Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 PM GMT

PDB ID	:	4KHP
Title	:	Structure of the Thermus thermophilus 30S ribosomal subunit in complex with de-6-MSA-pactamycin
Authors	:	Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2013-05-01
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

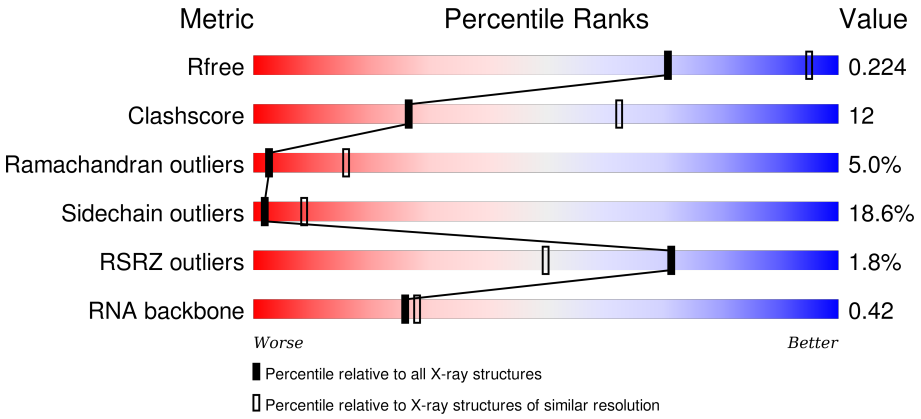
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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.



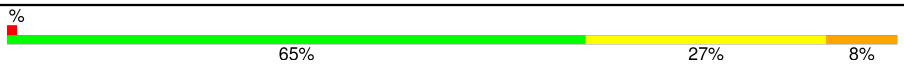
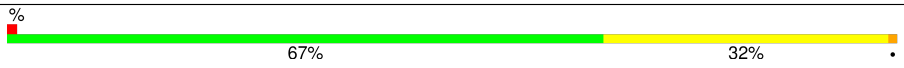
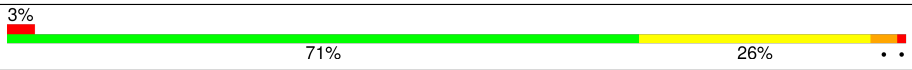
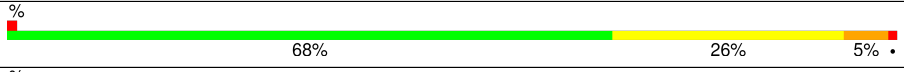
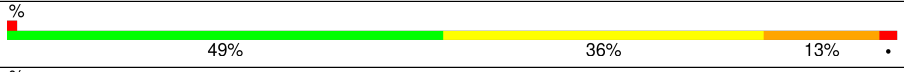
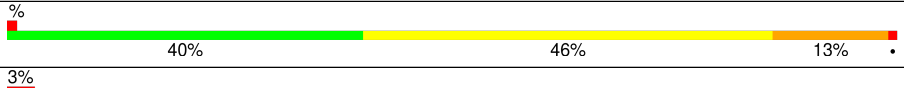
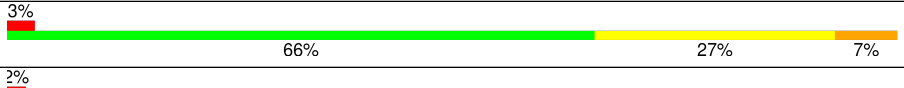
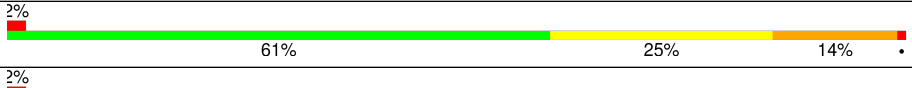
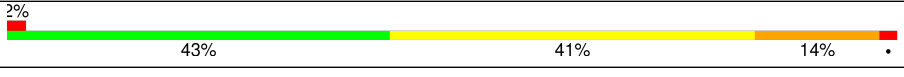
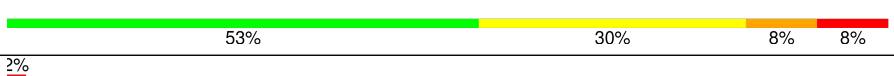
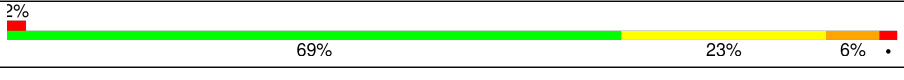
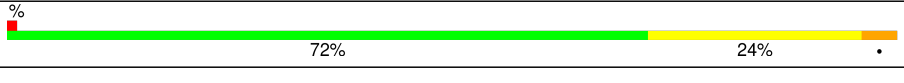
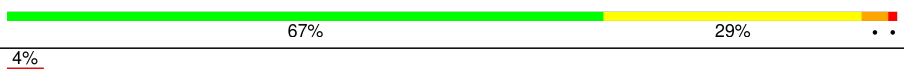
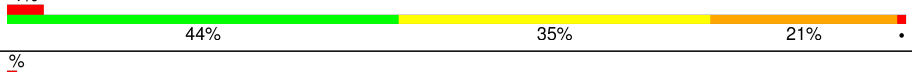
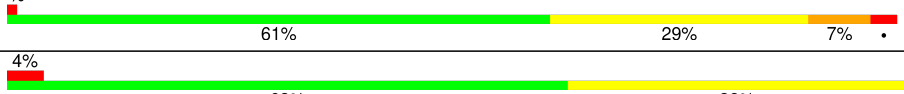
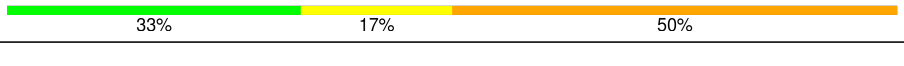
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	A	1506	2% 51% 35% 12% •
2	B	234	3% 47% 39% 12% •
3	C	206	62% 31% 5% •
4	D	208	63% 28% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	150	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	98	
11	K	119	
12	L	125	
13	M	120	
14	N	60	
15	O	88	
16	P	83	
17	Q	99	
18	R	70	
19	S	78	
20	T	99	
21	U	24	
22	X	6	

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
23	PAR	A	1602	-	-	-	X
23	PAR	A	1603	-	-	-	X
23	PAR	A	1605	-	-	-	X
23	PAR	A	1606	-	-	-	X
23	PAR	A	1607	-	-	-	X
25	MG	A	1609	-	-	-	X
25	MG	A	1610	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1614	-	-	-	X
25	MG	A	1617	-	-	-	X
25	MG	A	1620	-	-	-	X
25	MG	A	1622	-	-	-	X
25	MG	A	1632	-	-	-	X
25	MG	A	1633	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	1636	-	-	-	X
25	MG	A	1639	-	-	-	X
25	MG	A	1645	-	-	-	X
25	MG	A	1647	-	-	-	X
25	MG	A	1651	-	-	-	X
25	MG	A	1652	-	-	-	X
25	MG	A	1654	-	-	-	X
25	MG	A	1659	-	-	-	X
25	MG	A	1661	-	-	-	X
25	MG	A	1667	-	-	-	X
25	MG	A	1682	-	-	-	X
25	MG	A	1685	-	-	-	X
25	MG	A	1703	-	-	-	X
25	MG	D	301	-	-	-	X
25	MG	E	201	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52032 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1506	32368	14408	5997	10458	1505	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	A	G	CONFLICT	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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

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

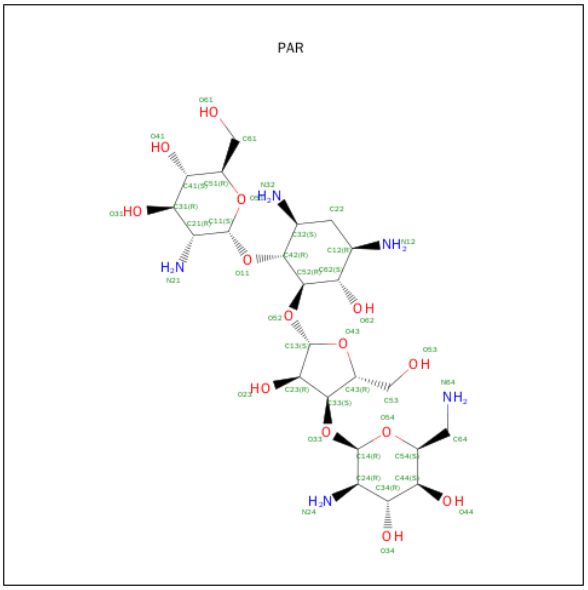
- Molecule 21 is a protein called 30S Ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called Fragment of messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 23 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



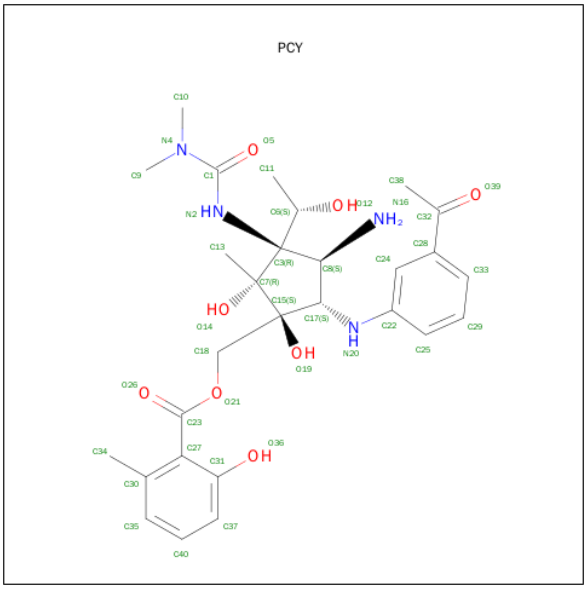
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			42	23	5	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C N O 42 23 5 14	0	0
23	A	1	Total C N O 42 23 5 14	0	0
23	A	1	Total C N O 42 23 5 14	0	0
23	A	1	Total C N O 42 23 5 14	0	0
23	A	1	Total C N O 42 23 5 14	0	0
23	A	1	Total C N O 42 23 5 14	0	0

- Molecule 24 is DE-6-MSA-PACTAMYCIN (three-letter code: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C N O 30 20 4 6	0	0

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	S	1	Total Mg 1 1	0	0
25	A	99	Total Mg 99 99	0	0

Continued on next page...

Continued from previous page...

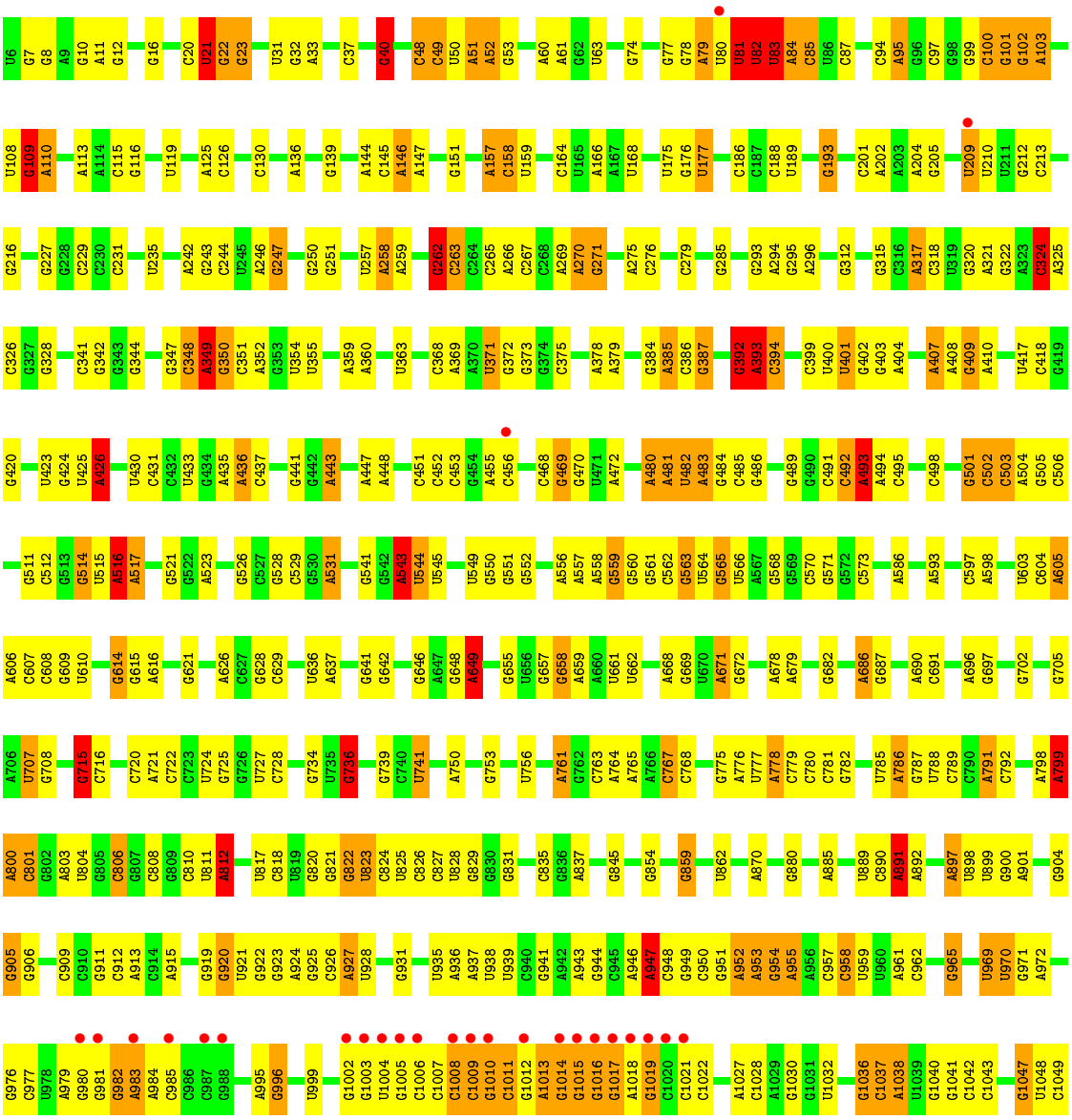
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	D	1	Total Mg 1 1	0	0
25	K	1	Total Mg 1 1	0	0
25	E	1	Total Mg 1 1	0	0

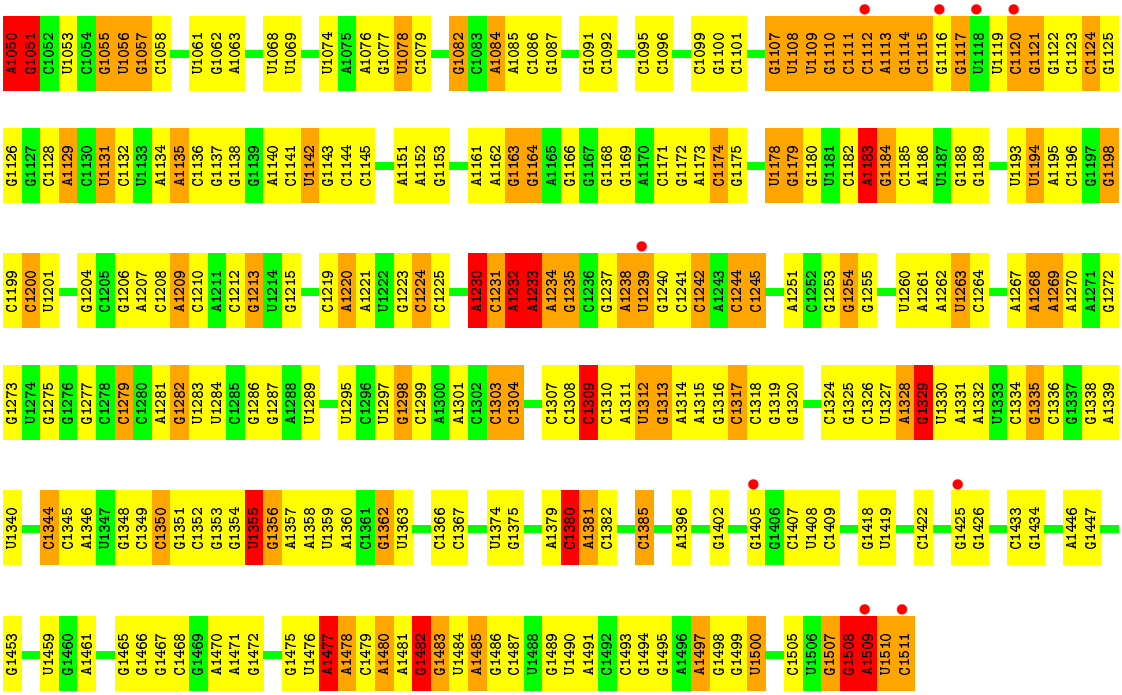
3 Residue-property plots (i)

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

- Molecule 1: 16S Ribosomal RNA

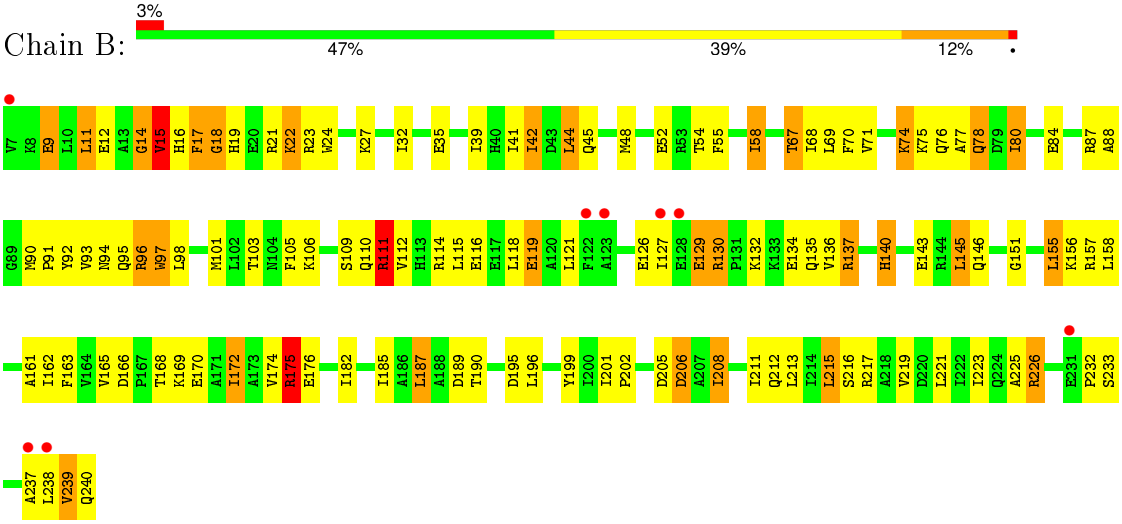
Chain A: 





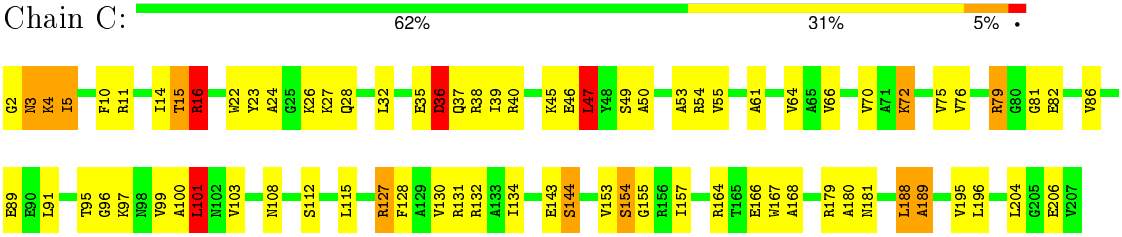
- Molecule 2: 30S Ribosomal protein S2

Chain B:



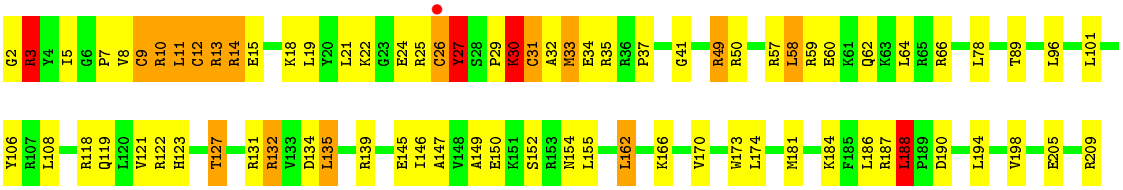
- Molecule 3: 30S Ribosomal protein S3

Chain C:

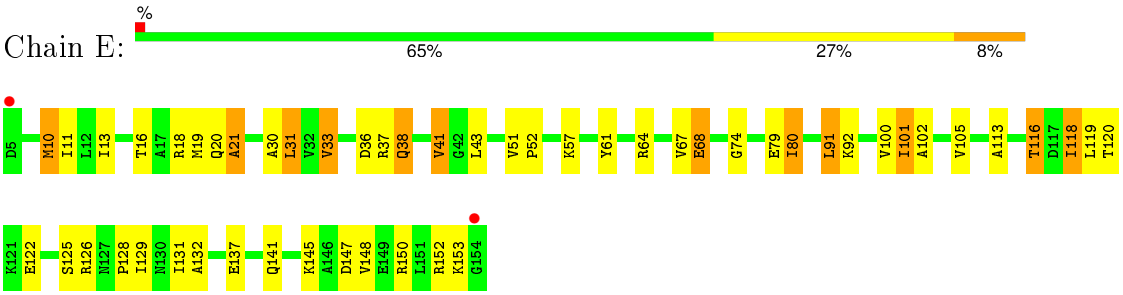


- Molecule 4: 30S Ribosomal protein S4

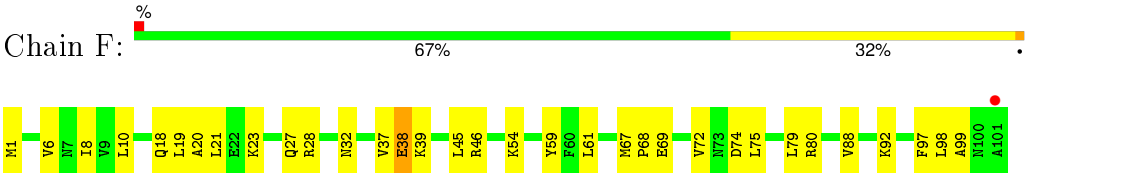
Chain D:



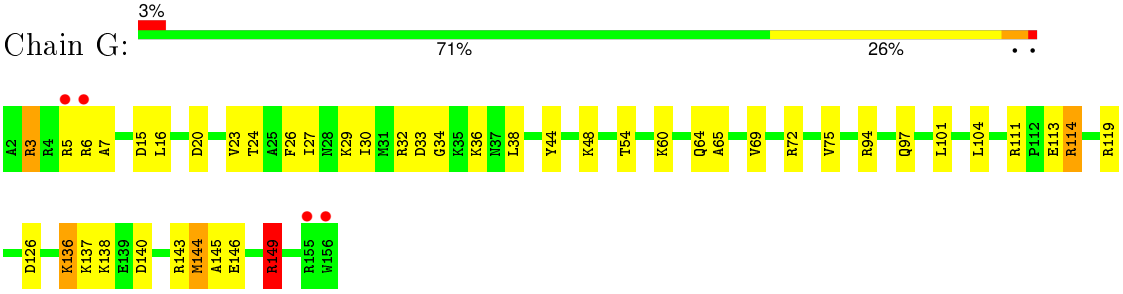
- Molecule 5: 30S Ribosomal protein S5



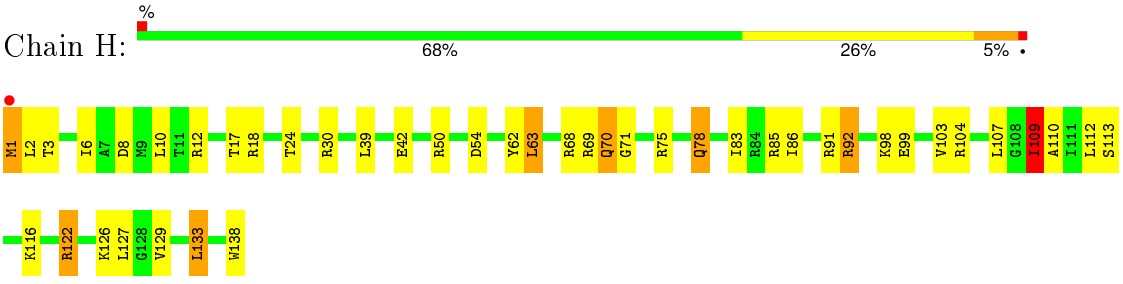
- Molecule 6: 30S Ribosomal protein S6



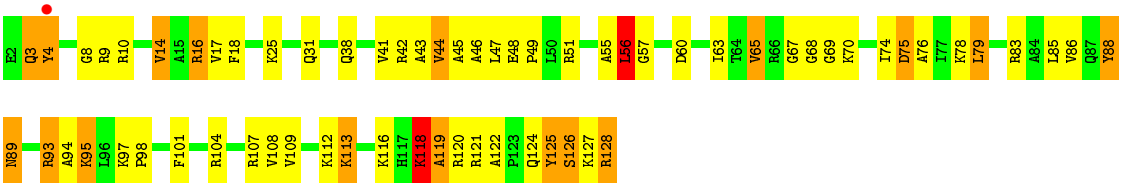
- Molecule 7: 30S Ribosomal protein S7



- Molecule 8: 30S Ribosomal protein S8

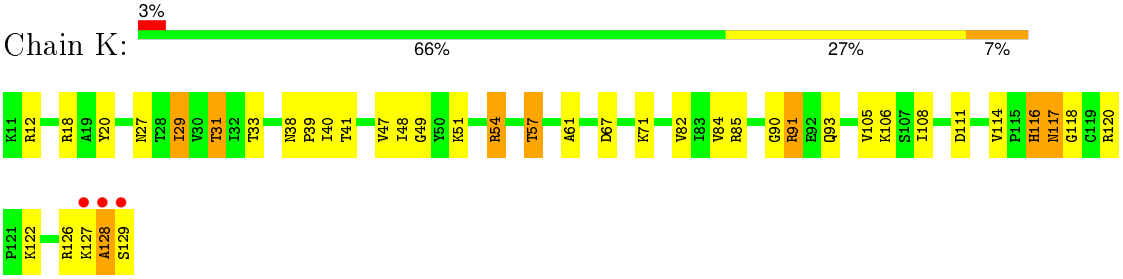


- Molecule 9: 30S Ribosomal protein S9

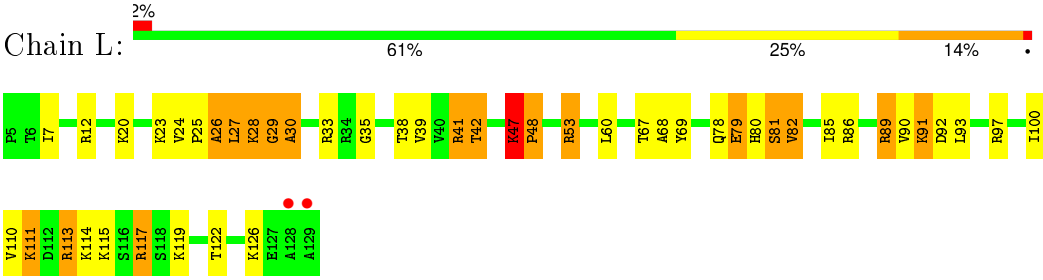


• Molecule 10: 30S Ribosomal protein S10

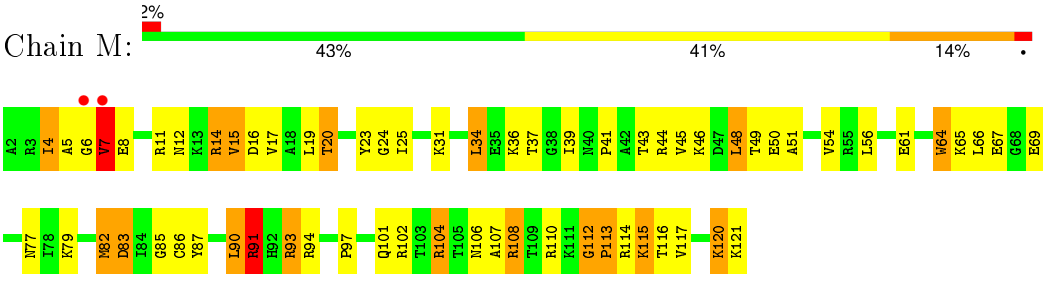
• Molecule 11: 30S Ribosomal protein S11



• Molecule 12: 30S Ribosomal protein S12

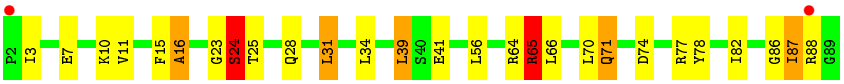


• Molecule 13: 30S Ribosomal protein S13

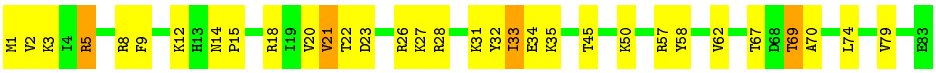


• Molecule 14: 30S Ribosomal protein S14

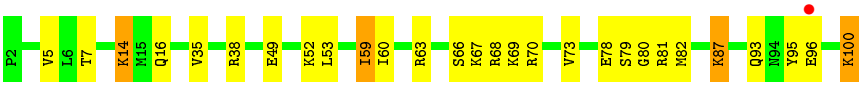
• Molecule 15: 30S Ribosomal protein S15



• Molecule 16: 30S Ribosomal protein S16

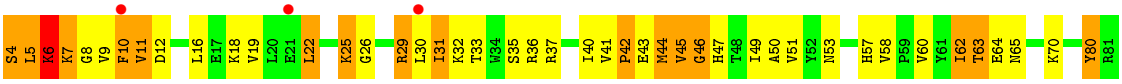


• Molecule 17: 30S Ribosomal protein S17

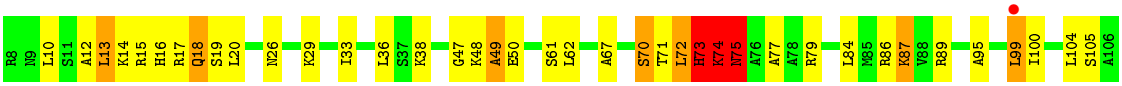


• Molecule 18: 30S Ribosomal protein S18

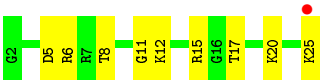
• Molecule 19: 30S Ribosomal protein S19



• Molecule 20: 30S Ribosomal protein S20

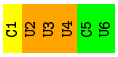


• Molecule 21: 30S Ribosomal protein THX



- Molecule 22: Fragment of messenger RNA

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.00Å 401.00Å 176.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 3.10 29.67 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.67-3.10) 91.5 (29.67-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, R_{free}	0.185 , 0.226 0.187 , 0.224	Depositor DCC
R_{free} test set	11726 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	75.3	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 234683 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	52032	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PAR, PCY, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.55	14/36233 (0.0%)	0.94	127/56552 (0.2%)
2	B	0.59	0/1935	0.89	2/2609 (0.1%)
3	C	0.64	0/1636	0.86	1/2205 (0.0%)
4	D	0.68	2/1733 (0.1%)	0.96	3/2318 (0.1%)
5	E	0.72	0/1162	0.96	0/1564
6	F	0.50	0/856	0.76	0/1154
7	G	0.51	0/1276	0.79	1/1709 (0.1%)
8	H	0.73	0/1136	0.97	1/1527 (0.1%)
9	I	0.52	0/1029	0.85	0/1378
10	J	0.59	0/807	0.93	2/1085 (0.2%)
11	K	0.58	0/900	0.85	1/1213 (0.1%)
12	L	0.70	0/991	1.00	4/1327 (0.3%)
13	M	0.56	0/965	0.93	2/1292 (0.2%)
14	N	0.74	0/501	1.10	2/664 (0.3%)
15	O	0.56	0/745	0.87	1/992 (0.1%)
16	P	0.67	0/716	0.89	1/963 (0.1%)
17	Q	0.64	0/836	0.86	0/1117
18	R	0.53	0/579	0.83	0/768
19	S	0.55	0/642	0.80	0/865
20	T	0.63	0/765	0.95	0/1007
21	U	0.61	0/212	0.86	0/277
22	X	0.58	0/128	0.85	0/196
All	All	0.58	16/55783 (0.0%)	0.92	148/82782 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
11	K	0	1
12	L	0	2
14	N	0	1
19	S	0	1
20	T	0	3
All	All	0	11

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	U	O3'-P	9.75	1.72	1.61
1	A	83	U	O3'-P	8.72	1.71	1.61
1	A	799	A	O3'-P	-6.81	1.52	1.61
1	A	1057	G	O3'-P	-6.41	1.53	1.61
4	D	12	CYS	CA-CB	6.18	1.67	1.53
1	A	1230	A	O3'-P	5.86	1.68	1.61
1	A	21	U	O3'-P	-5.76	1.54	1.61
1	A	1213	G	O3'-P	-5.73	1.54	1.61
1	A	371	U	O3'-P	-5.72	1.54	1.61
1	A	1235	G	O3'-P	-5.67	1.54	1.61
1	A	1232	A	O3'-P	5.43	1.67	1.61
1	A	493	A	O3'-P	-5.26	1.54	1.61
1	A	81	U	O3'-P	5.20	1.67	1.61
4	D	12	CYS	CB-SG	5.07	1.90	1.82
1	A	786	A	O3'-P	-5.07	1.55	1.61
1	A	242	A	O3'-P	-5.06	1.55	1.61

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1477	A	O5'-P-OP1	-12.26	94.67	105.70
1	A	767	C	O5'-P-OP2	-12.24	94.68	105.70
1	A	812	A	O5'-P-OP2	-11.96	94.93	105.70
1	A	492	C	C2'-C3'-O3'	10.89	133.46	109.50
1	A	399	C	O5'-P-OP2	-9.77	96.91	105.70
1	A	1050	A	C2'-C3'-O3'	9.62	130.66	109.50
1	A	605	A	O5'-P-OP2	9.49	122.08	110.70
1	A	558	A	O5'-P-OP1	-9.10	97.51	105.70
1	A	469	G	C2'-C3'-O3'	8.97	129.24	109.50
1	A	320	G	O5'-P-OP1	-8.88	97.71	105.70
1	A	82	U	C2'-C3'-O3'	8.77	128.78	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	U	O5'-P-OP1	-8.69	97.88	105.70
1	A	324	C	O5'-P-OP1	-8.63	97.93	105.70
1	A	1047	G	C2'-C3'-O3'	-8.51	90.78	109.50
1	A	565	G	O5'-P-OP2	-8.49	98.06	105.70
1	A	516	A	C2'-C3'-O3'	8.36	127.90	109.50
1	A	605	A	O5'-P-OP1	-8.36	98.18	105.70
1	A	1099	C	O5'-P-OP2	-8.21	98.31	105.70
1	A	835	C	O5'-P-OP2	-8.02	98.48	105.70
1	A	109	G	C2'-C3'-O3'	7.97	127.04	109.50
1	A	294	A	O5'-P-OP2	7.94	120.23	110.70
1	A	741	U	O5'-P-OP2	-7.88	98.61	105.70
1	A	1508	G	O5'-P-OP2	-7.84	98.64	105.70
1	A	756	U	O5'-P-OP2	-7.80	98.68	105.70
1	A	83	U	N1-C1'-C2'	7.72	124.04	114.00
1	A	262	G	C2'-C3'-O3'	7.70	126.43	109.50
1	A	736	G	O5'-P-OP2	-7.66	98.81	105.70
1	A	1233	A	O5'-P-OP1	-7.60	98.86	105.70
1	A	1277	G	O5'-P-OP1	-7.55	98.90	105.70
1	A	715	G	O5'-P-OP2	-7.54	98.91	105.70
1	A	101	G	O5'-P-OP2	7.46	119.66	110.70
1	A	859	G	O5'-P-OP2	-7.45	98.99	105.70
1	A	543	A	O5'-P-OP2	-7.44	99.00	105.70
1	A	1061	U	O5'-P-OP1	-7.37	99.06	105.70
1	A	22	G	O5'-P-OP2	-7.25	99.18	105.70
1	A	493	A	C2'-C3'-O3'	7.23	125.41	109.50
1	A	468	C	O5'-P-OP1	-7.20	99.22	105.70
1	A	82	U	P-O3'-C3'	7.16	128.29	119.70
1	A	63	U	O5'-P-OP2	-7.12	99.29	105.70
1	A	1329	G	O5'-P-OP2	-7.12	99.30	105.70
1	A	927	A	O5'-P-OP2	7.11	119.23	110.70
1	A	102	G	C5'-C4'-O4'	7.04	117.55	109.10
1	A	209	U	C2'-C3'-O3'	7.03	124.97	109.50
1	A	1233	A	C2'-C3'-O3'	7.02	124.94	109.50
4	D	12	CYS	N-CA-C	-6.83	92.56	111.00
13	M	114	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	1498	G	O5'-P-OP1	-6.73	99.64	105.70
14	N	24	CYS	CA-CB-SG	6.70	126.06	114.00
1	A	573	C	O5'-P-OP2	-6.69	99.67	105.70
1	A	1497	A	O5'-P-OP2	-6.69	99.68	105.70
1	A	1509	A	O5'-P-OP1	-6.68	99.69	105.70
1	A	360	A	O5'-P-OP1	-6.61	99.75	105.70
1	A	116	G	O5'-P-OP1	-6.60	99.76	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	58	ASP	CB-CG-OD1	6.50	124.15	118.30
10	J	60	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	948	C	O5'-P-OP2	6.44	118.43	110.70
1	A	891	A	C2'-C3'-O3'	6.39	123.92	113.70
1	A	812	A	O5'-P-OP1	6.37	118.34	110.70
1	A	100	C	O5'-P-OP1	6.35	118.32	110.70
1	A	671	A	C2'-C3'-O3'	6.33	123.83	113.70
1	A	1183	A	C2'-C3'-O3'	6.33	123.82	113.70
1	A	119	U	O5'-P-OP2	-6.32	100.02	105.70
1	A	102	G	O4'-C4'-C3'	-6.28	97.72	104.00
1	A	1267	A	O5'-P-OP1	-6.27	100.05	105.70
1	A	359	A	O5'-P-OP2	-6.27	100.06	105.70
1	A	806	C	O5'-P-OP1	-6.24	100.08	105.70
1	A	349	A	O5'-P-OP2	-6.24	100.09	105.70
11	K	120	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	1055	G	O5'-P-OP2	-6.17	100.14	105.70
1	A	1499	G	O5'-P-OP2	-6.14	100.18	105.70
1	A	22	G	O5'-P-OP1	6.13	118.05	110.70
1	A	558	A	O5'-P-OP2	6.11	118.03	110.70
1	A	1131	U	O5'-P-OP2	-6.09	100.22	105.70
1	A	598	A	C2'-C3'-O3'	6.01	123.32	113.70
1	A	831	G	O5'-P-OP2	-6.00	100.30	105.70
1	A	387	G	C2'-C3'-O3'	5.99	123.28	113.70
1	A	649	A	O5'-P-OP2	-5.97	100.33	105.70
1	A	318	C	O5'-P-OP2	-5.96	100.33	105.70
14	N	44	LEU	CB-CG-CD2	5.96	121.13	111.00
1	A	393	A	O5'-P-OP2	-5.93	100.36	105.70
7	G	149	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	1477	A	O5'-P-OP2	5.91	117.80	110.70
1	A	1251	A	O5'-P-OP2	-5.89	100.40	105.70
1	A	441	G	O5'-P-OP1	-5.88	100.41	105.70
1	A	1056	U	O5'-P-OP2	-5.86	100.43	105.70
1	A	1277	G	O5'-P-OP2	5.85	117.72	110.70
1	A	491	C	O5'-P-OP1	-5.81	100.47	105.70
12	L	92	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	806	C	O5'-P-OP2	5.74	117.58	110.70
1	A	1055	G	O5'-P-OP1	5.73	117.58	110.70
1	A	897	A	O5'-P-OP2	-5.71	100.56	105.70
1	A	1028	C	C2'-C3'-O3'	5.71	122.83	113.70
1	A	100	C	O5'-P-OP2	-5.70	100.57	105.70
1	A	82	U	O4'-C1'-N1	5.70	112.76	108.20
1	A	1344	C	O5'-P-OP2	5.66	117.50	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1062	G	N9-C1'-C2'	5.65	121.35	114.00
8	H	92	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	822	G	O5'-P-OP2	-5.63	100.63	105.70
1	A	686	A	N9-C1'-C2'	5.63	121.32	114.00
1	A	401	U	C2'-C3'-O3'	5.61	122.67	113.70
3	C	4	LYS	N-CA-C	5.58	126.06	111.00
1	A	229	C	O5'-P-OP2	5.58	117.39	110.70
1	A	724	U	O5'-P-OP2	-5.57	100.69	105.70
1	A	1329	G	O5'-P-OP1	5.56	117.37	110.70
1	A	166	A	O5'-P-OP2	5.54	117.36	110.70
1	A	1309	C	O5'-P-OP1	5.51	117.31	110.70
1	A	658	G	O5'-P-OP1	-5.49	100.76	105.70
2	B	111	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	947	A	O5'-P-OP1	-5.44	100.80	105.70
15	O	65	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	1380	C	O4'-C1'-N1	5.43	112.55	108.20
1	A	491	C	O5'-P-OP2	5.40	117.18	110.70
12	L	117	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	808	C	O5'-P-OP2	-5.38	100.86	105.70
1	A	1487	C	O5'-P-OP2	-5.36	100.88	105.70
1	A	512	C	C2'-C3'-O3'	5.35	122.26	113.70
1	A	682	G	O5'-P-OP2	-5.31	100.92	105.70
1	A	948	C	O5'-P-OP1	-5.28	100.95	105.70
1	A	1086	C	O5'-P-OP2	-5.28	100.95	105.70
1	A	392	G	P-O5'-C5'	-5.26	112.48	120.90
1	A	1367	C	O5'-P-OP1	-5.25	100.97	105.70
1	A	1224	C	O5'-P-OP1	-5.25	100.97	105.70
1	A	1051	G	O5'-P-OP2	-5.23	101.00	105.70
1	A	791	A	C2'-C3'-O3'	5.19	122.01	113.70
1	A	593	A	O5'-P-OP1	-5.18	101.03	105.70
1	A	965	G	O5'-P-OP2	-5.18	101.03	105.70
1	A	109	G	N9-C1'-C2'	5.18	120.74	114.00
1	A	1355	U	C2'-C3'-O3'	5.18	121.98	113.70
4	D	188	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	40	G	N9-C1'-C2'	-5.13	106.35	112.00
1	A	443	A	O5'-P-OP2	-5.13	101.08	105.70
1	A	348	C	O5'-P-OP1	-5.12	101.09	105.70
1	A	384	G	C4'-C3'-O3'	-5.12	98.64	109.40
1	A	1273	G	O5'-P-OP2	-5.12	101.09	105.70
1	A	293	G	O5'-P-OP2	-5.10	101.11	105.70
1	A	1062	G	O5'-P-OP2	5.10	116.82	110.70
2	B	175	ARG	NE-CZ-NH1	5.08	122.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	12	CYS	N-CA-CB	5.08	119.74	110.60
13	M	93	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	317	A	O5'-P-OP2	-5.05	101.15	105.70
1	A	642	G	O5'-P-OP2	-5.05	101.15	105.70
12	L	119	LYS	N-CA-C	-5.05	97.36	111.00
1	A	426	A	C2'-C3'-O3'	5.05	121.78	113.70
1	A	1030	G	O5'-P-OP2	-5.04	101.16	105.70
12	L	60	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	1309	C	O5'-P-OP2	-5.02	101.18	105.70
16	P	23	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	1482	G	O5'-P-OP2	5.02	116.72	110.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	LYS	Peptide
4	D	31	CYS	Peptide
8	H	109	ILE	Peptide
11	K	116	HIS	Peptide
12	L	26	ALA	Peptide
12	L	80	HIS	Peptide
14	N	27	CYS	Peptide
19	S	8	GLY	Peptide
20	T	12	ALA	Peptide
20	T	74	LYS	Peptide
20	T	75	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32368	0	16339	525	0
2	B	1900	0	1951	85	0
3	C	1612	0	1677	40	0
4	D	1703	0	1763	62	0
5	E	1146	0	1207	43	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	843	0	857	20	0
7	G	1257	0	1296	22	0
8	H	1116	0	1177	24	0
9	I	1011	0	1043	49	0
10	J	794	0	840	46	0
11	K	885	0	904	21	0
12	L	975	0	1062	36	0
13	M	955	0	1021	35	0
14	N	492	0	529	30	0
15	O	734	0	771	13	0
16	P	700	0	720	24	0
17	Q	823	0	891	16	0
18	R	574	0	644	14	0
19	S	629	0	652	36	0
20	T	763	0	861	24	0
21	U	208	0	221	4	0
22	X	117	0	64	2	0
23	A	294	0	315	40	0
24	A	30	0	31	5	0
25	A	99	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	K	1	0	0	0	0
25	S	1	0	0	0	0
All	All	52032	0	36836	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1080) 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)
1:A:1231:C:H2'	1:A:1232:A:C8	1.70	1.18
23:A:1606:PAR:H33	23:A:1606:PAR:N24	1.24	1.16
1:A:1287:G:N2	1:A:1313:G:O2'	1.80	1.13
23:A:1606:PAR:N24	23:A:1606:PAR:C33	2.18	1.06
5:E:101:ILE:HD11	5:E:119:LEU:HD23	1.31	1.06
14:N:27:CYS:SG	14:N:27:CYS:O	2.20	0.98
1:A:1232:A:O2'	1:A:1233:A:H8	1.46	0.97
1:A:1231:C:C2'	1:A:1232:A:C8	2.45	0.96
12:L:28:LYS:O	12:L:30:ALA:N	1.98	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.46	0.95
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.97	0.94
1:A:1230:A:H4'	1:A:1231:C:OP1	1.66	0.93
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.03	0.92
4:D:10:ARG:O	4:D:10:ARG:HG2	1.69	0.92
14:N:24:CYS:HB2	14:N:40:CYS:H	1.36	0.90
23:A:1606:PAR:H241	23:A:1606:PAR:C33	1.79	0.89
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.55	0.88
3:C:154:SER:OG	3:C:155:GLY:N	1.98	0.88
1:A:423:U:OP1	4:D:13:ARG:NH2	2.08	0.86
1:A:1232:A:O2'	1:A:1233:A:C8	2.21	0.84
12:L:90:VAL:O	12:L:91:LYS:HB3	1.77	0.84
8:H:17:THR:HB	8:H:78:GLN:OE1	1.76	0.84
1:A:1231:C:H42	1:A:1269:A:N6	1.77	0.83
1:A:77:G:H1	1:A:87:C:H5	1.24	0.82
1:A:1374:U:H2'	1:A:1375:G:C8	2.14	0.82
1:A:1230:A:H1'	1:A:1231:C:H5'	1.61	0.82
1:A:275:A:OP2	17:Q:95:TYR:OH	1.97	0.82
1:A:1232:A:HO2'	1:A:1233:A:H8	0.84	0.82
1:A:1043:C:C5	3:C:2:GLY:HA3	2.14	0.82
1:A:953:A:H4'	1:A:954:G:H5"	1.61	0.81
1:A:636:U:O4	1:A:736:G:O2'	1.98	0.81
1:A:779:C:H5"	1:A:780:C:OP2	1.81	0.81
19:S:45:VAL:O	19:S:47:HIS:N	2.14	0.80
1:A:1232:A:OP1	1:A:1232:A:O4'	1.98	0.80
1:A:906:G:O2'	1:A:1511:C:OP1	1.99	0.80
1:A:1380:C:O2'	1:A:1381:A:OP1	2.00	0.79
1:A:1210:C:OP1	13:M:108:ARG:NH2	2.16	0.79
5:E:10:MET:SD	5:E:13:ILE:HG23	2.23	0.78
1:A:1338:G:H2'	1:A:1339:A:C8	2.18	0.78
1:A:1231:C:H41	1:A:1354:G:C4'	1.97	0.78
1:A:1231:C:H3'	1:A:1232:A:C5	2.18	0.77
19:S:6:LYS:HG2	19:S:7:LYS:HE3	1.66	0.77
3:C:23:TYR:CD1	3:C:24:ALA:N	2.53	0.77
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.66	0.76
23:A:1606:PAR:O62	23:A:1606:PAR:O53	2.02	0.76
4:D:25:ARG:O	4:D:27:TYR:N	2.19	0.76
1:A:231:C:H5'	17:Q:70:ARG:HG2	1.67	0.76
12:L:27:LEU:O	12:L:29:GLY:N	2.18	0.75
1:A:1108:U:C6	1:A:1108:U:H5"	2.21	0.75
13:M:17:VAL:O	13:M:20:THR:HB	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:C:N4	1:A:1242:C:O2	2.19	0.75
1:A:957:C:H3'	1:A:958:C:H5"	1.66	0.75
1:A:108:U:OP1	23:A:1607:PAR:H221	1.86	0.75
1:A:516:A:H5'	1:A:516:A:N3	2.00	0.75
13:M:87:TYR:O	13:M:90:LEU:O	2.03	0.75
1:A:1011:C:H3'	1:A:1012:G:H5"	1.69	0.75
23:A:1607:PAR:H11	23:A:1607:PAR:O52	1.87	0.74
10:J:50:ILE:HG12	14:N:41:ARG:HD3	1.68	0.74
1:A:1111:C:O2'	1:A:1113:A:N7	2.20	0.74
1:A:324:C:H2'	1:A:324:C:O2	1.88	0.74
1:A:324:C:O2	1:A:324:C:C2'	2.36	0.74
1:A:1011:C:H3'	1:A:1012:G:C5'	2.18	0.73
1:A:1233:A:HO2'	1:A:1234:A:H8	1.30	0.73
5:E:101:ILE:CD1	5:E:119:LEU:HD23	2.14	0.73
1:A:1239:U:H4'	1:A:1239:U:OP2	1.87	0.73
1:A:506:C:OP2	12:L:69:TYR:OH	2.06	0.73
1:A:1279:C:O2'	7:G:114:ARG:NH2	2.21	0.73
23:A:1605:PAR:O44	23:A:1605:PAR:H33	1.88	0.73
1:A:1231:C:N4	1:A:1354:G:H4'	2.04	0.73
4:D:18:LYS:HD2	4:D:31:CYS:HB2	1.70	0.73
1:A:1241:C:C4	1:A:1242:C:O2	2.41	0.73
8:H:1:MET:O	8:H:1:MET:HG2	1.87	0.73
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.71	0.72
1:A:905:G:O2'	1:A:1481:A:N7	2.20	0.72
1:A:371:U:OP1	16:P:69:THR:HG21	1.90	0.72
1:A:953:A:H4'	1:A:954:G:C5'	2.20	0.72
1:A:1480:A:H2	1:A:1483:G:N1	1.88	0.72
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.72	0.72
5:E:11:ILE:HG21	5:E:105:VAL:HG22	1.71	0.72
23:A:1606:PAR:H241	23:A:1606:PAR:H33	0.90	0.71
1:A:1040:G:H5"	3:C:154:SER:HB2	1.71	0.71
1:A:1298:G:H4'	14:N:18:VAL:HG11	1.73	0.71
20:T:72:LEU:O	20:T:73:HIS:O	2.09	0.71
14:N:27:CYS:HB3	14:N:43:CYS:HB3	1.71	0.71
5:E:152:ARG:NH2	8:H:107:LEU:O	2.24	0.70
1:A:1172:G:O2'	3:C:3:ASN:HB2	1.91	0.70
23:A:1604:PAR:H13	23:A:1604:PAR:C11	2.22	0.70
1:A:952:A:OP2	14:N:29:ARG:NH2	2.24	0.70
19:S:10:PHE:HE1	19:S:70:LYS:HE2	1.56	0.70
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.21	0.70
1:A:1231:C:N4	1:A:1354:G:C4'	2.54	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.74	0.69
23:A:1604:PAR:N24	23:A:1604:PAR:O23	2.25	0.69
1:A:1043:C:C4	3:C:2:GLY:HA3	2.28	0.69
1:A:1313:G:H4'	1:A:1313:G:OP1	1.92	0.69
4:D:13:ARG:O	4:D:15:GLU:N	2.26	0.69
1:A:1007:C:H2'	1:A:1008:C:O4'	1.93	0.69
1:A:262:G:O2'	1:A:263:C:OP2	2.09	0.69
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.76	0.69
16:P:26:ARG:HD2	16:P:31:LYS:O	1.92	0.69
1:A:952:A:OP2	14:N:41:ARG:NH1	2.25	0.68
23:A:1603:PAR:H13	23:A:1603:PAR:C21	2.22	0.68
23:A:1603:PAR:O23	23:A:1603:PAR:N21	2.26	0.68
9:I:9:ARG:CG	9:I:14:VAL:HG13	2.24	0.68
13:M:108:ARG:NH1	13:M:113:PRO:O	2.27	0.67
14:N:6:LEU:HD23	14:N:23:ARG:HH22	1.60	0.67
1:A:995:A:H2'	1:A:996:G:O4'	1.94	0.67
21:U:5:ASP:O	21:U:11:GLY:HA3	1.95	0.67
1:A:1295:U:O4	19:S:4:SER:N	2.27	0.67
1:A:1477:A:H5'	1:A:1477:A:C8	2.30	0.67
1:A:1017:G:H2'	1:A:1017:G:N3	2.10	0.67
2:B:32:ILE:HD11	2:B:190:THR:HG22	1.76	0.67
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.24	0.67
1:A:958:C:C5'	1:A:958:C:H6	2.07	0.67
1:A:1477:A:H5'	1:A:1477:A:H8	1.60	0.67
1:A:193:G:H8	1:A:193:G:H5"	1.59	0.67
1:A:1230:A:C4'	1:A:1231:C:OP1	2.42	0.67
1:A:1009:C:O2	1:A:1009:C:H2'	1.93	0.67
2:B:208:ILE:HD12	2:B:208:ILE:H	1.60	0.66
9:I:3:GLN:HE21	9:I:3:GLN:HA	1.58	0.66
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.75	0.66
12:L:24:VAL:HG12	12:L:24:VAL:O	1.94	0.66
15:O:87:ILE:HG22	15:O:88:ARG:H	1.60	0.66
12:L:110:VAL:O	12:L:122:THR:HG21	1.95	0.66
1:A:1109:U:H2'	1:A:1109:U:O2	1.96	0.66
1:A:1355:U:H2'	1:A:1356:G:O5'	1.96	0.66
1:A:1135:A:H4'	10:J:17:ASP:OD2	1.95	0.66
11:K:126:ARG:O	11:K:128:ALA:N	2.28	0.66
4:D:26:CYS:HA	4:D:31:CYS:HA	1.77	0.66
1:A:1422:C:OP1	20:T:38:LYS:NZ	2.22	0.66
13:M:49:THR:HG22	13:M:51:ALA:H	1.60	0.66
12:L:47:LYS:CB	12:L:48:PRO:CD	2.73	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:42:ARG:NH2	9:I:75:ASP:OD1	2.27	0.66
1:A:707:U:H2'	1:A:707:U:O2	1.96	0.66
1:A:928:U:OP2	13:M:102:ARG:HD2	1.96	0.65
10:J:56:HIS:O	10:J:58:ASP:O	2.15	0.65
1:A:931:G:N7	13:M:104:ARG:NH1	2.45	0.65
1:A:1289:U:O3'	13:M:110:ARG:HD2	1.97	0.65
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.77	0.65
5:E:100:VAL:HG13	5:E:118:ILE:CG2	2.27	0.65
24:A:1608:PCY:O5	24:A:1608:PCY:O19	2.06	0.65
1:A:235:U:O4	23:A:1603:PAR:H24	1.97	0.65
1:A:1242:C:H6	1:A:1242:C:H3'	1.62	0.65
1:A:958:C:H5'	1:A:958:C:H6	1.62	0.64
24:A:1608:PCY:H113	24:A:1608:PCY:H132	1.78	0.64
20:T:73:HIS:C	20:T:74:LYS:HG3	2.17	0.64
13:M:65:LYS:HE2	13:M:69:GLU:HB3	1.77	0.64
14:N:24:CYS:HB2	14:N:40:CYS:N	2.10	0.64
12:L:41:ARG:HG3	12:L:42:THR:N	2.12	0.64
1:A:1231:C:H41	1:A:1354:G:C2'	2.10	0.63
19:S:4:SER:O	19:S:5:LEU:HB2	1.98	0.63
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.81	0.63
5:E:101:ILE:HD11	5:E:119:LEU:CD2	2.19	0.63
1:A:49:C:OP1	23:A:1607:PAR:N12	2.32	0.63
23:A:1604:PAR:H13	23:A:1604:PAR:H11	1.79	0.63
1:A:982:G:N2	1:A:1021:C:C2	2.67	0.63
3:C:55:VAL:HG12	3:C:55:VAL:O	1.99	0.63
5:E:41:VAL:O	5:E:67:VAL:HG12	1.99	0.62
12:L:81:SER:O	12:L:106:ASP:HB2	1.99	0.62
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.34	0.62
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.81	0.62
8:H:42:GLU:HG3	8:H:109:ILE:HD11	1.82	0.62
1:A:1351:G:OP2	9:I:112:LYS:HG3	1.99	0.62
4:D:8:VAL:O	4:D:10:ARG:N	2.33	0.62
1:A:1171:C:OP1	10:J:51:ARG:NH2	2.27	0.62
2:B:80:ILE:HD11	2:B:211:ILE:HG22	1.81	0.62
23:A:1604:PAR:H322	23:A:1604:PAR:H51	1.64	0.62
5:E:68:GLU:HG3	5:E:68:GLU:O	1.98	0.62
1:A:1231:C:C3'	1:A:1232:A:C5	2.82	0.62
1:A:1107:G:C2	1:A:1110:G:N2	2.68	0.62
23:A:1603:PAR:C11	23:A:1603:PAR:H13	2.29	0.62
5:E:148:VAL:O	5:E:152:ARG:HG3	2.00	0.61
4:D:146:ILE:HD12	4:D:146:ILE:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.35	0.61
2:B:111:ARG:HG2	2:B:111:ARG:HH11	1.64	0.61
23:A:1606:PAR:O52	23:A:1606:PAR:N21	2.34	0.61
14:N:24:CYS:CB	14:N:40:CYS:HB3	2.30	0.61
23:A:1607:PAR:H321	23:A:1607:PAR:H121	1.49	0.61
8:H:70:GLN:HA	8:H:70:GLN:NE2	2.16	0.61
1:A:691:C:H4'	11:K:20:TYR:CD2	2.36	0.61
1:A:526:G:OP1	4:D:10:ARG:NH2	2.33	0.61
19:S:10:PHE:CE1	19:S:70:LYS:HE2	2.36	0.61
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.83	0.61
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.83	0.61
1:A:480:A:H4'	1:A:481:A:OP1	2.01	0.60
1:A:1233:A:O2'	1:A:1234:A:C8	2.51	0.60
8:H:70:GLN:HA	8:H:70:GLN:HE21	1.64	0.60
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.82	0.60
4:D:11:LEU:O	4:D:12:CYS:C	2.40	0.60
1:A:1244:C:H2'	1:A:1245:C:C6	2.37	0.60
1:A:246:A:H4'	1:A:247:G:O5'	2.01	0.60
23:A:1606:PAR:O62	23:A:1606:PAR:C53	2.49	0.60
14:N:44:LEU:O	14:N:44:LEU:HD23	2.01	0.60
1:A:1231:C:H41	1:A:1354:G:C1'	2.15	0.60
1:A:1307:C:O3'	21:U:17:THR:HG21	2.01	0.60
1:A:61:A:N1	1:A:101:G:O2'	2.30	0.60
2:B:239:VAL:O	2:B:240:GLN:HB2	2.02	0.59
10:J:57:LYS:HE2	10:J:60:ARG:HH22	1.66	0.59
9:I:88:TYR:O	9:I:89:ASN:HB2	2.02	0.59
10:J:9:ARG:O	10:J:16:LEU:HD21	2.02	0.59
20:T:75:ASN:C	20:T:75:ASN:HD22	2.05	0.59
1:A:168:U:H6	1:A:205:G:HO2'	1.50	0.59
3:C:5:ILE:O	3:C:5:ILE:HD12	2.03	0.59
9:I:65:VAL:HG13	9:I:65:VAL:O	2.02	0.59
1:A:1480:A:C2	1:A:1483:G:N1	2.68	0.59
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.84	0.59
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.84	0.59
1:A:1349:C:O2'	1:A:1350:C:H5'	2.03	0.59
1:A:1009:C:O5'	1:A:1010:G:H5'	2.03	0.59
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.85	0.59
9:I:118:LYS:O	9:I:119:ALA:HB3	2.01	0.59
10:J:38:ILE:CD1	10:J:71:LEU:HD23	2.32	0.59
1:A:87:C:O4'	1:A:87:C:O2	2.21	0.59
1:A:1311:A:C2'	1:A:1312:U:H5'	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:87:ARG:HG2	18:R:87:ARG:O	2.02	0.59
1:A:1231:C:H41	1:A:1354:G:H4'	1.64	0.59
13:M:5:ALA:O	13:M:7:VAL:N	2.36	0.59
1:A:87:C:O2	1:A:87:C:O5'	2.21	0.58
16:P:26:ARG:CD	16:P:31:LYS:O	2.50	0.58
3:C:72:LYS:HB3	3:C:75:VAL:HG23	1.85	0.58
13:M:112:GLY:O	13:M:113:PRO:C	2.42	0.58
1:A:1295:U:P	19:S:6:LYS:HG3	2.43	0.58
5:E:51:VAL:HB	5:E:52:PRO:CD	2.32	0.58
1:A:349:A:C8	1:A:349:A:H5'	2.38	0.58
1:A:77:G:N1	1:A:87:C:H5	1.99	0.58
1:A:521:G:OP1	12:L:113:ARG:NH2	2.36	0.58
1:A:946:A:H4'	1:A:947:A:OP2	2.03	0.58
6:F:28:ARG:O	6:F:32:ASN:HB2	2.03	0.58
1:A:407:A:OP2	4:D:25:ARG:NH2	2.37	0.58
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.39	0.58
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.84	0.58
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.84	0.58
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.84	0.58
1:A:1238:A:OP2	1:A:1261:A:N6	2.37	0.58
2:B:225:ALA:O	2:B:226:ARG:HB2	2.03	0.58
4:D:173:TRP:HB2	4:D:187:ARG:O	2.04	0.58
4:D:13:ARG:HA	4:D:33:MET:CE	2.34	0.58
1:A:649:A:H2'	1:A:716:C:O2	2.03	0.58
1:A:920:G:C2	1:A:921:U:C6	2.91	0.58
13:M:50:GLU:O	13:M:54:VAL:HG23	2.03	0.58
20:T:48:LYS:O	20:T:49:ALA:O	2.22	0.58
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.81	0.57
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.38	0.57
4:D:60:GLU:HG3	4:D:198:VAL:HG23	1.85	0.57
1:A:1303:C:H3'	1:A:1304:C:H5"	1.84	0.57
1:A:101:G:N7	20:T:15:ARG:NH2	2.41	0.57
2:B:211:ILE:O	2:B:215:LEU:HB2	2.03	0.57
1:A:349:A:C8	1:A:349:A:C5'	2.88	0.57
9:I:48:GLU:N	9:I:49:PRO:CD	2.68	0.57
1:A:937:A:C2	1:A:1204:G:O4'	2.58	0.57
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.85	0.57
20:T:72:LEU:O	20:T:73:HIS:C	2.43	0.57
2:B:172:ILE:H	2:B:172:ILE:HD12	1.70	0.57
2:B:98:LEU:N	2:B:98:LEU:HD23	2.17	0.57
1:A:1244:C:H2'	1:A:1245:C:H6	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:A:H4'	1:A:271:G:OP1	2.04	0.57
1:A:923:G:C2	1:A:924:A:C8	2.91	0.57
1:A:482:U:O2'	1:A:483:A:P	2.63	0.57
1:A:1208:C:N4	13:M:104:ARG:HG3	2.20	0.57
1:A:798:A:H2'	1:A:800:A:H5"	1.85	0.57
1:A:955:A:N6	1:A:1206:G:O5'	2.38	0.57
19:S:6:LYS:HG2	19:S:7:LYS:CE	2.34	0.57
1:A:1311:A:H2'	1:A:1312:U:H5'	1.86	0.57
9:I:120:ARG:O	9:I:122:ALA:N	2.37	0.57
1:A:354:U:H2'	1:A:355:U:C6	2.40	0.57
2:B:195:ASP:O	8:H:68:ARG:NH2	2.33	0.57
2:B:155:LEU:HD12	2:B:157:ARG:O	2.04	0.57
1:A:1507:G:H4'	1:A:1508:G:OP2	2.04	0.57
8:H:6:ILE:O	8:H:10:LEU:HG	2.05	0.56
1:A:443:A:C4	1:A:472:A:C2	2.93	0.56
19:S:18:LYS:O	19:S:22:LEU:HD23	2.04	0.56
1:A:1049:C:H2'	1:A:1050:A:H5'	1.85	0.56
1:A:1234:A:C8	1:A:1352:C:O2'	2.58	0.56
1:A:924:A:H2'	1:A:925:G:C8	2.40	0.56
7:G:65:ALA:O	7:G:69:VAL:HG23	2.05	0.56
2:B:129:GLU:OE1	2:B:130:ARG:N	2.38	0.56
11:K:85:ARG:NH1	11:K:111:ASP:OD2	2.38	0.56
1:A:201:C:OP1	20:T:61:SER:OG	2.22	0.56
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.20	0.56
12:L:29:GLY:O	12:L:30:ALA:C	2.43	0.56
4:D:8:VAL:CG1	4:D:21:LEU:HB2	2.35	0.56
13:M:11:ARG:HG2	13:M:12:ASN:N	2.20	0.56
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.85	0.56
17:Q:87:LYS:HA	17:Q:87:LYS:CE	2.35	0.56
10:J:78:ASN:O	10:J:79:ARG:NH1	2.39	0.56
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.70	0.56
14:N:27:CYS:HB3	14:N:43:CYS:CB	2.36	0.56
1:A:953:A:H5"	1:A:953:A:H8	1.71	0.56
1:A:430:U:H2'	1:A:431:C:C6	2.40	0.56
1:A:911:G:O6	7:G:3:ARG:NH2	2.37	0.56
4:D:152:SER:O	4:D:155:LEU:HD12	2.06	0.56
18:R:47:THR:HG22	18:R:47:THR:O	2.06	0.56
12:L:111:LYS:O	12:L:111:LYS:HE2	2.05	0.56
19:S:63:THR:OG1	19:S:64:GLU:N	2.39	0.56
13:M:14:ARG:HB3	13:M:16:ASP:OD1	2.06	0.56
2:B:96:ARG:NE	2:B:96:ARG:HA	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:U:OP1	19:S:6:LYS:HG3	2.06	0.55
1:A:501:G:N1	1:A:517:A:OP2	2.26	0.55
1:A:1231:C:H42	1:A:1269:A:H62	1.53	0.55
20:T:14:LYS:HE2	20:T:18:GLN:HE22	1.70	0.55
2:B:71:VAL:HG12	2:B:93:VAL:HB	1.88	0.55
7:G:32:ARG:O	7:G:34:GLY:N	2.40	0.55
19:S:6:LYS:CG	19:S:7:LYS:HE3	2.34	0.55
23:A:1604:PAR:N64	23:A:1604:PAR:O44	2.39	0.55
9:I:120:ARG:O	9:I:121:ARG:C	2.42	0.55
1:A:1269:A:H2	1:A:1335:G:N3	2.05	0.55
1:A:927:A:N7	13:M:106:ASN:ND2	2.54	0.55
1:A:764:A:C2	1:A:785:U:C5	2.95	0.55
1:A:1385:C:O2	1:A:1478:A:N1	2.39	0.55
18:R:31:LEU:HD23	18:R:31:LEU:H	1.71	0.55
1:A:604:C:H2'	1:A:605:A:O4'	2.06	0.55
13:M:19:LEU:HB3	13:M:25:ILE:HG21	1.89	0.54
19:S:9:VAL:O	19:S:11:VAL:N	2.40	0.54
20:T:29:LYS:O	20:T:33:ILE:HG13	2.07	0.54
1:A:950:C:OP2	10:J:57:LYS:NZ	2.40	0.54
4:D:33:MET:HE2	4:D:37:PRO:HA	1.89	0.54
23:A:1603:PAR:O53	23:A:1603:PAR:O52	2.25	0.54
1:A:350:G:C2	1:A:351:C:C6	2.96	0.54
6:F:69:GLU:O	6:F:72:VAL:HG12	2.08	0.54
1:A:1005:G:H2'	1:A:1005:G:N3	2.22	0.54
1:A:1310:C:H2'	1:A:1311:A:O4'	2.08	0.54
10:J:23:ILE:O	10:J:23:ILE:HG22	2.07	0.54
12:L:25:PRO:C	12:L:27:LEU:N	2.61	0.54
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.88	0.54
1:A:925:G:H2'	1:A:926:C:O4'	2.08	0.54
1:A:250:G:OP1	17:Q:67:LYS:O	2.25	0.54
10:J:84:GLN:HE21	10:J:84:GLN:H	1.56	0.54
1:A:657:G:H2'	1:A:658:G:C8	2.43	0.54
1:A:788:U:H5"	1:A:789:C:OP2	2.07	0.54
1:A:483:A:H4'	1:A:484:G:OP1	2.07	0.54
2:B:67:THR:HG21	2:B:155:LEU:CD2	2.37	0.54
1:A:1233:A:N3	1:A:1234:A:N7	2.56	0.54
12:L:89:ARG:HA	12:L:97:ARG:HA	1.89	0.54
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.26	0.54
1:A:1074:U:O2	1:A:1076:A:C8	2.61	0.54
2:B:185:ILE:HA	2:B:199:TYR:O	2.08	0.54
1:A:690:A:H1'	11:K:29:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:G:H5"	1:A:1254:G:H8	1.72	0.54
1:A:1124:C:H2'	1:A:1125:G:C8	2.42	0.54
1:A:485:C:H2'	1:A:486:G:H8	1.73	0.54
1:A:1112:C:OP1	1:A:1113:A:H5'	2.08	0.54
12:L:23:LYS:O	12:L:24:VAL:HG23	2.07	0.54
1:A:775:G:C6	1:A:776:A:N7	2.76	0.54
1:A:954:G:N2	1:A:1345:C:OP2	2.36	0.54
1:A:715:G:H5'	1:A:750:A:H4'	1.89	0.54
4:D:170:VAL:HG13	4:D:174:LEU:HB2	1.89	0.54
1:A:258:A:H5'	20:T:74:LYS:HD3	1.90	0.53
1:A:586:A:C2	1:A:621:G:C2	2.96	0.53
1:A:8:G:O2'	5:E:120:THR:O	2.27	0.53
19:S:43:GLU:HA	19:S:45:VAL:HG13	1.90	0.53
23:A:1603:PAR:H13	23:A:1603:PAR:N21	2.23	0.53
10:J:86:MET:O	10:J:87:THR:HG23	2.08	0.53
20:T:16:HIS:O	20:T:19:SER:OG	2.20	0.53
4:D:11:LEU:C	4:D:13:ARG:N	2.61	0.53
1:A:1328:A:O4'	1:A:1330:U:C6	2.61	0.53
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.43	0.53
2:B:165:VAL:O	2:B:187:LEU:O	2.26	0.53
1:A:79:A:H61	1:A:85:C:H42	1.55	0.53
1:A:1049:C:C2'	1:A:1050:A:H5'	2.37	0.53
7:G:15:ASP:HB3	7:G:20:ASP:H	1.74	0.53
1:A:1142:U:C5	1:A:1164:G:C4	2.97	0.53
7:G:23:VAL:O	7:G:27:ILE:HG13	2.09	0.53
15:O:65:ARG:HH11	15:O:65:ARG:HG2	1.74	0.53
2:B:116:GLU:HA	2:B:119:GLU:HB2	1.89	0.53
9:I:118:LYS:O	9:I:119:ALA:CB	2.56	0.53
1:A:372:G:P	16:P:67:THR:HG21	2.49	0.53
1:A:564:U:H2'	1:A:565:G:O4'	2.09	0.53
3:C:22:TRP:O	3:C:22:TRP:CE3	2.61	0.53
1:A:97:C:P	20:T:17:ARG:HH21	2.31	0.53
20:T:73:HIS:C	20:T:74:LYS:CG	2.75	0.53
2:B:92:TYR:CE1	2:B:151:GLY:CA	2.92	0.53
10:J:45:ARG:O	10:J:46:ARG:O	2.26	0.53
1:A:11:A:OP2	5:E:126:ARG:HD2	2.09	0.53
1:A:661:U:H3	1:A:697:G:H22	1.55	0.53
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.89	0.53
2:B:69:LEU:HD13	2:B:91:PRO:HB2	1.89	0.53
16:P:22:THR:HA	16:P:33:ILE:HG13	1.91	0.53
19:S:45:VAL:HG23	19:S:46:GLY:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:C:OP1	23:A:1607:PAR:N32	2.42	0.53
1:A:1349:C:H2'	1:A:1350:C:C6	2.44	0.53
1:A:485:C:H2'	1:A:486:G:C8	2.44	0.53
4:D:121:VAL:O	4:D:134:ASP:HA	2.08	0.53
1:A:1234:A:H8	1:A:1352:C:O2'	1.92	0.52
1:A:1012:G:C8	1:A:1012:G:H3'	2.44	0.52
1:A:1349:C:H2'	1:A:1350:C:H6	1.73	0.52
1:A:1375:G:H21	1:A:1480:A:H8	1.58	0.52
10:J:50:ILE:HD13	10:J:50:ILE:H	1.74	0.52
1:A:349:A:H8	1:A:349:A:C5'	2.23	0.52
1:A:1315:A:H2'	1:A:1316:G:O4'	2.10	0.52
1:A:983:A:C8	1:A:1019:G:O6	2.62	0.52
2:B:136:VAL:O	2:B:140:HIS:HB2	2.09	0.52
2:B:9:GLU:N	2:B:12:GLU:OE1	2.43	0.52
9:I:79:LEU:HD23	9:I:101:PHE:O	2.09	0.52
8:H:116:LYS:HE3	8:H:127:LEU:HD12	1.90	0.52
1:A:1268:A:H2'	1:A:1269:A:H4'	1.91	0.52
1:A:40:G:C4	1:A:482:U:O4	2.62	0.52
17:Q:87:LYS:HE3	17:Q:87:LYS:HA	1.91	0.52
7:G:145:ALA:O	7:G:146:GLU:CB	2.57	0.52
1:A:1233:A:N6	1:A:1269:A:C5	2.77	0.52
1:A:1334:C:H2'	1:A:1335:G:C8	2.44	0.52
1:A:1355:U:C2'	1:A:1356:G:O5'	2.58	0.52
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.09	0.52
1:A:950:C:O3'	10:J:57:LYS:HG3	2.09	0.52
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.91	0.52
16:P:21:VAL:HG13	16:P:34:GLU:HB3	1.91	0.52
11:K:82:VAL:HG23	11:K:105:VAL:HG13	1.92	0.52
1:A:1232:A:C8	9:I:68:GLY:O	2.62	0.52
2:B:80:ILE:CD1	2:B:212:GLN:HA	2.40	0.52
4:D:149:ALA:O	4:D:152:SER:N	2.34	0.52
1:A:1253:G:H2'	1:A:1254:G:H5"	1.92	0.52
2:B:21:ARG:HB3	2:B:39:ILE:HA	1.92	0.52
1:A:626:A:N3	8:H:113:SER:OG	2.42	0.52
1:A:1232:A:O3'	9:I:67:GLY:HA2	2.10	0.52
1:A:1207:A:H2'	1:A:1208:C:C5	2.45	0.52
1:A:1263:U:OP2	1:A:1264:C:C5	2.63	0.52
1:A:734:G:N3	15:O:23:GLY:HA3	2.25	0.52
1:A:393:A:H3'	1:A:393:A:N3	2.24	0.52
1:A:1043:C:C5	3:C:2:GLY:CA	2.92	0.51
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.60	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:C:O2'	1:A:485:C:OP1	2.25	0.51
4:D:30:LYS:HB3	4:D:35:ARG:HD2	1.91	0.51
14:N:2:ALA:HB1	14:N:6:LEU:HD13	1.92	0.51
11:K:33:THR:HG22	11:K:39:PRO:HA	1.91	0.51
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.92	0.51
2:B:78:GLN:O	2:B:94:ASN:OD1	2.29	0.51
1:A:1037:C:OP2	1:A:1179:G:OP2	2.28	0.51
1:A:972:A:N3	1:A:972:A:H2'	2.26	0.51
1:A:1234:A:OP1	1:A:1234:A:C8	2.63	0.51
19:S:6:LYS:CD	19:S:7:LYS:HE3	2.40	0.51
1:A:765:A:H4'	1:A:1500:U:O2'	2.11	0.51
2:B:140:HIS:HA	2:B:143:GLU:HG2	1.91	0.51
1:A:1014:G:N3	1:A:1015:G:O6	2.43	0.51
2:B:35:GLU:HA	2:B:39:ILE:O	2.11	0.51
8:H:126:LYS:HG3	8:H:127:LEU:N	2.25	0.51
1:A:1234:A:O4'	1:A:1234:A:P	2.69	0.51
1:A:1287:G:H22	1:A:1313:G:C2'	2.17	0.51
1:A:969:U:C5	1:A:1194:U:H1'	2.45	0.51
14:N:24:CYS:HB2	14:N:40:CYS:CB	2.40	0.51
10:J:46:ARG:HA	10:J:63:PHE:O	2.11	0.51
1:A:100:C:O2	1:A:375:C:H4'	2.10	0.51
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.93	0.51
2:B:121:LEU:HD22	2:B:126:GLU:HB2	1.92	0.51
23:A:1607:PAR:N24	23:A:1607:PAR:O44	2.41	0.50
1:A:1008:C:H3'	1:A:1008:C:C6	2.47	0.50
1:A:1132:C:OP1	9:I:9:ARG:NH1	2.38	0.50
4:D:3:ARG:HG2	4:D:118:ARG:NE	2.26	0.50
1:A:1230:A:O2'	1:A:1230:A:N3	2.39	0.50
23:A:1606:PAR:H13	23:A:1606:PAR:N21	2.25	0.50
1:A:1111:C:H4'	9:I:16:ARG:HH22	1.76	0.50
1:A:1172:G:O2'	3:C:3:ASN:CB	2.59	0.50
16:P:57:ARG:NH1	16:P:79:VAL:O	2.44	0.50
15:O:23:GLY:O	15:O:24:SER:CB	2.59	0.50
1:A:1234:A:H2'	1:A:1234:A:N3	2.27	0.50
1:A:1329:G:N2	1:A:1356:G:H2'	2.26	0.50
9:I:4:TYR:CD2	9:I:88:TYR:CD2	3.00	0.50
8:H:103:VAL:HG21	8:H:109:ILE:O	2.11	0.50
1:A:482:U:O2'	1:A:483:A:OP2	2.27	0.50
11:K:48:ILE:HD13	11:K:48:ILE:N	2.26	0.50
11:K:54:ARG:O	11:K:57:THR:OG1	2.24	0.50
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:THR:O	3:C:16:ARG:HB2	2.12	0.50
1:A:1017:G:N3	1:A:1017:G:C2'	2.74	0.50
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.94	0.50
1:A:1418:G:H2'	1:A:1419:U:C6	2.46	0.50
19:S:12:ASP:OD2	19:S:35:SER:HB2	2.11	0.50
2:B:22:LYS:HA	2:B:22:LYS:HE2	1.93	0.50
2:B:80:ILE:HD12	2:B:212:GLN:HA	1.94	0.50
14:N:44:LEU:C	14:N:44:LEU:HD23	2.31	0.50
1:A:610:U:O4	23:A:1604:PAR:H641	2.11	0.50
1:A:1117:G:N2	1:A:1124:C:C2	2.79	0.50
1:A:485:C:O2'	1:A:486:G:H5'	2.12	0.50
1:A:659:A:H1'	11:K:116:HIS:CD2	2.47	0.50
1:A:386:C:O3'	16:P:28:ARG:NH2	2.45	0.50
1:A:1109:U:O2	1:A:1109:U:C2'	2.60	0.50
3:C:130:VAL:O	3:C:134:ILE:HG12	2.12	0.50
1:A:136:A:H1'	1:A:177:U:O2	2.12	0.50
1:A:778:A:H2'	1:A:779:C:C6	2.47	0.49
1:A:1331:A:OP2	9:I:118:LYS:NZ	2.42	0.49
1:A:828:U:H2'	1:A:829:G:O5'	2.12	0.49
1:A:81:U:O2	1:A:82:U:O2	2.29	0.49
11:K:29:ILE:C	11:K:29:ILE:HD12	2.33	0.49
1:A:1231:C:H5"	1:A:1232:A:N6	2.27	0.49
2:B:19:HIS:O	2:B:39:ILE:HG22	2.12	0.49
23:A:1604:PAR:HO53	23:A:1604:PAR:HO62	1.59	0.49
9:I:65:VAL:CG1	9:I:65:VAL:O	2.61	0.49
1:A:271:G:H5'	17:Q:14:LYS:HB3	1.94	0.49
1:A:82:U:HO2'	1:A:82:U:H6	1.60	0.49
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.94	0.49
2:B:213:LEU:O	2:B:213:LEU:HD23	2.12	0.49
1:A:1231:C:C6	9:I:69:GLY:HA2	2.48	0.49
19:S:9:VAL:C	19:S:10:PHE:CG	2.86	0.49
1:A:921:U:O2'	1:A:922:G:H5'	2.13	0.49
1:A:722:C:OP2	6:F:92:LYS:NZ	2.36	0.49
1:A:378:A:H2'	1:A:379:A:C8	2.46	0.49
13:M:70:LEU:O	13:M:73:GLU:N	2.46	0.49
1:A:1354:G:O2'	1:A:1355:U:H5'	2.13	0.49
1:A:1210:C:OP1	13:M:115:LYS:HE3	2.13	0.49
1:A:1238:A:H62	1:A:1260:U:H5'	1.77	0.49
1:A:608:C:H2'	1:A:609:G:H8	1.78	0.49
17:Q:100:LYS:HD2	17:Q:100:LYS:N	2.27	0.49
1:A:1011:C:C6	1:A:1012:G:H5"	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:1604:PAR:H13	23:A:1604:PAR:O11	2.13	0.49
1:A:899:U:O2	5:E:19:MET:HB2	2.13	0.49
1:A:961:A:N3	1:A:961:A:H3'	2.27	0.49
3:C:23:TYR:C	3:C:23:TYR:CD1	2.85	0.49
13:M:4:ILE:HG22	13:M:5:ALA:N	2.27	0.49
1:A:1325:G:H2'	1:A:1326:C:C6	2.48	0.49
1:A:1144:C:H2'	1:A:1145:C:C6	2.48	0.49
1:A:1509:A:O2'	1:A:1510:U:P	2.71	0.49
6:F:69:GLU:CD	6:F:69:GLU:H	2.16	0.49
1:A:1037:C:O2	1:A:1037:C:O2'	2.27	0.49
11:K:48:ILE:HG22	11:K:49:GLY:H	1.76	0.49
9:I:8:GLY:HA3	9:I:76:ALA:O	2.13	0.49
1:A:175:U:H2'	1:A:176:G:H5'	1.95	0.49
1:A:1040:G:H2'	1:A:1041:G:O4'	2.12	0.48
1:A:251:G:O6	1:A:262:G:O6	2.30	0.48
1:A:923:G:N3	1:A:923:G:H2'	2.27	0.48
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	1.95	0.48
1:A:1223:G:H2'	1:A:1224:C:C6	2.48	0.48
14:N:27:CYS:CB	14:N:43:CYS:HB3	2.43	0.48
1:A:48:C:P	23:A:1607:PAR:H322	2.37	0.48
1:A:690:A:O2'	11:K:31:THR:CG2	2.60	0.48
1:A:1143:G:O6	1:A:1163:G:O6	2.31	0.48
8:H:122:ARG:HB3	8:H:122:ARG:CZ	2.43	0.48
1:A:52:A:H4'	1:A:53:G:C5'	2.43	0.48
1:A:1254:G:H8	1:A:1254:G:C5'	2.26	0.48
1:A:1163:G:H8	1:A:1163:G:H5"	1.79	0.48
3:C:91:LEU:HB2	3:C:99:VAL:HG21	1.96	0.48
22:X:1:C:H3'	22:X:2:U:C6	2.49	0.48
13:M:64:TRP:O	13:M:66:LEU:HD12	2.13	0.48
1:A:1200:C:H2'	1:A:1201:U:C6	2.49	0.48
7:G:138:LYS:C	7:G:138:LYS:HD3	2.32	0.48
1:A:1231:C:N4	1:A:1354:G:C1'	2.75	0.48
15:O:23:GLY:O	15:O:24:SER:HB3	2.13	0.48
2:B:18:GLY:HA2	2:B:42:ILE:HG23	1.95	0.48
19:S:33:THR:HG22	19:S:49:ILE:CG2	2.43	0.48
1:A:1231:C:N4	1:A:1354:G:O4'	2.46	0.48
1:A:269:A:H2'	1:A:270:A:O5'	2.14	0.48
1:A:409:G:N7	4:D:35:ARG:NH1	2.62	0.48
2:B:42:ILE:HD11	2:B:202:PRO:C	2.33	0.48
2:B:55:PHE:HA	2:B:58:ILE:HG13	1.94	0.48
1:A:1116:G:C2	1:A:1125:G:N1	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:A:P	5:E:126:ARG:NH2	2.87	0.48
3:C:134:ILE:HD11	3:C:153:VAL:CG2	2.43	0.48
6:F:75:LEU:HD23	6:F:75:LEU:C	2.34	0.48
4:D:162:LEU:HG	4:D:181:MET:HG2	1.94	0.48
10:J:55:LYS:O	10:J:56:HIS:CG	2.67	0.48
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.95	0.48
1:A:702:G:C8	11:K:116:HIS:HB3	2.49	0.48
10:J:6:ILE:HG22	10:J:98:ILE:HG23	1.95	0.48
1:A:822:G:N2	1:A:827:C:C2	2.82	0.48
3:C:11:ARG:O	3:C:14:ILE:O	2.32	0.48
18:R:46:GLU:CD	18:R:46:GLU:H	2.17	0.48
1:A:1013:A:N3	1:A:1013:A:OP1	2.46	0.48
1:A:1350:C:C2	1:A:1351:G:C8	3.02	0.48
2:B:208:ILE:O	2:B:212:GLN:HB2	2.13	0.48
1:A:900:G:C6	1:A:901:A:C6	3.02	0.48
5:E:11:ILE:HD11	5:E:33:VAL:HG22	1.95	0.48
1:A:257:U:O2	1:A:259:A:C8	2.66	0.48
20:T:73:HIS:O	20:T:74:LYS:HG3	2.13	0.48
12:L:110:VAL:O	12:L:122:THR:CG2	2.62	0.48
16:P:20:VAL:HG21	16:P:32:TYR:CB	2.43	0.48
1:A:1225:C:H5"	21:U:8:THR:HG22	1.95	0.48
1:A:1348:G:C6	1:A:1349:C:C4	3.02	0.48
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.48	0.48
5:E:11:ILE:CG2	5:E:105:VAL:HG22	2.42	0.48
2:B:158:LEU:H	2:B:158:LEU:HD12	1.78	0.48
1:A:1408:U:H2'	1:A:1409:C:C6	2.49	0.47
24:A:1608:PCY:H133	24:A:1608:PCY:O5	2.14	0.47
9:I:4:TYR:N	9:I:4:TYR:CD1	2.81	0.47
19:S:51:VAL:O	19:S:57:HIS:HA	2.14	0.47
6:F:23:LYS:O	6:F:27:GLN:HG2	2.14	0.47
1:A:392:G:H2'	1:A:394:C:OP1	2.14	0.47
19:S:25:LYS:O	19:S:25:LYS:HG3	2.13	0.47
1:A:1242:C:C6	1:A:1242:C:H3'	2.44	0.47
2:B:165:VAL:HG23	2:B:166:ASP:N	2.29	0.47
1:A:1237:G:O2'	1:A:1240:G:O2'	2.14	0.47
13:M:37:THR:OG1	13:M:39:ILE:HG13	2.14	0.47
1:A:559:G:H4'	1:A:559:G:OP1	2.15	0.47
5:E:102:ALA:HB2	5:E:120:THR:HG21	1.96	0.47
1:A:257:U:OP2	20:T:79:ARG:NH2	2.46	0.47
8:H:107:LEU:N	8:H:107:LEU:HD23	2.30	0.47
1:A:372:G:OP2	16:P:67:THR:HG21	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:HIS:HA	2:B:143:GLU:CG	2.44	0.47
1:A:1036:G:N7	1:A:1182:C:H5'	2.30	0.47
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.96	0.47
16:P:14:ASN:N	16:P:15:PRO:HD3	2.29	0.47
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.44	0.47
3:C:35:GLU:O	3:C:37:GLN:N	2.46	0.47
1:A:943:A:C2	1:A:947:A:C2	3.02	0.47
11:K:48:ILE:HG22	11:K:49:GLY:N	2.29	0.47
1:A:81:U:H4'	1:A:82:U:OP1	2.15	0.47
4:D:188:LEU:CD2	4:D:188:LEU:H	2.28	0.47
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.45	0.47
10:J:8:LEU:HD13	10:J:20:ALA:CB	2.44	0.47
9:I:44:VAL:O	9:I:51:ARG:NH2	2.48	0.47
1:A:1446:A:H2'	1:A:1447:G:O4'	2.13	0.47
1:A:1114:G:C6	1:A:1115:C:N4	2.83	0.47
1:A:1184:G:C2'	1:A:1185:C:H5'	2.44	0.47
1:A:1014:G:N3	1:A:1015:G:N1	2.62	0.47
1:A:722:C:H6	1:A:722:C:O5'	1.98	0.47
1:A:1489:G:H2'	1:A:1490:U:O4'	2.14	0.47
1:A:312:G:OP2	1:A:347:G:O2'	2.33	0.47
1:A:648:G:H22	1:A:725:G:H1	1.63	0.47
1:A:781:C:O2'	1:A:782:G:H5'	2.14	0.47
1:A:696:A:H2'	1:A:697:G:O4'	2.15	0.47
16:P:20:VAL:CG2	16:P:32:TYR:HB2	2.45	0.47
9:I:112:LYS:HD2	9:I:113:LYS:O	2.15	0.47
9:I:3:GLN:C	9:I:4:TYR:CD1	2.88	0.47
1:A:386:C:H2'	1:A:387:G:C8	2.49	0.47
6:F:99:ALA:O	18:R:28:GLU:HA	2.14	0.47
15:O:71:GLN:HG3	15:O:78:TYR:CE1	2.50	0.47
1:A:1057:G:O3'	2:B:103:THR:CG2	2.63	0.47
3:C:66:VAL:O	3:C:66:VAL:HG12	2.15	0.47
4:D:9:CYS:HA	4:D:12:CYS:CB	2.43	0.47
1:A:1008:C:H3'	1:A:1008:C:H6	1.80	0.47
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.96	0.47
2:B:18:GLY:HA2	2:B:42:ILE:H	1.80	0.47
1:A:1058:C:H5'	2:B:103:THR:HG21	1.97	0.47
19:S:16:LEU:O	19:S:19:VAL:N	2.47	0.47
1:A:1362:G:O2'	1:A:1363:U:H5'	2.15	0.47
1:A:1101:C:H1'	1:A:1161:A:C4	2.50	0.47
10:J:38:ILE:HD12	10:J:71:LEU:HD23	1.97	0.46
19:S:22:LEU:O	19:S:26:GLY:HA3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ILE:O	2:B:185:ILE:HD12	2.15	0.46
1:A:1143:G:O6	1:A:1163:G:C6	2.68	0.46
22:X:3:U:H2'	22:X:4:U:OP2	2.15	0.46
1:A:1479:C:N4	1:A:1482:G:C2	2.83	0.46
15:O:7:GLU:O	15:O:11:VAL:HG23	2.15	0.46
1:A:1184:G:H2'	1:A:1185:C:H5'	1.95	0.46
1:A:1108:U:H6	1:A:1108:U:H5"	1.78	0.46
7:G:149:ARG:CG	7:G:149:ARG:HH11	2.28	0.46
9:I:55:ALA:O	9:I:57:GLY:N	2.49	0.46
1:A:1183:A:H4'	1:A:1184:G:O5'	2.16	0.46
1:A:1242:C:C3'	1:A:1242:C:C6	2.99	0.46
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.44	0.46
1:A:1263:U:OP2	1:A:1264:C:H5	1.98	0.46
1:A:157:A:C5	1:A:158:C:H1'	2.50	0.46
9:I:126:SER:HB2	9:I:128:ARG:OXT	2.15	0.46
17:Q:5:VAL:HG22	17:Q:60:ILE:HG13	1.97	0.46
18:R:53:ARG:HA	18:R:56:THR:OG1	2.15	0.46
19:S:42:PRO:O	19:S:44:MET:SD	2.73	0.46
13:M:20:THR:HA	13:M:25:ILE:HG22	1.98	0.46
1:A:958:C:H5'	1:A:958:C:C6	2.48	0.46
2:B:174:VAL:O	2:B:175:ARG:C	2.53	0.46
5:E:137:GLU:OE1	5:E:141:GLN:OE1	2.34	0.46
3:C:180:ALA:O	3:C:181:ASN:HB3	2.16	0.46
1:A:493:A:C8	1:A:493:A:H3'	2.51	0.46
8:H:17:THR:HG22	8:H:63:LEU:HG	1.98	0.46
1:A:1012:G:C3'	1:A:1012:G:C8	2.98	0.46
10:J:23:ILE:O	10:J:23:ILE:CG2	2.63	0.46
2:B:213:LEU:HD23	2:B:213:LEU:C	2.36	0.46
3:C:46:GLU:O	3:C:47:LEU:HB2	2.14	0.46
1:A:350:G:C2	1:A:351:C:C5	3.03	0.46
17:Q:67:LYS:O	17:Q:68:ARG:HG2	2.15	0.46
1:A:1161:A:H2'	1:A:1162:A:O4'	2.15	0.46
1:A:1131:U:H2'	1:A:1132:C:O4'	2.15	0.46
1:A:1135:A:OP1	10:J:68:HIS:CD2	2.69	0.46
1:A:351:C:H2'	1:A:352:A:O4'	2.15	0.46
1:A:20:C:OP1	5:E:125:SER:OG	2.23	0.46
1:A:1493:C:O2'	1:A:1494:G:H5'	2.15	0.46
10:J:35:SER:O	10:J:36:GLY:O	2.34	0.46
1:A:953:A:C5'	1:A:953:A:H8	2.29	0.46
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.50	0.46
12:L:41:ARG:HG3	12:L:42:THR:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:74:LEU:O	16:P:79:VAL:HG23	2.16	0.46
5:E:36:ASP:OD1	5:E:38:GLN:N	2.45	0.46
1:A:1358:A:O2'	7:G:29:LYS:NZ	2.49	0.46
6:F:6:VAL:HG12	6:F:8:ILE:CD1	2.45	0.46
23:A:1601:PAR:N64	23:A:1601:PAR:O44	2.48	0.46
1:A:1232:A:P	1:A:1232:A:O4'	2.73	0.46
1:A:981:G:H2'	1:A:982:G:C8	2.51	0.46
1:A:604:C:C2	4:D:135:LEU:HG	2.51	0.46
1:A:1408:U:H2'	1:A:1409:C:H6	1.80	0.46
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.31	0.46
2:B:11:LEU:HD13	2:B:217:ARG:HH22	1.80	0.46
1:A:1351:G:O2'	1:A:1352:C:H5'	2.15	0.46
15:O:74:ASP:CG	15:O:77:ARG:HG2	2.37	0.46
1:A:1078:U:H2'	1:A:1079:C:C6	2.50	0.46
1:A:1327:U:C4	1:A:1360:A:C2	3.04	0.46
9:I:93:ARG:O	9:I:95:LYS:N	2.49	0.45
6:F:45:LEU:O	6:F:46:ARG:HG3	2.16	0.45
1:A:544:U:H5'	1:A:550:G:N2	2.32	0.45
23:A:1606:PAR:C13	23:A:1606:PAR:N21	2.79	0.45
1:A:271:G:C5'	17:Q:14:LYS:HB3	2.46	0.45
2:B:22:LYS:HD2	2:B:22:LYS:N	2.31	0.45
1:A:531:A:OP2	4:D:2:GLY:N	2.49	0.45
1:A:426:A:P	4:D:22:LYS:HZ1	2.39	0.45
1:A:21:U:H2'	1:A:22:G:O4'	2.15	0.45
1:A:1329:G:C6	9:I:107:ARG:NH2	2.85	0.45
1:A:1231:C:N4	1:A:1354:G:O2'	2.48	0.45
1:A:1210:C:H4'	13:M:116:THR:HA	1.97	0.45
12:L:24:VAL:CG1	12:L:24:VAL:O	2.61	0.45
1:A:721:A:O2'	6:F:72:VAL:HG13	2.16	0.45
1:A:1471:A:OP2	23:A:1601:PAR:O41	2.34	0.45
1:A:727:U:H2'	1:A:728:C:C6	2.52	0.45
1:A:109:G:O2'	1:A:110:A:OP2	2.30	0.45
1:A:1329:G:H22	1:A:1356:G:H2'	1.81	0.45
14:N:43:CYS:SG	14:N:43:CYS:O	2.74	0.45
9:I:4:TYR:O	9:I:18:PHE:HA	2.17	0.45
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.98	0.45
2:B:67:THR:HG23	2:B:90:MET:CE	2.47	0.45
1:A:961:A:H5'	1:A:962:C:OP2	2.16	0.45
1:A:1151:A:C6	1:A:1152:A:C6	3.04	0.45
10:J:32:ALA:CB	10:J:76:ASN:HD22	2.29	0.45
1:A:1051:G:H8	1:A:1051:G:OP2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:C:O2'	10:J:56:HIS:ND1	2.48	0.45
1:A:1297:U:H2'	1:A:1298:G:O4'	2.17	0.45
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.47	0.45
10:J:84:GLN:HA	10:J:88:LEU:CB	2.47	0.45
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.52	0.45
13:M:45:VAL:HA	13:M:48:LEU:HD22	1.98	0.45
1:A:979:A:N3	1:A:979:A:H2'	2.31	0.45
1:A:1375:G:N2	1:A:1480:A:H8	2.14	0.45
12:L:111:LYS:N	12:L:111:LYS:HE2	2.32	0.45
8:H:86:ILE:HB	8:H:133:LEU:O	2.17	0.45
1:A:1038:A:N6	1:A:1188:G:C5	2.84	0.45
1:A:1380:C:O2	1:A:1380:C:O4'	2.34	0.45
1:A:715:G:OP1	1:A:750:A:H1'	2.17	0.45
1:A:1219:C:H4'	1:A:1316:G:N2	2.32	0.45
5:E:57:LYS:HG2	5:E:61:TYR:HE2	1.81	0.45
1:A:551:G:H2'	1:A:552:G:O4'	2.16	0.45
15:O:31:LEU:O	15:O:34:LEU:HB3	2.17	0.45
1:A:1002:G:N3	1:A:1002:G:H2'	2.32	0.45
3:C:100:ALA:O	3:C:101:LEU:HB2	2.15	0.45
1:A:1231:C:H3'	1:A:1232:A:C4	2.50	0.45
2:B:158:LEU:HD23	2:B:182:ILE:HD11	1.99	0.45
6:F:18:GLN:O	6:F:19:LEU:C	2.55	0.45
3:C:76:VAL:HG21	3:C:103:VAL:HG21	1.98	0.45
1:A:741:U:H5"	1:A:806:C:O2	2.17	0.45
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.32	0.45
1:A:1178:U:O2	1:A:1178:U:C2'	2.64	0.45
5:E:20:GLN:OE1	5:E:21:ALA:O	2.35	0.45
1:A:528:G:OP1	4:D:59:ARG:NH2	2.50	0.45
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.98	0.45
18:R:73:ALA:CB	18:R:79:LEU:HD12	2.44	0.45
1:A:1312:U:H4'	13:M:23:TYR:CE1	2.51	0.45
5:E:37:ARG:C	5:E:38:GLN:HG2	2.37	0.45
1:A:144:A:H2'	1:A:145:C:C6	2.51	0.45
1:A:1212:C:H2'	1:A:1213:G:H8	1.80	0.45
3:C:32:LEU:O	3:C:36:ASP:HB2	2.17	0.45
1:A:953:A:H5"	1:A:953:A:C8	2.51	0.44
1:A:953:A:C4'	1:A:954:G:H5"	2.41	0.44
10:J:15:THR:O	10:J:16:LEU:HD23	2.16	0.44
1:A:1057:G:O2'	1:A:1084:A:N1	2.36	0.44
20:T:49:ALA:HB2	20:T:99:LEU:HD12	1.98	0.44
1:A:502:C:HO2'	1:A:514:G:N2	2.14	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:C:O2'	1:A:279:C:H4'	2.17	0.44
12:L:115:LYS:O	12:L:117:ARG:N	2.49	0.44
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.87	0.44
1:A:927:A:C2	1:A:1215:G:N3	2.85	0.44
1:A:378:A:C2	1:A:379:A:C4	3.06	0.44
10:J:34:VAL:HG22	10:J:74:ILE:HG22	1.98	0.44
7:G:38:LEU:HD12	7:G:38:LEU:O	2.16	0.44
4:D:8:VAL:HG12	4:D:21:LEU:HB2	2.00	0.44
1:A:1040:G:H5"	3:C:154:SER:CB	2.42	0.44
5:E:100:VAL:HG13	5:E:118:ILE:HG21	2.00	0.44
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.50	0.44
5:E:122:GLU:O	5:E:126:ARG:NH1	2.50	0.44
1:A:1358:A:C5	1:A:1359:U:C5	3.06	0.44
6:F:37:VAL:HG12	6:F:38:GLU:O	2.18	0.44
14:N:4:LYS:O	14:N:7:ILE:HG13	2.18	0.44
3:C:188:LEU:HD13	3:C:195:VAL:HG13	1.99	0.44
1:A:83:U:H1'	1:A:84:A:OP2	2.16	0.44
10:J:57:LYS:CD	10:J:60:ARG:NH2	2.81	0.44
10:J:58:ASP:O	10:J:59:SER:HB3	2.18	0.44
2:B:145:LEU:HA	2:B:145:LEU:HD12	1.89	0.44
1:A:1407:C:H2'	1:A:1408:U:O4'	2.18	0.44
1:A:433:U:O2'	4:D:123:HIS:HD2	2.00	0.44
1:A:628:G:C5	1:A:629:C:C5	3.06	0.44
14:N:26:ARG:HH11	14:N:47:LEU:HD21	1.82	0.44
1:A:801:C:N3	1:A:1507:G:O6	2.50	0.44
1:A:1084:A:H4'	1:A:1085:A:O5'	2.18	0.44
1:A:321:A:OP2	20:T:70:SER:OG	2.32	0.44
7:G:16:LEU:HD13	9:I:41:VAL:HG12	1.98	0.44
1:A:1055:G:H2'	1:A:1056:U:C6	2.53	0.44
1:A:265:C:H2'	1:A:266:A:C8	2.52	0.44
1:A:295:G:C6	1:A:296:A:C6	3.06	0.44
1:A:1231:C:H5"	1:A:1232:A:C6	2.52	0.44
1:A:1008:C:C3'	1:A:1008:C:C6	3.01	0.44
10:J:38:ILE:HG13	10:J:71:LEU:HB3	2.00	0.44
10:J:40:LEU:HB2	10:J:69:ASN:HB2	2.00	0.44
14:N:30:ALA:O	14:N:33:VAL:HG22	2.18	0.44
10:J:31:GLY:HA3	10:J:81:THR:CG2	2.48	0.44
4:D:33:MET:CE	4:D:37:PRO:HA	2.48	0.44
9:I:4:TYR:CD2	9:I:88:TYR:CG	3.06	0.44
2:B:42:ILE:HD11	2:B:202:PRO:O	2.18	0.44
13:M:15:VAL:HG22	13:M:43:THR:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:GLU:O	3:C:86:VAL:HG23	2.17	0.44
1:A:1174:C:H2'	1:A:1175:G:O4'	2.17	0.44
1:A:1309:C:O3'	21:U:20:LYS:NZ	2.50	0.44
1:A:753:G:H4'	1:A:1491:A:H4'	2.00	0.44
1:A:678:A:H2'	1:A:679:A:O5'	2.18	0.44
1:A:1137:G:C4	1:A:1138:G:C8	3.06	0.44
8:H:78:GLN:HE21	8:H:78:GLN:HB2	1.58	0.44
1:A:1380:C:HO2'	1:A:1381:A:P	2.30	0.44
1:A:258:A:C6	1:A:259:A:C6	3.05	0.44
1:A:610:U:O4	23:A:1604:PAR:C64	2.66	0.44
2:B:189:ASP:OD2	2:B:205:ASP:OD1	2.36	0.44
1:A:146:A:H2'	1:A:147:A:O4'	2.18	0.44
1:A:614:G:H5'	1:A:615:G:OP2	2.17	0.44
1:A:16:G:OP1	1:A:1379:A:O2'	2.23	0.44
8:H:8:ASP:O	8:H:12:ARG:HG3	2.17	0.44
5:E:74:GLY:HA3	5:E:116:THR:OG1	2.17	0.44
1:A:641:G:H4'	15:O:28:GLN:HG2	1.98	0.44
2:B:215:LEU:O	2:B:219:VAL:HG23	2.18	0.43
13:M:90:LEU:HD23	13:M:90:LEU:H	1.83	0.43
2:B:19:HIS:O	2:B:39:ILE:CG2	2.66	0.43
9:I:48:GLU:N	9:I:49:PRO:HD2	2.32	0.43
1:A:1263:U:O4'	1:A:1263:U:O2	2.36	0.43
10:J:4:ILE:HD13	10:J:100:THR:HG22	2.00	0.43
1:A:1063:A:H5"	5:E:16:THR:HG21	1.99	0.43
1:A:786:A:H2'	1:A:787:G:O4'	2.18	0.43
18:R:32:ARG:HA	18:R:69:THR:HG21	2.00	0.43
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.99	0.43
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.99	0.43
2:B:67:THR:HG23	2:B:90:MET:HE2	2.00	0.43
1:A:1188:G:C6	1:A:1189:G:C5	3.07	0.43
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.48	0.43
1:A:859:G:P	12:L:12:ARG:HH22	2.41	0.43
1:A:1354:G:C2'	1:A:1355:U:H5'	2.49	0.43
3:C:23:TYR:CG	3:C:24:ALA:N	2.87	0.43
1:A:48:C:O2'	23:A:1607:PAR:H14	2.18	0.43
1:A:982:G:C2	1:A:983:A:N3	2.86	0.43
9:I:79:LEU:HD22	9:I:83:ARG:HD2	2.00	0.43
2:B:77:ALA:O	2:B:78:GLN:C	2.55	0.43
1:A:266:A:H2'	1:A:267:C:O4'	2.17	0.43
1:A:1120:C:O2'	1:A:1121:G:N2	2.51	0.43
5:E:128:PRO:O	5:E:129:ILE:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:A:N6	1:A:669:G:C6	2.86	0.43
2:B:41:ILE:HD12	2:B:41:ILE:N	2.34	0.43
4:D:14:ARG:HG3	4:D:15:GLU:N	2.33	0.43
4:D:31:CYS:C	4:D:33:MET:H	2.22	0.43
1:A:1477:A:C2	1:A:1478:A:C8	3.07	0.43
1:A:1219:C:C2'	1:A:1220:A:OP1	2.66	0.43
1:A:900:G:O2'	1:A:1381:A:N1	2.36	0.43
2:B:97:TRP:CE3	2:B:98:LEU:O	2.72	0.43
4:D:145:GLU:C	4:D:146:ILE:HD12	2.39	0.43
4:D:101:LEU:HD23	4:D:121:VAL:CG1	2.48	0.43
1:A:1137:G:C2	1:A:1138:G:C8	3.06	0.43
1:A:1485:A:C2	1:A:1486:G:C4	3.07	0.43
7:G:144:MET:CE	7:G:144:MET:HA	2.47	0.43
1:A:927:A:H2'	1:A:928:U:O4'	2.18	0.43
1:A:935:U:O2'	1:A:937:A:N7	2.37	0.43
14:N:36:PHE:O	14:N:36:PHE:CD1	2.72	0.43
5:E:38:GLN:HE21	5:E:38:GLN:HB3	1.64	0.43
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.52	0.43
1:A:52:A:H4'	1:A:53:G:O5'	2.19	0.43
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.83	0.43
6:F:75:LEU:HD23	6:F:79:LEU:HG	2.00	0.43
1:A:889:U:H2'	1:A:890:C:C6	2.53	0.43
16:P:58:TYR:O	16:P:62:VAL:HG22	2.19	0.43
15:O:15:PHE:O	15:O:16:ALA:O	2.37	0.43
12:L:35:GLY:O	12:L:82:VAL:HA	2.19	0.43
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.88	0.43
1:A:870:A:C2	1:A:885:A:C4	3.07	0.43
8:H:69:ARG:NH1	8:H:75:ARG:O	2.42	0.43
1:A:1040:G:C5	1:A:1186:A:C2	3.07	0.43
1:A:951:G:OP1	10:J:57:LYS:HE3	2.18	0.43
1:A:1295:U:OP2	19:S:6:LYS:HB3	2.19	0.43
1:A:1219:C:C4'	1:A:1316:G:N2	2.82	0.43
2:B:216:SER:OG	2:B:217:ARG:N	2.52	0.43
1:A:21:U:H6	1:A:21:U:O5'	2.02	0.43
19:S:49:ILE:HD12	19:S:49:ILE:H	1.84	0.43
16:P:20:VAL:CG2	16:P:32:TYR:CB	2.97	0.43
9:I:55:ALA:O	9:I:56:LEU:C	2.57	0.43
9:I:97:LYS:HB3	9:I:98:PRO:HD3	2.00	0.43
3:C:95:THR:O	3:C:97:LYS:N	2.43	0.43
13:M:82:MET:SD	13:M:83:ASP:N	2.92	0.43
1:A:1095:C:O2	3:C:179:ARG:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:C:H2'	1:A:189:U:O4'	2.19	0.43
1:A:130:C:O2	16:P:1:MET:HB2	2.19	0.43
4:D:8:VAL:CG1	4:D:21:LEU:CB	2.96	0.42
10:J:59:SER:C	10:J:60:ARG:HG3	2.39	0.42
1:A:780:C:O2'	24:A:1608:PCY:C9	2.67	0.42
1:A:921:U:C2'	1:A:922:G:H5'	2.48	0.42
1:A:11:A:O2'	1:A:12:G:H5'	2.19	0.42
7:G:145:ALA:O	7:G:146:GLU:HB2	2.19	0.42
1:A:385:A:C6	1:A:386:C:H1'	2.54	0.42
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.99	0.42
2:B:134:GLU:HA	2:B:137:ARG:HB3	2.00	0.42
1:A:1324:C:H4'	9:I:125:TYR:HB2	2.01	0.42
2:B:109:SER:O	2:B:112:VAL:N	2.52	0.42
9:I:116:LYS:N	9:I:116:LYS:HD3	2.34	0.42
14:N:44:LEU:C	14:N:44:LEU:CD2	2.88	0.42
19:S:11:VAL:HG11	19:S:41:VAL:CG2	2.49	0.42
2:B:74:LYS:HE3	2:B:166:ASP:HB2	2.01	0.42
1:A:969:U:O2'	1:A:970:U:H5'	2.19	0.42
17:Q:93:GLN:O	17:Q:96:GLU:HG3	2.18	0.42
1:A:1198:G:H5"	14:N:5:ALA:CB	2.48	0.42
1:A:1476:U:H4'	1:A:1497:A:C2	2.55	0.42
13:M:24:GLY:C	13:M:25:ILE:HD12	2.40	0.42
1:A:1016:G:O2'	1:A:1017:G:OP1	2.32	0.42
4:D:198:VAL:O	4:D:198:VAL:HG13	2.18	0.42
16:P:70:ALA:O	16:P:74:LEU:HG	2.19	0.42
6:F:19:LEU:HD23	6:F:19:LEU:C	2.40	0.42
3:C:188:LEU:O	3:C:189:ALA:HB2	2.19	0.42
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.55	0.42
11:K:61:ALA:HB2	11:K:90:GLY:HA3	2.00	0.42
1:A:1087:G:P	2:B:111:ARG:HD2	2.59	0.42
11:K:108:ILE:O	18:R:87:ARG:N	2.49	0.42
6:F:19:LEU:HD23	6:F:20:ALA:N	2.33	0.42
1:A:436:A:H5"	1:A:437:C:OP2	2.19	0.42
10:J:54:PHE:O	10:J:55:LYS:C	2.58	0.42
1:A:49:C:OP1	23:A:1607:PAR:H62	2.20	0.42
1:A:1110:G:H5"	1:A:1111:C:OP2	2.19	0.42
1:A:193:G:C8	1:A:193:G:H5"	2.46	0.42
8:H:109:ILE:HG23	8:H:110:ALA:N	2.35	0.42
1:A:1163:G:C8	1:A:1163:G:H5"	2.54	0.42
1:A:608:C:H2'	1:A:609:G:C8	2.53	0.42
18:R:37:VAL:HG11	18:R:78:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:36:ARG:NH1	19:S:53:ASN:HA	2.34	0.42
2:B:14:GLY:O	2:B:15:VAL:HG13	2.19	0.42
10:J:90:LEU:N	10:J:91:PRO:CD	2.82	0.42
20:T:89:ARG:NH1	20:T:105:SER:O	2.38	0.42
2:B:70:PHE:O	2:B:92:TYR:HA	2.20	0.42
1:A:765:A:C5	1:A:786:A:C2	3.08	0.42
4:D:3:ARG:HG2	4:D:118:ARG:CZ	2.50	0.42
19:S:29:ARG:C	19:S:31:ILE:H	2.23	0.42
1:A:570:C:O2'	1:A:571:G:H5'	2.19	0.42
1:A:526:G:H5'	4:D:41:GLY:HA3	2.01	0.42
1:A:1331:A:P	9:I:118:LYS:NZ	2.93	0.42
10:J:78:ASN:N	10:J:78:ASN:HD22	2.18	0.42
10:J:79:ARG:HA	10:J:79:ARG:HD3	1.88	0.42
1:A:1263:U:OP2	1:A:1264:C:N4	2.51	0.42
8:H:69:ARG:HD3	8:H:75:ARG:O	2.20	0.42
1:A:1184:G:H21	14:N:43:CYS:HB3	1.84	0.42
12:L:69:TYR:CG	12:L:90:VAL:HG21	2.53	0.42
9:I:17:VAL:HG22	9:I:63:ILE:HG12	2.02	0.42
1:A:662:U:H1'	1:A:761:A:O3'	2.20	0.42
4:D:13:ARG:HA	4:D:33:MET:HE3	2.02	0.42
19:S:5:LEU:HA	19:S:6:LYS:NZ	2.35	0.42
1:A:1111:C:H1'	1:A:1129:A:H61	1.85	0.42
1:A:1289:U:O3'	13:M:110:ARG:CD	2.66	0.42
1:A:890:C:O2'	1:A:891:A:H5'	2.20	0.42
1:A:606:A:C8	1:A:607:C:C5	3.08	0.42
1:A:1078:U:H5"	1:A:1092:C:O2	2.19	0.42
18:R:37:VAL:CG1	18:R:78:LEU:HB3	2.50	0.42
1:A:606:A:C8	1:A:607:C:C6	3.08	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.93	0.42
1:A:799:A:O2'	1:A:1505:C:H1'	2.20	0.42
1:A:503:C:H2'	1:A:504:A:C8	2.55	0.42
4:D:25:ARG:C	4:D:27:TYR:N	2.74	0.41
13:M:106:ASN:O	13:M:107:ALA:HB3	2.20	0.41
1:A:296:A:O5'	1:A:296:A:H8	2.03	0.41
20:T:26:ASN:ND2	20:T:71:THR:HA	2.34	0.41
1:A:812:A:OP1	1:A:812:A:H4'	2.19	0.41
1:A:94:C:H2'	1:A:95:A:O4'	2.20	0.41
5:E:101:ILE:O	5:E:120:THR:HG23	2.20	0.41
12:L:29:GLY:O	12:L:30:ALA:O	2.38	0.41
1:A:49:C:H4'	1:A:50:U:OP2	2.20	0.41
12:L:38:THR:O	12:L:79:GLU:HG2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLN:OE1	2:B:95:GLN:NE2	2.52	0.41
6:F:6:VAL:HG12	6:F:8:ILE:HD12	2.01	0.41
1:A:103:A:C6	1:A:322:G:C6	3.08	0.41
14:N:24:CYS:CB	14:N:40:CYS:CB	2.97	0.41
1:A:1344:C:H2'	1:A:1345:C:H5"	2.02	0.41
1:A:983:A:N7	1:A:1019:G:O6	2.52	0.41
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.03	0.41
8:H:62:TYR:N	8:H:62:TYR:CD2	2.87	0.41
1:A:1286:G:C6	1:A:1287:G:N1	2.89	0.41
1:A:1382:C:C2	1:A:1480:A:N6	2.88	0.41
5:E:41:VAL:HG22	5:E:113:ALA:HB2	2.02	0.41
1:A:101:G:O6	20:T:15:ARG:NE	2.53	0.41
5:E:51:VAL:HB	5:E:52:PRO:HD2	2.01	0.41
10:J:45:ARG:NH2	14:N:36:PHE:CD2	2.88	0.41
1:A:898:U:H2'	1:A:899:U:C6	2.55	0.41
9:I:43:ALA:O	9:I:45:ALA:N	2.53	0.41
1:A:562:C:H2'	1:A:563:G:O4'	2.20	0.41
1:A:528:G:OP2	4:D:66:ARG:NH2	2.51	0.41
1:A:125:A:H1'	1:A:259:A:O2'	2.19	0.41
1:A:349:A:H8	1:A:349:A:H5"	1.85	0.41
4:D:64:LEU:HB2	4:D:198:VAL:HG21	2.03	0.41
1:A:763:C:N4	1:A:764:A:C6	2.88	0.41
1:A:1117:G:C2	1:A:1125:G:N1	2.89	0.41
2:B:187:LEU:HD23	2:B:201:ILE:O	2.20	0.41
16:P:3:LYS:O	16:P:21:VAL:HA	2.20	0.41
4:D:162:LEU:HD13	4:D:162:LEU:HA	1.93	0.41
1:A:1069:U:H3	1:A:1082:G:H22	1.67	0.41
3:C:157:ILE:HD11	3:C:166:GLU:HB2	2.02	0.41
1:A:1329:G:OP2	9:I:107:ARG:HG2	2.20	0.41
1:A:1135:A:C6	1:A:1136:C:C4	3.09	0.41
1:A:1208:C:H4'	1:A:1209:A:OP1	2.20	0.41
1:A:720:C:H2'	1:A:721:A:C8	2.55	0.41
1:A:690:A:O2'	11:K:31:THR:HG21	2.21	0.41
1:A:1125:G:H2'	1:A:1126:G:O4'	2.20	0.41
1:A:1140:A:C6	1:A:1162:A:C6	3.09	0.41
1:A:1137:G:N3	1:A:1138:G:C8	2.88	0.41
2:B:15:VAL:C	2:B:16:HIS:CG	2.94	0.41
1:A:791:A:H2'	1:A:792:C:C6	2.55	0.41
1:A:451:C:H2'	1:A:452:C:C6	2.55	0.41
12:L:68:ALA:HB1	12:L:100:ILE:HD12	2.02	0.41
4:D:13:ARG:HG2	4:D:33:MET:HE3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:U:O2'	1:A:51:A:H2'	2.21	0.41
1:A:1314:A:C2	1:A:1315:A:C4	3.08	0.41
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.53	0.41
18:R:43:PHE:HA	18:R:51:LEU:HD12	2.03	0.41
20:T:50:GLU:HA	20:T:100:ILE:HB	2.02	0.41
1:A:1335:G:O2'	1:A:1336:C:H5'	2.21	0.41
12:L:27:LEU:HG	12:L:28:LYS:N	2.35	0.41
4:D:15:GLU:OE2	4:D:59:ARG:NH1	2.54	0.41
10:J:84:GLN:HA	10:J:88:LEU:HB2	2.03	0.41
1:A:690:A:C2'	11:K:31:THR:HG21	2.50	0.41
1:A:543:A:OP1	5:E:126:ARG:NH2	2.52	0.41
1:A:378:A:H2'	1:A:379:A:H8	1.85	0.41
1:A:1042:C:O3'	14:N:45:ARG:NH2	2.52	0.41
1:A:1234:A:O4'	1:A:1234:A:OP1	2.39	0.41
1:A:1231:C:N4	1:A:1270:A:H61	2.18	0.41
1:A:954:G:C8	1:A:1340:U:C2	3.09	0.41
19:S:6:LYS:HD2	19:S:6:LYS:N	2.36	0.41
1:A:52:A:OP2	23:A:1607:PAR:N24	2.54	0.41
1:A:1132:C:P	9:I:9:ARG:NH1	2.94	0.41
9:I:4:TYR:CE2	9:I:88:TYR:CG	3.09	0.41
5:E:118:ILE:O	5:E:118:ILE:HG23	2.20	0.41
5:E:31:LEU:HD22	5:E:43:LEU:CD1	2.47	0.41
4:D:127:THR:HA	4:D:132:ARG:HA	2.03	0.41
11:K:33:THR:HB	11:K:38:ASN:O	2.21	0.41
17:Q:59:ILE:HD13	17:Q:59:ILE:HA	1.70	0.41
16:P:20:VAL:HG21	16:P:32:TYR:CG	2.56	0.41
23:A:1601:PAR:H531	23:A:1601:PAR:H21	2.02	0.41
1:A:1327:U:C2	1:A:1360:A:N1	2.89	0.41
2:B:105:PHE:O	2:B:106:LYS:C	2.59	0.41
17:Q:80:GLY:O	17:Q:82:MET:N	2.54	0.41
9:I:46:ALA:HB2	9:I:74:ILE:HG23	2.03	0.41
12:L:86:ARG:HB3	12:L:101:VAL:CG2	2.51	0.41
2:B:68:ILE:HD13	2:B:161:ALA:HB3	2.03	0.41
23:A:1607:PAR:N64	23:A:1607:PAR:O44	2.54	0.41
1:A:935:U:H6	1:A:935:U:O5'	2.04	0.41
1:A:85:C:H6	1:A:85:C:O5'	2.04	0.41
1:A:1014:G:H1'	1:A:1015:G:N1	2.36	0.41
1:A:452:C:H2'	1:A:453:C:H6	1.85	0.41
1:A:817:U:H2'	1:A:818:C:C6	2.56	0.41
1:A:400:U:H2'	1:A:401:U:C6	2.56	0.41
1:A:403:G:H2'	1:A:404:A:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:C:O5'	1:A:1185:C:H6	2.04	0.40
1:A:1132:C:P	9:I:9:ARG:HH11	2.43	0.40
1:A:1254:G:C8	1:A:1254:G:C5'	3.04	0.40
4:D:101:LEU:HD23	4:D:121:VAL:HG13	2.03	0.40
1:A:373:G:OP1	16:P:3:LYS:HD3	2.20	0.40
1:A:821:G:C2	1:A:828:U:O2	2.74	0.40
1:A:1357:A:C2'	1:A:1358:A:H5'	2.51	0.40
1:A:22:G:H2'	1:A:23:G:C8	2.56	0.40
2:B:15:VAL:H	2:B:16:HIS:CE1	2.39	0.40
1:A:810:C:H2'	1:A:811:U:C6	2.56	0.40
1:A:1467:G:H2'	1:A:1468:C:O4'	2.20	0.40
1:A:767:C:O2'	1:A:768:C:H5'	2.21	0.40
4:D:49:ARG:O	4:D:50:ARG:C	2.60	0.40
5:E:102:ALA:HB2	5:E:120:THR:CG2	2.52	0.40
3:C:23:TYR:CE1	3:C:24:ALA:C	2.95	0.40
1:A:108:U:H5"	23:A:1607:PAR:O62	2.21	0.40
13:M:90:LEU:O	13:M:91:ARG:CB	2.70	0.40
13:M:97:PRO:HA	13:M:110:ARG:HD3	2.03	0.40
1:A:1179:G:OP1	1:A:1180:G:OP2	2.39	0.40
1:A:1014:G:N3	1:A:1015:G:C6	2.90	0.40
3:C:134:ILE:HD11	3:C:153:VAL:HG23	2.03	0.40
7:G:136:LYS:C	7:G:138:LYS:H	2.21	0.40
19:S:49:ILE:HD12	19:S:49:ILE:N	2.36	0.40
1:A:433:U:O2'	4:D:123:HIS:CD2	2.74	0.40
12:L:53:ARG:HB3	12:L:93:LEU:HD11	2.02	0.40
1:A:1009:C:H4'	1:A:1010:G:H8	1.86	0.40
1:A:982:G:N2	1:A:1021:C:O2	2.53	0.40
4:D:146:ILE:N	4:D:146:ILE:CD1	2.82	0.40
1:A:603:U:C2	4:D:135:LEU:HD22	2.57	0.40
7:G:15:ASP:HB2	7:G:20:ASP:O	2.22	0.40
1:A:372:G:H5"	16:P:5:ARG:HB2	2.04	0.40
1:A:1037:C:O2	1:A:1037:C:C2'	2.70	0.40
1:A:392:G:H8	1:A:392:G:C5'	2.35	0.40
14:N:15:LYS:C	14:N:16:PHE:CG	2.95	0.40
1:A:823:U:C2'	1:A:823:U:O2	2.69	0.40
1:A:1231:C:H1'	9:I:70:LYS:HD2	2.02	0.40
1:A:900:G:N3	1:A:1381:A:H2	2.19	0.40
2:B:172:ILE:O	2:B:176:GLU:HG3	2.20	0.40
1:A:296:A:H1'	1:A:549:U:O2	2.21	0.40
1:A:1396:A:C2	1:A:1466:G:C2	3.09	0.40
1:A:1282:G:C6	1:A:1317:C:C6	3.10	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:C:OP2	1:A:1272:G:N2	2.54	0.40
1:A:780:C:C1'	24:A:1608:PCY:H92	2.52	0.40
14:N:41:ARG:HA	14:N:44:LEU:HD13	2.03	0.40
1:A:610:U:OP1	16:P:35:LYS:NZ	2.55	0.40
9:I:31:GLN:HB2	9:I:31:GLN:HE21	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/234 (99%)	180 (78%)	39 (17%)	13 (6%)	2 13
3	C	204/206 (99%)	156 (76%)	33 (16%)	15 (7%)	1 7
4	D	206/208 (99%)	172 (84%)	23 (11%)	11 (5%)	2 14
5	E	148/150 (99%)	127 (86%)	20 (14%)	1 (1%)	26 65
6	F	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	9 38
7	G	153/155 (99%)	128 (84%)	22 (14%)	3 (2%)	9 38
8	H	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	26 65
9	I	125/127 (98%)	99 (79%)	15 (12%)	11 (9%)	1 5
10	J	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	2 15
11	K	117/119 (98%)	102 (87%)	8 (7%)	7 (6%)	2 11
12	L	123/125 (98%)	98 (80%)	16 (13%)	9 (7%)	1 7
13	M	118/120 (98%)	88 (75%)	17 (14%)	13 (11%)	0 3
14	N	58/60 (97%)	40 (69%)	12 (21%)	6 (10%)	1 4
15	O	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	4 24
16	P	81/83 (98%)	73 (90%)	8 (10%)	0	100 100
17	Q	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	9 37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	R	68/70 (97%)	60 (88%)	7 (10%)	1 (2%)	13 46
19	S	76/78 (97%)	55 (72%)	15 (20%)	6 (8%)	1 6
20	T	97/99 (98%)	81 (84%)	7 (7%)	9 (9%)	1 4
21	U	22/24 (92%)	20 (91%)	2 (9%)	0	100 100
All	All	2342/2382 (98%)	1924 (82%)	300 (13%)	118 (5%)	3 16

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	18	GLY
2	B	44	LEU
2	B	226	ARG
2	B	237	ALA
2	B	239	VAL
3	C	36	ASP
3	C	47	LEU
3	C	79	ARG
3	C	101	LEU
3	C	127	ARG
3	C	154	SER
4	D	3	ARG
4	D	13	ARG
4	D	14	ARG
4	D	26	CYS
4	D	27	TYR
4	D	29	PRO
4	D	30	LYS
6	F	39	LYS
7	G	33	ASP
7	G	137	LYS
9	I	56	LEU
10	J	46	ARG
11	K	12	ARG
11	K	117	ASN
11	K	127	LYS
12	L	27	LEU
12	L	29	GLY
12	L	30	ALA
12	L	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	6	GLY
13	M	67	GLU
13	M	83	ASP
13	M	91	ARG
13	M	113	PRO
14	N	27	CYS
15	O	16	ALA
17	Q	49	GLU
17	Q	81	ARG
19	S	6	LYS
19	S	42	PRO
19	S	80	TYR
20	T	49	ALA
20	T	74	LYS
20	T	95	ALA
20	T	99	LEU
2	B	14	GLY
2	B	78	GLN
2	B	110	GLN
3	C	16	ARG
3	C	189	ALA
3	C	206	GLU
4	D	10	ARG
6	F	38	GLU
7	G	7	ALA
9	I	78	LYS
9	I	119	ALA
10	J	36	GLY
10	J	55	LYS
11	K	27	ASN
11	K	91	ARG
12	L	91	LYS
13	M	14	ARG
13	M	46	LYS
14	N	28	GLY
14	N	32	SER
14	N	44	LEU
19	S	45	VAL
19	S	46	GLY
20	T	73	HIS
2	B	9	GLU
5	E	21	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	89	ASN
9	I	94	ALA
11	K	128	ALA
12	L	28	LYS
13	M	112	GLY
15	O	24	SER
20	T	13	LEU
20	T	47	GLY
2	B	130	ARG
4	D	166	LYS
8	H	71	GLY
9	I	118	LYS
10	J	67	THR
13	M	71	ARG
14	N	26	ARG
15	O	86	GLY
18	R	87	ARG
20	T	87	LYS
2	B	232	PRO
3	C	4	LYS
3	C	53	ALA
4	D	5	ILE
4	D	32	ALA
10	J	59	SER
12	L	26	ALA
12	L	82	VAL
13	M	120	LYS
3	C	39	ILE
3	C	61	ALA
3	C	81	GLY
9	I	125	TYR
9	I	127	LYS
14	N	16	PHE
19	S	10	PHE
20	T	75	ASN
9	I	65	VAL
9	I	109	VAL
11	K	118	GLY
13	M	4	ILE
12	L	48	PRO
13	M	7	VAL
3	C	96	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	44	VAL
13	M	85	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/202 (100%)	154 (76%)	48 (24%)	1 3
3	C	160/160 (100%)	130 (81%)	30 (19%)	2 8
4	D	180/180 (100%)	149 (83%)	31 (17%)	2 11
5	E	115/115 (100%)	97 (84%)	18 (16%)	3 13
6	F	90/90 (100%)	84 (93%)	6 (7%)	20 56
7	G	126/126 (100%)	106 (84%)	20 (16%)	3 13
8	H	119/119 (100%)	97 (82%)	22 (18%)	2 9
9	I	98/98 (100%)	74 (76%)	24 (24%)	1 3
10	J	88/88 (100%)	71 (81%)	17 (19%)	2 8
11	K	90/90 (100%)	74 (82%)	16 (18%)	2 10
12	L	104/104 (100%)	88 (85%)	16 (15%)	3 14
13	M	96/96 (100%)	69 (72%)	27 (28%)	0 1
14	N	49/49 (100%)	36 (74%)	13 (26%)	0 2
15	O	79/79 (100%)	67 (85%)	12 (15%)	3 14
16	P	72/72 (100%)	62 (86%)	10 (14%)	4 19
17	Q	94/94 (100%)	81 (86%)	13 (14%)	4 19
18	R	61/61 (100%)	50 (82%)	11 (18%)	2 10
19	S	69/69 (100%)	50 (72%)	19 (28%)	0 1
20	T	76/76 (100%)	63 (83%)	13 (17%)	2 11
21	U	19/19 (100%)	15 (79%)	4 (21%)	1 6
All	All	1987/1987 (100%)	1617 (81%)	370 (19%)	2 9

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
2	B	15	VAL
2	B	17	PHE
2	B	22	LYS
2	B	23	ARG
2	B	24	TRP
2	B	27	LYS
2	B	42	ILE
2	B	44	LEU
2	B	45	GLN
2	B	48	MET
2	B	52	GLU
2	B	58	ILE
2	B	67	THR
2	B	74	LYS
2	B	75	LYS
2	B	76	GLN
2	B	80	ILE
2	B	87	ARG
2	B	96	ARG
2	B	97	TRP
2	B	111	ARG
2	B	119	GLU
2	B	127	ILE
2	B	129	GLU
2	B	132	LYS
2	B	135	GLN
2	B	137	ARG
2	B	140	HIS
2	B	145	LEU
2	B	146	GLN
2	B	155	LEU
2	B	156	LYS
2	B	163	PHE
2	B	168	THR
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	175	ARG
2	B	187	LEU
2	B	196	LEU
2	B	206	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	208	ILE
2	B	215	LEU
2	B	221	LEU
2	B	223	ILE
2	B	233	SER
2	B	238	LEU
3	C	3	ASN
3	C	5	ILE
3	C	15	THR
3	C	16	ARG
3	C	26	LYS
3	C	27	LYS
3	C	28	GLN
3	C	36	ASP
3	C	38	ARG
3	C	40	ARG
3	C	45	LYS
3	C	47	LEU
3	C	49	SER
3	C	54	ARG
3	C	64	VAL
3	C	72	LYS
3	C	79	ARG
3	C	89	GLU
3	C	101	LEU
3	C	127	ARG
3	C	128	PHE
3	C	131	ARG
3	C	132	ARG
3	C	143	GLU
3	C	144	SER
3	C	164	ARG
3	C	167	TRP
3	C	188	LEU
3	C	196	LEU
3	C	204	LEU
4	D	3	ARG
4	D	9	CYS
4	D	11	LEU
4	D	19	LEU
4	D	24	GLU
4	D	27	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	30	LYS
4	D	33	MET
4	D	34	GLU
4	D	49	ARG
4	D	58	LEU
4	D	89	THR
4	D	96	LEU
4	D	106	TYR
4	D	108	LEU
4	D	119	GLN
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	132	ARG
4	D	135	LEU
4	D	139	ARG
4	D	150	GLU
4	D	154	ASN
4	D	162	LEU
4	D	184	LYS
4	D	186	LEU
4	D	188	LEU
4	D	190	ASP
4	D	194	LEU
4	D	209	ARG
5	E	10	MET
5	E	18	ARG
5	E	31	LEU
5	E	33	VAL
5	E	38	GLN
5	E	41	VAL
5	E	64	ARG
5	E	68	GLU
5	E	79	GLU
5	E	80	ILE
5	E	91	LEU
5	E	101	ILE
5	E	116	THR
5	E	118	ILE
5	E	145	LYS
5	E	147	ASP
5	E	150	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	153	LYS
6	F	1	MET
6	F	21	LEU
6	F	54	LYS
6	F	61	LEU
6	F	74	ASP
6	F	98	LEU
7	G	3	ARG
7	G	5	ARG
7	G	6	ARG
7	G	24	THR
7	G	36	LYS
7	G	48	LYS
7	G	54	THR
7	G	60	LYS
7	G	64	GLN
7	G	72	ARG
7	G	75	VAL
7	G	94	ARG
7	G	97	GLN
7	G	104	LEU
7	G	114	ARG
7	G	136	LYS
7	G	140	ASP
7	G	143	ARG
7	G	144	MET
7	G	149	ARG
8	H	1	MET
8	H	2	LEU
8	H	3	THR
8	H	18	ARG
8	H	24	THR
8	H	30	ARG
8	H	39	LEU
8	H	50	ARG
8	H	54	ASP
8	H	63	LEU
8	H	70	GLN
8	H	78	GLN
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	98	LYS
8	H	99	GLU
8	H	109	ILE
8	H	112	LEU
8	H	122	ARG
8	H	129	VAL
8	H	133	LEU
9	I	3	GLN
9	I	4	TYR
9	I	10	ARG
9	I	14	VAL
9	I	16	ARG
9	I	25	LYS
9	I	38	GLN
9	I	47	LEU
9	I	56	LEU
9	I	60	ASP
9	I	75	ASP
9	I	79	LEU
9	I	85	LEU
9	I	86	VAL
9	I	88	TYR
9	I	93	ARG
9	I	95	LYS
9	I	104	ARG
9	I	108	VAL
9	I	113	LYS
9	I	118	LYS
9	I	124	GLN
9	I	126	SER
9	I	128	ARG
10	J	13	HIS
10	J	19	SER
10	J	22	LYS
10	J	38	ILE
10	J	50	ILE
10	J	55	LYS
10	J	57	LYS
10	J	66	ARG
10	J	70	ARG
10	J	73	ASP
10	J	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	84	GLN
10	J	87	THR
10	J	92	THR
10	J	96	ILE
10	J	97	GLU
10	J	98	ILE
11	K	18	ARG
11	K	29	ILE
11	K	31	THR
11	K	47	VAL
11	K	51	LYS
11	K	54	ARG
11	K	57	THR
11	K	67	ASP
11	K	84	VAL
11	K	91	ARG
11	K	93	GLN
11	K	106	LYS
11	K	114	VAL
11	K	117	ASN
11	K	122	LYS
11	K	129	SER
12	L	20	LYS
12	L	33	ARG
12	L	41	ARG
12	L	42	THR
12	L	47	LYS
12	L	53	ARG
12	L	67	THR
12	L	78	GLN
12	L	79	GLU
12	L	81	SER
12	L	85	ILE
12	L	89	ARG
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
12	L	126	LYS
13	M	7	VAL
13	M	8	GLU
13	M	15	VAL
13	M	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	31	LYS
13	M	34	LEU
13	M	36	LYS
13	M	44	ARG
13	M	48	LEU
13	M	56	LEU
13	M	61	GLU
13	M	64	TRP
13	M	77	ASN
13	M	79	LYS
13	M	82	MET
13	M	86	CYS
13	M	90	LEU
13	M	91	ARG
13	M	93	ARG
13	M	94	ARG
13	M	101	GLN
13	M	104	ARG
13	M	108	ARG
13	M	115	LYS
13	M	117	VAL
13	M	120	LYS
13	M	121	LYS
14	N	3	ARG
14	N	4	LYS
14	N	7	ILE
14	N	8	GLU
14	N	15	LYS
14	N	16	PHE
14	N	17	LYS
14	N	24	CYS
14	N	26	ARG
14	N	27	CYS
14	N	33	VAL
14	N	35	ARG
14	N	41	ARG
15	O	3	ILE
15	O	10	LYS
15	O	24	SER
15	O	31	LEU
15	O	39	LEU
15	O	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	64	ARG
15	O	65	ARG
15	O	66	LEU
15	O	71	GLN
15	O	82	ILE
15	O	87	ILE
16	P	2	VAL
16	P	5	ARG
16	P	8	ARG
16	P	12	LYS
16	P	21	VAL
16	P	27	LYS
16	P	33	ILE
16	P	45	THR
16	P	50	LYS
16	P	69	THR
17	Q	7	THR
17	Q	14	LYS
17	Q	16	GLN
17	Q	35	VAL
17	Q	38	ARG
17	Q	52	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	63	ARG
17	Q	78	GLU
17	Q	79	SER
17	Q	87	LYS
17	Q	100	LYS
18	R	25	THR
18	R	31	LEU
18	R	36	ASN
18	R	37	VAL
18	R	59	SER
18	R	72	ARG
18	R	76	LEU
18	R	82	THR
18	R	83	GLU
18	R	84	LYS
18	R	87	ARG
19	S	4	SER
19	S	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	6	LYS
19	S	7	LYS
19	S	11	VAL
19	S	22	LEU
19	S	25	LYS
19	S	29	ARG
19	S	30	LEU
19	S	31	ILE
19	S	32	LYS
19	S	37	ARG
19	S	44	MET
19	S	58	VAL
19	S	60	VAL
19	S	62	ILE
19	S	63	THR
19	S	65	ASN
19	S	80	TYR
20	T	10	LEU
20	T	13	LEU
20	T	18	GLN
20	T	36	LEU
20	T	62	LEU
20	T	70	SER
20	T	72	LEU
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
20	T	86	ARG
20	T	87	LYS
20	T	104	LEU
21	U	6	ARG
21	U	12	LYS
21	U	15	ARG
21	U	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	GLN
2	B	78	GLN
2	B	95	GLN
2	B	110	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	135	GLN
2	B	212	GLN
3	C	102	ASN
4	D	42	GLN
4	D	45	GLN
4	D	77	ASN
4	D	123	HIS
5	E	38	GLN
8	H	70	GLN
9	I	3	GLN
9	I	31	GLN
10	J	68	HIS
10	J	76	ASN
10	J	78	ASN
11	K	78	GLN
11	K	99	GLN
11	K	116	HIS
11	K	117	ASN
16	P	13	HIS
16	P	14	ASN
20	T	16	HIS
20	T	18	GLN
20	T	26	ASN
20	T	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1506 (99%)	339 (22%)	66 (4%)
22	X	5/6 (83%)	3 (60%)	0
All	All	1510/1512 (99%)	342 (22%)	66 (4%)

All (342) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	10	G
1	A	21	U
1	A	23	G
1	A	32	G
1	A	33	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	G
1	A	48	C
1	A	49	C
1	A	51	A
1	A	52	A
1	A	60	A
1	A	74	G
1	A	78	G
1	A	79	A
1	A	80	U
1	A	81	U
1	A	82	U
1	A	83	U
1	A	84	A
1	A	85	C
1	A	95	A
1	A	99	G
1	A	102	G
1	A	103	A
1	A	110	A
1	A	115	C
1	A	126	C
1	A	139	G
1	A	146	A
1	A	151	G
1	A	157	A
1	A	158	C
1	A	164	C
1	A	177	U
1	A	186	C
1	A	193	G
1	A	202	A
1	A	204	A
1	A	209	U
1	A	210	U
1	A	212	G
1	A	213	C
1	A	216	G
1	A	227	G
1	A	243	G
1	A	247	G
1	A	258	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	G
1	A	263	C
1	A	270	A
1	A	271	G
1	A	276	C
1	A	285	G
1	A	315	G
1	A	317	A
1	A	324	C
1	A	325	A
1	A	326	C
1	A	328	G
1	A	341	C
1	A	342	G
1	A	344	G
1	A	348	C
1	A	349	A
1	A	350	G
1	A	363	U
1	A	368	C
1	A	369	A
1	A	385	A
1	A	392	G
1	A	393	A
1	A	394	C
1	A	402	G
1	A	407	A
1	A	408	A
1	A	409	G
1	A	410	A
1	A	417	U
1	A	418	C
1	A	420	G
1	A	425	U
1	A	426	A
1	A	435	A
1	A	436	A
1	A	447	A
1	A	448	A
1	A	455	A
1	A	456	C
1	A	469	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	470	G
1	A	481	A
1	A	482	U
1	A	483	A
1	A	489	G
1	A	492	C
1	A	493	A
1	A	494	A
1	A	495	C
1	A	498	C
1	A	501	G
1	A	502	C
1	A	503	C
1	A	505	G
1	A	511	G
1	A	515	U
1	A	516	A
1	A	517	A
1	A	523	A
1	A	529	C
1	A	531	A
1	A	541	G
1	A	544	U
1	A	545	U
1	A	556	A
1	A	557	A
1	A	559	G
1	A	560	G
1	A	561	G
1	A	563	G
1	A	566	U
1	A	568	G
1	A	597	C
1	A	614	G
1	A	616	A
1	A	637	A
1	A	646	G
1	A	649	A
1	A	655	G
1	A	672	G
1	A	687	G
1	A	705	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	707	U
1	A	708	G
1	A	715	G
1	A	736	G
1	A	739	G
1	A	761	A
1	A	778	A
1	A	799	A
1	A	800	A
1	A	801	C
1	A	803	A
1	A	804	U
1	A	812	A
1	A	820	G
1	A	823	U
1	A	824	C
1	A	825	U
1	A	826	C
1	A	837	A
1	A	845	G
1	A	854	G
1	A	880	G
1	A	892	A
1	A	897	A
1	A	904	G
1	A	905	G
1	A	912	C
1	A	913	A
1	A	915	A
1	A	919	G
1	A	920	G
1	A	936	A
1	A	938	U
1	A	939	U
1	A	941	G
1	A	944	G
1	A	947	A
1	A	949	G
1	A	952	A
1	A	953	A
1	A	954	G
1	A	955	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	958	C
1	A	959	U
1	A	965	G
1	A	969	U
1	A	970	U
1	A	971	G
1	A	976	G
1	A	977	C
1	A	980	G
1	A	982	G
1	A	983	A
1	A	984	A
1	A	985	C
1	A	996	G
1	A	999	U
1	A	1003	G
1	A	1006	C
1	A	1008	C
1	A	1009	C
1	A	1010	G
1	A	1011	C
1	A	1013	A
1	A	1014	G
1	A	1015	G
1	A	1016	G
1	A	1017	G
1	A	1018	A
1	A	1019	G
1	A	1022	C
1	A	1027	A
1	A	1032	U
1	A	1036	G
1	A	1037	C
1	A	1038	A
1	A	1048	U
1	A	1050	A
1	A	1051	G
1	A	1053	U
1	A	1068	U
1	A	1077	G
1	A	1078	U
1	A	1082	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1084	A
1	A	1091	G
1	A	1096	C
1	A	1100	G
1	A	1107	G
1	A	1108	U
1	A	1109	U
1	A	1110	G
1	A	1111	C
1	A	1112	C
1	A	1113	A
1	A	1114	G
1	A	1115	C
1	A	1117	G
1	A	1119	U
1	A	1120	C
1	A	1121	G
1	A	1122	G
1	A	1123	C
1	A	1124	C
1	A	1128	C
1	A	1129	A
1	A	1134	A
1	A	1135	A
1	A	1141	C
1	A	1142	U
1	A	1153	G
1	A	1163	G
1	A	1164	G
1	A	1166	G
1	A	1168	G
1	A	1169	G
1	A	1173	A
1	A	1174	C
1	A	1178	U
1	A	1179	G
1	A	1183	A
1	A	1184	G
1	A	1193	U
1	A	1194	U
1	A	1195	A
1	A	1196	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1198	G
1	A	1199	C
1	A	1200	C
1	A	1209	A
1	A	1220	A
1	A	1221	A
1	A	1230	A
1	A	1231	C
1	A	1232	A
1	A	1233	A
1	A	1234	A
1	A	1235	G
1	A	1238	A
1	A	1239	U
1	A	1242	C
1	A	1244	C
1	A	1245	C
1	A	1254	G
1	A	1255	G
1	A	1262	A
1	A	1263	U
1	A	1268	A
1	A	1269	A
1	A	1275	G
1	A	1279	C
1	A	1281	A
1	A	1282	G
1	A	1283	U
1	A	1284	U
1	A	1298	G
1	A	1299	C
1	A	1301	A
1	A	1303	C
1	A	1304	C
1	A	1308	C
1	A	1312	U
1	A	1313	G
1	A	1318	C
1	A	1319	G
1	A	1320	G
1	A	1328	A
1	A	1329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1332	A
1	A	1335	G
1	A	1346	A
1	A	1350	C
1	A	1353	G
1	A	1355	U
1	A	1356	G
1	A	1362	G
1	A	1366	C
1	A	1380	C
1	A	1381	A
1	A	1385	C
1	A	1402	G
1	A	1405	G
1	A	1425	G
1	A	1426	G
1	A	1433	C
1	A	1434	G
1	A	1453	G
1	A	1459	U
1	A	1461	A
1	A	1465	G
1	A	1470	A
1	A	1472	G
1	A	1475	G
1	A	1477	A
1	A	1478	A
1	A	1480	A
1	A	1482	G
1	A	1483	G
1	A	1484	U
1	A	1485	A
1	A	1495	G
1	A	1500	U
1	A	1507	G
1	A	1508	G
1	A	1509	A
1	A	1510	U
1	A	1511	C
22	X	2	U
22	X	3	U
22	X	4	U

All (66) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	31	U
1	A	80	U
1	A	81	U
1	A	82	U
1	A	83	U
1	A	102	G
1	A	109	G
1	A	113	A
1	A	209	U
1	A	262	G
1	A	270	A
1	A	325	A
1	A	349	A
1	A	417	U
1	A	424	G
1	A	425	U
1	A	426	A
1	A	455	A
1	A	469	G
1	A	480	A
1	A	482	U
1	A	492	C
1	A	493	A
1	A	514	G
1	A	516	A
1	A	531	A
1	A	543	A
1	A	544	U
1	A	559	G
1	A	671	A
1	A	686	A
1	A	707	U
1	A	777	U
1	A	824	C
1	A	862	U
1	A	891	A
1	A	909	C
1	A	949	G
1	A	952	A
1	A	958	C
1	A	970	U
1	A	1004	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1016	G
1	A	1027	A
1	A	1032	U
1	A	1047	G
1	A	1050	A
1	A	1107	G
1	A	1112	C
1	A	1128	C
1	A	1134	A
1	A	1173	A
1	A	1178	U
1	A	1183	A
1	A	1221	A
1	A	1230	A
1	A	1233	A
1	A	1234	A
1	A	1283	U
1	A	1301	A
1	A	1309	C
1	A	1317	C
1	A	1319	G
1	A	1477	A
1	A	1482	G
1	A	1507	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 111 ligands modelled in this entry, 103 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
23	PAR	A	1601	-	45,45,45	0.79	1 (2%)	59,67,67	1.82	12 (20%)
23	PAR	A	1602	-	45,45,45	0.82	1 (2%)	59,67,67	1.63	14 (23%)
23	PAR	A	1603	-	45,45,45	0.79	2 (4%)	59,67,67	1.97	10 (16%)
23	PAR	A	1604	-	45,45,45	0.87	2 (4%)	59,67,67	1.81	12 (20%)
23	PAR	A	1605	-	45,45,45	0.83	0	59,67,67	1.90	12 (20%)
23	PAR	A	1606	-	45,45,45	0.75	0	59,67,67	1.85	15 (25%)
23	PAR	A	1607	-	45,45,45	1.13	4 (8%)	59,67,67	2.01	19 (32%)
24	PCY	A	1608	-	26,31,42	1.32	2 (7%)	24,49,65	1.47	4 (16%)

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
23	PAR	A	1601	-	-	0/18/94/94	0/4/4/4
23	PAR	A	1602	-	-	0/18/94/94	0/4/4/4
23	PAR	A	1603	-	-	1/18/94/94	0/4/4/4
23	PAR	A	1604	-	-	0/18/94/94	0/4/4/4
23	PAR	A	1605	-	-	1/18/94/94	0/4/4/4
23	PAR	A	1606	-	-	1/18/94/94	0/4/4/4
23	PAR	A	1607	-	-	0/18/94/94	1/4/4/4
24	PCY	A	1608	-	-	0/26/60/67	0/2/2/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1608	PCY	C28-C32	-4.04	1.42	1.49
23	A	1607	PAR	C31-C21	-3.90	1.48	1.53
24	A	1608	PCY	C22-N20	-3.29	1.33	1.39
23	A	1604	PAR	C13-C23	-3.27	1.48	1.52
23	A	1601	PAR	C13-C23	-2.48	1.49	1.52
23	A	1607	PAR	C22-C32	-2.42	1.48	1.53
23	A	1607	PAR	C24-N24	-2.35	1.43	1.47
23	A	1603	PAR	C34-C24	-2.25	1.50	1.53
23	A	1607	PAR	C44-C54	-2.18	1.48	1.53
23	A	1603	PAR	C13-C23	-2.13	1.50	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1602	PAR	C24-N24	-2.09	1.44	1.47
23	A	1604	PAR	O54-C54	-2.08	1.39	1.44

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1603	PAR	O34-C34-C24	-5.92	100.31	110.31
23	A	1604	PAR	O54-C54-C64	-5.37	95.61	106.10
23	A	1603	PAR	C14-O33-C33	-5.10	104.69	118.01
23	A	1607	PAR	O53-C53-C43	-4.87	95.25	111.33
23	A	1607	PAR	O11-C11-C21	-4.66	99.33	107.96
23	A	1603	PAR	O54-C54-C44	-4.54	101.15	109.68
23	A	1606	PAR	C31-C41-C51	-4.52	102.31	110.20
23	A	1604	PAR	C14-O33-C33	-4.42	106.45	118.01
23	A	1601	PAR	C31-C21-N21	-4.18	103.12	110.86
23	A	1607	PAR	C14-O54-C54	-4.12	105.75	113.75
24	A	1608	PCY	C8-C3-N2	-3.89	104.21	112.42
23	A	1606	PAR	C64-C54-C44	-3.88	105.84	113.17
23	A	1601	PAR	O23-C23-C13	-3.84	100.98	111.67
23	A	1607	PAR	C34-C24-N24	-3.78	103.85	110.86
23	A	1605	PAR	C14-C24-N24	-3.71	103.73	111.10
23	A	1607	PAR	O43-C13-C23	-3.62	99.69	104.78
23	A	1607	PAR	C11-O11-C42	-3.59	108.62	118.01
23	A	1607	PAR	O54-C54-C44	-3.56	103.00	109.68
23	A	1605	PAR	O62-C62-C52	-3.54	101.50	109.87
23	A	1601	PAR	O34-C34-C24	-3.50	104.40	110.31
23	A	1603	PAR	O44-C44-C34	-3.41	102.67	110.34
23	A	1607	PAR	C64-C54-C44	-3.35	106.84	113.17
23	A	1606	PAR	O34-C34-C24	-3.33	104.68	110.31
24	A	1608	PCY	C8-C17-N20	-3.28	108.25	113.17
23	A	1602	PAR	O34-C34-C24	-3.20	104.91	110.31
23	A	1601	PAR	O34-C34-C44	-3.13	103.29	110.34
23	A	1607	PAR	O62-C62-C12	-2.95	104.40	109.87
23	A	1602	PAR	O23-C23-C13	-2.95	103.46	111.67
23	A	1601	PAR	O31-C31-C21	-2.92	105.38	110.31
23	A	1602	PAR	O62-C62-C12	-2.91	104.47	109.87
23	A	1607	PAR	C14-C24-N24	-2.90	105.34	111.10
23	A	1606	PAR	O62-C62-C12	-2.80	104.68	109.87
23	A	1602	PAR	C62-C12-N12	-2.79	105.82	110.78
23	A	1601	PAR	C13-O52-C52	-2.70	110.94	118.01
23	A	1603	PAR	O33-C14-O54	-2.66	103.96	110.68
23	A	1607	PAR	C23-C33-C43	-2.66	98.30	103.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1604	PAR	O44-C44-C54	-2.63	102.28	109.24
23	A	1605	PAR	C64-C54-C44	-2.62	108.21	113.17
23	A	1607	PAR	C22-C32-N32	-2.59	102.73	110.94
23	A	1602	PAR	C31-C21-N21	-2.43	106.35	110.86
23	A	1604	PAR	O11-C11-C21	-2.40	103.53	107.96
23	A	1602	PAR	C34-C24-N24	-2.38	106.44	110.86
23	A	1603	PAR	C31-C21-N21	-2.35	106.50	110.86
23	A	1602	PAR	O43-C13-C23	-2.33	101.51	104.78
23	A	1601	PAR	O33-C33-C43	-2.33	102.41	111.83
23	A	1607	PAR	O43-C43-C53	-2.31	104.16	109.17
23	A	1605	PAR	O41-C41-C31	-2.31	105.14	110.34
23	A	1605	PAR	C31-C21-N21	-2.24	106.71	110.86
23	A	1602	PAR	C14-O54-C54	-2.23	109.42	113.75
24	A	1608	PCY	O5-C1-N4	-2.21	118.06	122.16
23	A	1602	PAR	C34-C44-C54	-2.17	106.41	110.20
23	A	1607	PAR	O44-C44-C54	-2.17	103.48	109.24
23	A	1606	PAR	O44-C44-C54	-2.11	103.65	109.24
23	A	1606	PAR	O44-C44-C34	-2.08	105.66	110.34
23	A	1607	PAR	C11-C21-C31	-2.07	104.07	109.95
23	A	1602	PAR	O54-C54-C44	-2.03	105.87	109.68
23	A	1604	PAR	O34-C34-C44	2.08	115.02	110.34
23	A	1601	PAR	O62-C62-C12	2.11	113.78	109.87
23	A	1602	PAR	O52-C13-C23	2.12	112.17	107.75
23	A	1606	PAR	C11-C21-N21	2.14	115.37	111.10
23	A	1604	PAR	O51-C11-C21	2.19	115.40	110.47
23	A	1607	PAR	O43-C43-C33	2.21	109.96	104.86
23	A	1601	PAR	C11-C21-C31	2.25	116.34	109.95
24	A	1608	PCY	C10-N4-C9	2.27	122.67	115.74
23	A	1606	PAR	O52-C13-C23	2.31	112.55	107.75
23	A	1606	PAR	O51-C51-C61	2.32	112.22	106.36
23	A	1605	PAR	O54-C14-C24	2.39	115.83	110.47
23	A	1606	PAR	O31-C31-C41	2.43	115.81	110.34
23	A	1607	PAR	O51-C11-C21	2.44	115.94	110.47
23	A	1602	PAR	C22-C32-C42	2.45	116.06	109.53
23	A	1605	PAR	O11-C11-C21	2.60	112.78	107.96
23	A	1605	PAR	O52-C13-C23	2.63	113.22	107.75
23	A	1603	PAR	O52-C52-C42	2.68	114.50	107.49
23	A	1605	PAR	O31-C31-C21	2.81	115.05	110.31
23	A	1607	PAR	O54-C54-C64	2.83	111.64	106.10
23	A	1607	PAR	C14-C24-C34	2.84	118.01	109.95
23	A	1606	PAR	C13-O52-C52	2.84	125.42	118.01
23	A	1605	PAR	C52-C42-C32	2.89	118.09	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	1604	PAR	C23-C33-C43	3.01	108.96	103.29
23	A	1604	PAR	C11-O51-C51	3.07	119.70	113.75
23	A	1601	PAR	O54-C54-C64	3.11	112.18	106.10
23	A	1606	PAR	O11-C11-C21	3.12	113.75	107.96
23	A	1603	PAR	C14-C24-N24	3.16	117.38	111.10
23	A	1604	PAR	O54-C14-C24	3.19	117.63	110.47
23	A	1601	PAR	C34-C44-C54	3.38	116.09	110.20
23	A	1604	PAR	O51-C51-C41	3.46	116.17	109.68
23	A	1602	PAR	O54-C54-C64	3.66	113.25	106.10
23	A	1606	PAR	O54-C54-C64	3.76	113.45	106.10
23	A	1604	PAR	C34-C44-C54	3.87	116.95	110.20
23	A	1605	PAR	O54-C54-C64	4.09	114.10	106.10
23	A	1604	PAR	O52-C52-C42	4.71	119.80	107.49
23	A	1606	PAR	O52-C52-C62	4.74	119.40	107.17
23	A	1602	PAR	C22-C12-C62	4.94	117.69	110.11
23	A	1603	PAR	C64-C54-C44	5.05	122.72	113.17
23	A	1601	PAR	C14-O54-C54	5.07	123.59	113.75
23	A	1603	PAR	O33-C14-C24	5.24	117.66	107.96
23	A	1606	PAR	C34-C44-C54	5.36	119.55	110.20
23	A	1605	PAR	C14-O54-C54	7.32	127.95	113.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1603	PAR	C52-O52-C13-C23
23	A	1605	PAR	C52-O52-C13-C23
23	A	1606	PAR	C33-O33-C14-C24

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1607	PAR	C12-C22-C32-C42-C52-C62

7 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1601	PAR	3	0
23	A	1603	PAR	6	0
23	A	1604	PAR	9	0
23	A	1605	PAR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	1606	PAR	9	0
23	A	1607	PAR	12	0
24	A	1608	PCY	5	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1506/1506 (100%)	-0.23	35 (2%) 64 40	39, 69, 142, 245	0
2	B	234/234 (100%)	-0.08	8 (3%) 49 24	53, 98, 168, 194	0
3	C	206/206 (100%)	-0.35	0 100 100	55, 95, 139, 157	0
4	D	208/208 (100%)	-0.44	1 (0%) 91 83	53, 80, 113, 134	0
5	E	150/150 (100%)	-0.47	2 (1%) 79 62	41, 65, 98, 136	0
6	F	101/101 (100%)	-0.27	1 (0%) 84 69	72, 101, 131, 172	0
7	G	155/155 (100%)	-0.32	4 (2%) 59 35	65, 96, 145, 196	0
8	H	138/138 (100%)	-0.49	1 (0%) 89 78	40, 61, 91, 131	0
9	I	127/127 (100%)	-0.27	1 (0%) 87 75	51, 103, 140, 219	0
10	J	98/98 (100%)	-0.03	1 (1%) 84 69	61, 126, 174, 199	0
11	K	119/119 (100%)	-0.23	3 (2%) 61 37	53, 78, 113, 164	0
12	L	125/125 (100%)	-0.38	2 (1%) 74 55	39, 76, 112, 179	0
13	M	120/120 (100%)	-0.18	2 (1%) 73 52	60, 97, 144, 183	0
14	N	60/60 (100%)	-0.36	0 100 100	62, 85, 113, 131	0
15	O	88/88 (100%)	-0.37	2 (2%) 64 40	55, 82, 121, 155	0
16	P	83/83 (100%)	-0.54	0 100 100	50, 67, 99, 140	0
17	Q	99/99 (100%)	-0.49	1 (1%) 84 69	42, 72, 106, 142	0
18	R	70/70 (100%)	-0.36	0 100 100	61, 81, 123, 157	0
19	S	78/78 (100%)	0.03	3 (3%) 44 21	72, 114, 168, 186	0
20	T	99/99 (100%)	-0.40	1 (1%) 84 69	51, 78, 136, 162	0
21	U	24/24 (100%)	0.13	1 (4%) 40 19	67, 82, 111, 134	0
22	X	6/6 (100%)	0.03	0 100 100	59, 75, 131, 138	0
All	All	3894/3894 (100%)	-0.28	69 (1%) 71 50	39, 79, 145, 245	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	7	VAL	6.4
11	K	129	SER	6.3
1	A	1012	G	5.7
11	K	128	ALA	5.6
19	S	30	LEU	5.4
7	G	156	TRP	5.2
1	A	1017	G	5.2
7	G	155	ARG	4.6
1	A	1003	G	4.3
1	A	985	C	4.1
1	A	983	A	4.0
2	B	237	ALA	4.0
1	A	1019	G	4.0
1	A	1112	C	3.8
6	F	101	ALA	3.8
1	A	980	G	3.7
2	B	128	GLU	3.6
1	A	981	G	3.6
8	H	1	MET	3.6
1	A	1006	C	3.3
1	A	1020	C	3.3
2	B	231	GLU	3.3
1	A	1014	G	3.1
11	K	127	LYS	3.0
21	U	25	LYS	3.0
12	L	128	ALA	2.9
13	M	6	GLY	2.7
1	A	1009	C	2.7
1	A	1016	G	2.7
9	I	4	TYR	2.7
1	A	1002	G	2.7
1	A	1004	U	2.7
4	D	26	CYS	2.6
1	A	1118	U	2.6
15	O	88	ARG	2.6
1	A	1018	A	2.6
1	A	1509	A	2.5
1	A	1405	G	2.5
2	B	238	LEU	2.5
2	B	122	PHE	2.5
2	B	123	ALA	2.5
1	A	456	C	2.5
1	A	1005	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1425	G	2.5
15	O	2	PRO	2.4
5	E	154	GLY	2.4
1	A	1021	C	2.4
1	A	1239	U	2.4
5	E	5	ASP	2.3
1	A	1008	C	2.3
1	A	1010	G	2.3
1	A	1015	G	2.3
1	A	80	U	2.2
13	M	7	VAL	2.2
7	G	5	ARG	2.2
10	J	32	ALA	2.2
1	A	1511	C	2.2
19	S	10	PHE	2.2
2	B	127	ILE	2.2
1	A	1116	G	2.2
12	L	129	ALA	2.1
19	S	21	GLU	2.1
1	A	988	G	2.1
17	Q	96	GLU	2.1
1	A	209	U	2.0
1	A	987	C	2.0
7	G	6	ARG	2.0
1	A	1120	C	2.0
20	T	99	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1622	1/1	0.93	0.45	28.56	38,38,38,38	0
25	MG	A	1661	1/1	0.93	1.01	25.06	60,60,60,60	0
25	MG	A	1651	1/1	0.98	0.55	23.99	42,42,42,42	0
25	MG	A	1617	1/1	0.98	0.43	22.86	35,35,35,35	0
25	MG	A	1610	1/1	0.99	0.57	19.68	42,42,42,42	0
25	MG	A	1659	1/1	0.88	0.42	19.49	36,36,36,36	1
25	MG	A	1632	1/1	0.92	0.71	19.38	56,56,56,56	0
25	MG	A	1703	1/1	0.77	0.51	18.13	88,88,88,88	0
25	MG	D	301	1/1	0.81	0.47	17.00	93,93,93,93	0
25	MG	A	1620	1/1	0.95	0.30	16.34	34,34,34,34	0
25	MG	A	1634	1/1	0.98	0.31	14.72	44,44,44,44	0
25	MG	A	1614	1/1	0.98	0.45	13.87	31,31,31,31	0
25	MG	A	1609	1/1	0.94	0.34	13.66	45,45,45,45	0
25	MG	A	1639	1/1	0.94	0.34	13.30	47,47,47,47	0
25	MG	A	1647	1/1	0.98	0.32	10.80	34,34,34,34	0
25	MG	E	201	1/1	0.95	0.41	8.11	39,39,39,39	0
25	MG	A	1645	1/1	0.94	0.23	6.35	34,34,34,34	0
25	MG	A	1633	1/1	0.95	0.60	5.97	52,52,52,52	0
25	MG	A	1685	1/1	0.84	0.26	5.66	46,46,46,46	0
25	MG	A	1654	1/1	0.97	0.23	5.62	26,26,26,26	0
25	MG	A	1682	1/1	0.93	0.21	5.59	52,52,52,52	0
25	MG	A	1636	1/1	0.90	0.20	4.84	46,46,46,46	0
23	PAR	A	1605	42/42	0.91	0.25	4.79	58,75,85,89	42
23	PAR	A	1607	42/42	0.93	0.25	4.58	11,15,17,19	42
23	PAR	A	1602	42/42	0.96	0.19	4.53	32,41,50,61	42
25	MG	A	1667	1/1	0.81	0.29	4.07	39,39,39,39	0
23	PAR	A	1606	42/42	0.86	0.27	3.71	38,44,55,56	42
23	PAR	A	1603	42/42	0.90	0.21	3.52	53,84,97,117	42
25	MG	A	1652	1/1	0.97	0.25	3.51	49,49,49,49	0
25	MG	A	1683	1/1	0.86	0.20	1.93	44,44,44,44	1
25	MG	A	1699	1/1	0.90	0.31	1.79	55,55,55,55	0
25	MG	A	1644	1/1	0.95	0.17	1.18	41,41,41,41	0
23	PAR	A	1604	42/42	0.94	0.22	1.08	64,79,104,137	0
25	MG	A	1655	1/1	0.93	0.18	1.08	39,39,39,39	1
24	PCY	A	1608	30/40	0.96	0.21	0.65	50,59,68,76	0
25	MG	A	1657	1/1	0.97	0.17	0.61	23,23,23,23	0
25	MG	A	1700	1/1	0.93	0.17	0.35	52,52,52,52	0
23	PAR	A	1601	42/42	0.96	0.15	0.18	52,59,74,83	0
25	MG	A	1640	1/1	0.97	0.17	-0.08	36,36,36,36	0
25	MG	A	1674	1/1	0.90	0.13	-1.36	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1650	1/1	0.99	0.12	-1.94	37,37,37,37	0
25	MG	A	1623	1/1	0.94	0.10	-2.01	57,57,57,57	0
25	MG	A	1677	1/1	0.81	0.59	-	58,58,58,58	0
25	MG	A	1681	1/1	0.99	0.37	-	36,36,36,36	0
25	MG	A	1665	1/1	0.88	0.12	-	40,40,40,40	0
25	MG	A	1690	1/1	0.85	0.16	-	54,54,54,54	0
25	MG	A	1689	1/1	0.89	0.34	-	52,52,52,52	0
25	MG	A	1664	1/1	0.95	0.24	-	61,61,61,61	0
25	MG	A	1613	1/1	0.97	0.16	-	56,56,56,56	1
25	MG	A	1638	1/1	0.97	0.26	-	40,40,40,40	0
25	MG	A	1627	1/1	0.92	0.47	-	50,50,50,50	0
25	MG	A	1615	1/1	0.96	0.68	-	38,38,38,38	0
25	MG	A	1629	1/1	0.96	0.37	-	42,42,42,42	0
25	MG	A	1706	1/1	0.82	0.49	-	71,71,71,71	0
25	MG	A	1691	1/1	0.71	0.34	-	69,69,69,69	0
25	MG	A	1680	1/1	0.96	0.25	-	36,36,36,36	1
25	MG	A	1676	1/1	0.82	0.27	-	51,51,51,51	0
25	MG	A	1669	1/1	0.94	0.63	-	57,57,57,57	0
25	MG	A	1686	1/1	0.90	0.39	-	42,42,42,42	1
25	MG	A	1692	1/1	0.91	0.37	-	65,65,65,65	0
25	MG	A	1616	1/1	0.98	0.67	-	40,40,40,40	0
25	MG	A	1630	1/1	0.92	0.44	-	33,33,33,33	1
25	MG	A	1628	1/1	0.96	0.34	-	39,39,39,39	0
25	MG	A	1642	1/1	0.91	0.21	-	43,43,43,43	0
25	MG	A	1684	1/1	0.43	0.63	-	67,67,67,67	1
25	MG	A	1658	1/1	0.85	0.41	-	41,41,41,41	1
25	MG	A	1646	1/1	0.99	0.26	-	34,34,34,34	0
25	MG	A	1611	1/1	0.93	0.26	-	37,37,37,37	0
25	MG	A	1693	1/1	0.92	0.29	-	52,52,52,52	0
25	MG	A	1688	1/1	0.79	0.36	-	49,49,49,49	0
25	MG	A	1673	1/1	0.96	0.13	-	41,41,41,41	1
25	MG	A	1625	1/1	0.95	0.28	-	50,50,50,50	0
25	MG	A	1696	1/1	0.88	0.25	-	54,54,54,54	0
25	MG	A	1695	1/1	0.93	0.34	-	64,64,64,64	0
25	MG	A	1641	1/1	0.94	0.17	-	42,42,42,42	0
25	MG	S	101	1/1	0.94	0.10	-	58,58,58,58	0
25	MG	A	1694	1/1	0.85	0.73	-	61,61,61,61	0
25	MG	A	1619	1/1	0.94	0.13	-	25,25,25,25	0
25	MG	A	1656	1/1	0.98	0.37	-	50,50,50,50	0
25	MG	A	1653	1/1	0.97	0.50	-	30,30,30,30	0
25	MG	A	1621	1/1	0.94	0.24	-	45,45,45,45	0
25	MG	A	1702	1/1	0.82	0.14	-	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1698	1/1	0.97	0.44	-	53,53,53,53	0
25	MG	A	1626	1/1	0.97	0.34	-	31,31,31,31	0
25	MG	A	1687	1/1	0.94	0.45	-	43,43,43,43	1
25	MG	A	1662	1/1	0.90	0.68	-	48,48,48,48	0
25	MG	A	1705	1/1	0.90	0.30	-	61,61,61,61	0
25	MG	A	1678	1/1	0.90	0.17	-	54,54,54,54	0
25	MG	A	1618	1/1	0.87	0.49	-	56,56,56,56	0
25	MG	A	1707	1/1	0.77	0.43	-	67,67,67,67	0
25	MG	A	1666	1/1	0.96	0.36	-	47,47,47,47	0
25	MG	A	1631	1/1	0.97	0.19	-	36,36,36,36	0
25	MG	A	1660	1/1	0.93	0.48	-	61,61,61,61	0
25	MG	A	1635	1/1	0.98	0.12	-	42,42,42,42	0
25	MG	A	1697	1/1	0.67	0.38	-	63,63,63,63	0
25	MG	A	1671	1/1	0.85	0.48	-	57,57,57,57	1
25	MG	A	1648	1/1	0.96	0.43	-	43,43,43,43	0
25	MG	A	1643	1/1	0.91	0.45	-	59,59,59,59	0
25	MG	A	1704	1/1	0.96	0.08	-	53,53,53,53	0
25	MG	A	1668	1/1	0.97	0.47	-	39,39,39,39	1
25	MG	A	1637	1/1	0.89	0.27	-	59,59,59,59	0
25	MG	A	1670	1/1	0.74	0.50	-	49,49,49,49	1
25	MG	A	1675	1/1	0.87	0.38	-	63,63,63,63	0
25	MG	A	1612	1/1	0.97	0.73	-	46,46,46,46	0
25	MG	A	1679	1/1	0.95	0.25	-	61,61,61,61	0
25	MG	A	1701	1/1	0.79	0.60	-	68,68,68,68	0
25	MG	A	1624	1/1	0.87	0.09	-	38,38,38,38	0
25	MG	A	1649	1/1	0.98	0.14	-	53,53,53,53	1
25	MG	A	1663	1/1	0.89	0.75	-	64,64,64,64	0
25	MG	A	1672	1/1	0.94	0.46	-	65,65,65,65	0
25	MG	K	201	1/1	0.96	0.59	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.