Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:02 AM EDT

PDB ID	:	6NY6
Title	:	Structure of dimeric Escherichia coli toxin YoeB bound to the Thermus thermophilus 30S ribosome
Authors	:	Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-02-11
Resolution	:	3.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

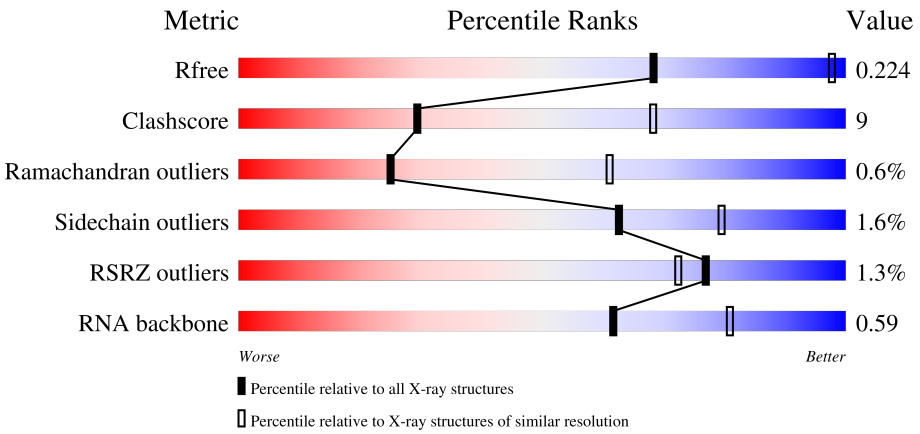
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)
RNA backbone	3102	1028 (4.46-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1523	49% 39% 10% ••
2	B	256	% 69% 22% • 8%
3	C	239	% 70% 15% 14%
4	D	209	72% 26% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	162	77% 15% 7%
6	F	101	77% 22%
7	G	156	84% 15%
8	H	138	74% 25%
9	I	128	2% 73% 25%
10	J	105	5% 57% 29% 5% 9%
11	K	129	73% 16% 10%
12	L	132	2% 73% 19% 8%
13	M	126	3% 67% 22% 8%
14	N	61	2% 59% 39%
15	O	89	76% 21%
16	P	88	3% 82% 14% 5%
17	Q	105	% 64% 31% 5%
18	R	88	73% 7% 20%
19	S	93	2% 74% 15% 10%
20	T	106	63% 28% 7%
21	U	27	19% 70% 22% 7%
22	Y	84	13% 73% 27%
22	Z	84	10% 74% 25%

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	MG	A	1604	-	-	-	X
23	MG	A	1609	-	-	-	X
23	MG	A	1610	-	-	-	X
23	MG	A	1612	-	-	-	X
23	MG	A	1613	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1615	-	-	-	X
23	MG	A	1616	-	-	-	X
23	MG	A	1617	-	-	-	X
23	MG	A	1618	-	-	-	X
23	MG	A	1619	-	-	-	X
23	MG	A	1620	-	-	-	X
23	MG	A	1622	-	-	-	X
23	MG	A	1625	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1634	-	-	-	X
23	MG	A	1649	-	-	-	X
23	MG	A	1653	-	-	-	X
23	MG	A	1660	-	-	-	X
23	MG	A	1661	-	-	-	X
23	MG	A	1665	-	-	-	X
23	MG	A	1677	-	-	-	X
23	MG	A	1678	-	-	-	X
23	MG	A	1679	-	-	-	X
23	MG	A	1681	-	-	-	X
23	MG	A	1683	-	-	-	X
23	MG	A	1689	-	-	-	X
23	MG	A	1691	-	-	-	X
23	MG	A	1692	-	-	-	X
23	MG	A	1694	-	-	-	X
23	MG	A	1696	-	-	-	X
23	MG	A	1698	-	-	-	X
23	MG	A	1699	-	-	-	X
23	MG	A	1703	-	-	-	X
23	MG	A	1707	-	-	-	X
23	MG	A	1708	-	-	-	X
23	MG	A	1717	-	-	-	X
23	MG	A	1718	-	-	-	X
23	MG	A	1719	-	-	-	X
23	MG	A	1724	-	-	-	X
23	MG	A	1731	-	-	-	X
23	MG	A	1732	-	-	-	X
23	MG	A	1734	-	-	-	X
23	MG	A	1735	-	-	-	X
23	MG	A	1737	-	-	-	X
23	MG	A	1738	-	-	-	X
23	MG	A	1746	-	-	-	X
23	MG	A	1758	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1766	-	-	-	X
23	MG	A	1767	-	-	-	X
23	MG	A	1776	-	-	-	X
23	MG	A	1778	-	-	-	X
23	MG	A	1779	-	-	-	X
23	MG	A	1780	-	-	-	X
23	MG	E	201	-	-	-	X
24	SF4	D	301	-	-	X	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 53243 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1513	32514	14472	6016	10513	1513	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1915	1223	343	344	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	205	1605	1011	313	280	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	151	1155	729	218	204	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	837	528	154	152	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	137	1108	700	214	192	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	126	998	633	193	172	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	96	777	487	153	136	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	116	864	537	164	160	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	122	956	603	193	159	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	116	928	574	191	161	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	87	729	457	146	124	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	84	705	446	140	118	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	100	834	534	155	143	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	84	674	430	126	116	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	U	25	217	134	52	31	0	0	0

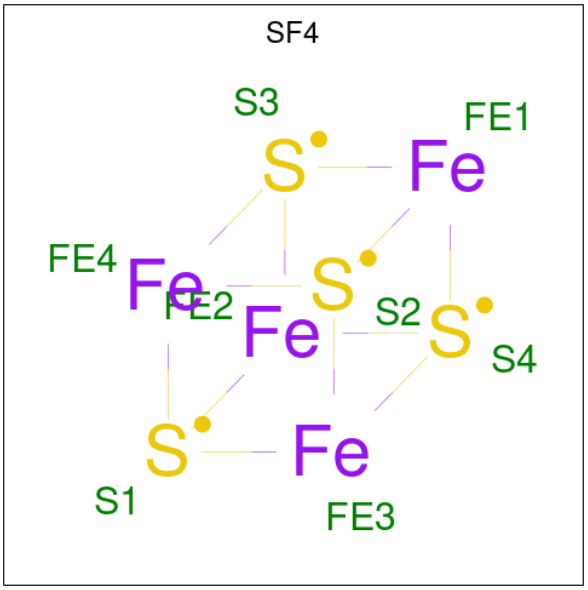
- Molecule 22 is a protein called Toxin YoeB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	Y	84	722	464	126	130	2	0	0	0
22	Z	84	723	464	126	131	2	0	0	0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
23	A	182	182	182	0	0
23	B	1	1	1	0	0
23	E	1	1	1	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
24	D	1	8	4	4	0	0

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

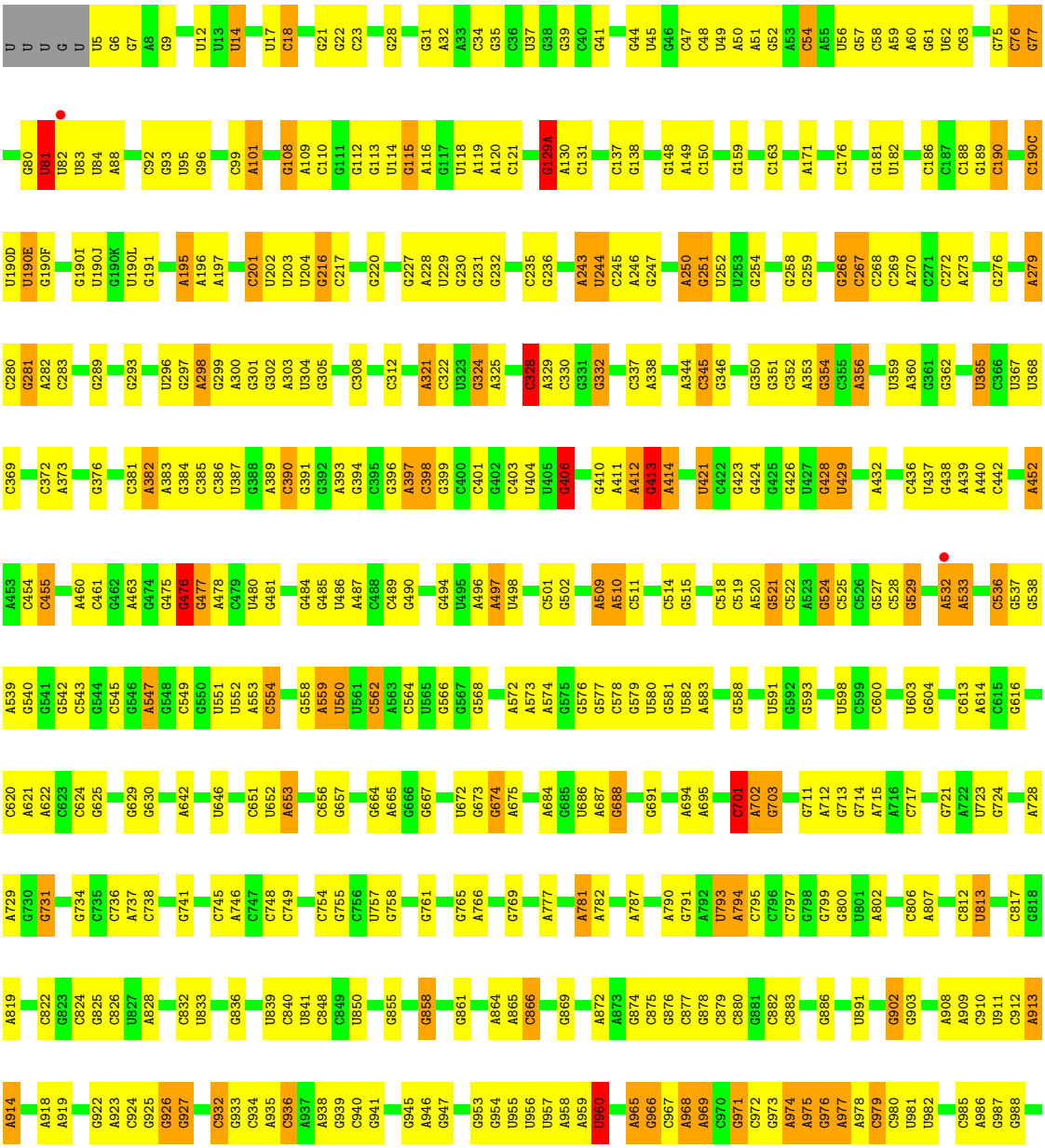
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
25	N	1	1	1	0	0

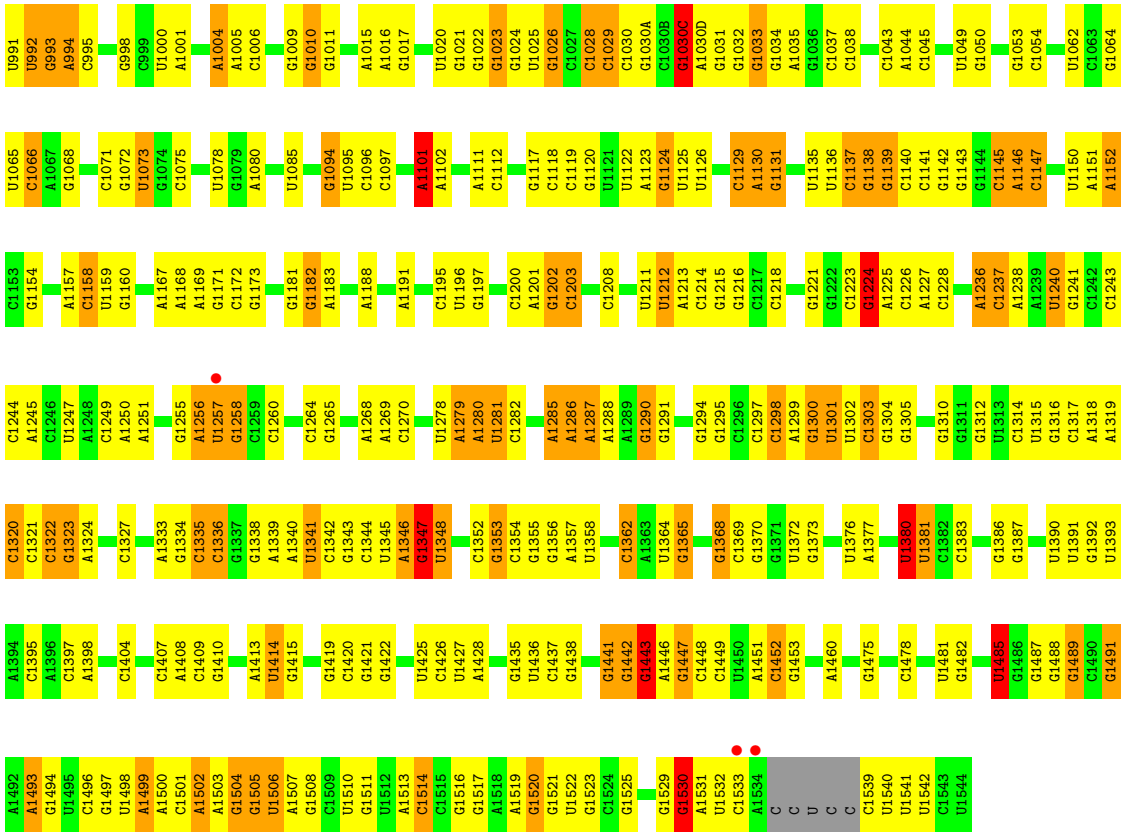
3 Residue-property plots (i)

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

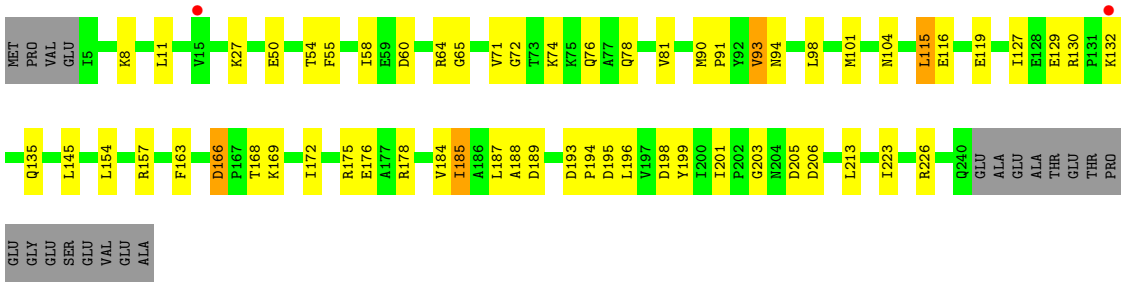
Chain A:





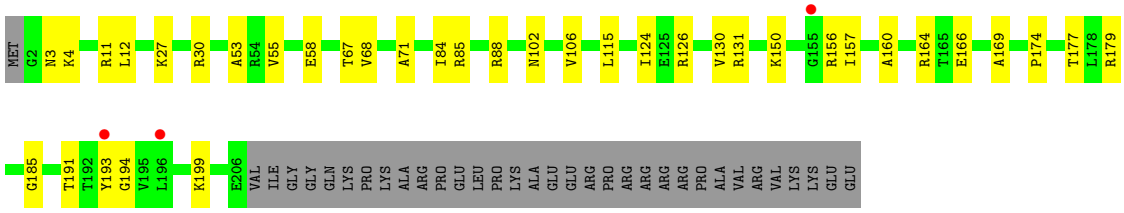
- Molecule 2: 30S ribosomal protein S2

Chain B:



- Molecule 3: 30S ribosomal protein S3

Chain C:



- Molecule 4: 30S ribosomal protein S4

Chain D: 72% 26%

MET G2 R3 C9 C12 R13 R14 K18 L19 Y20 L21 K22 G23 E24 R25 C26 K30 C31 A32 M33 E34 R35 Y38 G41 A55 V56 R57 E60 K63 I67 R73 E81 V88 E98 N103 V104 V105 Y106 R107 L108 V112 R115 Q116

A117 R118 Q119 R122 R132 R139 V140 R141 P142 E150 R153 N154 L155 R159 L162 L174 V178 E179 G180 M181 K182 F185 L194 A195 L196 P197 V198 L202 F206 R209

- Molecule 5: 30S ribosomal protein S5

Chain E: 77% 15% 7%

MET PRO GLU THR D5 E8 K9 M10 I11 R14 L31 V32 V33 V34 G74 E79 S87 P93 A94 A102 P106 R107 L112 T116 L119 S125 L142 R143 T144 D147 L151 E155 ALA HIS ALA GLN ALA GLN GLY

- Molecule 6: 30S ribosomal protein S6

Chain F: 77% 22%

M1 E5 L14 Q18 E22 K23 E24 I25 I26 Q27 R28 A35 R36 Y50 Y63 Q64 V65 E66 E69 R80 I81 R82 D83 N84 R87 V88 N100 ALA

- Molecule 7: 30S ribosomal protein S7

Chain G: 84% 15%

MET A2 R3 R4 D15 L16 G19 D20 V23 T24 I27 M31 K35 K36 K63 V66 V69 K70 P71 R76 Q96 L99 A100 A116 R119 D140 R143 W156

- Molecule 8: 30S ribosomal protein S8

Chain H: 74% 25%

MET L2 T3 D4 A7 L10 T11 R12 I13 R14 N15 A16 T17 R30 E33 E34 R37 E49 R50 K56 L59 Y62 R68 R69 R75 Q78 V79 R85 P89 G90 R91 R92 V93 Y94 V97 R105 I111 L112 S113 L119 T120 D121

R122 E123 I134 W138

- Molecule 9: 30S ribosomal protein S9

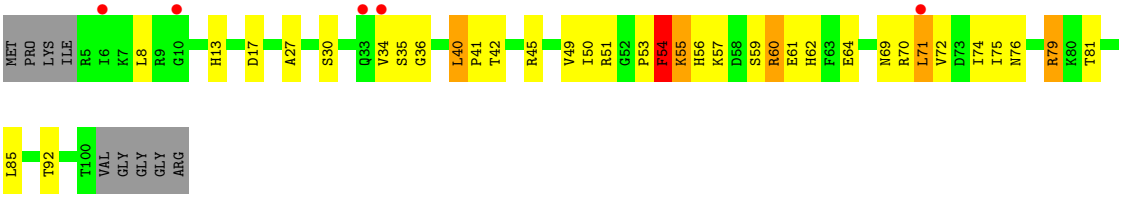
Chain I: 2% 73% 25%

MET E2 Q3 Y4 Y5 R9 R10 A13 V14 A15 R16 R20 P21 G22 K25 V28 G39 A45 E48 P49 L50 R51 L56 F59 D60 I63 T64 G68 I81 A82 R83 L99 G100 F101 D105 V108 K112 K113 R120 R121 A122

K127 ARG

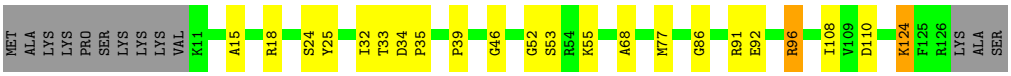
• Molecule 10: 30S ribosomal protein S10

Chain J:



• Molecule 11: 30S ribosomal protein S11

Chain K:

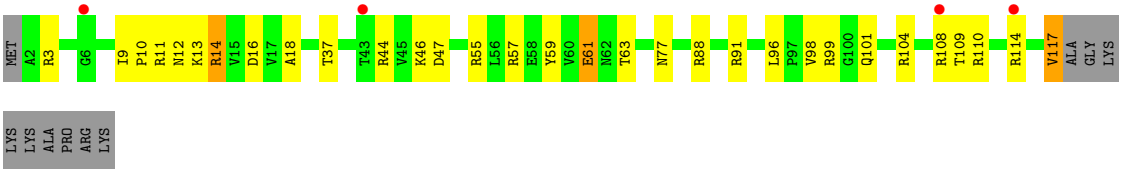


• Molecule 12: 30S ribosomal protein S12

Chain L:

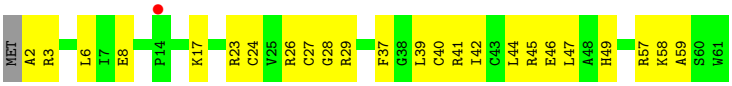
• Molecule 13: 30S ribosomal protein S13

Chain M:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:

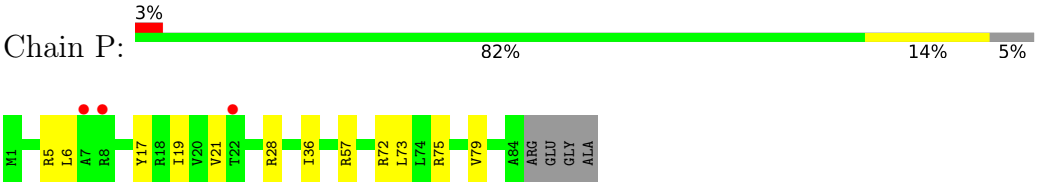


• Molecule 15: 30S ribosomal protein S15

Chain O:

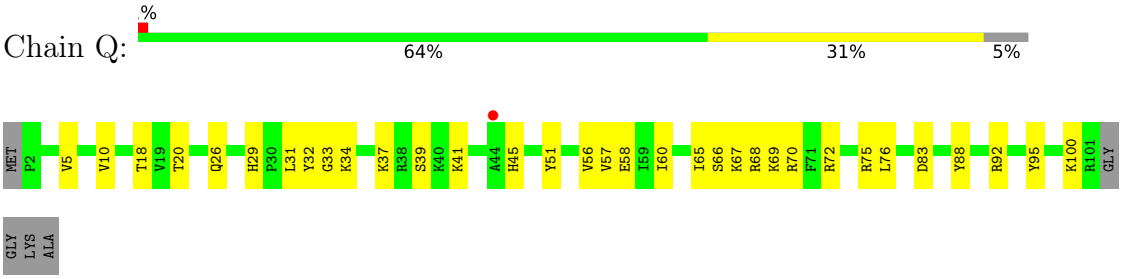
• Molecule 16: 30S ribosomal protein S16

Chain P:



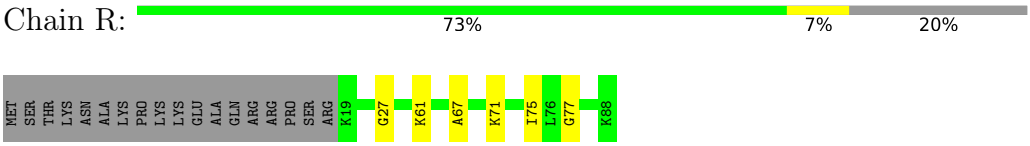
• Molecule 17: 30S ribosomal protein S17

Chain Q:



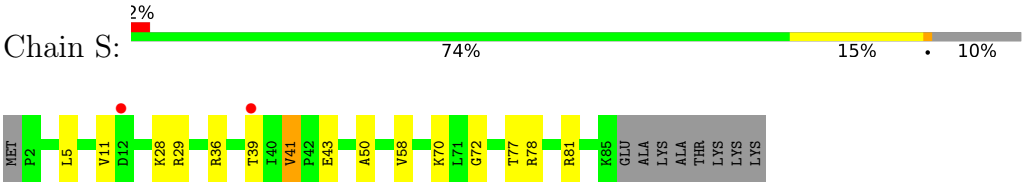
• Molecule 18: 30S ribosomal protein S18

Chain R:



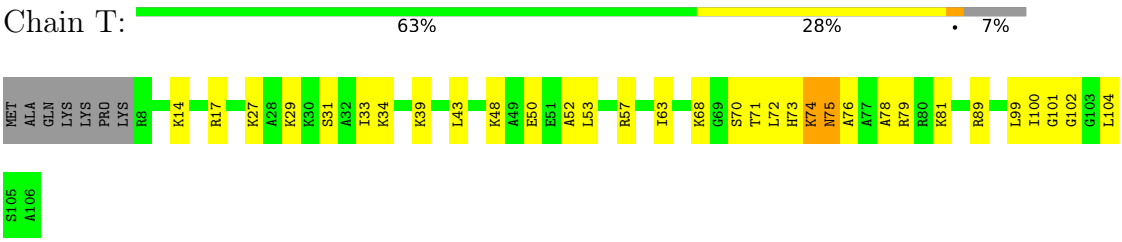
• Molecule 19: 30S ribosomal protein S19

Chain S:



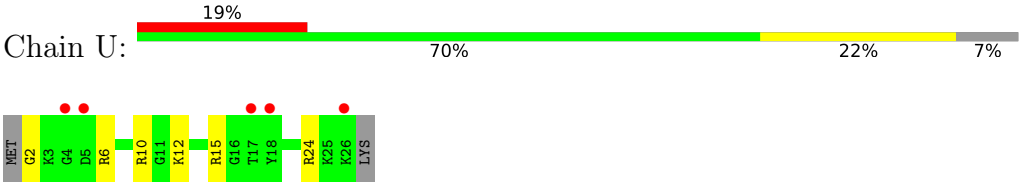
• Molecule 20: 30S ribosomal protein S20

Chain T:



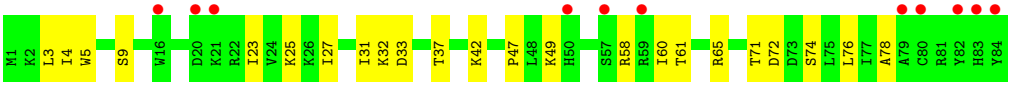
• Molecule 21: 30S ribosomal protein Thx

Chain U:



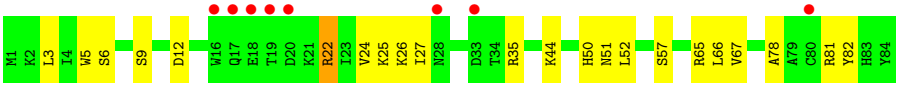
• Molecule 22: Toxin YoeB

Chain Y:



- Molecule 22: Toxin YoeB

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.71Å 401.71Å 175.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.74 49.83 – 3.74	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.83-3.74) 90.4 (49.83-3.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_3406	Depositor
R, R_{free}	0.206 , 0.224 0.206 , 0.224	Depositor DCC
R_{free} test set	7170 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	142.5	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 109.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53243	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.85	5/36349 (0.0%)	1.11	146/56729 (0.3%)
2	B	0.48	1/1950 (0.1%)	0.67	0/2630
3	C	0.39	0/1629	0.63	0/2195
4	D	0.46	0/1733	0.61	0/2318
5	E	0.47	0/1171	0.63	0/1576
6	F	0.41	0/850	0.58	0/1147
7	G	0.37	0/1276	0.57	0/1709
8	H	0.54	0/1128	0.62	0/1517
9	I	0.36	0/1017	0.69	0/1365
10	J	0.39	0/790	0.93	3/1063 (0.3%)
11	K	0.41	0/879	0.58	0/1187
12	L	0.47	0/972	0.72	1/1301 (0.1%)
13	M	0.42	0/938	0.69	0/1258
14	N	0.46	0/501	0.77	1/664 (0.2%)
15	O	0.44	0/740	0.52	0/987
16	P	0.47	0/721	0.67	0/970
17	Q	0.47	0/847	0.61	0/1131
18	R	0.41	0/579	0.60	0/768
19	S	0.37	0/689	0.69	0/926
20	T	0.36	0/765	0.69	0/1007
21	U	0.35	0/221	0.58	0/288
22	Y	0.35	0/742	0.63	0/1002
22	Z	0.33	0/743	0.69	0/1002
All	All	0.73	6/57230 (0.0%)	0.99	151/84740 (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
1	A	0	1
10	J	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1443	G	C6-O6	30.32	1.51	1.24
1	A	1443	G	C6-N1	22.77	1.55	1.39
1	A	701	C	C1'-N1	12.11	1.67	1.48
1	A	1030(C)	G	C1'-N9	10.04	1.63	1.48
1	A	476	G	C1'-N9	-9.74	1.33	1.46
2	B	166	ASP	C-N	8.79	1.50	1.34

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	G	N9-C1'-C2'	-23.22	83.81	114.00
1	A	1030(C)	G	C4-N9-C1'	19.78	152.21	126.50
1	A	1030(C)	G	C8-N9-C1'	-19.73	101.35	127.00
1	A	476	G	C8-N9-C1'	-16.27	105.84	127.00
1	A	1443	G	N1-C6-O6	15.89	129.43	119.90
10	J	54	PHE	C-N-CA	13.32	155.00	121.70
1	A	476	G	C4-N9-C1'	12.73	143.05	126.50
1	A	328	C	N1-C2-O2	10.70	125.32	118.90
1	A	1443	G	C5-C6-O6	-10.09	122.55	128.60
1	A	476	G	C3'-C2'-C1'	9.60	109.18	101.50
1	A	190(C)	C	N3-C2-O2	-9.47	115.27	121.90
1	A	328	C	C2-N1-C1'	9.47	129.22	118.80
1	A	328	C	N3-C2-O2	-9.40	115.32	121.90
1	A	159	G	N1-C6-O6	-8.52	114.79	119.90
1	A	190(C)	C	N1-C2-O2	8.44	123.97	118.90
1	A	369	C	N1-C2-O2	8.38	123.93	118.90
1	A	159	G	C5-C6-O6	7.87	133.32	128.60
1	A	129(A)	G	C5-C6-O6	-7.56	124.06	128.60
1	A	701	C	C2-N1-C1'	-7.47	110.58	118.80
14	N	44	LEU	CA-CB-CG	7.42	132.36	115.30
1	A	1158	C	C2-N1-C1'	7.39	126.93	118.80
1	A	1030	C	N3-C2-O2	-7.29	116.80	121.90
1	A	369	C	N3-C2-O2	-7.23	116.84	121.90
1	A	328	C	C6-N1-C2	-7.14	117.44	120.30
1	A	83	U	N3-C2-O2	-7.12	117.22	122.20
1	A	83	U	N1-C2-O2	7.11	127.77	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	936	C	N1-C2-O2	7.05	123.13	118.90
1	A	365	U	C2-N1-C1'	6.99	126.09	117.70
1	A	1443	G	C5-C6-N1	-6.96	108.02	111.50
1	A	972	C	C6-N1-C2	-6.95	117.52	120.30
1	A	1158	C	N1-C2-O2	6.91	123.04	118.90
1	A	110	C	N1-C2-O2	6.87	123.02	118.90
1	A	129(A)	G	N3-C4-N9	6.85	130.11	126.00
1	A	129(A)	G	C6-C5-N7	-6.82	126.31	130.40
1	A	1028	C	N1-C2-O2	6.78	122.97	118.90
1	A	701	C	C6-N1-C1'	6.61	128.73	120.80
1	A	283	C	N1-C2-O2	6.57	122.84	118.90
1	A	18	C	C6-N1-C2	-6.56	117.67	120.30
1	A	1030(C)	G	O4'-C1'-N9	6.55	113.44	108.20
10	J	71	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	476	G	P-O3'-C3'	6.43	127.41	119.70
1	A	328	C	C6-N1-C1'	-6.39	113.13	120.80
1	A	1029	C	N3-C2-O2	-6.34	117.46	121.90
1	A	1485	U	N1-C2-O2	6.30	127.21	122.80
1	A	413	G	C4-N9-C1'	6.29	134.67	126.50
1	A	1346	A	P-O3'-C3'	6.27	127.22	119.70
1	A	37	U	N3-C2-O2	-6.23	117.84	122.20
1	A	1485	U	N3-C2-O2	-6.15	117.90	122.20
1	A	1037	C	C5-C6-N1	6.12	124.06	121.00
1	A	1029	C	C6-N1-C2	-6.11	117.86	120.30
1	A	536	C	C6-N1-C2	-6.07	117.87	120.30
1	A	369	C	C6-N1-C2	-6.06	117.88	120.30
1	A	754	C	C2-N1-C1'	6.04	125.44	118.80
1	A	129(A)	G	N1-C6-O6	6.02	123.51	119.90
1	A	1147	C	N1-C2-O2	5.99	122.50	118.90
1	A	129(A)	G	C4-N9-C1'	5.98	134.27	126.50
1	A	58	C	C6-N1-C2	-5.93	117.93	120.30
1	A	1228	C	C6-N1-C2	-5.91	117.94	120.30
1	A	1028	C	N3-C2-O2	-5.91	117.76	121.90
1	A	536	C	C5-C6-N1	5.85	123.93	121.00
1	A	1066	C	N1-C2-O2	5.85	122.41	118.90
1	A	413	G	N3-C4-N9	5.84	129.50	126.00
1	A	81	U	C2-N1-C1'	-5.81	110.73	117.70
1	A	1383	C	N1-C2-O2	5.81	122.39	118.90
1	A	14	U	C2-N1-C1'	-5.76	110.79	117.70
1	A	455	C	N1-C2-O2	5.73	122.34	118.90
1	A	14	U	C6-N1-C1'	5.73	129.22	121.20
1	A	413	G	N3-C4-C5	-5.69	125.75	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1158	C	C6-N1-C1'	-5.68	113.99	120.80
1	A	18	C	C5-C6-N1	5.59	123.79	121.00
1	A	1224	G	C4-N9-C1'	-5.59	119.24	126.50
1	A	1026	G	N3-C4-N9	5.58	129.35	126.00
1	A	965	A	P-O3'-C3'	5.58	126.39	119.70
1	A	118	U	C2-N1-C1'	-5.57	111.02	117.70
1	A	110	C	N3-C2-O2	-5.56	118.01	121.90
1	A	118	U	C6-N1-C1'	5.55	128.97	121.20
10	J	60	ARG	N-CA-C	5.54	125.96	111.00
1	A	283	C	C6-N1-C2	-5.53	118.09	120.30
1	A	54	C	N1-C2-O2	5.52	122.21	118.90
1	A	536	C	C2-N1-C1'	5.51	124.86	118.80
1	A	1158	C	N3-C2-O2	-5.50	118.05	121.90
1	A	1101	A	P-O3'-C3'	5.46	126.25	119.70
1	A	129(A)	G	C8-N9-C1'	-5.43	119.94	127.00
1	A	365	U	C6-N1-C1'	-5.42	113.61	121.20
1	A	1514	C	C6-N1-C2	-5.42	118.13	120.30
1	A	82	U	N1-C2-O2	5.41	126.59	122.80
1	A	1033	G	N1-C6-O6	-5.41	116.66	119.90
1	A	932	C	C6-N1-C2	-5.40	118.14	120.30
1	A	1073	U	N3-C2-O2	-5.40	118.42	122.20
1	A	833	U	N3-C2-O2	-5.40	118.42	122.20
1	A	1030	C	C6-N1-C2	-5.39	118.14	120.30
1	A	108	G	C4-N9-C1'	5.39	133.51	126.50
1	A	866	C	C6-N1-C2	-5.36	118.16	120.30
1	A	477	G	C4-N9-C1'	5.36	133.47	126.50
1	A	328	C	C5-C6-N1	5.35	123.68	121.00
1	A	129(A)	G	N3-C4-C5	-5.34	125.93	128.60
1	A	1449	C	N1-C2-O2	5.34	122.10	118.90
1	A	924	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1539	C	N1-C2-O2	5.31	122.09	118.90
1	A	1285	A	P-O3'-C3'	5.31	126.07	119.70
1	A	1249	C	C6-N1-C2	-5.30	118.18	120.30
1	A	1414	U	N3-C2-O2	-5.30	118.49	122.20
1	A	674	G	N7-C8-N9	5.30	115.75	113.10
1	A	536	C	N1-C2-O2	5.29	122.08	118.90
1	A	312	C	C2-N1-C1'	-5.29	112.99	118.80
1	A	54	C	N3-C2-O2	-5.28	118.21	121.90
1	A	528	C	N1-C2-O2	5.27	122.06	118.90
1	A	620	C	N1-C2-O2	5.26	122.06	118.90
1	A	1203	C	C6-N1-C2	-5.26	118.19	120.30
1	A	1448	C	C6-N1-C2	-5.26	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1530	G	C4-N9-C1'	-5.24	119.69	126.50
1	A	1224	G	C6-C5-N7	5.23	133.54	130.40
1	A	1224	G	C8-N9-C1'	5.20	133.76	127.00
1	A	1228	C	N1-C2-O2	5.20	122.02	118.90
1	A	1228	C	C2-N1-C1'	5.19	124.51	118.80
1	A	477	G	C8-N9-C1'	-5.19	120.25	127.00
1	A	1224	G	N3-C4-N9	-5.19	122.89	126.00
1	A	1208	C	N1-C2-O2	5.18	122.01	118.90
1	A	1303	C	N1-C2-O2	5.18	122.01	118.90
1	A	1380	U	P-O3'-C3'	5.17	125.90	119.70
1	A	1203	C	N1-C2-O2	5.17	122.00	118.90
1	A	267	C	C2-N1-C1'	5.16	124.48	118.80
1	A	190	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1347	G	P-O3'-C3'	5.14	125.86	119.70
1	A	1237	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1449	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1195	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1203	C	C5-C6-N1	5.12	123.56	121.00
1	A	406	G	N3-C4-N9	5.12	129.07	126.00
1	A	913	A	P-O3'-C3'	5.10	125.82	119.70
12	L	47	LYS	N-CA-C	5.10	124.76	111.00
1	A	1341	U	C6-N1-C1'	5.09	128.33	121.20
1	A	201	C	C5-C6-N1	5.08	123.54	121.00
1	A	1372	U	N3-C2-O2	-5.07	118.65	122.20
1	A	115	G	P-O3'-C3'	5.07	125.78	119.70
1	A	891	U	N3-C2-O2	-5.06	118.66	122.20
1	A	1395	C	C2-N1-C1'	5.06	124.36	118.80
1	A	404	U	N3-C2-O2	-5.05	118.66	122.20
1	A	442	C	N1-C2-O2	5.05	121.93	118.90
1	A	1038	C	N1-C2-O2	5.05	121.93	118.90
1	A	308	C	N1-C2-O2	5.05	121.93	118.90
1	A	1530	G	C8-N9-C1'	5.04	133.55	127.00
1	A	82	U	N3-C2-O2	-5.04	118.67	122.20
1	A	283	C	N3-C2-O2	-5.04	118.37	121.90
1	A	1228	C	C5-C6-N1	5.04	123.52	121.00
1	A	386	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1037	C	C6-N1-C2	-5.03	118.29	120.30
1	A	960	U	C2-N1-C1'	5.02	123.72	117.70
1	A	413	G	C8-N9-C1'	-5.01	120.49	127.00
1	A	529	G	C8-N9-C1'	5.01	133.51	127.00
1	A	554	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	476	G	Sidechain
10	J	54	PHE	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	32514	0	16412	531	25
2	B	1915	0	1969	38	1
3	C	1605	0	1668	26	0
4	D	1703	0	1765	52	0
5	E	1155	0	1213	15	0
6	F	837	0	852	15	0
7	G	1257	0	1296	17	0
8	H	1108	0	1165	26	0
9	I	998	0	1024	26	0
10	J	777	0	815	30	1
11	K	864	0	881	15	0
12	L	956	0	1046	29	0
13	M	928	0	987	20	0
14	N	492	0	530	32	0
15	O	729	0	768	15	0
16	P	705	0	725	7	0
17	Q	834	0	904	26	0
18	R	574	0	644	6	0
19	S	674	0	699	12	0
20	T	763	0	861	25	0
21	U	217	0	234	4	0
22	Y	722	0	713	17	0
22	Z	723	0	713	12	0
23	A	182	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
24	D	8	0	0	7	0
25	N	1	0	0	0	0
All	All	53243	0	37884	836	27

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

All (836) 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)
14:N:24:CYS:HB2	14:N:40:CYS:SG	1.79	1.21
14:N:24:CYS:CB	14:N:40:CYS:SG	2.35	1.15
1:A:129(A):G:N1	1:A:190(C):C:O2	1.85	1.08
12:L:8:ASN:CG	17:Q:34:LYS:HZ3	1.60	1.02
1:A:246:A:H62	1:A:281:G:N2	1.60	0.98
12:L:8:ASN:CG	17:Q:34:LYS:NZ	2.16	0.98
1:A:925:G:H1	1:A:1391:U:H3	1.12	0.96
1:A:1419:G:H1	1:A:1481:U:H3	1.04	0.92
1:A:246:A:H62	1:A:281:G:H21	0.95	0.91
14:N:24:CYS:CB	14:N:40:CYS:HG	1.86	0.88
14:N:29:ARG:HB2	14:N:40:CYS:SG	2.13	0.88
1:A:1425:U:H3	1:A:1475:G:H1	1.21	0.88
1:A:246:A:N6	1:A:281:G:H21	1.72	0.87
14:N:29:ARG:HG3	14:N:40:CYS:SG	2.14	0.86
1:A:1238:A:H62	1:A:1301:U:H3	1.22	0.85
1:A:1415:G:H1	1:A:1485:U:H3	1.25	0.84
1:A:476:G:H2'	1:A:477:G:C8	2.13	0.84
1:A:476:G:HO2'	1:A:477:G:H8	1.28	0.82
1:A:912:C:OP1	12:L:46:LYS:NZ	2.12	0.82
1:A:927:G:H1	1:A:1390:U:H3	1.27	0.80
22:Z:57:SER:HA	22:Z:66:LEU:O	1.80	0.79
1:A:782:A:OP1	1:A:1521:G:N2	2.15	0.78
1:A:1131:G:H1	1:A:1143:G:H21	1.32	0.77
1:A:979:C:OP1	1:A:1223:C:N4	2.18	0.77
1:A:321:A:H61	1:A:332:G:H1	1.31	0.77
10:J:8:LEU:O	10:J:69:ASN:HA	1.84	0.76
1:A:1530:G:C6	1:A:1531:A:N6	2.54	0.76
1:A:1250:A:H4'	9:I:68:GLY:H	1.52	0.75
1:A:293:G:H1	1:A:304:U:H3	1.30	0.75
1:A:673:G:O3'	6:F:87:ARG:NH2	2.20	0.75
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.19	0.74
1:A:476:G:C2'	1:A:477:G:C8	2.70	0.74
1:A:938:A:H5'	7:G:76:ARG:HH22	1.53	0.73
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.70	0.72
1:A:28:G:O2'	1:A:296:U:OP1	2.07	0.72
1:A:476:G:C2'	1:A:477:G:H8	2.02	0.72
14:N:29:ARG:CG	14:N:40:CYS:SG	2.78	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:A:OP2	1:A:428:G:N2	2.21	0.71
1:A:1030(A):G:N1	1:A:1030(C):G:H5"	2.06	0.71
1:A:509:A:H5'	4:D:55:ALA:HB2	1.73	0.71
1:A:302:G:O3'	12:L:17:LYS:NZ	2.23	0.70
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.23	0.70
10:J:40:LEU:HD22	10:J:69:ASN:HB2	1.73	0.70
1:A:1022:G:N2	1:A:1023:G:N7	2.40	0.69
14:N:29:ARG:CB	14:N:40:CYS:SG	2.79	0.69
1:A:1504:G:H8	1:A:1504:G:H5"	1.57	0.69
1:A:593:G:H1	1:A:646:U:H3	1.38	0.69
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.25	0.69
1:A:581:G:O3'	15:O:64:ARG:NH2	2.24	0.69
1:A:1504:G:H5"	1:A:1504:G:C8	2.28	0.68
1:A:1530:G:N1	1:A:1531:A:N6	2.41	0.68
1:A:440:A:H62	1:A:494:G:H21	1.42	0.67
1:A:579:G:H5'	1:A:728:A:H1'	1.76	0.67
1:A:452:A:N6	1:A:480:U:N3	2.43	0.67
1:A:109:A:H62	1:A:324:G:H21	1.43	0.66
1:A:191:G:O2'	20:T:101:GLY:O	2.12	0.66
1:A:520:A:H62	1:A:529:G:H21	1.41	0.66
1:A:1238:A:N6	1:A:1301:U:H3	1.93	0.66
21:U:6:ARG:HE	21:U:15:ARG:HE	1.43	0.66
2:B:166:ASP:HB2	2:B:205:ASP:HB2	1.77	0.66
1:A:673:G:H2'	1:A:674:G:C8	2.31	0.66
1:A:1510:U:H3	1:A:1525:G:H1	1.43	0.65
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.77	0.65
1:A:1288:A:N3	1:A:1352:C:O2'	2.29	0.65
20:T:43:LEU:HD22	20:T:52:ALA:HB2	1.78	0.65
2:B:78:GLN:HG3	2:B:94:ASN:HB2	1.76	0.65
1:A:1010:G:H2'	1:A:1011:G:H8	1.61	0.64
1:A:452:A:N6	1:A:480:U:H3	1.95	0.64
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.30	0.64
2:B:187:LEU:HA	2:B:201:ILE:HB	1.79	0.64
12:L:60:LEU:HD12	12:L:62:SER:H	1.62	0.64
1:A:1356:G:H2'	1:A:1357:A:C8	2.32	0.64
14:N:24:CYS:HB3	14:N:40:CYS:SG	2.36	0.64
1:A:954:G:H21	1:A:1227:A:H62	1.46	0.64
1:A:279:A:OP2	17:Q:95:TYR:OH	2.15	0.63
14:N:24:CYS:SG	14:N:27:CYS:HB2	2.37	0.63
1:A:59:A:H5"	1:A:387:U:H5"	1.79	0.63
1:A:150:C:H42	1:A:171:A:H62	1.44	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:U:H2'	1:A:553:A:H8	1.62	0.63
1:A:958:A:N3	1:A:985:C:O2'	2.29	0.63
1:A:476:G:C8	1:A:476:G:C4'	2.80	0.63
1:A:189:G:H1	1:A:190(J):U:H3	1.47	0.63
1:A:674:G:H2'	1:A:675:A:H8	1.63	0.63
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.80	0.63
1:A:325:A:OP2	20:T:70:SER:OG	2.09	0.62
1:A:1404:C:C2	1:A:1499:A:C6	2.88	0.62
12:L:8:ASN:ND2	17:Q:34:LYS:NZ	2.47	0.62
1:A:947:G:O3'	13:M:109:THR:OG1	2.17	0.62
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.81	0.62
1:A:21:G:H2'	1:A:22:G:C8	2.35	0.62
1:A:953:G:N7	13:M:104:ARG:NH2	2.48	0.62
1:A:664:G:H22	1:A:741:G:H1	1.47	0.62
1:A:1119:C:H2'	1:A:1120:G:H8	1.64	0.61
1:A:1238:A:N7	1:A:1301:U:O4	2.33	0.61
1:A:359:U:H2'	1:A:360:A:H8	1.66	0.61
4:D:18:LYS:HE2	4:D:18:LYS:HA	1.81	0.61
11:K:33:THR:OG1	11:K:34:ASP:N	2.33	0.61
13:M:108:ARG:HE	13:M:114:ARG:HD3	1.66	0.61
4:D:9:CYS:SG	24:D:301:SF4:S2	2.99	0.61
1:A:558:G:OP2	1:A:559:A:O2'	2.15	0.61
1:A:21:G:H2'	1:A:22:G:H8	1.65	0.61
1:A:52:G:H1	1:A:359:U:H3	1.49	0.61
10:J:40:LEU:HB2	10:J:71:LEU:HD22	1.81	0.61
1:A:476:G:O2'	1:A:477:G:C8	2.54	0.60
1:A:1236:A:OP1	21:U:2:GLY:N	2.34	0.60
1:A:1286:A:H2'	1:A:1287:A:H4'	1.81	0.60
4:D:154:ASN:HA	4:D:159:ARG:HH21	1.65	0.60
14:N:24:CYS:SG	14:N:27:CYS:N	2.74	0.60
9:I:10:ARG:O	9:I:13:ALA:HB3	2.01	0.60
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.84	0.60
1:A:1202:G:N2	14:N:27:CYS:SG	2.73	0.60
1:A:476:G:O2'	1:A:477:G:H8	1.84	0.60
1:A:946:A:O2'	1:A:1333:A:N3	2.35	0.60
1:A:195:A:O5'	20:T:68:LYS:NZ	2.35	0.60
10:J:53:PRO:HB3	14:N:42:ILE:HG12	1.84	0.59
1:A:1321:C:O2'	19:S:78:ARG:NH1	2.35	0.59
4:D:31:CYS:SG	24:D:301:SF4:S1	2.92	0.59
1:A:328:C:H4'	1:A:329:A:H5'	1.83	0.59
1:A:426:G:OP1	4:D:38:TYR:OH	2.19	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:ALA:HA	11:K:77:MET:HA	1.84	0.59
1:A:976:G:OP2	1:A:1358:U:O2'	2.09	0.59
4:D:30:LYS:HA	4:D:35:ARG:HE	1.67	0.59
7:G:24:THR:HA	7:G:27:ILE:HD12	1.85	0.59
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.67	0.59
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.33	0.59
1:A:1281:U:H5'	1:A:1282:C:H5	1.68	0.59
2:B:115:LEU:HD12	2:B:145:LEU:HB3	1.82	0.59
1:A:406:G:N3	4:D:119:GLN:NE2	2.48	0.59
1:A:603:U:H2'	1:A:604:G:C8	2.38	0.59
1:A:603:U:H2'	1:A:604:G:H8	1.67	0.59
1:A:321:A:N6	1:A:332:G:H1	1.99	0.59
1:A:1413:A:H2	1:A:1487:G:H22	1.51	0.59
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.83	0.59
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.84	0.59
11:K:92:GLU:OE1	11:K:96:ARG:NH1	2.36	0.59
20:T:89:ARG:HD3	20:T:104:LEU:HD21	1.84	0.59
1:A:1009:G:H1	1:A:1020:U:H3	1.51	0.58
1:A:1119:C:OP1	9:I:83:ARG:NH1	2.36	0.58
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.84	0.58
1:A:489:C:OP1	4:D:132:ARG:NH2	2.36	0.58
1:A:691:G:H1	11:K:52:GLY:HA2	1.67	0.58
1:A:973:G:H3'	1:A:974:A:H5"	1.85	0.58
11:K:32:ILE:HD11	11:K:68:ALA:HB1	1.83	0.58
1:A:452:A:N6	1:A:480:U:C2	2.71	0.58
1:A:303:A:P	12:L:17:LYS:HZ3	2.25	0.58
1:A:656:C:O2'	15:O:28:GLN:OE1	2.18	0.58
22:Y:61:THR:O	22:Y:65:ARG:NH1	2.37	0.58
1:A:269:C:H2'	1:A:270:A:H8	1.68	0.58
1:A:667:G:H4'	15:O:51:HIS:CE1	2.39	0.58
1:A:992:U:H3	1:A:1044:A:H62	1.51	0.58
1:A:1414:U:H2'	1:A:1415:G:H8	1.69	0.58
4:D:24:GLU:HG2	4:D:112:VAL:HG21	1.86	0.58
10:J:8:LEU:HD13	10:J:70:ARG:HB2	1.85	0.58
10:J:35:SER:OG	10:J:72:VAL:O	2.22	0.58
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.85	0.58
1:A:438:G:H21	1:A:497:A:H62	1.51	0.57
1:A:624:C:H2'	1:A:625:G:H8	1.69	0.57
1:A:1247:U:H3	1:A:1290:G:H1	1.52	0.57
1:A:1427:U:H2'	1:A:1428:A:H8	1.69	0.57
14:N:57:ARG:NH1	14:N:58:LYS:O	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:G:OP1	1:A:766:A:H1'	2.04	0.57
10:J:30:SER:O	10:J:81:THR:OG1	2.21	0.57
1:A:501:C:H2'	1:A:502:G:H8	1.70	0.57
1:A:250:A:H4'	1:A:251:G:O5'	2.04	0.57
1:A:1073:U:O2	2:B:104:ASN:ND2	2.37	0.57
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.52	0.57
1:A:657:G:H4'	15:O:28:GLN:HG2	1.86	0.57
9:I:51:ARG:HH22	9:I:56:LEU:HA	1.70	0.57
1:A:547:A:OP2	4:D:2:GLY:N	2.37	0.56
1:A:412:A:OP2	4:D:35:ARG:NH2	2.38	0.56
1:A:946:A:H2'	1:A:947:G:C8	2.40	0.56
6:F:87:ARG:NH1	18:R:75:ILE:O	2.38	0.56
15:O:9:GLN:HA	15:O:12:ILE:HD12	1.86	0.56
1:A:1139:G:H4'	1:A:1140:C:H5'	1.88	0.56
11:K:52:GLY:H	11:K:55:LYS:HE3	1.69	0.56
1:A:99:C:H2'	1:A:101:A:C8	2.40	0.56
1:A:410:G:H21	1:A:432:A:H62	1.53	0.56
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.87	0.56
1:A:421:U:O2	3:C:126:ARG:NH1	2.39	0.56
1:A:582:U:P	15:O:64:ARG:HH22	2.29	0.56
1:A:908:A:H2'	1:A:909:A:H8	1.70	0.56
1:A:797:C:OP1	11:K:124:LYS:NZ	2.38	0.56
1:A:824:C:H2'	1:A:825:G:H8	1.71	0.56
1:A:902:G:H2'	1:A:903:G:H8	1.71	0.56
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.70	0.56
13:M:117:VAL:HG12	13:M:117:VAL:O	2.05	0.56
1:A:76:C:H5"	1:A:76:C:H6	1.70	0.56
1:A:1391:U:H2'	1:A:1392:G:C8	2.41	0.56
1:A:994:A:O2'	14:N:8:GLU:OE1	2.24	0.56
1:A:945:G:H21	1:A:1334:G:H4'	1.71	0.55
8:H:91:ARG:NE	17:Q:32:TYR:O	2.34	0.55
10:J:51:ARG:HG2	10:J:61:GLU:HB2	1.88	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:861:G:HO2'	1:A:874:G:HO2'	1.54	0.55
2:B:11:LEU:HG	2:B:213:LEU:HD11	1.88	0.55
17:Q:88:TYR:OH	17:Q:92:ARG:NH1	2.39	0.55
1:A:148:G:H2'	1:A:149:A:H8	1.71	0.55
1:A:514:C:H2'	1:A:515:G:H8	1.72	0.55
1:A:806:C:H2'	1:A:807:A:H8	1.71	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.55
1:A:1499:A:H2'	1:A:1500:A:H8	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:NH2	3:C:177:THR:O	2.39	0.55
12:L:74:GLY:O	12:L:102:ARG:NH1	2.34	0.55
16:P:72:ARG:HE	16:P:73:LEU:HD22	1.71	0.55
1:A:1342:C:H2'	1:A:1343:G:C8	2.42	0.55
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.89	0.55
20:T:27:LYS:NZ	20:T:31:SER:OG	2.39	0.55
1:A:272:C:H2'	1:A:273:A:H8	1.72	0.55
1:A:62:U:OP1	1:A:385:C:O2'	2.24	0.55
1:A:1356:G:H2'	1:A:1357:A:H8	1.71	0.55
4:D:32:ALA:HB3	24:D:301:SF4:S4	2.47	0.55
11:K:18:ARG:NH2	11:K:35:PRO:O	2.40	0.55
1:A:1499:A:H1'	1:A:1520:G:H5'	1.88	0.55
1:A:542:G:H5'	4:D:41:GLY:HA3	1.89	0.54
4:D:18:LYS:NZ	24:D:301:SF4:S4	2.80	0.54
7:G:71:PRO:HG3	7:G:99:LEU:HD11	1.88	0.54
11:K:24:SER:OG	11:K:25:TYR:N	2.38	0.54
14:N:26:ARG:NH2	14:N:46:GLU:OE1	2.40	0.54
1:A:975:A:H4'	1:A:976:G:H5'	1.88	0.54
1:A:1318:A:H4'	19:S:11:VAL:HG11	1.88	0.54
14:N:3:ARG:NH2	14:N:27:CYS:O	2.40	0.54
1:A:92:C:H2'	1:A:93:G:C8	2.43	0.54
1:A:412:A:N3	4:D:35:ARG:NH1	2.55	0.54
1:A:1297:C:H4'	1:A:1298:C:H5'	1.90	0.54
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.89	0.54
3:C:131:ARG:NH1	3:C:166:GLU:OE1	2.41	0.54
11:K:18:ARG:HB3	11:K:33:THR:HG23	1.88	0.54
1:A:1151:A:H5"	10:J:42:THR:HG23	1.88	0.54
5:E:33:VAL:HG13	5:E:112:LEU:HD22	1.90	0.54
1:A:6:G:H4'	1:A:298:A:H4'	1.89	0.54
1:A:269:C:H2'	1:A:270:A:C8	2.41	0.54
7:G:71:PRO:O	7:G:96:GLN:NE2	2.39	0.54
17:Q:18:THR:OG1	17:Q:69:LYS:NZ	2.35	0.54
1:A:578:C:O2'	1:A:728:A:N3	2.40	0.54
4:D:26:CYS:HA	24:D:301:SF4:S1	2.48	0.54
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.89	0.54
1:A:113:G:H1'	1:A:354:G:H5'	1.90	0.54
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.54
1:A:911:U:OP2	12:L:97:ARG:NH2	2.36	0.54
1:A:1251:A:N3	1:A:1369:C:O2'	2.37	0.54
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.89	0.54
1:A:1129:C:H4'	1:A:1130:A:OP2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:LYS:HA	3:C:30:ARG:HH22	1.73	0.54
1:A:1167:A:H2'	1:A:1168:A:C8	2.42	0.54
4:D:18:LYS:HD2	24:D:301:SF4:S1	2.48	0.54
2:B:130:ARG:O	2:B:135:GLN:NE2	2.41	0.54
9:I:22:GLY:H	9:I:59:PHE:HA	1.73	0.54
17:Q:41:LYS:NZ	17:Q:88:TYR:OH	2.38	0.54
1:A:651:C:O2'	1:A:652:U:H5'	2.08	0.53
2:B:127:ILE:O	2:B:135:GLN:NE2	2.41	0.53
1:A:1427:U:H2'	1:A:1428:A:C8	2.43	0.53
4:D:105:VAL:HG23	4:D:117:ALA:HB1	1.89	0.53
14:N:45:ARG:O	14:N:49:HIS:ND1	2.42	0.53
2:B:54:THR:HG23	2:B:199:TYR:HB3	1.91	0.53
1:A:80:G:H3'	1:A:81:U:H5"	1.91	0.53
1:A:757:U:O2'	1:A:879:C:O2	2.25	0.53
1:A:826:C:O2	8:H:15:ASN:ND2	2.41	0.53
11:K:86:GLY:O	11:K:91:ARG:NH1	2.41	0.53
1:A:359:U:H2'	1:A:360:A:C8	2.44	0.53
1:A:393:A:H2'	1:A:394:G:H8	1.74	0.53
1:A:524:G:H2'	1:A:525:C:C6	2.44	0.53
1:A:580:U:H3	1:A:761:G:H1	1.57	0.53
1:A:736:C:H2'	1:A:737:A:C8	2.44	0.53
1:A:1404:C:C2	1:A:1499:A:N6	2.76	0.53
4:D:19:LEU:HD23	4:D:67:ILE:HD13	1.90	0.53
4:D:98:GLU:HA	4:D:103:ASN:HD22	1.74	0.53
1:A:148:G:H2'	1:A:149:A:C8	2.43	0.53
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.42	0.53
1:A:92:C:H2'	1:A:93:G:H8	1.74	0.52
1:A:543:C:OP1	4:D:14:ARG:HD3	2.08	0.52
1:A:1152:A:H5"	10:J:13:HIS:HD2	1.74	0.52
1:A:362:G:OP2	12:L:34:ARG:NH2	2.41	0.52
6:F:1:MET:N	6:F:69:GLU:OE1	2.41	0.52
6:F:100:ASN:ND2	18:R:27:GLY:O	2.41	0.52
10:J:34:VAL:HA	10:J:74:ILE:HD13	1.90	0.52
1:A:452:A:N7	1:A:480:U:O4	2.42	0.52
1:A:591:U:OP2	8:H:30:ARG:NH1	2.43	0.52
1:A:1191:A:H5"	3:C:4:LYS:HE3	1.91	0.52
1:A:1391:U:H2'	1:A:1392:G:H8	1.73	0.52
17:Q:58:GLU:OE1	17:Q:75:ARG:NH2	2.42	0.52
1:A:1441:G:H21	1:A:1460:A:H62	1.56	0.52
1:A:1124:G:O2'	1:A:1145:C:N4	2.43	0.52
9:I:112:LYS:NZ	9:I:113:LYS:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:H1	1:A:850:U:H3	1.56	0.52
1:A:1327:C:OP1	21:U:12:LYS:NZ	2.37	0.52
2:B:76:GLN:NE2	2:B:206:ASP:OD1	2.42	0.52
3:C:71:ALA:HA	3:C:106:VAL:HG22	1.92	0.52
13:M:16:ASP:OD1	13:M:16:ASP:N	2.42	0.52
1:A:520:A:H62	1:A:529:G:N2	2.08	0.52
1:A:1031:G:H2'	1:A:1032:G:C8	2.45	0.52
1:A:34:C:H2'	1:A:35:G:H8	1.74	0.52
1:A:356:A:N3	1:A:368:U:O2'	2.40	0.52
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.43	0.52
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.52
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.90	0.52
7:G:116:ALA:HA	7:G:119:ARG:HE	1.75	0.52
1:A:390:C:H2'	1:A:391:G:C8	2.44	0.52
2:B:55:PHE:HD2	2:B:58:ILE:HD11	1.75	0.52
1:A:1287:A:H2	1:A:1353:G:H1'	1.75	0.51
19:S:28:LYS:O	19:S:29:ARG:NH1	2.40	0.51
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.51
1:A:1147:C:O2	9:I:16:ARG:NH1	2.43	0.51
1:A:56:U:H2'	1:A:57:G:H8	1.75	0.51
1:A:985:C:H2'	1:A:986:A:H8	1.75	0.51
1:A:1009:G:N2	1:A:1020:U:O2	2.38	0.51
1:A:1224:G:O2'	1:A:1322:C:OP1	2.26	0.51
2:B:8:LYS:HG2	2:B:11:LEU:HD22	1.92	0.51
22:Z:12:ASP:OD2	22:Z:12:ASP:N	2.38	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.45	0.51
1:A:12:U:H3	1:A:22:G:H1	1.57	0.51
1:A:532:A:H62	3:C:193:TYR:CB	2.24	0.51
1:A:1203:C:H5'	14:N:3:ARG:HH21	1.76	0.51
11:K:91:ARG:NH2	11:K:110:ASP:OD1	2.40	0.51
1:A:501:C:OP1	12:L:117:ARG:NH1	2.35	0.51
1:A:925:G:O6	1:A:1391:U:O4	2.28	0.51
2:B:98:LEU:H	2:B:101:MET:HE3	1.75	0.51
19:S:50:ALA:HA	19:S:58:VAL:O	2.11	0.51
1:A:673:G:H1'	18:R:75:ILE:HD12	1.93	0.51
1:A:75:G:H2'	1:A:76:C:H5"	1.91	0.51
1:A:558:G:C8	1:A:559:A:H2'	2.46	0.51
12:L:33:ARG:H	12:L:85:ILE:HG22	1.74	0.51
1:A:227:G:H2'	1:A:228:A:C8	2.45	0.51
1:A:401:C:O2'	1:A:621:A:N3	2.38	0.51
1:A:1216:G:OP1	14:N:2:ALA:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:C:O3'	2:B:175:ARG:NH2	2.41	0.51
2:B:50:GLU:O	2:B:54:THR:OG1	2.24	0.50
4:D:12:CYS:HB3	4:D:18:LYS:HE2	1.92	0.50
10:J:51:ARG:HH22	14:N:58:LYS:HZ1	1.59	0.50
19:S:41:VAL:HG13	19:S:43:GLU:H	1.75	0.50
1:A:300:A:H8	1:A:300:A:O5'	1.95	0.50
1:A:1256:A:O2'	1:A:1257:U:O4'	2.27	0.50
4:D:150:GLU:HG2	4:D:153:ARG:HE	1.74	0.50
20:T:43:LEU:HD21	20:T:48:LYS:HB3	1.93	0.50
1:A:243:A:H4'	1:A:244:U:O5'	2.12	0.50
1:A:398:C:H2'	1:A:399:G:H8	1.75	0.50
2:B:27:LYS:HD2	2:B:193:ASP:HB2	1.93	0.50
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.92	0.50
22:Y:71:THR:HB	22:Y:74:SER:HB2	1.93	0.50
1:A:1342:C:H2'	1:A:1343:G:H8	1.75	0.50
1:A:258:G:H2'	1:A:259:G:H8	1.76	0.50
1:A:463:A:OP1	16:P:75:ARG:NH2	2.45	0.50
1:A:1530:G:N1	1:A:1531:A:C6	2.80	0.50
8:H:17:THR:O	8:H:78:GLN:NE2	2.37	0.50
1:A:538:G:H4'	12:L:114:LYS:HE3	1.92	0.50
1:A:539:A:H2'	1:A:540:G:C8	2.47	0.50
1:A:1314:C:H2'	1:A:1315:U:C6	2.47	0.50
1:A:932:C:O3'	7:G:4:ARG:NH2	2.42	0.50
1:A:933:G:O6	7:G:3:ARG:NH1	2.44	0.50
1:A:1004:A:H5"	1:A:1025:U:C4	2.47	0.50
1:A:1256:A:O2'	1:A:1257:U:O5'	2.29	0.50
5:E:5:ASP:OD1	5:E:5:ASP:N	2.45	0.50
20:T:78:ALA:HA	20:T:81:LYS:HD3	1.94	0.50
1:A:95:U:H2'	1:A:96:G:H8	1.77	0.50
4:D:18:LYS:HD3	4:D:19:LEU:H	1.77	0.50
1:A:231:G:H2'	1:A:232:G:H8	1.76	0.50
1:A:1033:G:H2'	1:A:1034:G:H8	1.77	0.50
6:F:80:ARG:NH2	6:F:88:VAL:O	2.38	0.50
12:L:8:ASN:CG	17:Q:34:LYS:HZ2	2.14	0.50
17:Q:66:SER:OG	17:Q:67:LYS:N	2.45	0.50
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.45	0.49
1:A:560:U:H5'	1:A:566:G:N2	2.27	0.49
1:A:1298:C:H4'	1:A:1299:A:C4	2.47	0.49
1:A:195:A:H4'	20:T:68:LYS:HD3	1.94	0.49
1:A:946:A:H2'	1:A:947:G:H8	1.76	0.49
1:A:1443:G:C2'	1:A:1443:G:N3	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:ILE:HD13	3:C:166:GLU:HG2	1.94	0.49
7:G:66:VAL:HA	7:G:69:VAL:HG12	1.94	0.49
17:Q:51:TYR:HE1	17:Q:76:LEU:HB2	1.77	0.49
1:A:790:A:H2'	1:A:791:G:C8	2.47	0.49
1:A:1256:A:N6	1:A:1278:U:O2	2.43	0.49
4:D:19:LEU:HB3	4:D:21:LEU:HD21	1.94	0.49
4:D:23:GLY:N	4:D:26:CYS:SG	2.85	0.49
8:H:111:ILE:HG23	8:H:134:ILE:HB	1.92	0.49
13:M:37:THR:O	13:M:55:ARG:NH2	2.45	0.49
22:Z:6:SER:N	22:Z:9:SER:OG	2.45	0.49
1:A:1404:C:N3	1:A:1499:A:N6	2.60	0.49
6:F:14:LEU:HD11	6:F:18:GLN:HB3	1.95	0.49
4:D:63:LYS:HD2	4:D:198:VAL:HG12	1.94	0.49
5:E:8:GLU:HG2	5:E:34:VAL:HG12	1.94	0.49
6:F:22:GLU:OE2	6:F:84:ASN:ND2	2.44	0.49
17:Q:10:VAL:HA	17:Q:20:THR:O	2.12	0.49
20:T:75:ASN:O	20:T:79:ARG:N	2.44	0.49
1:A:1314:C:H2'	1:A:1315:U:H6	1.78	0.49
5:E:151:LEU:HD12	8:H:79:VAL:HG12	1.94	0.49
8:H:7:ALA:HA	8:H:10:LEU:HD12	1.93	0.49
1:A:793:U:O2	1:A:1516:G:H4'	2.13	0.49
1:A:977:A:H2'	1:A:978:A:H5"	1.93	0.49
1:A:981:U:H6	1:A:981:U:O5'	1.96	0.49
13:M:13:LYS:HD3	13:M:44:ARG:HG2	1.95	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.49
1:A:1129:C:H4'	1:A:1130:A:H5'	1.95	0.49
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.95	0.49
2:B:27:LYS:HG3	2:B:194:PRO:HD2	1.94	0.49
8:H:119:LEU:HB3	8:H:123:GLU:HG3	1.94	0.49
15:O:7:GLU:OE2	15:O:38:ARG:NH2	2.46	0.49
1:A:782:A:H62	1:A:800:G:H21	1.61	0.49
1:A:1015:A:H2'	1:A:1016:A:C8	2.48	0.49
1:A:190:C:H42	1:A:190(I):G:H1	1.60	0.48
1:A:701:C:H4'	1:A:702:A:H5"	1.95	0.48
1:A:858:G:O6	1:A:869:G:C8	2.66	0.48
1:A:1025:U:H2'	1:A:1026:G:H8	1.78	0.48
4:D:60:GLU:HG3	4:D:202:LEU:HD12	1.95	0.48
1:A:45:U:H3	1:A:396:G:H1	1.60	0.48
1:A:129(A):G:C6	1:A:190(C):C:O2	2.64	0.48
1:A:1020:U:H2'	1:A:1021:G:H8	1.78	0.48
1:A:1236:A:H4'	1:A:1304:G:H4'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:PRO:HA	8:H:92:ARG:HE	1.79	0.48
1:A:908:A:H2'	1:A:909:A:C8	2.49	0.48
4:D:18:LYS:HA	4:D:18:LYS:CE	2.42	0.48
1:A:1096:C:H2'	1:A:1097:C:H6	1.79	0.48
1:A:1294:G:H2'	1:A:1295:G:H8	1.78	0.48
1:A:188:C:H2'	1:A:189:G:H8	1.79	0.48
1:A:1355:G:H2'	1:A:1356:G:C8	2.49	0.48
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.32	0.48
1:A:1505:G:O2'	1:A:1506:U:OP2	2.27	0.48
7:G:31:MET:HG3	7:G:35:LYS:H	1.78	0.48
1:A:1287:A:H2'	1:A:1288:A:C8	2.48	0.48
5:E:102:ALA:O	5:E:107:ARG:NH2	2.47	0.48
9:I:25:LYS:NZ	9:I:60:ASP:OD2	2.46	0.48
1:A:1119:C:H2'	1:A:1120:G:C8	2.47	0.48
1:A:1181:G:O2'	1:A:1182:G:O4'	2.28	0.48
1:A:1256:A:H61	1:A:1278:U:H1'	1.79	0.48
5:E:10:MET:HA	5:E:32:VAL:HG23	1.96	0.48
14:N:29:ARG:HD2	14:N:42:ILE:HD12	1.95	0.48
1:A:869:G:H4'	1:A:872:A:C8	2.49	0.48
1:A:966:G:H2'	1:A:967:C:C6	2.49	0.48
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.48
1:A:1522:U:H2'	1:A:1523:G:H8	1.78	0.48
5:E:87:SER:OG	5:E:125:SER:OG	2.32	0.48
7:G:140:ASP:OD1	7:G:143:ARG:NH2	2.47	0.48
22:Z:67:VAL:HB	22:Z:78:ALA:HB3	1.96	0.48
1:A:298:A:H2'	1:A:299:G:C8	2.49	0.48
1:A:522:C:OP2	12:L:69:TYR:OH	2.25	0.48
1:A:864:A:H2'	1:A:865:A:C8	2.49	0.48
1:A:345:C:O2	1:A:346:G:N2	2.44	0.47
1:A:489:C:H2'	1:A:490:G:H8	1.79	0.47
1:A:886:G:H1	1:A:911:U:H3	1.60	0.47
1:A:993:G:O2'	1:A:994:A:N7	2.42	0.47
1:A:1034:G:H2'	1:A:1035:A:H8	1.79	0.47
22:Y:3:LEU:HB2	22:Z:5:TRP:HB2	1.95	0.47
1:A:436:C:H2'	1:A:437:U:H6	1.78	0.47
1:A:672:U:H3	1:A:734:G:H1	1.62	0.47
10:J:40:LEU:HD12	10:J:71:LEU:HD13	1.96	0.47
1:A:113:G:H2'	1:A:114:U:H6	1.79	0.47
1:A:406:G:O3'	4:D:3:ARG:NH1	2.48	0.47
1:A:545:C:O2'	1:A:549:C:OP1	2.33	0.47
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.46	0.47
22:Y:9:SER:HB3	22:Y:78:ALA:HA	1.96	0.47
1:A:876:G:O5'	8:H:14:ARG:NH1	2.48	0.47
1:A:1071:C:H2'	1:A:1072:G:H8	1.78	0.47
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.15	0.47
4:D:21:LEU:N	24:D:301:SF4:S3	2.79	0.47
16:P:6:LEU:HD13	16:P:17:TYR:CG	2.49	0.47
17:Q:5:VAL:HG12	17:Q:60:ILE:HD13	1.96	0.47
1:A:1172:C:H2'	1:A:1173:G:H8	1.80	0.47
1:A:1244:C:H2'	1:A:1245:A:H8	1.77	0.47
1:A:77:G:H1	1:A:92:C:H42	1.61	0.47
1:A:229:U:H2'	1:A:230:G:H8	1.80	0.47
1:A:1112:C:H1'	3:C:179:ARG:HE	1.80	0.47
1:A:1244:C:H2'	1:A:1245:A:C8	2.49	0.47
1:A:1268:A:H2'	1:A:1269:A:C8	2.50	0.47
1:A:1499:A:C1'	1:A:1520:G:H5'	2.44	0.47
1:A:1513:A:H2'	1:A:1514:C:C6	2.50	0.47
3:C:55:VAL:HG12	3:C:68:VAL:HG22	1.97	0.47
4:D:3:ARG:HD2	4:D:115:ARG:HD2	1.96	0.47
4:D:154:ASN:OD1	4:D:154:ASN:N	2.44	0.47
15:O:85:LEU:HB3	15:O:87:ILE:HG12	1.95	0.47
20:T:53:LEU:HD22	20:T:100:ILE:HG23	1.96	0.47
1:A:188:C:H4'	20:T:89:ARG:HH12	1.80	0.47
1:A:538:G:H5'	12:L:114:LYS:HB2	1.97	0.47
1:A:1073:U:O2'	2:B:104:ASN:OD1	2.29	0.47
1:A:1368:G:OP1	10:J:62:HIS:NE2	2.40	0.47
13:M:57:ARG:O	13:M:61:GLU:HB2	2.15	0.47
13:M:96:LEU:O	13:M:110:ARG:NH1	2.46	0.47
1:A:694:A:H5'	11:K:53:SER:HB3	1.96	0.47
1:A:979:C:H2'	1:A:979:C:O2	2.15	0.47
1:A:1437:C:H2'	1:A:1438:G:H8	1.80	0.47
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.39	0.47
17:Q:100:LYS:HE2	17:Q:100:LYS:HB3	1.82	0.47
1:A:376:G:O3'	16:P:5:ARG:NH1	2.40	0.46
1:A:429:U:H3'	4:D:9:CYS:SG	2.55	0.46
1:A:600:C:OP1	8:H:97:VAL:HG22	2.15	0.46
1:A:436:C:H2'	1:A:437:U:C6	2.50	0.46
1:A:673:G:H2'	1:A:674:G:H8	1.79	0.46
1:A:969:A:H4'	10:J:55:LYS:HE3	1.98	0.46
1:A:1150:U:H4'	10:J:41:PRO:HB3	1.96	0.46
1:A:1443:G:N3	1:A:1443:G:H2'	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1496:C:H2'	1:A:1497:G:O4'	2.16	0.46
1:A:112:G:H5'	1:A:389:A:O2'	2.16	0.46
1:A:877:C:H2'	1:A:878:G:H8	1.80	0.46
3:C:84:ILE:HG23	3:C:85:ARG:HD3	1.97	0.46
1:A:137:C:H2'	1:A:138:G:H8	1.80	0.46
1:A:642:A:N3	8:H:113:SER:OG	2.46	0.46
1:A:1281:U:H5'	1:A:1282:C:C5	2.49	0.46
1:A:1414:U:H2'	1:A:1415:G:C8	2.50	0.46
1:A:1531:A:H2'	1:A:1532:U:C6	2.51	0.46
3:C:124:ILE:HD13	3:C:130:VAL:HB	1.97	0.46
1:A:119:A:H4'	1:A:120:A:C8	2.50	0.46
1:A:537:G:OP1	12:L:113:ARG:NH2	2.47	0.46
1:A:713:G:H2'	1:A:714:G:C8	2.51	0.46
1:A:794:A:H2'	1:A:795:C:C6	2.50	0.46
1:A:337:C:H2'	1:A:338:A:C8	2.51	0.46
1:A:911:U:H2'	1:A:912:C:C6	2.50	0.46
1:A:1141:C:H2'	1:A:1142:G:H8	1.81	0.46
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.46
1:A:1488:G:O2'	1:A:1489:G:H5'	2.14	0.46
7:G:15:ASP:HB3	7:G:19:GLY:H	1.79	0.46
1:A:35:G:O2'	12:L:118:SER:O	2.28	0.46
1:A:397:A:H5'	1:A:398:C:OP1	2.15	0.46
1:A:411:A:OP1	4:D:30:LYS:NZ	2.43	0.46
1:A:882:C:O2'	1:A:883:C:H5'	2.16	0.46
1:A:955:U:H2'	1:A:956:U:C6	2.50	0.46
1:A:1043:C:H2'	1:A:1044:A:H8	1.81	0.46
4:D:81:GLU:OE1	4:D:139:ARG:NH2	2.45	0.46
17:Q:29:HIS:HB3	17:Q:33:GLY:H	1.81	0.46
20:T:33:ILE:HD12	20:T:63:ILE:HG13	1.97	0.46
1:A:1386:G:H2'	1:A:1387:G:H8	1.80	0.46
5:E:144:THR:HG23	5:E:147:ASP:H	1.80	0.46
1:A:296:U:H2'	1:A:297:G:C8	2.51	0.46
16:P:19:ILE:HG13	16:P:36:ILE:HG13	1.97	0.46
1:A:190(L):U:H2'	1:A:191:G:H8	1.80	0.46
1:A:1212:U:O2'	1:A:1213:A:O4'	2.30	0.46
3:C:84:ILE:O	3:C:88:ARG:HB2	2.15	0.46
10:J:17:ASP:OD2	10:J:70:ARG:NH1	2.49	0.46
20:T:71:THR:OG1	20:T:72:LEU:N	2.48	0.46
1:A:1137:C:H4'	1:A:1138:G:N2	2.30	0.45
2:B:188:ALA:O	2:B:203:GLY:N	2.48	0.45
2:B:223:ILE:HA	2:B:226:ARG:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.98	0.45
2:B:184:VAL:HG23	2:B:198:ASP:H	1.80	0.45
5:E:94:ALA:HB2	5:E:119:LEU:HG	1.98	0.45
1:A:293:G:C6	1:A:305:G:N1	2.84	0.45
1:A:509:A:H4'	1:A:510:A:OP1	2.17	0.45
1:A:598:U:H4'	8:H:94:TYR:CD2	2.52	0.45
1:A:973:G:OP1	10:J:57:LYS:NZ	2.32	0.45
1:A:1028:C:H2'	1:A:1029:C:C6	2.51	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.45
1:A:1409:C:H2'	1:A:1410:G:C8	2.52	0.45
2:B:163:PHE:HA	2:B:185:ILE:O	2.17	0.45
20:T:57:ARG:NE	20:T:102:GLY:O	2.41	0.45
9:I:10:ARG:NH1	9:I:105:ASP:OD1	2.49	0.45
19:S:29:ARG:HA	19:S:29:ARG:HD3	1.79	0.45
1:A:702:A:H3'	1:A:703:G:C5'	2.47	0.45
1:A:956:U:H3	1:A:960:U:H3	1.64	0.45
1:A:1010:G:H2'	1:A:1011:G:C8	2.47	0.45
1:A:1494:G:H5'	22:Y:47:PRO:HG2	1.98	0.45
2:B:60:ASP:HB3	2:B:64:ARG:HE	1.80	0.45
12:L:102:ARG:NH2	12:L:109:GLY:O	2.38	0.45
15:O:29:VAL:HG23	15:O:63:ARG:HG3	1.99	0.45
20:T:74:LYS:O	20:T:76:ALA:N	2.49	0.45
1:A:235:C:H2'	1:A:236:G:H8	1.81	0.45
1:A:621:A:H2'	1:A:622:A:H8	1.81	0.45
7:G:16:LEU:HD21	9:I:45:ALA:HB2	1.99	0.45
15:O:29:VAL:HG11	15:O:81:LEU:HD21	1.98	0.45
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.41	0.45
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.98	0.45
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.81	0.45
14:N:3:ARG:NH1	14:N:28:GLY:O	2.50	0.45
1:A:299:G:O5'	1:A:299:G:H8	1.99	0.45
1:A:410:G:OP1	4:D:30:LYS:NZ	2.37	0.45
1:A:728:A:H2'	1:A:729:A:H8	1.81	0.45
1:A:985:C:H2'	1:A:986:A:C8	2.51	0.45
4:D:162:LEU:HD12	4:D:178:VAL:HG23	1.98	0.45
4:D:194:LEU:HG	4:D:196:LEU:HD23	1.99	0.45
1:A:971:G:C8	1:A:1365:G:H4'	2.52	0.45
1:A:1237:C:O2'	1:A:1300:G:N2	2.39	0.45
1:A:1338:G:H2'	1:A:1339:A:C8	2.52	0.45
1:A:1407:C:H2'	1:A:1408:A:H8	1.81	0.45
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:50:GLU:HB2	20:T:99:LEU:HD13	1.98	0.45
1:A:76:C:H6	1:A:76:C:C5'	2.29	0.45
1:A:362:G:N2	1:A:365:U:OP2	2.50	0.45
1:A:954:G:H2'	1:A:955:U:C6	2.52	0.45
1:A:1101:A:C8	2:B:172:ILE:HD11	2.52	0.45
5:E:142:LEU:O	5:E:143:ARG:NH1	2.44	0.45
1:A:17:U:H2'	1:A:18:C:C6	2.52	0.44
1:A:129(A):G:N3	1:A:190(E):U:H5"	2.32	0.44
1:A:519:C:O3'	22:Y:42:LYS:NZ	2.49	0.44
1:A:968:A:C8	1:A:1062:U:H4'	2.52	0.44
1:A:1030(A):G:C2	1:A:1030(C):G:H5"	2.51	0.44
3:C:174:PRO:O	3:C:177:THR:OG1	2.35	0.44
22:Z:22:ARG:HA	22:Z:25:LYS:HD2	2.00	0.44
22:Z:24:VAL:HA	22:Z:27:ILE:HD12	1.99	0.44
8:H:34:GLU:OE1	8:H:37:ARG:NH1	2.51	0.44
4:D:30:LYS:HG2	4:D:35:ARG:HH21	1.82	0.44
14:N:24:CYS:HB3	14:N:29:ARG:N	2.32	0.44
22:Y:4:ILE:HB	22:Y:76:LEU:HA	1.99	0.44
1:A:22:G:H2'	1:A:23:C:C6	2.52	0.44
1:A:476:G:C3'	1:A:477:G:H8	2.31	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	1.99	0.44
1:A:1085:U:C2	1:A:1094:G:O6	2.70	0.44
1:A:1315:U:H2'	1:A:1316:G:O4'	2.18	0.44
1:A:1422:G:H1	1:A:1478:C:H42	1.64	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.44
1:A:216:G:H2'	1:A:217:C:C6	2.53	0.44
1:A:1482:G:O5'	1:A:1482:G:H8	2.00	0.44
2:B:178:ARG:NH2	2:B:196:LEU:O	2.51	0.44
5:E:11:ILE:HB	5:E:31:LEU:HD23	1.98	0.44
8:H:3:THR:OG1	8:H:4:ASP:N	2.50	0.44
8:H:33:GLU:HG2	8:H:59:LEU:HD21	1.99	0.44
1:A:21:G:H21	1:A:914:A:H62	1.65	0.44
1:A:1295:G:O2'	13:M:14:ARG:NH1	2.45	0.44
3:C:157:ILE:HD12	3:C:164:ARG:HG3	1.99	0.44
9:I:25:LYS:N	9:I:60:ASP:OD1	2.44	0.44
10:J:64:GLU:HB3	14:N:59:ALA:HB2	1.98	0.44
1:A:653:A:P	8:H:56:LYS:HZ1	2.41	0.44
2:B:189:ASP:OD1	2:B:189:ASP:N	2.51	0.44
2:B:195:ASP:O	8:H:68:ARG:NH2	2.43	0.44
3:C:156:ARG:NE	3:C:160:ALA:O	2.46	0.44
18:R:67:ALA:O	18:R:71:LYS:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:5:TRP:HB2	22:Z:3:LEU:HB3	1.99	0.44
22:Y:60:ILE:HG22	22:Y:61:THR:HG23	1.99	0.44
1:A:454:C:H2'	1:A:455:C:H5'	2.00	0.44
1:A:1376:U:H2'	1:A:1377:A:C8	2.53	0.44
1:A:1437:C:H2'	1:A:1438:G:C8	2.53	0.44
7:G:69:VAL:HG13	7:G:100:ALA:HB1	1.99	0.44
14:N:23:ARG:NH1	14:N:28:GLY:O	2.51	0.44
1:A:176:C:OP1	20:T:29:LYS:NZ	2.35	0.44
1:A:186:C:H5'	20:T:78:ALA:HB1	2.00	0.44
1:A:1340:A:H2'	1:A:1341:U:O4'	2.18	0.44
2:B:71:VAL:HA	2:B:93:VAL:HG23	1.99	0.44
1:A:188:C:H2'	1:A:189:G:C8	2.53	0.43
1:A:736:C:H2'	1:A:737:A:H8	1.82	0.43
1:A:957:U:P	19:S:81:ARG:HH21	2.41	0.43
1:A:1335:C:C5'	1:A:1336:C:H5'	2.48	0.43
1:A:701:C:H4'	1:A:702:A:C5'	2.48	0.43
1:A:1300:G:HO2'	1:A:1301:U:P	2.40	0.43
1:A:538:G:OP2	12:L:115:LYS:HE2	2.18	0.43
1:A:781:A:C8	1:A:802:A:N1	2.86	0.43
1:A:1522:U:H2'	1:A:1523:G:C8	2.53	0.43
7:G:20:ASP:HB3	7:G:23:VAL:HG12	2.00	0.43
8:H:69:ARG:NH2	8:H:75:ARG:O	2.52	0.43
1:A:266:G:H5"	1:A:268:C:H41	1.84	0.43
1:A:910:C:P	12:L:97:ARG:HH22	2.41	0.43
1:A:959:A:C2	1:A:1221:G:N2	2.86	0.43
1:A:1493:A:H1'	22:Y:49:LYS:HE2	2.01	0.43
1:A:1504:G:H4'	1:A:1505:G:H5'	2.00	0.43
13:M:3:ARG:HA	13:M:9:ILE:HG12	1.99	0.43
17:Q:66:SER:HB3	17:Q:69:LYS:HE3	2.01	0.43
1:A:476:G:O2'	1:A:477:G:O4'	2.32	0.43
1:A:674:G:H2'	1:A:675:A:C8	2.47	0.43
1:A:922:G:H2'	1:A:923:A:C8	2.53	0.43
22:Y:25:LYS:O	22:Y:25:LYS:NZ	2.38	0.43
22:Z:12:ASP:HB2	22:Z:81:ARG:HB3	2.00	0.43
1:A:532:A:H62	3:C:193:TYR:HB3	1.83	0.43
1:A:1380:U:H1'	1:A:1381:U:OP2	2.18	0.43
6:F:82:ARG:HG3	6:F:84:ASN:H	1.84	0.43
1:A:108:G:H5'	1:A:109:A:H5"	2.00	0.43
1:A:272:C:H2'	1:A:273:A:C8	2.53	0.43
1:A:390:C:H4'	16:P:28:ARG:HH21	1.84	0.43
1:A:629:G:H2'	1:A:630:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:G:O2'	8:H:12:ARG:NH2	2.51	0.43
1:A:932:C:H5'	7:G:4:ARG:HE	1.83	0.43
1:A:1343:G:H2'	1:A:1344:C:C6	2.54	0.43
3:C:191:THR:OG1	3:C:194:GLY:N	2.52	0.43
20:T:29:LYS:O	20:T:33:ILE:HG12	2.18	0.43
22:Z:22:ARG:O	22:Z:26:LYS:HG2	2.19	0.43
1:A:321:A:O2'	1:A:322:C:H5'	2.19	0.43
1:A:616:G:OP2	4:D:141:ARG:NH2	2.52	0.43
1:A:1118:C:O3'	9:I:83:ARG:NH2	2.39	0.43
1:A:1442:G:H2'	1:A:1442:G:O5'	2.19	0.43
1:A:1491:G:H4'	1:A:1491:G:OP1	2.18	0.43
1:A:1510:U:H2'	1:A:1511:G:H8	1.83	0.43
8:H:121:ASP:N	8:H:121:ASP:OD1	2.52	0.43
1:A:521:G:OP2	12:L:54:LYS:NZ	2.48	0.43
1:A:745:C:H2'	1:A:746:A:C8	2.54	0.43
1:A:978:A:C5	1:A:1319:A:C2	3.06	0.43
9:I:45:ALA:HA	9:I:48:GLU:HG2	2.01	0.43
22:Y:33:ASP:OD1	22:Y:42:LYS:N	2.49	0.43
22:Z:57:SER:OG	22:Z:65:ARG:NE	2.44	0.43
1:A:737:A:H2'	1:A:738:C:C6	2.54	0.43
1:A:1264:C:H2'	1:A:1265:G:H8	1.83	0.43
1:A:1435:G:H2'	1:A:1436:U:H6	1.83	0.43
22:Y:72:ASP:OD1	22:Y:72:ASP:N	2.52	0.43
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.42
16:P:57:ARG:NE	16:P:79:VAL:O	2.45	0.42
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.19	0.42
1:A:562:C:O2	12:L:16:GLU:N	2.51	0.42
1:A:985:C:C2	1:A:1221:G:N2	2.87	0.42
1:A:1122:U:O4	1:A:1123:A:N6	2.51	0.42
1:A:1481:U:H2'	1:A:1482:G:O4'	2.19	0.42
1:A:880:C:OP1	12:L:12:ARG:NH1	2.50	0.42
3:C:53:ALA:HB2	3:C:115:LEU:HD21	2.02	0.42
15:O:3:ILE:HD11	15:O:38:ARG:HG3	2.01	0.42
1:A:382:A:H2'	1:A:383:A:C8	2.54	0.42
1:A:745:C:H2'	1:A:746:A:H8	1.84	0.42
1:A:861:G:O6	1:A:869:G:N2	2.52	0.42
1:A:1101:A:N6	2:B:176:GLU:OE2	2.51	0.42
1:A:1221:G:O3'	19:S:77:THR:HG21	2.18	0.42
1:A:1500:A:H5"	1:A:1508:G:H5"	2.00	0.42
6:F:5:GLU:HA	6:F:63:TYR:O	2.19	0.42
9:I:49:PRO:HG2	9:I:81:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:C:H2'	1:A:1097:C:C6	2.55	0.42
1:A:1312:G:H5'	19:S:5:LEU:HD11	2.00	0.42
1:A:1392:G:H2'	1:A:1393:U:C6	2.55	0.42
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.02	0.42
1:A:542:G:H5'	4:D:41:GLY:CA	2.49	0.42
1:A:684:A:O2'	11:K:39:PRO:O	2.28	0.42
1:A:711:G:H2'	1:A:712:A:H8	1.85	0.42
1:A:1016:A:H2'	1:A:1017:G:O4'	2.19	0.42
1:A:1172:C:H2'	1:A:1173:G:C8	2.55	0.42
1:A:1447:G:O5'	1:A:1447:G:H8	2.03	0.42
1:A:1502:A:H2	1:A:1505:G:H22	1.68	0.42
1:A:1507:A:H2'	1:A:1508:G:C8	2.54	0.42
2:B:116:GLU:HA	2:B:119:GLU:HB2	2.02	0.42
13:M:12:ASN:HA	13:M:46:LYS:HG3	2.01	0.42
1:A:14:U:N3	1:A:17:U:OP2	2.53	0.42
1:A:150:C:N4	1:A:171:A:H62	2.12	0.42
1:A:553:A:H2'	1:A:554:C:C6	2.55	0.42
1:A:737:A:H2'	1:A:738:C:H6	1.84	0.42
1:A:1393:U:O2'	1:A:1501:C:O2'	2.33	0.42
15:O:29:VAL:O	15:O:33:THR:OG1	2.29	0.42
20:T:89:ARG:HA	20:T:89:ARG:HD2	1.84	0.42
22:Y:23:ILE:O	22:Y:27:ILE:HG12	2.19	0.42
1:A:987:G:H2'	1:A:988:G:H8	1.84	0.42
1:A:1043:C:H2'	1:A:1044:A:C8	2.54	0.42
1:A:1255:G:O2'	1:A:1258:G:N3	2.41	0.42
22:Y:27:ILE:O	22:Y:31:ILE:HG12	2.18	0.42
1:A:403:C:H4'	4:D:122:ARG:NH1	2.35	0.42
1:A:613:C:H2'	1:A:614:A:H8	1.85	0.42
1:A:728:A:H2'	1:A:729:A:C8	2.55	0.42
1:A:982:U:H5"	14:N:6:LEU:HD21	2.02	0.42
1:A:1425:U:H2'	1:A:1426:C:C6	2.54	0.42
1:A:381:C:H2'	1:A:382:A:O4'	2.20	0.42
1:A:486:U:H2'	1:A:487:A:H8	1.85	0.42
1:A:836:G:OP1	18:R:61:LYS:NZ	2.35	0.42
1:A:1226:C:P	13:M:91:ARG:HH12	2.43	0.42
1:A:1320:C:N3	19:S:72:GLY:HA3	2.35	0.42
3:C:185:GLY:O	3:C:199:LYS:HA	2.20	0.42
14:N:37:PHE:HB3	14:N:39:LEU:HD12	2.01	0.42
1:A:188:C:H4'	20:T:89:ARG:NH1	2.34	0.41
1:A:280:C:N3	17:Q:39:SER:OG	2.44	0.41
1:A:476:G:C3'	1:A:477:G:C8	3.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:G:N2	1:A:813:U:OP2	2.53	0.41
1:A:1101:A:N7	2:B:172:ILE:HD11	2.35	0.41
1:A:1111:A:N1	3:C:177:THR:HG22	2.34	0.41
6:F:35:ALA:HB1	6:F:65:VAL:HG21	2.01	0.41
13:M:47:ASP:OD1	13:M:47:ASP:N	2.53	0.41
1:A:533:A:C5	1:A:536:C:C4	3.08	0.41
1:A:1080:A:H5'	5:E:14:ARG:NH2	2.35	0.41
1:A:1347:G:N2	1:A:1373:G:H2'	2.34	0.41
1:A:1354:C:H2'	1:A:1355:G:H8	1.85	0.41
1:A:757:U:H2'	1:A:758:G:O4'	2.20	0.41
1:A:1145:C:H1'	1:A:1146:A:N7	2.36	0.41
1:A:1499:A:H2'	1:A:1500:A:C8	2.55	0.41
1:A:229:U:H2'	1:A:230:G:C8	2.55	0.41
1:A:582:U:H2'	1:A:583:A:H8	1.85	0.41
1:A:621:A:H2'	1:A:622:A:C8	2.55	0.41
1:A:927:G:N2	1:A:1390:U:O2	2.42	0.41
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.86	0.41
13:M:59:TYR:O	13:M:63:THR:OG1	2.26	0.41
20:T:14:LYS:HA	20:T:17:ARG:HG2	2.02	0.41
1:A:5:U:O2'	1:A:6:G:OP2	2.33	0.41
1:A:657:G:H21	15:O:22:THR:HG23	1.86	0.41
1:A:1347:G:H1'	1:A:1348:U:OP2	2.20	0.41
10:J:59:SER:OG	10:J:60:ARG:N	2.51	0.41
15:O:29:VAL:HG21	15:O:67:LEU:HD21	2.01	0.41
20:T:75:ASN:OD1	20:T:75:ASN:N	2.50	0.41
1:A:580:U:O4	1:A:761:G:O6	2.38	0.41
1:A:1167:A:H8	1:A:1167:A:P	2.43	0.41
1:A:532:A:N3	1:A:532:A:H2'	2.35	0.41
1:A:1264:C:H2'	1:A:1265:G:C8	2.56	0.41
6:F:36:ARG:NH2	6:F:66:GLU:OE1	2.52	0.41
22:Y:33:ASP:O	22:Y:37:THR:N	2.47	0.41
1:A:411:A:H2'	1:A:413:G:C8	2.56	0.41
1:A:875:C:O2'	8:H:14:ARG:NH1	2.52	0.41
1:A:978:A:OP2	1:A:1362:C:N4	2.50	0.41
1:A:1130:A:O5'	9:I:20:ARG:NH2	2.54	0.41
1:A:1135:U:H4'	1:A:1136:U:H5	1.86	0.41
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.36	0.41
1:A:1347:G:H3'	9:I:108:VAL:O	2.21	0.41
1:A:1409:C:H2'	1:A:1410:G:H8	1.85	0.41
1:A:1504:G:OP2	1:A:1507:A:H4'	2.20	0.41
8:H:33:GLU:OE1	8:H:50:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:P	4:D:73:ARG:HH21	2.44	0.41
1:A:537:G:O3'	12:L:113:ARG:NH1	2.54	0.41
1:A:551:U:H2'	1:A:552:U:C6	2.55	0.41
1:A:910:C:OP1	12:L:97:ARG:NH1	2.42	0.41
1:A:1168:A:H2'	1:A:1169:A:C8	2.56	0.41
1:A:1357:A:H61	1:A:1365:G:H1	1.68	0.41
2:B:129:GLU:HG3	2:B:130:ARG:HD2	2.03	0.41
2:B:178:ARG:HD3	2:B:178:ARG:HA	1.68	0.41
3:C:58:GLU:HG2	10:J:92:THR:HG21	2.03	0.41
6:F:24:GLU:HG2	6:F:28:ARG:HE	1.86	0.41
10:J:75:ILE:HG22	10:J:76:ASN:H	1.86	0.41
13:M:11:ARG:HG2	13:M:12:ASN:H	1.86	0.41
17:Q:65:ILE:HB	17:Q:69:LYS:HD2	2.03	0.41
1:A:390:C:H2'	1:A:391:G:H8	1.85	0.41
1:A:1279:A:H5"	1:A:1280:A:OP1	2.21	0.41
1:A:1316:G:N2	1:A:1319:A:OP2	2.53	0.41
2:B:90:MET:HA	2:B:91:PRO:HD3	1.96	0.41
10:J:50:ILE:HD12	10:J:50:ILE:H	1.86	0.41
1:A:538:G:OP1	12:L:115:LYS:HB2	2.22	0.40
1:A:926:G:H3'	1:A:1505:G:N2	2.36	0.40
1:A:939:G:H2'	1:A:940:C:C6	2.57	0.40
1:A:992:U:O2'	1:A:993:G:OP2	2.28	0.40
1:A:1373:G:H5"	7:G:36:LYS:HE3	2.01	0.40
1:A:1392:G:O2'	1:A:1502:A:H5"	2.20	0.40
15:O:74:ASP:HB3	15:O:77:ARG:HD3	2.03	0.40
19:S:39:THR:HG22	19:S:70:LYS:HE2	2.03	0.40
22:Z:51:ASN:HB3	22:Z:52:LEU:HD12	2.03	0.40
1:A:17:U:H2'	1:A:18:C:H6	1.85	0.40
1:A:574:A:N3	1:A:883:C:H1'	2.36	0.40
1:A:580:U:H2'	1:A:581:G:O4'	2.22	0.40
1:A:757:U:H1'	1:A:879:C:H1'	2.02	0.40
1:A:1000:U:H2'	1:A:1001:A:C8	2.56	0.40
1:A:1320:C:H42	19:S:36:ARG:HE	1.68	0.40
1:A:1420:C:H2'	1:A:1421:G:H8	1.85	0.40
9:I:99:LEU:HB3	9:I:101:PHE:CD2	2.56	0.40
17:Q:45:HIS:H	17:Q:72:ARG:HA	1.86	0.40
1:A:246:A:N6	1:A:281:G:N2	2.43	0.40
1:A:688:G:H5'	11:K:46:GLY:HA3	2.03	0.40
1:A:988:G:N1	1:A:1218:C:N3	2.70	0.40
10:J:45:ARG:HE	10:J:45:ARG:HB3	1.72	0.40
20:T:39:LYS:HD3	20:T:39:LYS:HA	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:42:LYS:O	22:Y:58:ARG:NH1	2.55	0.40
1:A:398:C:H2'	1:A:399:G:C8	2.55	0.40
1:A:475:G:H2'	1:A:476:G:C8	2.56	0.40
1:A:757:U:OP1	1:A:822:C:O2'	2.37	0.40
1:A:832:C:N4	1:A:855:G:O6	2.54	0.40
4:D:23:GLY:HA3	4:D:112:VAL:HG22	2.03	0.40
4:D:108:LEU:HD22	4:D:174:LEU:HD13	2.02	0.40
8:H:105:ARG:HA	8:H:105:ARG:HD2	1.93	0.40
9:I:9:ARG:HG2	9:I:14:VAL:HG12	2.03	0.40
10:J:51:ARG:O	14:N:45:ARG:NH1	2.54	0.40
1:A:35:G:OP1	12:L:104:VAL:HG11	2.22	0.40
1:A:714:G:H2'	1:A:715:A:C8	2.56	0.40
1:A:865:A:H2'	1:A:866:C:C6	2.56	0.40
1:A:1287:A:N3	1:A:1353:G:O2'	2.45	0.40
3:C:67:THR:HG22	3:C:102:ASN:HB2	2.02	0.40
4:D:180:GLY:O	4:D:182:LYS:NZ	2.54	0.40
6:F:22:GLU:O	6:F:26:ILE:HG12	2.21	0.40
12:L:8:ASN:CB	17:Q:34:LYS:HZ2	2.35	0.40
17:Q:26:GLN:HG2	17:Q:37:LYS:HB3	2.03	0.40
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	2.03	0.40

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:U:N3	1:A:1542:U:O4[3_545]	1.57	0.63
1:A:84:U:O2	1:A:1542:U:N3[3_545]	1.62	0.58
1:A:703:G:N1	1:A:1452:C:C4[4_554]	1.64	0.56
1:A:703:G:N1	1:A:1452:C:C5[4_554]	1.67	0.53
1:A:703:G:C6	1:A:1452:C:N3[4_554]	1.75	0.45
1:A:703:G:O6	1:A:1452:C:C2[4_554]	1.75	0.45
1:A:703:G:C2	1:A:1452:C:C5[4_554]	1.82	0.38
1:A:92:C:O2	1:A:1338:G:N2[3_545]	1.85	0.35
1:A:703:G:N2	1:A:1452:C:C5[4_554]	1.87	0.33
1:A:701:C:C6	1:A:1452:C:C4[4_554]	1.90	0.30
1:A:701:C:N1	1:A:1452:C:N3[4_554]	1.95	0.25
1:A:703:G:C2	1:A:1452:C:C4[4_554]	1.97	0.23
1:A:703:G:O6	1:A:1452:C:N3[4_554]	1.99	0.21
1:A:701:C:C5	1:A:1452:C:C5[4_554]	2.01	0.19
1:A:703:G:O6	1:A:1452:C:O2[4_554]	2.02	0.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLY:O	2:B:157:ARG:CD[7_555]	2.03	0.17
1:A:701:C:N1	1:A:1452:C:C4[4_554]	2.05	0.15
1:A:703:G:N3	1:A:1452:C:N4[4_554]	2.06	0.14
1:A:703:G:C6	1:A:1452:C:C4[4_554]	2.07	0.13
1:A:701:C:C6	1:A:1452:C:N4[4_554]	2.12	0.08
1:A:703:G:N1	1:A:1452:C:C6[4_554]	2.12	0.08
1:A:703:G:N1	1:A:1452:C:N3[4_554]	2.12	0.08
10:J:79:ARG:CD	10:J:79:ARG:CD[8_665]	2.14	0.06
1:A:701:C:C2	1:A:1452:C:C2[4_554]	2.16	0.04
1:A:703:G:C4	1:A:1452:C:N4[4_554]	2.17	0.03
1:A:703:G:C2	1:A:1452:C:N4[4_554]	2.18	0.02
1:A:88:A:C5	1:A:1542:U:O4[3_545]	2.19	0.01

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	234/256 (91%)	204 (87%)	30 (13%)	0	100	100
3	C	203/239 (85%)	176 (87%)	26 (13%)	1 (0%)	29	65
4	D	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	65
5	E	149/162 (92%)	143 (96%)	6 (4%)	0	100	100
6	F	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	H	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
9	I	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	J	94/105 (90%)	75 (80%)	15 (16%)	4 (4%)	2	25
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	L	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	56
13	M	114/126 (90%)	102 (90%)	11 (10%)	1 (1%)	17	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	43
15	O	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	P	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	R	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	S	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
20	T	97/106 (92%)	85 (88%)	9 (9%)	3 (3%)	4	33
21	U	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
22	Y	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
22	Z	82/84 (98%)	76 (93%)	4 (5%)	2 (2%)	6	37
All	All	2501/2706 (92%)	2281 (91%)	206 (8%)	14 (1%)	25	61

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
20	T	74	LYS
20	T	75	ASN
3	C	12	LEU
10	J	56	HIS
12	L	105	TYR
14	N	17	LYS
22	Z	50	HIS
22	Z	82	TYR
10	J	54	PHE
20	T	73	HIS
4	D	155	LEU
13	M	14	ARG
10	J	40	LEU

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	204/220 (93%)	198 (97%)	6 (3%)	42	66
3	C	159/188 (85%)	159 (100%)	0	100	100
4	D	180/181 (99%)	174 (97%)	6 (3%)	38	64
5	E	116/123 (94%)	115 (99%)	1 (1%)	78	88
6	F	90/90 (100%)	90 (100%)	0	100	100
7	G	126/127 (99%)	125 (99%)	1 (1%)	81	89
8	H	118/119 (99%)	118 (100%)	0	100	100
9	I	97/99 (98%)	96 (99%)	1 (1%)	76	86
10	J	86/92 (94%)	85 (99%)	1 (1%)	71	84
11	K	88/99 (89%)	85 (97%)	3 (3%)	37	64
12	L	103/109 (94%)	102 (99%)	1 (1%)	76	86
13	M	94/101 (93%)	91 (97%)	3 (3%)	39	64
14	N	49/50 (98%)	49 (100%)	0	100	100
15	O	79/80 (99%)	78 (99%)	1 (1%)	69	82
16	P	72/74 (97%)	71 (99%)	1 (1%)	67	82
17	Q	95/97 (98%)	93 (98%)	2 (2%)	53	74
18	R	61/77 (79%)	61 (100%)	0	100	100
19	S	73/80 (91%)	72 (99%)	1 (1%)	67	82
20	T	76/82 (93%)	75 (99%)	1 (1%)	69	82
21	U	20/22 (91%)	19 (95%)	1 (5%)	24	55
22	Y	78/78 (100%)	77 (99%)	1 (1%)	69	82
22	Z	78/78 (100%)	75 (96%)	3 (4%)	33	61
All	All	2142/2266 (94%)	2108 (98%)	34 (2%)	62	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	74	LYS
2	B	93	VAL
2	B	115	LEU
2	B	168	THR
2	B	169	LYS
2	B	185	ILE
4	D	19	LEU
4	D	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	22	LYS
4	D	33	MET
4	D	88	VAL
4	D	154	ASN
5	E	31	LEU
7	G	63	LYS
9	I	64	THR
10	J	79	ARG
11	K	96	ARG
11	K	108	ILE
11	K	124	LYS
12	L	21	LYS
13	M	61	GLU
13	M	77	ASN
13	M	117	VAL
15	O	10	LYS
16	P	21	VAL
17	Q	31	LEU
17	Q	56	VAL
19	S	41	VAL
20	T	34	LYS
21	U	24	ARG
22	Y	32	LYS
22	Z	22	ARG
22	Z	35	ARG
22	Z	44	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
13	M	77	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1523 (99%)	279 (18%)	47 (3%)

All (279) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	54	C
1	A	63	C
1	A	76	C
1	A	77	G
1	A	81	U
1	A	101	A
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	190(E)	U
1	A	190(F)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	C
1	A	279	A
1	A	281	G
1	A	282	A
1	A	289	G
1	A	298	A
1	A	301	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	373	A
1	A	382	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	423	G
1	A	424	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	476	G
1	A	478	A
1	A	481	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	485	G
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	588	G
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	787	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	941	G
1	A	960	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	979	C
1	A	980	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	995	C
1	A	998	G
1	A	1004	A
1	A	1005	A
1	A	1006	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1010	G
1	A	1023	G
1	A	1024	G
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1045	C
1	A	1049	U
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1183	A
1	A	1196	U
1	A	1197	G
1	A	1200	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1236	A
1	A	1240	U
1	A	1241	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1298	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1364	U
1	A	1365	G
1	A	1368	G
1	A	1370	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1381	U
1	A	1398	A
1	A	1441	G
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1485	U
1	A	1489	G
1	A	1491	G
1	A	1493	A
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	281	G
1	A	372	C
1	A	413	G
1	A	428	G
1	A	484	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	496	A
1	A	509	A
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	819	A
1	A	913	A
1	A	965	A
1	A	991	U
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1101	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1441	G
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1498	U
1	A	1504	G
1	A	1505	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	1541	1	18,21,22	1.23	1 (5%)	22,30,33	1.71	4 (18%)
1	PSU	A	1540	1	18,21,22	1.12	1 (5%)	22,30,33	1.75	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1541	PSU	C6-C5	4.19	1.40	1.35
1	A	1540	PSU	C6-C5	3.63	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	C4-N3-C2	-4.52	119.83	126.34
1	A	1541	PSU	C4-N3-C2	-4.46	119.91	126.34
1	A	1540	PSU	N1-C2-N3	4.33	120.04	115.13
1	A	1541	PSU	N1-C2-N3	4.27	119.97	115.13
1	A	1540	PSU	O2-C2-N1	-2.58	119.95	122.79
1	A	1541	PSU	O2-C2-N1	-2.57	119.97	122.79
1	A	1541	PSU	C6-N1-C2	-2.33	120.31	122.68
1	A	1540	PSU	C6-N1-C2	-2.08	120.55	122.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1541	PSU	C2'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 186 ligands modelled in this entry, 185 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	SF4	D	301	4	0,12,12	-	-	-		

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
24	SF4	D	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	301	SF4	7	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1511/1523 (99%)	-0.45	5 (0%)	94	93	90, 147, 260, 421	0
2	B	236/256 (92%)	-0.25	2 (0%)	86	83	118, 180, 289, 354	0
3	C	205/239 (85%)	-0.30	3 (1%)	73	68	151, 217, 273, 325	0
4	D	208/209 (99%)	-0.24	0	100	100	117, 162, 211, 236	0
5	E	151/162 (93%)	-0.20	0	100	100	99, 137, 180, 240	0
6	F	100/101 (99%)	-0.50	0	100	100	133, 182, 222, 246	0
7	G	155/156 (99%)	-0.37	0	100	100	142, 199, 246, 274	0
8	H	137/138 (99%)	-0.31	0	100	100	87, 124, 161, 190	0
9	I	126/128 (98%)	0.24	2 (1%)	72	66	139, 212, 286, 326	0
10	J	96/105 (91%)	0.47	5 (5%)	27	24	165, 256, 318, 339	0
11	K	116/129 (89%)	-0.32	0	100	100	117, 159, 224, 272	0
12	L	122/132 (92%)	0.08	2 (1%)	72	66	100, 155, 209, 293	0
13	M	116/126 (92%)	0.12	4 (3%)	45	38	159, 191, 243, 346	0
14	N	60/61 (98%)	0.14	1 (1%)	70	64	180, 207, 257, 273	0
15	O	87/89 (97%)	-0.30	0	100	100	99, 144, 189, 201	0
16	P	84/88 (95%)	0.26	3 (3%)	42	36	117, 150, 191, 239	0
17	Q	100/105 (95%)	0.05	1 (1%)	82	78	107, 136, 182, 230	0
18	R	70/88 (79%)	-0.36	0	100	100	118, 156, 207, 220	0
19	S	84/93 (90%)	0.01	2 (2%)	59	52	173, 225, 264, 279	0
20	T	99/106 (93%)	0.03	0	100	100	121, 164, 241, 269	0
21	U	25/27 (92%)	1.01	5 (20%)	1	1	179, 222, 254, 262	0
22	Y	84/84 (100%)	0.67	11 (13%)	3	4	184, 252, 296, 327	0
22	Z	84/84 (100%)	0.62	8 (9%)	8	7	262, 313, 356, 402	0
All	All	4056/4229 (95%)	-0.21	54 (1%)	77	72	87, 166, 279, 421	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	15	ALA	4.9
1	A	1533	C	4.4
22	Y	84	TYR	4.1
22	Z	19	THR	4.0
13	M	43	THR	3.9
22	Y	20	ASP	3.9
22	Y	80	CYS	3.7
22	Y	16	TRP	3.6
21	U	18	TYR	3.6
1	A	1534	A	3.4
21	U	17	THR	3.2
22	Y	59	ARG	3.1
14	N	14	PRO	3.1
10	J	33	GLN	3.0
10	J	34	VAL	3.0
22	Y	50	HIS	3.0
22	Y	57	SER	2.8
22	Z	80	CYS	2.8
2	B	132	LYS	2.7
1	A	532	A	2.7
22	Z	18	GLU	2.6
9	I	16	ARG	2.6
3	C	196	LEU	2.6
22	Z	17	GLN	2.6
21	U	26	LYS	2.6
1	A	82	U	2.5
10	J	6	ILE	2.5
22	Z	28	ASN	2.5
22	Z	16	TRP	2.5
10	J	71	LEU	2.4
10	J	10	GLY	2.4
13	M	108	ARG	2.4
12	L	32	PHE	2.4
16	P	22	THR	2.3
17	Q	44	ALA	2.3
22	Z	20	ASP	2.3
1	A	1257	U	2.3
2	B	15	VAL	2.3
19	S	12	ASP	2.3
22	Y	79	ALA	2.3
21	U	5	ASP	2.3
3	C	193	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	Y	21	LYS	2.2
19	S	39	THR	2.1
22	Y	83	HIS	2.1
16	P	7	ALA	2.1
3	C	155	GLY	2.1
13	M	6	GLY	2.1
22	Y	82	TYR	2.1
16	P	8	ARG	2.0
22	Z	33	ASP	2.0
13	M	114	ARG	2.0
21	U	4	GLY	2.0
12	L	33	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.82	0.42	192,201,210,210	0
1	PSU	A	1540	20/21	0.88	0.49	260,288,300,318	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1717	1/1	-0.04	1.29	153,153,153,153	0
23	MG	A	1712	1/1	-0.03	0.35	157,157,157,157	0
23	MG	A	1665	1/1	0.04	1.16	129,129,129,129	0
23	MG	A	1618	1/1	0.06	1.18	169,169,169,169	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1615	1/1	0.12	1.28	164,164,164,164	0
23	MG	A	1731	1/1	0.17	0.50	124,124,124,124	0
23	MG	A	1604	1/1	0.23	1.12	145,145,145,145	0
23	MG	A	1779	1/1	0.25	0.89	160,160,160,160	0
23	MG	A	1620	1/1	0.30	0.86	168,168,168,168	0
23	MG	A	1622	1/1	0.36	1.07	133,133,133,133	0
23	MG	A	1736	1/1	0.36	0.36	179,179,179,179	0
23	MG	A	1757	1/1	0.36	0.23	105,105,105,105	0
23	MG	A	1719	1/1	0.36	1.01	173,173,173,173	0
23	MG	A	1758	1/1	0.37	0.95	146,146,146,146	0
23	MG	A	1627	1/1	0.38	0.40	196,196,196,196	0
23	MG	A	1699	1/1	0.38	0.42	163,163,163,163	0
23	MG	A	1724	1/1	0.43	0.71	100,100,100,100	0
23	MG	A	1626	1/1	0.44	1.07	83,83,83,83	0
23	MG	A	1681	1/1	0.48	0.57	100,100,100,100	0
23	MG	A	1696	1/1	0.50	0.65	157,157,157,157	0
23	MG	A	1738	1/1	0.54	0.46	100,100,100,100	0
23	MG	A	1679	1/1	0.55	0.77	156,156,156,156	0
23	MG	A	1613	1/1	0.55	0.70	137,137,137,137	0
23	MG	A	1734	1/1	0.56	0.63	107,107,107,107	0
23	MG	A	1614	1/1	0.56	0.30	84,84,84,84	0
23	MG	A	1677	1/1	0.57	0.82	180,180,180,180	0
23	MG	A	1762	1/1	0.59	0.36	144,144,144,144	0
23	MG	E	201	1/1	0.59	0.87	85,85,85,85	0
23	MG	A	1781	1/1	0.62	0.30	156,156,156,156	0
23	MG	A	1711	1/1	0.62	0.36	158,158,158,158	0
23	MG	A	1610	1/1	0.63	0.48	143,143,143,143	0
23	MG	A	1676	1/1	0.63	0.19	188,188,188,188	0
23	MG	A	1692	1/1	0.63	1.39	171,171,171,171	0
23	MG	A	1638	1/1	0.63	0.38	133,133,133,133	0
23	MG	A	1716	1/1	0.65	0.39	87,87,87,87	0
23	MG	A	1625	1/1	0.65	0.54	171,171,171,171	0
23	MG	A	1619	1/1	0.65	2.04	141,141,141,141	0
23	MG	A	1735	1/1	0.65	0.67	134,134,134,134	0
23	MG	A	1678	1/1	0.66	2.07	143,143,143,143	0
23	MG	A	1755	1/1	0.66	0.24	134,134,134,134	0
23	MG	A	1695	1/1	0.67	0.20	115,115,115,115	0
23	MG	A	1708	1/1	0.67	0.66	134,134,134,134	0
23	MG	A	1767	1/1	0.68	0.50	137,137,137,137	0
23	MG	A	1617	1/1	0.68	1.14	145,145,145,145	0
23	MG	A	1694	1/1	0.68	0.63	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1691	1/1	0.68	0.61	95,95,95,95	0
23	MG	A	1661	1/1	0.69	1.15	75,75,75,75	0
23	MG	A	1683	1/1	0.69	0.43	149,149,149,149	0
23	MG	A	1612	1/1	0.70	0.79	179,179,179,179	0
23	MG	A	1737	1/1	0.70	0.42	87,87,87,87	0
23	MG	A	1732	1/1	0.70	1.65	134,134,134,134	0
23	MG	A	1776	1/1	0.70	1.95	153,153,153,153	0
23	MG	A	1744	1/1	0.70	0.19	153,153,153,153	0
23	MG	A	1780	1/1	0.70	0.56	156,156,156,156	0
23	MG	A	1673	1/1	0.70	0.20	188,188,188,188	0
23	MG	A	1603	1/1	0.70	0.38	159,159,159,159	0
23	MG	B	301	1/1	0.72	0.12	150,150,150,150	0
23	MG	A	1698	1/1	0.72	0.43	95,95,95,95	0
23	MG	A	1649	1/1	0.73	0.84	116,116,116,116	0
23	MG	A	1689	1/1	0.73	0.61	126,126,126,126	0
23	MG	A	1718	1/1	0.73	0.60	168,168,168,168	0
23	MG	A	1682	1/1	0.73	0.35	182,182,182,182	0
23	MG	A	1609	1/1	0.74	1.19	84,84,84,84	0
23	MG	A	1705	1/1	0.74	0.32	144,144,144,144	0
23	MG	A	1707	1/1	0.74	1.25	146,146,146,146	0
23	MG	A	1741	1/1	0.74	0.35	136,136,136,136	0
23	MG	A	1634	1/1	0.75	0.87	154,154,154,154	0
23	MG	A	1746	1/1	0.76	0.46	171,171,171,171	0
23	MG	A	1658	1/1	0.77	0.36	185,185,185,185	0
23	MG	A	1763	1/1	0.77	0.16	112,112,112,112	0
23	MG	A	1616	1/1	0.77	0.43	136,136,136,136	0
23	MG	A	1766	1/1	0.78	0.41	128,128,128,128	0
23	MG	A	1653	1/1	0.79	0.70	115,115,115,115	0
23	MG	A	1663	1/1	0.79	0.14	123,123,123,123	0
23	MG	A	1778	1/1	0.79	1.32	141,141,141,141	0
23	MG	A	1660	1/1	0.79	0.81	100,100,100,100	0
23	MG	A	1703	1/1	0.80	0.62	74,74,74,74	0
23	MG	A	1636	1/1	0.80	0.45	61,61,61,61	0
23	MG	A	1765	1/1	0.80	0.28	101,101,101,101	0
23	MG	A	1728	1/1	0.81	0.14	140,140,140,140	0
23	MG	A	1715	1/1	0.81	0.69	106,106,106,106	0
23	MG	A	1764	1/1	0.81	0.51	138,138,138,138	0
23	MG	A	1740	1/1	0.81	0.56	146,146,146,146	0
23	MG	A	1672	1/1	0.81	1.58	110,110,110,110	0
23	MG	A	1742	1/1	0.81	0.77	123,123,123,123	0
23	MG	A	1771	1/1	0.81	1.32	168,168,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1769	1/1	0.82	0.59	99,99,99,99	0
23	MG	A	1624	1/1	0.83	0.34	121,121,121,121	0
23	MG	A	1706	1/1	0.83	0.52	136,136,136,136	0
23	MG	A	1768	1/1	0.83	0.39	106,106,106,106	0
23	MG	A	1628	1/1	0.83	0.65	132,132,132,132	0
23	MG	A	1720	1/1	0.83	0.79	86,86,86,86	0
23	MG	A	1693	1/1	0.83	1.06	128,128,128,128	0
23	MG	A	1606	1/1	0.84	1.94	148,148,148,148	0
23	MG	A	1685	1/1	0.84	0.40	73,73,73,73	0
23	MG	A	1675	1/1	0.84	0.30	79,79,79,79	0
23	MG	A	1739	1/1	0.84	0.36	118,118,118,118	0
25	ZN	N	101	1/1	0.85	0.13	165,165,165,165	0
23	MG	A	1640	1/1	0.86	0.42	157,157,157,157	0
23	MG	A	1723	1/1	0.86	0.33	157,157,157,157	0
23	MG	A	1782	1/1	0.86	0.07	87,87,87,87	0
23	MG	A	1664	1/1	0.87	0.93	100,100,100,100	0
23	MG	A	1602	1/1	0.87	1.75	196,196,196,196	0
23	MG	A	1690	1/1	0.87	0.15	82,82,82,82	0
23	MG	A	1729	1/1	0.87	0.93	124,124,124,124	0
23	MG	A	1648	1/1	0.87	0.38	123,123,123,123	0
23	MG	A	1761	1/1	0.87	0.91	139,139,139,139	0
23	MG	A	1601	1/1	0.88	0.10	148,148,148,148	0
23	MG	A	1714	1/1	0.88	0.68	101,101,101,101	0
23	MG	A	1688	1/1	0.88	0.86	77,77,77,77	0
23	MG	A	1710	1/1	0.88	1.34	104,104,104,104	0
23	MG	A	1745	1/1	0.88	1.11	110,110,110,110	0
23	MG	A	1670	1/1	0.88	0.28	95,95,95,95	0
23	MG	A	1772	1/1	0.88	0.29	167,167,167,167	0
23	MG	A	1752	1/1	0.88	1.43	120,120,120,120	0
23	MG	A	1611	1/1	0.89	0.33	154,154,154,154	0
23	MG	A	1651	1/1	0.89	0.30	118,118,118,118	0
23	MG	A	1702	1/1	0.89	0.28	90,90,90,90	0
23	MG	A	1759	1/1	0.90	0.97	134,134,134,134	0
23	MG	A	1684	1/1	0.90	0.30	80,80,80,80	0
23	MG	A	1680	1/1	0.90	0.20	138,138,138,138	0
23	MG	A	1647	1/1	0.90	0.12	84,84,84,84	0
23	MG	A	1701	1/1	0.90	0.22	147,147,147,147	0
23	MG	A	1671	1/1	0.90	0.38	185,185,185,185	0
23	MG	A	1657	1/1	0.90	0.63	71,71,71,71	0
23	MG	A	1635	1/1	0.91	0.86	103,103,103,103	0
23	MG	A	1773	1/1	0.91	0.13	82,82,82,82	0
23	MG	A	1686	1/1	0.91	0.19	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1632	1/1	0.91	0.51	58,58,58,58	0
23	MG	A	1637	1/1	0.91	0.73	87,87,87,87	0
23	MG	A	1727	1/1	0.91	0.40	99,99,99,99	0
23	MG	A	1753	1/1	0.91	0.18	115,115,115,115	0
23	MG	A	1621	1/1	0.91	0.47	73,73,73,73	0
23	MG	A	1659	1/1	0.91	0.70	154,154,154,154	0
23	MG	A	1730	1/1	0.91	0.14	96,96,96,96	0
23	MG	A	1650	1/1	0.91	0.11	81,81,81,81	0
23	MG	A	1722	1/1	0.92	0.10	204,204,204,204	0
23	MG	A	1747	1/1	0.92	0.36	140,140,140,140	0
23	MG	A	1760	1/1	0.92	0.27	103,103,103,103	0
23	MG	A	1645	1/1	0.92	0.59	76,76,76,76	0
23	MG	A	1655	1/1	0.92	0.92	88,88,88,88	0
23	MG	A	1643	1/1	0.92	1.35	84,84,84,84	0
23	MG	A	1756	1/1	0.92	0.29	137,137,137,137	0
23	MG	A	1721	1/1	0.92	0.27	94,94,94,94	0
23	MG	A	1775	1/1	0.93	0.32	114,114,114,114	0
23	MG	A	1674	1/1	0.93	0.30	89,89,89,89	0
23	MG	A	1709	1/1	0.93	0.54	122,122,122,122	0
23	MG	A	1726	1/1	0.93	0.44	143,143,143,143	0
23	MG	A	1669	1/1	0.93	0.24	165,165,165,165	0
23	MG	A	1605	1/1	0.93	0.18	205,205,205,205	0
23	MG	A	1639	1/1	0.93	1.18	125,125,125,125	0
23	MG	A	1748	1/1	0.93	0.21	83,83,83,83	0
23	MG	A	1654	1/1	0.93	0.47	84,84,84,84	0
23	MG	A	1623	1/1	0.93	0.22	186,186,186,186	0
23	MG	A	1777	1/1	0.94	0.99	71,71,71,71	0
23	MG	A	1725	1/1	0.94	0.18	76,76,76,76	0
23	MG	A	1751	1/1	0.94	0.73	98,98,98,98	0
23	MG	A	1642	1/1	0.94	0.56	67,67,67,67	0
23	MG	A	1667	1/1	0.94	0.44	88,88,88,88	0
23	MG	A	1668	1/1	0.94	0.32	176,176,176,176	0
23	MG	A	1607	1/1	0.94	0.55	124,124,124,124	0
23	MG	A	1608	1/1	0.94	0.91	56,56,56,56	0
23	MG	A	1697	1/1	0.94	0.58	137,137,137,137	0
23	MG	A	1770	1/1	0.95	0.52	184,184,184,184	0
23	MG	A	1630	1/1	0.95	1.24	82,82,82,82	0
23	MG	A	1631	1/1	0.95	0.27	55,55,55,55	0
23	MG	A	1652	1/1	0.95	0.63	146,146,146,146	0
23	MG	A	1641	1/1	0.95	0.29	73,73,73,73	0
23	MG	A	1749	1/1	0.96	0.19	96,96,96,96	0
23	MG	A	1656	1/1	0.96	0.60	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1633	1/1	0.97	0.42	65,65,65,65	0
23	MG	A	1704	1/1	0.97	0.46	98,98,98,98	0
23	MG	A	1750	1/1	0.97	0.53	93,93,93,93	0
23	MG	A	1687	1/1	0.97	0.08	57,57,57,57	0
23	MG	A	1774	1/1	0.97	0.85	102,102,102,102	0
23	MG	A	1666	1/1	0.97	0.62	110,110,110,110	0
23	MG	A	1733	1/1	0.97	0.15	156,156,156,156	0
23	MG	A	1662	1/1	0.97	1.11	83,83,83,83	0
23	MG	A	1754	1/1	0.98	0.30	150,150,150,150	0
23	MG	A	1700	1/1	0.98	0.35	94,94,94,94	0
23	MG	A	1713	1/1	0.99	0.10	71,71,71,71	0
23	MG	A	1644	1/1	0.99	0.56	67,67,67,67	0
23	MG	A	1743	1/1	0.99	0.42	165,165,165,165	0
23	MG	A	1629	1/1	0.99	0.27	117,117,117,117	0
24	SF4	D	301	8/8	0.99	0.14	114,138,170,287	0
23	MG	A	1646	1/1	0.99	0.16	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.