	0.93	0.11	36,36,36,36	1
60	MG	A	3043	1/1	0.93	0.08	39,39,39,39	0
60	MG	a	1780	1/1	0.93	0.10	54,54,54,54	0
60	MG	A	3623	1/1	0.93	0.23	57,57,57,57	0
60	MG	A	3260	1/1	0.93	0.12	44,44,44,44	1
60	MG	a	1784	1/1	0.93	0.24	52,52,52,52	0
60	MG	A	3285	1/1	0.93	0.08	31,31,31,31	0
60	MG	A	3558	1/1	0.93	0.12	53,53,53,53	0
60	MG	A	3632	1/1	0.93	0.10	35,35,35,35	1
60	MG	A	3491	1/1	0.93	0.18	39,39,39,39	0
60	MG	A	3261	1/1	0.93	0.14	46,46,46,46	0
60	MG	A	3347	1/1	0.93	0.07	37,37,37,37	1
60	MG	n	103	1/1	0.93	0.14	55,55,55,55	0
60	MG	A	3639	1/1	0.93	0.11	36,36,36,36	0
60	MG	x	103	1/1	0.93	0.07	62,62,62,62	0
60	MG	x	104	1/1	0.93	0.17	43,43,43,43	0
60	MG	A	3140	1/1	0.93	0.18	48,48,48,48	0
60	MG	A	3122	1/1	0.93	0.10	51,51,51,51	1
60	MG	A	3430	1/1	0.93	0.10	43,43,43,43	0
60	MG	A	3506	1/1	0.93	0.06	41,41,41,41	0
60	MG	a	1694	1/1	0.94	0.15	41,41,41,41	0
60	MG	A	3105	1/1	0.94	0.13	28,28,28,28	1
60	MG	a	1617	1/1	0.94	0.14	47,47,47,47	0
60	MG	A	3028	1/1	0.94	0.06	57,57,57,57	0
60	MG	a	1619	1/1	0.94	0.06	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3051	1/1	0.94	0.17	54,54,54,54	0
60	MG	A	3466	1/1	0.94	0.11	49,49,49,49	0
60	MG	A	3065	1/1	0.94	0.18	64,64,64,64	0
60	MG	a	1706	1/1	0.94	0.12	48,48,48,48	0
60	MG	a	1624	1/1	0.94	0.07	39,39,39,39	0
60	MG	A	3392	1/1	0.94	0.07	42,42,42,42	0
60	MG	A	3007	1/1	0.94	0.10	35,35,35,35	0
60	MG	B	208	1/1	0.94	0.12	64,64,64,64	0
60	MG	A	3053	1/1	0.94	0.08	35,35,35,35	0
60	MG	B	210	1/1	0.94	0.07	44,44,44,44	0
60	MG	A	3476	1/1	0.94	0.07	58,58,58,58	0
60	MG	A	3159	1/1	0.94	0.09	45,45,45,45	1
60	MG	a	1724	1/1	0.94	0.13	42,42,42,42	0
60	MG	a	1725	1/1	0.94	0.13	51,51,51,51	0
60	MG	A	3040	1/1	0.94	0.10	31,31,31,31	1
60	MG	A	3093	1/1	0.94	0.21	50,50,50,50	0
60	MG	A	3204	1/1	0.94	0.07	39,39,39,39	0
60	MG	A	3409	1/1	0.94	0.07	35,35,35,35	0
60	MG	A	3411	1/1	0.94	0.10	39,39,39,39	0
60	MG	a	1737	1/1	0.94	0.16	46,46,46,46	0
60	MG	A	3494	1/1	0.94	0.07	35,35,35,35	0
60	MG	a	1743	1/1	0.94	0.10	45,45,45,45	0
60	MG	A	3416	1/1	0.94	0.07	31,31,31,31	0
60	MG	a	1746	1/1	0.94	0.06	49,49,49,49	0
60	MG	A	3417	1/1	0.94	0.11	43,43,43,43	0
60	MG	A	3503	1/1	0.94	0.09	53,53,53,53	0
60	MG	A	3504	1/1	0.94	0.09	25,25,25,25	0
60	MG	a	1752	1/1	0.94	0.19	43,43,43,43	0
60	MG	a	1647	1/1	0.94	0.06	35,35,35,35	0
60	MG	A	3334	1/1	0.94	0.11	57,57,57,57	0
60	MG	A	3137	1/1	0.94	0.16	35,35,35,35	0
60	MG	A	3206	1/1	0.94	0.07	50,50,50,50	0
60	MG	A	3138	1/1	0.94	0.05	31,31,31,31	0
60	MG	A	3116	1/1	0.94	0.14	47,47,47,47	0
60	MG	A	3427	1/1	0.94	0.10	49,49,49,49	0
60	MG	A	3025	1/1	0.94	0.12	51,51,51,51	1
60	MG	A	3247	1/1	0.94	0.10	46,46,46,46	1
60	MG	A	3210	1/1	0.94	0.22	30,30,30,30	0
60	MG	A	3177	1/1	0.94	0.17	39,39,39,39	0
60	MG	A	3521	1/1	0.94	0.07	35,35,35,35	1
60	MG	A	3354	1/1	0.94	0.07	53,53,53,53	0
60	MG	A	3178	1/1	0.94	0.20	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3526	1/1	0.94	0.13	29,29,29,29	0
60	MG	A	3527	1/1	0.94	0.11	45,45,45,45	0
60	MG	a	1775	1/1	0.94	0.11	53,53,53,53	1
60	MG	A	3042	1/1	0.94	0.08	40,40,40,40	0
60	MG	A	3033	1/1	0.94	0.07	59,59,59,59	1
60	MG	A	3181	1/1	0.94	0.22	49,49,49,49	0
60	MG	A	3079	1/1	0.94	0.08	18,18,18,18	0
60	MG	A	3026	1/1	0.94	0.12	43,43,43,43	0
60	MG	A	3293	1/1	0.94	0.14	48,48,48,48	0
60	MG	A	3048	1/1	0.94	0.05	35,35,35,35	0
60	MG	A	3444	1/1	0.94	0.11	39,39,39,39	0
60	MG	A	3015	1/1	0.94	0.07	45,45,45,45	0
60	MG	A	3620	1/1	0.94	0.06	29,29,29,29	0
60	MG	A	3365	1/1	0.94	0.08	35,35,35,35	0
60	MG	A	3299	1/1	0.94	0.12	35,35,35,35	0
60	MG	A	3224	1/1	0.94	0.09	34,34,34,34	0
60	MG	A	3371	1/1	0.94	0.06	40,40,40,40	0
60	MG	v	101	1/1	0.94	0.10	35,35,35,35	1
60	MG	x	101	1/1	0.94	0.16	29,29,29,29	1
60	MG	A	3303	1/1	0.94	0.09	57,57,57,57	0
60	MG	A	3380	1/1	0.94	0.08	45,45,45,45	0
60	MG	A	3458	1/1	0.94	0.11	38,38,38,38	0
60	MG	x	105	1/1	0.94	0.06	51,51,51,51	0
60	MG	A	3549	1/1	0.94	0.09	47,47,47,47	0
60	MG	A	3062	1/1	0.94	0.11	41,41,41,41	0
60	MG	A	3638	1/1	0.94	0.08	38,38,38,38	0
60	MG	A	3226	1/1	0.94	0.20	45,45,45,45	0
60	MG	A	3239	1/1	0.95	0.26	51,51,51,51	0
60	MG	A	3445	1/1	0.95	0.11	42,42,42,42	1
60	MG	a	1697	1/1	0.95	0.11	34,34,34,34	0
60	MG	a	1699	1/1	0.95	0.10	56,56,56,56	0
60	MG	a	1610	1/1	0.95	0.23	32,32,32,32	1
60	MG	A	3447	1/1	0.95	0.11	47,47,47,47	0
60	MG	A	3533	1/1	0.95	0.15	52,52,52,52	0
60	MG	A	3187	1/1	0.95	0.17	31,31,31,31	0
60	MG	A	3373	1/1	0.95	0.06	34,34,34,34	0
60	MG	A	3310	1/1	0.95	0.14	37,37,37,37	0
60	MG	A	3080	1/1	0.95	0.10	48,48,48,48	0
60	MG	A	3315	1/1	0.95	0.07	37,37,37,37	0
60	MG	A	3243	1/1	0.95	0.09	52,52,52,52	0
60	MG	A	3317	1/1	0.95	0.06	52,52,52,52	0
60	MG	A	3385	1/1	0.95	0.05	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3460	1/1	0.95	0.05	41,41,41,41	0
60	MG	A	3641	1/1	0.95	0.07	32,32,32,32	1
60	MG	A	3643	1/1	0.95	0.14	34,34,34,34	0
60	MG	a	1722	1/1	0.95	0.14	51,51,51,51	0
60	MG	a	1723	1/1	0.95	0.12	48,48,48,48	0
60	MG	A	3216	1/1	0.95	0.17	31,31,31,31	0
60	MG	A	3272	1/1	0.95	0.17	55,55,55,55	0
60	MG	a	1727	1/1	0.95	0.06	49,49,49,49	0
60	MG	A	3113	1/1	0.95	0.16	29,29,29,29	1
60	MG	A	3322	1/1	0.95	0.06	42,42,42,42	1
60	MG	a	1630	1/1	0.95	0.19	44,44,44,44	0
60	MG	A	3393	1/1	0.95	0.12	41,41,41,41	0
60	MG	A	3059	1/1	0.95	0.07	37,37,37,37	1
60	MG	a	1734	1/1	0.95	0.04	33,33,33,33	0
60	MG	a	1736	1/1	0.95	0.05	46,46,46,46	0
60	MG	A	3165	1/1	0.95	0.17	42,42,42,42	0
60	MG	a	1740	1/1	0.95	0.08	58,58,58,58	0
60	MG	A	3399	1/1	0.95	0.09	44,44,44,44	0
60	MG	a	1742	1/1	0.95	0.09	58,58,58,58	0
60	MG	A	3400	1/1	0.95	0.13	42,42,42,42	0
60	MG	A	3166	1/1	0.95	0.08	40,40,40,40	0
60	MG	A	3475	1/1	0.95	0.07	41,41,41,41	0
60	MG	A	3129	1/1	0.95	0.10	35,35,35,35	1
60	MG	A	3477	1/1	0.95	0.06	21,21,21,21	0
60	MG	a	1750	1/1	0.95	0.10	41,41,41,41	0
60	MG	A	3001	1/1	0.95	0.12	51,51,51,51	0
60	MG	A	3483	1/1	0.95	0.05	31,31,31,31	0
60	MG	A	3484	1/1	0.95	0.19	41,41,41,41	0
60	MG	D	302	1/1	0.95	0.13	43,43,43,43	0
60	MG	A	3281	1/1	0.95	0.06	43,43,43,43	0
60	MG	a	1757	1/1	0.95	0.07	46,46,46,46	0
60	MG	A	3487	1/1	0.95	0.05	35,35,35,35	0
60	MG	a	1650	1/1	0.95	0.20	47,47,47,47	0
60	MG	A	3566	1/1	0.95	0.09	55,55,55,55	0
60	MG	A	3170	1/1	0.95	0.20	33,33,33,33	0
60	MG	a	1763	1/1	0.95	0.06	34,34,34,34	1
60	MG	A	3489	1/1	0.95	0.09	27,27,27,27	0
60	MG	A	3337	1/1	0.95	0.09	48,48,48,48	0
60	MG	a	1766	1/1	0.95	0.16	49,49,49,49	0
60	MG	A	3414	1/1	0.95	0.08	47,47,47,47	0
60	MG	A	3339	1/1	0.95	0.09	54,54,54,54	0
60	MG	A	3103	1/1	0.95	0.07	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3575	1/1	0.95	0.07	39,39,39,39	1
60	MG	A	3074	1/1	0.95	0.09	29,29,29,29	0
60	MG	A	3202	1/1	0.95	0.05	36,36,36,36	0
60	MG	A	3499	1/1	0.95	0.10	36,36,36,36	0
60	MG	A	3500	1/1	0.95	0.07	30,30,30,30	0
60	MG	A	3502	1/1	0.95	0.08	44,44,44,44	0
60	MG	A	3345	1/1	0.95	0.11	48,48,48,48	0
60	MG	A	3286	1/1	0.95	0.25	48,48,48,48	0
60	MG	A	3176	1/1	0.95	0.06	37,37,37,37	0
60	MG	A	3352	1/1	0.95	0.13	39,39,39,39	0
60	MG	A	3067	1/1	0.95	0.08	34,34,34,34	0
60	MG	A	3590	1/1	0.95	0.10	63,63,63,63	0
60	MG	X	101	1/1	0.95	0.07	50,50,50,50	0
60	MG	A	3510	1/1	0.95	0.13	48,48,48,48	0
60	MG	A	3258	1/1	0.95	0.07	41,41,41,41	0
60	MG	A	3096	1/1	0.95	0.04	27,27,27,27	0
60	MG	A	3023	1/1	0.95	0.10	34,34,34,34	0
60	MG	A	3152	1/1	0.95	0.10	48,48,48,48	0
60	MG	n	102	1/1	0.95	0.10	28,28,28,28	0
60	MG	A	3296	1/1	0.95	0.06	31,31,31,31	0
60	MG	A	3077	1/1	0.95	0.10	24,24,24,24	1
60	MG	a	1682	1/1	0.95	0.10	45,45,45,45	0
60	MG	A	3109	1/1	0.95	0.09	25,25,25,25	1
60	MG	A	3139	1/1	0.95	0.09	37,37,37,37	0
60	MG	A	3522	1/1	0.95	0.06	28,28,28,28	0
60	MG	A	3211	1/1	0.95	0.13	50,50,50,50	0
60	MG	x	106	1/1	0.95	0.11	56,56,56,56	1
60	MG	A	3440	1/1	0.95	0.06	45,45,45,45	0
60	MG	A	3304	1/1	0.95	0.08	53,53,53,53	0
60	MG	A	3069	1/1	0.95	0.09	30,30,30,30	0
60	MG	A	3306	1/1	0.95	0.15	33,33,33,33	0
60	MG	z	702	1/1	0.95	0.06	57,57,57,57	0
60	MG	D	301	1/1	0.96	0.04	21,21,21,21	0
60	MG	a	1634	1/1	0.96	0.27	53,53,53,53	0
60	MG	a	1719	1/1	0.96	0.16	48,48,48,48	0
60	MG	a	1720	1/1	0.96	0.08	48,48,48,48	0
60	MG	A	3150	1/1	0.96	0.15	54,54,54,54	0
60	MG	D	303	1/1	0.96	0.12	24,24,24,24	1
60	MG	A	3161	1/1	0.96	0.08	34,34,34,34	1
60	MG	A	3539	1/1	0.96	0.06	21,21,21,21	0
60	MG	a	1639	1/1	0.96	0.07	48,48,48,48	0
60	MG	A	3162	1/1	0.96	0.05	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3592	1/1	0.96	0.12	41,41,41,41	1
60	MG	A	3136	1/1	0.96	0.06	32,32,32,32	0
60	MG	A	3245	1/1	0.96	0.05	45,45,45,45	0
60	MG	F	305	1/1	0.96	0.06	46,46,46,46	0
60	MG	A	3596	1/1	0.96	0.09	44,44,44,44	1
60	MG	a	1735	1/1	0.96	0.07	37,37,37,37	0
60	MG	A	3038	1/1	0.96	0.08	29,29,29,29	0
60	MG	G	202	1/1	0.96	0.09	48,48,48,48	0
60	MG	A	3598	1/1	0.96	0.14	29,29,29,29	0
60	MG	A	3338	1/1	0.96	0.07	20,20,20,20	0
60	MG	A	3410	1/1	0.96	0.09	44,44,44,44	0
60	MG	A	3546	1/1	0.96	0.07	53,53,53,53	0
60	MG	A	3547	1/1	0.96	0.07	41,41,41,41	0
60	MG	a	1745	1/1	0.96	0.07	40,40,40,40	0
60	MG	A	3366	1/1	0.96	0.08	19,19,19,19	1
60	MG	A	3412	1/1	0.96	0.15	44,44,44,44	0
60	MG	A	3413	1/1	0.96	0.07	35,35,35,35	0
60	MG	A	3273	1/1	0.96	0.11	37,37,37,37	1
60	MG	A	3552	1/1	0.96	0.07	48,48,48,48	0
60	MG	A	3611	1/1	0.96	0.09	46,46,46,46	0
60	MG	A	3456	1/1	0.96	0.09	46,46,46,46	1
60	MG	A	3340	1/1	0.96	0.09	45,45,45,45	0
60	MG	A	3616	1/1	0.96	0.10	45,45,45,45	0
60	MG	a	1756	1/1	0.96	0.09	52,52,52,52	0
60	MG	A	3370	1/1	0.96	0.14	39,39,39,39	0
60	MG	A	3509	1/1	0.96	0.19	45,45,45,45	0
60	MG	A	3341	1/1	0.96	0.10	30,30,30,30	0
60	MG	a	1760	1/1	0.96	0.05	38,38,38,38	0
60	MG	A	3047	1/1	0.96	0.05	29,29,29,29	0
60	MG	A	3512	1/1	0.96	0.07	44,44,44,44	0
60	MG	A	3625	1/1	0.96	0.04	45,45,45,45	0
60	MG	A	3626	1/1	0.96	0.09	30,30,30,30	1
60	MG	A	3078	1/1	0.96	0.13	27,27,27,27	1
60	MG	6	103	1/1	0.96	0.08	41,41,41,41	0
60	MG	A	3377	1/1	0.96	0.09	26,26,26,26	0
60	MG	8	101	1/1	0.96	0.09	35,35,35,35	0
60	MG	A	3222	1/1	0.96	0.05	39,39,39,39	0
60	MG	A	3425	1/1	0.96	0.16	54,54,54,54	0
60	MG	A	3073	1/1	0.96	0.07	32,32,32,32	0
60	MG	A	3346	1/1	0.96	0.09	57,57,57,57	0
60	MG	A	3567	1/1	0.96	0.06	38,38,38,38	1
60	MG	a	1774	1/1	0.96	0.04	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3030	1/1	0.96	0.06	33,33,33,33	0
60	MG	a	1685	1/1	0.96	0.06	46,46,46,46	0
60	MG	A	3640	1/1	0.96	0.05	30,30,30,30	1
60	MG	a	1687	1/1	0.96	0.09	29,29,29,29	0
60	MG	A	3471	1/1	0.96	0.08	65,65,65,65	0
60	MG	a	1781	1/1	0.96	0.05	46,46,46,46	0
60	MG	A	3642	1/1	0.96	0.08	38,38,38,38	1
60	MG	A	3472	1/1	0.96	0.18	25,25,25,25	0
60	MG	A	3571	1/1	0.96	0.08	38,38,38,38	1
60	MG	A	3349	1/1	0.96	0.07	42,42,42,42	0
60	MG	B	202	1/1	0.96	0.10	52,52,52,52	0
60	MG	A	3279	1/1	0.96	0.07	30,30,30,30	1
60	MG	A	3172	1/1	0.96	0.17	49,49,49,49	0
60	MG	A	3390	1/1	0.96	0.05	36,36,36,36	0
60	MG	f	201	1/1	0.96	0.12	53,53,53,53	0
60	MG	l	201	1/1	0.96	0.11	31,31,31,31	0
60	MG	A	3529	1/1	0.96	0.05	59,59,59,59	0
60	MG	A	3478	1/1	0.96	0.18	50,50,50,50	0
60	MG	A	3300	1/1	0.96	0.07	42,42,42,42	0
60	MG	a	1702	1/1	0.96	0.21	42,42,42,42	0
60	MG	v	102	1/1	0.96	0.10	42,42,42,42	0
60	MG	a	1622	1/1	0.96	0.05	36,36,36,36	0
60	MG	A	3005	1/1	0.96	0.09	31,31,31,31	1
60	MG	A	3325	1/1	0.96	0.04	23,23,23,23	0
60	MG	A	3327	1/1	0.96	0.07	30,30,30,30	0
60	MG	a	1707	1/1	0.96	0.07	34,34,34,34	0
60	MG	A	3583	1/1	0.96	0.12	46,46,46,46	0
60	MG	A	3584	1/1	0.96	0.06	39,39,39,39	0
60	MG	A	3302	1/1	0.96	0.07	22,22,22,22	0
60	MG	A	3397	1/1	0.96	0.12	38,38,38,38	0
60	MG	A	3587	1/1	0.96	0.09	23,23,23,23	1
60	MG	B	218	1/1	0.96	0.11	49,49,49,49	0
60	MG	A	3330	1/1	0.97	0.06	37,37,37,37	1
60	MG	A	3595	1/1	0.97	0.05	27,27,27,27	0
60	MG	a	1668	1/1	0.97	0.04	30,30,30,30	0
60	MG	A	3387	1/1	0.97	0.05	26,26,26,26	0
60	MG	A	3009	1/1	0.97	0.10	52,52,52,52	0
60	MG	A	3389	1/1	0.97	0.05	33,33,33,33	0
60	MG	a	1672	1/1	0.97	0.08	41,41,41,41	0
60	MG	A	3003	1/1	0.97	0.11	32,32,32,32	0
60	MG	A	3013	1/1	0.97	0.08	24,24,24,24	0
60	MG	A	3429	1/1	0.97	0.07	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3153	1/1	0.97	0.12	45,45,45,45	0
60	MG	a	1613	1/1	0.97	0.13	29,29,29,29	0
60	MG	A	3185	1/1	0.97	0.12	32,32,32,32	0
60	MG	A	3516	1/1	0.97	0.11	25,25,25,25	1
60	MG	A	3469	1/1	0.97	0.07	48,48,48,48	0
60	MG	A	3090	1/1	0.97	0.12	43,43,43,43	0
60	MG	A	3608	1/1	0.97	0.05	32,32,32,32	0
60	MG	A	3609	1/1	0.97	0.08	31,31,31,31	0
60	MG	A	3171	1/1	0.97	0.09	31,31,31,31	0
60	MG	A	3017	1/1	0.97	0.06	41,41,41,41	0
60	MG	E	301	1/1	0.97	0.06	33,33,33,33	0
60	MG	E	302	1/1	0.97	0.05	32,32,32,32	0
60	MG	A	3398	1/1	0.97	0.05	37,37,37,37	0
60	MG	A	3288	1/1	0.97	0.07	45,45,45,45	0
60	MG	A	3614	1/1	0.97	0.07	39,39,39,39	0
60	MG	A	3615	1/1	0.97	0.10	34,34,34,34	0
60	MG	F	304	1/1	0.97	0.15	28,28,28,28	1
60	MG	A	3070	1/1	0.97	0.04	10,10,10,10	0
60	MG	A	3617	1/1	0.97	0.06	45,45,45,45	0
60	MG	A	3018	1/1	0.97	0.10	27,27,27,27	0
60	MG	a	1698	1/1	0.97	0.18	49,49,49,49	0
60	MG	A	3439	1/1	0.97	0.09	50,50,50,50	0
60	MG	a	1633	1/1	0.97	0.14	32,32,32,32	0
60	MG	A	3621	1/1	0.97	0.21	48,48,48,48	0
60	MG	A	3479	1/1	0.97	0.10	41,41,41,41	0
60	MG	a	1776	1/1	0.97	0.13	52,52,52,52	0
60	MG	A	3480	1/1	0.97	0.07	41,41,41,41	0
60	MG	O	202	1/1	0.97	0.05	50,50,50,50	0
60	MG	A	3403	1/1	0.97	0.07	37,37,37,37	0
60	MG	A	3192	1/1	0.97	0.05	26,26,26,26	0
60	MG	A	3405	1/1	0.97	0.12	32,32,32,32	0
60	MG	a	1709	1/1	0.97	0.05	36,36,36,36	0
60	MG	A	3193	1/1	0.97	0.05	27,27,27,27	0
60	MG	Q	202	1/1	0.97	0.07	33,33,33,33	0
60	MG	A	3486	1/1	0.97	0.08	44,44,44,44	0
60	MG	A	3631	1/1	0.97	0.20	24,24,24,24	1
60	MG	a	1645	1/1	0.97	0.11	42,42,42,42	0
60	MG	a	1788	1/1	0.97	0.06	43,43,43,43	1
60	MG	A	3213	1/1	0.97	0.06	34,34,34,34	1
60	MG	A	3035	1/1	0.97	0.07	30,30,30,30	1
60	MG	A	3634	1/1	0.97	0.07	42,42,42,42	1
60	MG	A	3635	1/1	0.97	0.16	29,29,29,29	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	m	201	1/1	0.97	0.19	38,38,38,38	1
60	MG	m	202	1/1	0.97	0.12	56,56,56,56	0
60	MG	A	3446	1/1	0.97	0.06	26,26,26,26	0
60	MG	A	3490	1/1	0.97	0.06	40,40,40,40	0
60	MG	A	3095	1/1	0.97	0.07	32,32,32,32	0
60	MG	A	3375	1/1	0.97	0.07	35,35,35,35	0
60	MG	A	3019	1/1	0.97	0.09	20,20,20,20	0
60	MG	A	3378	1/1	0.97	0.11	41,41,41,41	0
60	MG	A	3046	1/1	0.97	0.11	29,29,29,29	0
60	MG	a	1658	1/1	0.97	0.08	30,30,30,30	0
60	MG	A	3497	1/1	0.97	0.07	38,38,38,38	1
60	MG	A	3351	1/1	0.97	0.07	33,33,33,33	0
60	MG	A	3021	1/1	0.97	0.07	34,34,34,34	0
60	MG	A	3200	1/1	0.97	0.06	39,39,39,39	0
60	MG	A	3419	1/1	0.97	0.05	30,30,30,30	1
60	MG	A	3457	1/1	0.97	0.04	24,24,24,24	0
60	MG	A	3329	1/1	0.97	0.06	33,33,33,33	1
60	MG	a	1739	1/1	0.97	0.06	42,42,42,42	0
61	ZN	4	501	1/1	0.97	0.05	79,79,79,79	0
62	SF4	d	302	8/8	0.97	0.05	60,65,70,71	2
63	GCP	z	703	32/32	0.97	0.07	47,57,62,63	13
60	MG	A	3407	1/1	0.98	0.06	30,30,30,30	0
60	MG	A	3379	1/1	0.98	0.07	36,36,36,36	0
60	MG	A	3582	1/1	0.98	0.04	21,21,21,21	1
60	MG	D	306	1/1	0.98	0.06	25,25,25,25	0
60	MG	A	3507	1/1	0.98	0.05	42,42,42,42	0
60	MG	a	1607	1/1	0.98	0.12	42,42,42,42	1
60	MG	a	1608	1/1	0.98	0.08	23,23,23,23	0
60	MG	a	1708	1/1	0.98	0.07	40,40,40,40	0
60	MG	A	3331	1/1	0.98	0.06	31,31,31,31	0
60	MG	A	3120	1/1	0.98	0.16	26,26,26,26	0
60	MG	E	304	1/1	0.98	0.04	35,35,35,35	0
60	MG	E	305	1/1	0.98	0.04	23,23,23,23	1
60	MG	A	3627	1/1	0.98	0.09	25,25,25,25	0
60	MG	A	3112	1/1	0.98	0.06	44,44,44,44	0
60	MG	A	3311	1/1	0.98	0.09	41,41,41,41	0
60	MG	a	1716	1/1	0.98	0.04	36,36,36,36	0
60	MG	A	3294	1/1	0.98	0.08	25,25,25,25	1
60	MG	A	3313	1/1	0.98	0.07	29,29,29,29	0
60	MG	A	3314	1/1	0.98	0.05	48,48,48,48	0
60	MG	A	3515	1/1	0.98	0.12	47,47,47,47	0
60	MG	a	1721	1/1	0.98	0.04	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3241	1/1	0.98	0.05	20,20,20,20	0
60	MG	A	3481	1/1	0.98	0.05	46,46,46,46	0
60	MG	A	3186	1/1	0.98	0.07	33,33,33,33	0
60	MG	A	3230	1/1	0.98	0.13	40,40,40,40	0
60	MG	a	1726	1/1	0.98	0.04	43,43,43,43	0
60	MG	A	3363	1/1	0.98	0.06	35,35,35,35	0
60	MG	a	1728	1/1	0.98	0.05	33,33,33,33	0
60	MG	A	3298	1/1	0.98	0.07	34,34,34,34	0
60	MG	A	3045	1/1	0.98	0.14	20,20,20,20	0
60	MG	A	3198	1/1	0.98	0.07	20,20,20,20	0
60	MG	A	3524	1/1	0.98	0.06	49,49,49,49	1
60	MG	A	3601	1/1	0.98	0.03	33,33,33,33	0
60	MG	A	3424	1/1	0.98	0.11	20,20,20,20	0
60	MG	A	3455	1/1	0.98	0.05	28,28,28,28	0
60	MG	A	3168	1/1	0.98	0.09	23,23,23,23	0
60	MG	A	3565	1/1	0.98	0.03	35,35,35,35	0
60	MG	a	1738	1/1	0.98	0.05	35,35,35,35	0
60	MG	A	3426	1/1	0.98	0.05	36,36,36,36	0
60	MG	a	1684	1/1	0.98	0.05	31,31,31,31	0
60	MG	A	3396	1/1	0.98	0.04	26,26,26,26	0
60	MG	A	3031	1/1	0.98	0.06	33,33,33,33	0
60	MG	A	3324	1/1	0.98	0.06	38,38,38,38	0
60	MG	a	1688	1/1	0.98	0.03	32,32,32,32	0
60	MG	A	3495	1/1	0.98	0.04	35,35,35,35	0
60	MG	A	3287	1/1	0.98	0.04	35,35,35,35	0
60	MG	A	3372	1/1	0.98	0.12	41,41,41,41	0
60	MG	A	3401	1/1	0.98	0.13	36,36,36,36	0
60	MG	A	3348	1/1	0.98	0.04	30,30,30,30	0
60	MG	A	3004	1/1	0.98	0.15	40,40,40,40	1
60	MG	A	3501	1/1	0.98	0.05	24,24,24,24	0
60	MG	A	3125	1/1	0.98	0.12	22,22,22,22	1
60	MG	B	217	1/1	0.98	0.06	40,40,40,40	0
60	MG	A	3163	1/1	0.98	0.04	26,26,26,26	0
61	ZN	5	103	1/1	0.98	0.03	54,54,54,54	0
60	MG	A	3619	1/1	0.98	0.08	16,16,16,16	0
60	MG	A	3156	1/1	0.98	0.08	26,26,26,26	0
60	MG	A	3174	1/1	0.99	0.13	25,25,25,25	0
60	MG	A	3086	1/1	0.99	0.10	21,21,21,21	0
60	MG	a	1747	1/1	0.99	0.03	38,38,38,38	0
60	MG	A	3383	1/1	0.99	0.03	28,28,28,28	0
60	MG	A	3326	1/1	0.99	0.04	32,32,32,32	0
60	MG	A	3376	1/1	0.99	0.04	31,31,31,31	0

Continued on next page...

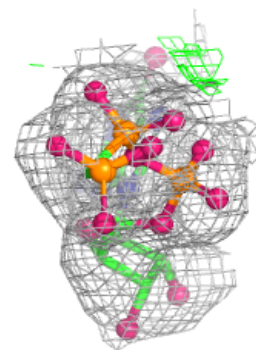
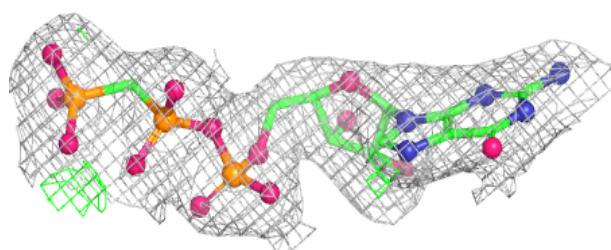
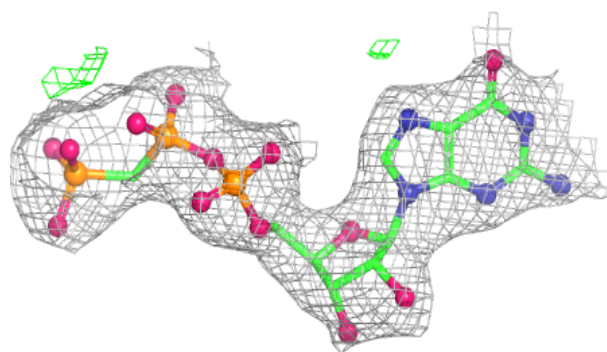
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	A	3459	1/1	0.99	0.11	33,33,33,33	0
60	MG	A	3369	1/1	0.99	0.03	31,31,31,31	0
60	MG	A	3308	1/1	0.99	0.09	14,14,14,14	0
60	MG	A	3020	1/1	0.99	0.05	26,26,26,26	0
61	ZN	Y	501	1/1	0.99	0.02	63,63,63,63	0
60	MG	A	3473	1/1	0.99	0.04	27,27,27,27	0
60	MG	A	3318	1/1	0.99	0.07	42,42,42,42	1
61	ZN	6	102	1/1	0.99	0.15	72,72,72,72	0
61	ZN	9	102	1/1	0.99	0.12	49,49,49,49	1
61	ZN	n	104	1/1	0.99	0.02	44,44,44,44	0
60	MG	a	1652	1/1	0.99	0.08	20,20,20,20	0
60	MG	A	3629	1/1	0.99	0.03	21,21,21,21	0
60	MG	A	3415	1/1	1.00	0.04	34,34,34,34	0

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

Electron density around GCP z 703:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.