



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 2WWA
EMDB ID: : EMD-1651
Title : Cryo-EM structure of idle yeast Ssh1 complex bound to the yeast 80S ribosome
Authors : Becker, T.; Mandon, E.; Bhushan, S.; Jarasch, A.; Armache, J.P.; Funes, S.; Jossinet, F.; Gumbart, J.; Mielke, T.; Berninghausen, O.; Schulten, K.; Westhof, E.; Gilmore, R.; Beckmann, R.
Deposited on : 2009-10-22
Resolution : 8.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

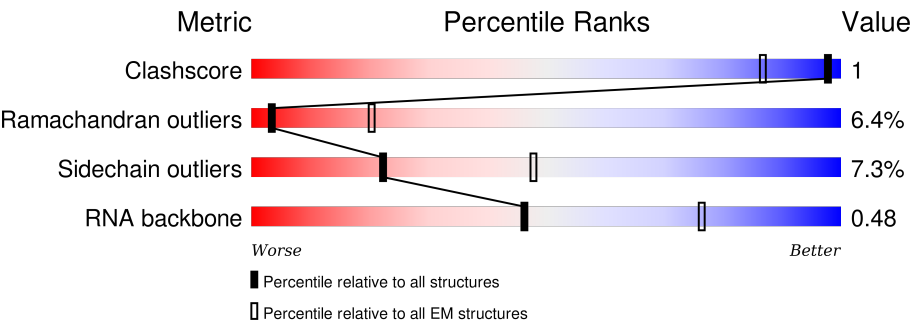
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	490	91% 8% ..
2	B	80	73% .. 25%
3	C	87	22% . 76%
4	D	63	54% 44% .
5	E	34	71% 29%
6	F	25	100%
7	G	18	94% 6%
8	H	362	57% 12% 5% . 26%

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Mol	Chain	Length	Quality of chain
9	I	184	<div><div></div><div>70%10%••17%</div></div>
10	J	189	<div><div></div><div>27%•72%</div></div>
11	K	142	<div><div></div><div>54%•42%</div></div>
12	L	127	<div><div></div><div>80%17%•</div></div>
13	M	113	<div><div></div><div>63%8%•26%</div></div>
14	N	120	<div><div></div><div>46%8%••43%</div></div>
15	O	51	<div><div></div><div>53%16%••27%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14301 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called SEC SIXTY-ONE PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	490	Total	C	N	O	S	0	0
			3770	2487	603	671	9		

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	60	Total	C	N	O	S	0	0
			472	318	76	77	1		

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	21	Total	C	N	O	0	0
			162	112	24	26		

- Molecule 4 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	63	Total	C	N	O	P	0	0
			1347	603	245	436	63		

- Molecule 5 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	34	Total	C	N	O	P	0	0
			740	332	148	226	34		

- Molecule 6 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	25	Total	C	N	O	P	0	0
			536	239	99	173	25		

- Molecule 7 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	18	Total	C	N	O	P	0	0
			379	169	64	128	18		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	269	Total	C	N	O	S	0	0
			2039	1281	391	363	4		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	153	Total	C	N	O	S	0	0
			1212	756	236	219	1		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	53	Total	C	N	O	S	0	0
			410	254	83	72	1		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	83	Total	C	N	O	S	0	0
			663	424	111	126	2		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	127	Total	C	N	O	S	0	0
			1002	630	193	178	1		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	84	Total	C	N	O	S	0	0
			706	447	140	118	1		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	69	Total	C	N	O	S	0	0
			547	345	101	99	2		

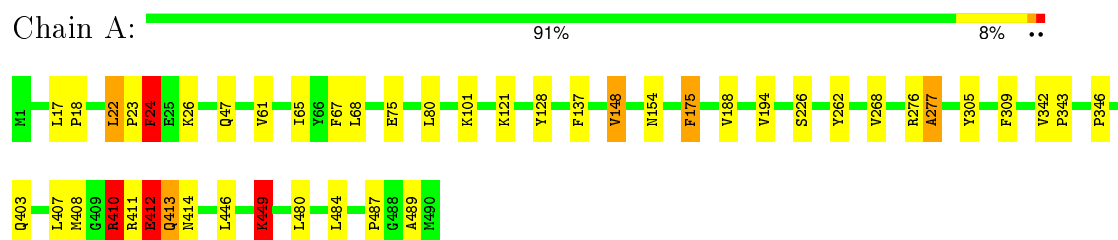
- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	37	Total	C	N	O	S	0	0
			316	200	66	48	2		

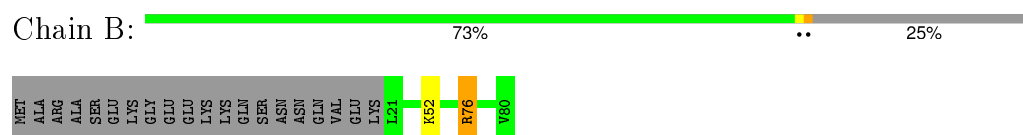
3 Residue-property plots

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. 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. 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.

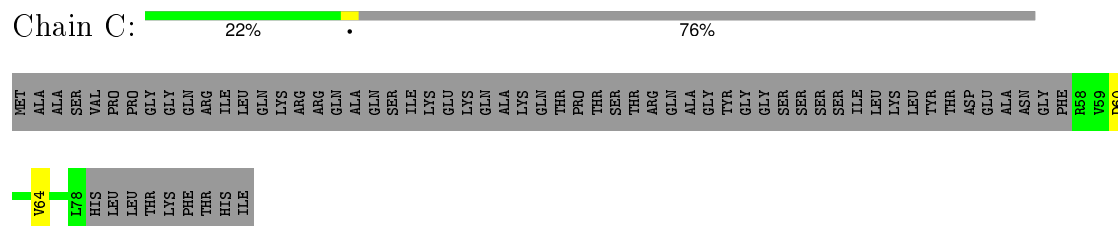
- Molecule 1: SEC SIXTY-ONE PROTEIN HOMOLOG



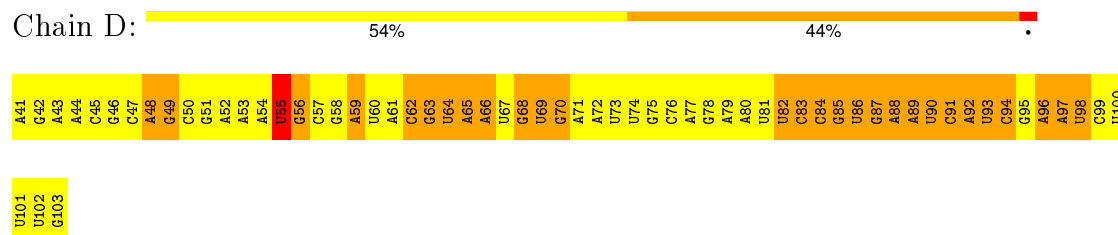
- Molecule 2: PROTEIN TRANSPORT PROTEIN SSS1



- Molecule 3: PROTEIN TRANSPORT PROTEIN SEB2



- Molecule 4: 25S RRNA



- Molecule 5: 25S RRNA



ASP
ARG
ALA
ARG
ALA
SER
GLN
ARG
VAL
ALA
GLU
LYS
ARG
ASP
ALA
LEU
LEU
GLU
ASP
ALA

• Molecule 11: 60S RIBOSOMAL PROTEIN L25

Chain K: 54% 42%

MET
ALA
PRO
SER
LYS
ALA
THR
ALA
LYS
LYS
VAL
VAL
LYS
GLY
THR
ASN
GLY
LYS
LYS
ALA
LEU
LYS
VAL
VAL
THR
SER
SER
ALA
THR
PHE
ARG
LEU
PRO
LYS
THR
LEU
LYS
LEU
ALA
ARG
ALA
PRO
LYS
TYR
ALA
SER
LYS
VAL
VAL
PRO
HIS
TYR
ASN
ARG
L57
V62

Q65
K74
K100
K109
D131
I139
GLY
TYR
ILE

• Molecule 12: 60S RIBOSOMAL PROTEIN L26-A

Chain L: 80% 17%

K1
L6
S10
D11
P23
S24
S36
K37
I45
K46
R52
V56
L57
K64
F78
K84
V85
T86
K87
E88
S94
V95
P96
I97
I106
T107
K122
K125
L126
E127

• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A

Chain M: 63% 8% 26%

MET
ALA
GLY
LEU
LYS
ASP
VAL
VAL
T9
S24
F25
K26
K27
R28
K38
D47
R62
R77
K78
R79
E82
K86
P90
S91
T92
VAL
GLU
PRO
VAL
LEU
VAL
ALA
SER
ALA
LYS
GLY
LEU
GLN
THR
VAL
VAL
GLU
ASP
ALA

• Molecule 14: 60S RIBOSOMAL PROTEIN L35

Chain N: 46% 8% 43%

K1
V4
K5
L9
K14
D23
Q34
K35
L36
R38
P39
S40
R63
R67
Q68
L69
TYR
LYS
GLY
LYS
LYS
LYS
TYR
GLN
PRO
LYS
ASP
LEU
ARG
ALA
LYS
LYS
THR
ARG
ALA
LEU
ARG
ARG
ALA
LEU
THR
PHE
GLU
ALA
SER
GLN
VAL
THR
GLU
LYS
GLN
ARG

LYS
LYS
GLN
ILE
ALA
PHE
PRO
GLN
ARG
LYS
TYR
ALA
ILE
LYS
ALA

• Molecule 15: 60S RIBOSOMAL PROTEIN L39

Chain O: 53% 16% 27%

K1
K5
S6
K17
P22
L23
P24
Q25
W26
T31
T34
I35
R36
Y37
ASN
ALA
LYS
LYS
ARG
ARG
ASN
TRP
ARG
ARG
THR
LYS
MET
ASN
ILE

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163	Depositor

5 Model quality

5.1 Standard geometry

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.90	0/3848	1.03	10/5234 (0.2%)
10	J	1.01	0/412	0.90	0/551
11	K	0.90	0/670	0.96	0/903
12	L	1.01	0/1013	1.17	3/1351 (0.2%)
13	M	1.09	0/719	1.19	5/959 (0.5%)
14	N	1.06	1/549 (0.2%)	1.33	9/733 (1.2%)
15	O	1.08	0/321	1.31	3/426 (0.7%)
2	B	0.89	0/481	0.91	0/648
3	C	0.96	0/164	0.89	0/222
4	D	1.59	0/1508	2.60	196/2348 (8.3%)
5	E	1.59	0/833	2.65	118/1298 (9.1%)
6	F	1.60	0/599	2.41	71/932 (7.6%)
7	G	1.54	0/421	2.27	50/653 (7.7%)
8	H	0.99	0/2079	1.31	22/2817 (0.8%)
9	I	1.03	0/1235	1.27	9/1662 (0.5%)
All	All	1.14	1/14852 (0.0%)	1.61	496/20737 (2.4%)

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	3
12	L	0	1
14	N	0	2
15	O	0	2
4	D	0	2
8	H	0	2
9	I	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	69	LEU	C-O	-12.06	1.00	1.23

All (496) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	532	A	P-O3'-C3'	18.42	141.80	119.70
4	D	69	U	P-O3'-C3'	14.68	137.31	119.70
4	D	65	A	P-O3'-C3'	13.79	136.25	119.70
4	D	90	U	P-O3'-C3'	13.58	136.00	119.70
5	E	555	A	N1-C6-N6	13.40	126.64	118.60
4	D	96	A	P-O3'-C3'	13.29	135.65	119.70
4	D	54	A	N1-C6-N6	13.23	126.54	118.60
4	D	53	A	N1-C6-N6	13.16	126.50	118.60
4	D	55	U	P-O3'-C3'	12.99	135.29	119.70
5	E	533	A	N1-C6-N6	12.94	126.37	118.60
6	F	1673	A	N1-C6-N6	12.68	126.21	118.60
4	D	77	A	N1-C6-N6	12.61	126.17	118.60
6	F	1662	A	N1-C6-N6	12.58	126.15	118.60
4	D	65	A	N1-C6-N6	12.57	126.14	118.60
6	F	1661	A	N1-C6-N6	12.56	126.13	118.60
5	E	545	A	N1-C6-N6	12.40	126.04	118.60
5	E	536	A	N1-C6-N6	12.39	126.03	118.60
4	D	88	A	N1-C6-N6	12.36	126.02	118.60
4	D	79	A	N1-C6-N6	12.32	125.99	118.60
4	D	97	A	N1-C6-N6	12.21	125.92	118.60
5	E	535	A	N1-C6-N6	12.14	125.89	118.60
4	D	41	A	N1-C6-N6	12.14	125.88	118.60
4	D	44	A	N1-C6-N6	12.13	125.88	118.60
5	E	554	A	N1-C6-N6	12.13	125.88	118.60
6	F	1667	A	N1-C6-N6	12.12	125.87	118.60
4	D	80	A	N1-C6-N6	12.08	125.85	118.60
4	D	71	A	N1-C6-N6	12.05	125.83	118.60
4	D	43	A	N1-C6-N6	12.02	125.81	118.60
4	D	96	A	N1-C6-N6	11.99	125.79	118.60
5	E	549	A	N1-C6-N6	11.96	125.78	118.60
5	E	547	A	N1-C6-N6	11.91	125.75	118.60
5	E	543	A	N1-C6-N6	11.90	125.74	118.60
5	E	556	A	N1-C6-N6	11.89	125.73	118.60
5	E	531	A	N1-C6-N6	11.80	125.68	118.60
4	D	61	A	N1-C6-N6	11.80	125.68	118.60
4	D	72	A	N1-C6-N6	11.80	125.68	118.60
4	D	48	A	N1-C6-N6	11.74	125.64	118.60
5	E	557	A	N1-C6-N6	11.73	125.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	530	A	N1-C6-N6	11.68	125.61	118.60
4	D	89	A	N1-C6-N6	11.65	125.59	118.60
7	G	1915	A	N1-C6-N6	11.65	125.59	118.60
4	D	66	A	N1-C6-N6	11.62	125.57	118.60
7	G	1918	A	N1-C6-N6	11.56	125.54	118.60
5	E	544	A	N1-C6-N6	11.51	125.51	118.60
5	E	560	A	P-O3'-C3'	11.42	133.41	119.70
5	E	553	A	N1-C6-N6	11.41	125.44	118.60
6	F	1664	A	N1-C6-N6	11.37	125.42	118.60
4	D	59	A	N1-C6-N6	11.36	125.41	118.60
5	E	560	A	N1-C6-N6	11.31	125.39	118.60
4	D	52	A	N1-C6-N6	11.30	125.38	118.60
4	D	92	A	N1-C6-N6	11.21	125.33	118.60
4	D	93	U	P-O3'-C3'	11.11	133.03	119.70
6	F	1656	A	N1-C6-N6	11.04	125.22	118.60
5	E	542	A	N1-C6-N6	11.02	125.21	118.60
4	D	89	A	P-O3'-C3'	10.95	132.84	119.70
5	E	532	A	N1-C6-N6	10.64	124.99	118.60
4	D	50	C	O4'-C1'-N1	9.58	115.86	108.20
4	D	63	G	N1-C6-O6	9.35	125.51	119.90
6	F	1668	G	N1-C6-O6	9.10	125.36	119.90
4	D	49	G	N1-C6-O6	9.00	125.30	119.90
4	D	46	G	N1-C6-O6	8.99	125.29	119.90
4	D	58	G	N1-C6-O6	8.94	125.27	119.90
5	E	534	G	N1-C6-O6	8.94	125.27	119.90
6	F	1675	G	N1-C6-O6	8.89	125.23	119.90
5	E	541	G	N1-C6-O6	8.84	125.20	119.90
4	D	87	G	N1-C6-O6	8.83	125.20	119.90
6	F	1677	G	N1-C6-O6	8.82	125.19	119.90
4	D	103	G	N1-C6-O6	8.82	125.19	119.90
7	G	1924	G	N1-C6-O6	8.82	125.19	119.90
5	E	546	G	N1-C6-O6	8.80	125.18	119.90
4	D	85	G	N1-C6-O6	8.75	125.15	119.90
7	G	1927	G	N1-C6-O6	8.70	125.12	119.90
4	D	70	G	N1-C6-O6	8.66	125.10	119.90
4	D	56	G	N1-C6-O6	8.61	125.07	119.90
7	G	1928	G	N1-C6-O6	8.60	125.06	119.90
5	E	558	G	N1-C6-O6	8.59	125.05	119.90
4	D	90	U	O4'-C1'-N1	8.58	115.06	108.20
5	E	529	G	N1-C6-O6	8.57	125.04	119.90
5	E	552	G	N1-C6-O6	8.53	125.02	119.90
6	F	1678	G	N1-C6-O6	8.51	125.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1658	G	N1-C6-O6	8.51	125.00	119.90
7	G	1912	G	N1-C6-O6	8.50	125.00	119.90
4	D	57	C	O4'-C1'-N1	8.47	114.98	108.20
6	F	1665	G	N1-C6-O6	8.46	124.98	119.90
4	D	45	C	O4'-C1'-N1	8.46	114.97	108.20
5	E	548	G	N1-C6-O6	8.46	124.97	119.90
6	F	1672	G	N1-C6-O6	8.42	124.95	119.90
4	D	68	G	N1-C6-O6	8.42	124.95	119.90
8	H	54	GLU	C-N-CA	8.42	142.76	121.70
4	D	75	G	N1-C6-O6	8.40	124.94	119.90
5	E	550	G	N1-C6-O6	8.40	124.94	119.90
14	N	37	SER	N-CA-CB	8.38	123.08	110.50
6	F	1657	C	O4'-C1'-N1	8.35	114.88	108.20
4	D	42	G	N1-C6-O6	8.30	124.88	119.90
7	G	1916	G	N1-C6-O6	8.29	124.88	119.90
4	D	51	G	N1-C6-O6	8.22	124.83	119.90
4	D	92	A	O4'-C1'-N9	8.15	114.72	108.20
6	F	1671	G	N1-C6-O6	8.05	124.73	119.90
8	H	75	PRO	C-N-CA	7.99	141.68	121.70
4	D	78	G	N1-C6-O6	7.99	124.69	119.90
7	G	1914	C	O4'-C1'-N1	7.99	114.59	108.20
8	H	60	THR	N-CA-CB	7.95	125.41	110.30
4	D	95	G	N1-C6-O6	7.95	124.67	119.90
7	G	1925	C	O4'-C1'-N1	7.95	114.56	108.20
8	H	59	GLN	C-N-CA	7.93	141.52	121.70
4	D	91	C	O4'-C1'-N1	7.92	114.53	108.20
7	G	1920	C	O4'-C1'-N1	7.91	114.53	108.20
6	F	1674	C	O4'-C1'-N1	7.91	114.53	108.20
4	D	69	U	O4'-C1'-N1	7.90	114.52	108.20
6	F	1666	C	O4'-C1'-N1	7.85	114.48	108.20
4	D	76	C	O4'-C1'-N1	7.80	114.44	108.20
7	G	1913	C	O4'-C1'-N1	7.79	114.43	108.20
5	E	558	G	C5-C6-O6	-7.79	123.93	128.60
7	G	1929	C	O4'-C1'-N1	7.78	114.43	108.20
7	G	1919	C	O4'-C1'-N1	7.78	114.42	108.20
4	D	99	C	O4'-C1'-N1	7.74	114.39	108.20
4	D	80	A	O4'-C1'-N9	7.73	114.38	108.20
5	E	537	C	O4'-C1'-N1	7.62	114.30	108.20
5	E	528	U	O4'-C1'-N1	7.55	114.24	108.20
4	D	102	U	O4'-C1'-N1	7.51	114.21	108.20
7	G	1917	C	O4'-C1'-N1	7.48	114.18	108.20
5	E	540	U	O4'-C1'-N1	7.46	114.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1922	U	O4'-C1'-N1	7.42	114.14	108.20
6	F	1654	C	O4'-C1'-N1	7.41	114.13	108.20
6	F	1676	U	O4'-C1'-N1	7.39	114.11	108.20
4	D	46	G	C5-C6-O6	-7.37	124.18	128.60
6	F	1655	C	O4'-C1'-N1	7.36	114.08	108.20
8	H	89	ALA	N-CA-CB	7.34	120.38	110.10
4	D	75	G	C4-N9-C1'	7.32	136.01	126.50
4	D	63	G	C5-C6-O6	-7.30	124.22	128.60
4	D	100	U	O4'-C1'-N1	7.23	113.98	108.20
4	D	81	U	O4'-C1'-N1	7.21	113.97	108.20
6	F	1663	C	O4'-C1'-N1	7.20	113.96	108.20
6	F	1668	G	C5-C6-O6	-7.14	124.32	128.60
6	F	1670	U	O4'-C1'-N1	7.13	113.91	108.20
5	E	534	G	C5-C6-O6	-7.12	124.33	128.60
4	D	55	U	O4'-C1'-N1	7.11	113.89	108.20
4	D	101	U	O4'-C1'-N1	7.09	113.87	108.20
9	I	56	ARG	C-N-CA	7.09	139.42	121.70
5	E	561	C	O4'-C1'-N1	7.06	113.85	108.20
4	D	63	G	P-O3'-C3'	7.04	128.15	119.70
7	G	1926	U	O4'-C1'-N1	7.03	113.82	108.20
5	E	539	U	O4'-C1'-N1	7.00	113.80	108.20
4	D	103	G	C5-C6-O6	-6.98	124.41	128.60
4	D	85	G	C5-C6-O6	-6.95	124.43	128.60
5	E	555	A	C5-C6-N6	-6.94	118.15	123.70
9	I	37	ASN	N-CA-CB	6.93	123.07	110.60
4	D	58	G	C5-C6-O6	-6.92	124.45	128.60
4	D	53	A	C4-C5-C6	6.90	120.45	117.00
4	D	95	G	O4'-C1'-N9	6.89	113.71	108.20
5	E	551	U	O4'-C1'-N1	6.86	113.69	108.20
5	E	538	U	O4'-C1'-N1	6.86	113.69	108.20
4	D	47	C	O4'-C1'-N1	6.86	113.69	108.20
4	D	67	U	O4'-C1'-N1	6.86	113.69	108.20
4	D	87	G	C5-C6-O6	-6.85	124.49	128.60
6	F	1660	C	O4'-C1'-N1	6.81	113.65	108.20
6	F	1675	G	O4'-C1'-N9	6.79	113.63	108.20
4	D	70	G	C5-C6-O6	-6.77	124.53	128.60
9	I	36	ILE	C-N-CA	6.76	138.60	121.70
4	D	98	U	O4'-C1'-N1	6.75	113.60	108.20
12	L	84	LYS	C-N-CA	6.75	138.57	121.70
5	E	541	G	C5-C6-O6	-6.74	124.56	128.60
4	D	77	A	C4-C5-C6	6.73	120.37	117.00
7	G	1924	G	C5-C6-O6	-6.71	124.58	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	184	SER	C-N-CA	6.69	138.43	121.70
6	F	1673	A	C4-C5-C6	6.68	120.34	117.00
4	D	78	G	O4'-C1'-N9	6.68	113.54	108.20
5	E	533	A	C4-C5-C6	6.67	120.34	117.00
4	D	49	G	C5-C6-O6	-6.64	124.61	128.60
8	H	214	GLY	C-N-CA	6.63	138.26	121.70
7	G	1928	G	C5-C6-O6	-6.62	124.62	128.60
6	F	1661	A	C4-C5-C6	6.59	120.30	117.00
4	D	56	G	O4'-C1'-N9	6.58	113.47	108.20
5	E	536	A	C5-C6-N6	-6.57	118.44	123.70
5	E	546	G	C5-C6-O6	-6.56	124.67	128.60
6	F	1677	G	C5-C6-O6	-6.56	124.66	128.60
4	D	74	U	O4'-C1'-N1	6.55	113.44	108.20
4	D	89	A	O4'-C1'-N9	6.54	113.43	108.20
6	F	1659	U	O4'-C1'-N1	6.53	113.43	108.20
7	G	1921	U	O4'-C1'-N1	6.53	113.42	108.20
7	G	1912	G	C5-C6-O6	-6.52	124.69	128.60
4	D	68	G	C5-C6-O6	-6.52	124.69	128.60
4	D	54	A	C5-C6-N6	-6.51	118.49	123.70
6	F	1658	G	C5-C6-O6	-6.50	124.70	128.60
14	N	39	PRO	C-N-CA	6.49	137.93	121.70
7	G	1927	G	C5-C6-O6	-6.49	124.71	128.60
4	D	56	G	C5-C6-O6	-6.48	124.71	128.60
7	G	1923	U	O4'-C1'-N1	6.48	113.39	108.20
5	E	548	G	C5-C6-O6	-6.47	124.72	128.60
6	F	1672	G	C5-C6-O6	-6.45	124.73	128.60
6	F	1675	G	C5-C6-O6	-6.43	124.74	128.60
5	E	529	G	C5-C6-O6	-6.43	124.74	128.60
5	E	550	G	C5-C6-O6	-6.42	124.75	128.60
6	F	1662	A	C4-C5-C6	6.40	120.20	117.00
4	D	68	G	O4'-C1'-N9	6.38	113.30	108.20
6	F	1678	G	C5-C6-O6	-6.37	124.78	128.60
4	D	51	G	C5-C6-O6	-6.36	124.79	128.60
4	D	64	U	O4'-C1'-N1	6.35	113.28	108.20
4	D	61	A	C4-C5-C6	6.35	120.17	117.00
5	E	544	A	C4-C5-C6	6.35	120.17	117.00
5	E	552	G	C5-C6-O6	-6.34	124.80	128.60
4	D	93	U	O4'-C1'-N1	6.32	113.25	108.20
8	H	75	PRO	CA-C-N	6.31	131.09	117.20
4	D	95	G	C5-C6-O6	-6.30	124.82	128.60
4	D	82	U	O4'-C1'-N1	6.29	113.24	108.20
4	D	78	G	C5-C6-O6	-6.29	124.83	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	PHE	CB-CG-CD1	6.29	125.20	120.80
5	E	548	G	O4'-C1'-N9	6.29	113.23	108.20
7	G	1916	G	C5-C6-O6	-6.28	124.83	128.60
4	D	65	A	C4-C5-C6	6.27	120.13	117.00
4	D	53	A	C5-C6-N6	-6.25	118.70	123.70
12	L	10	SER	C-N-CA	6.24	137.29	121.70
4	D	41	A	C4-C5-C6	6.23	120.12	117.00
6	F	1673	A	C5-C6-N6	-6.23	118.72	123.70
5	E	549	A	C4-C5-C6	6.21	120.11	117.00
4	D	88	A	C4-C5-C6	6.20	120.10	117.00
5	E	560	A	O4'-C1'-N9	6.20	113.16	108.20
4	D	97	A	C4-C5-C6	6.19	120.09	117.00
14	N	67	ARG	NE-CZ-NH2	6.18	123.39	120.30
4	D	96	A	C4-C5-C6	6.17	120.08	117.00
4	D	91	C	N3-C4-C5	-6.15	119.44	121.90
4	D	54	A	C4-C5-C6	6.15	120.08	117.00
5	E	543	A	C4-C5-C6	6.15	120.07	117.00
1	A	24	PHE	CB-CG-CD2	6.14	125.10	120.80
5	E	531	A	C4-C5-C6	6.14	120.07	117.00
4	D	59	A	C4-C5-C6	6.13	120.06	117.00
6	F	1671	G	C5-C6-O6	-6.12	124.93	128.60
4	D	48	A	C4-C5-C6	6.12	120.06	117.00
5	E	545	A	C4-C5-C6	6.11	120.06	117.00
4	D	42	G	C5-C6-O6	-6.10	124.94	128.60
4	D	66	A	C4-C5-C6	6.10	120.05	117.00
5	E	556	A	C4-C5-C6	6.09	120.05	117.00
4	D	75	G	C8-N9-C1'	-6.08	119.10	127.00
5	E	547	A	C4-C5-C6	6.08	120.04	117.00
6	F	1654	C	N3-C4-N4	6.08	122.25	118.00
5	E	535	A	C4-C5-C6	6.07	120.04	117.00
6	F	1667	A	C4-C5-C6	6.07	120.03	117.00
4	D	73	U	O4'-C1'-N1	6.07	113.05	108.20
4	D	44	A	C5-C6-N6	-6.06	118.85	123.70
4	D	75	G	C5-C6-O6	-6.04	124.98	128.60
6	F	1665	G	C5-C6-O6	-6.03	124.98	128.60
5	E	536	A	O4'-C1'-N9	6.03	113.03	108.20
4	D	71	A	C4-C5-C6	6.02	120.01	117.00
6	F	1658	G	O4'-C1'-N9	5.99	112.99	108.20
5	E	533	A	C5-C6-N6	-5.98	118.91	123.70
1	A	137	PHE	CB-CG-CD2	-5.98	116.61	120.80
4	D	43	A	C4-C5-C6	5.98	119.99	117.00
6	F	1671	G	O4'-C1'-N9	5.98	112.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	41	A	C5-C6-N6	-5.98	118.92	123.70
5	E	557	A	C4-C5-C6	5.97	119.99	117.00
5	E	555	A	C4-C5-C6	5.97	119.99	117.00
5	E	554	A	C4-C5-C6	5.97	119.98	117.00
5	E	533	A	C5-C6-N1	-5.96	114.72	117.70
13	M	24	SER	N-CA-CB	5.96	119.44	110.50
4	D	79	A	C4-C5-C6	5.96	119.98	117.00
4	D	88	A	C5-C6-N6	-5.95	118.94	123.70
6	F	1661	A	C5-C6-N6	-5.94	118.95	123.70
5	E	553	A	C4-C5-C6	5.93	119.97	117.00
7	G	1915	A	C4-C5-C6	5.92	119.96	117.00
5	E	542	A	C4-C5-C6	5.92	119.96	117.00
4	D	62	C	O4'-C1'-N1	5.91	112.93	108.20
4	D	65	A	C5-C6-N6	-5.91	118.97	123.70
5	E	559	U	O4'-C1'-N1	5.89	112.91	108.20
4	D	44	A	C4-C5-C6	5.88	119.94	117.00
7	G	1918	A	C4-C5-C6	5.88	119.94	117.00
4	D	52	A	C4-C5-C6	5.88	119.94	117.00
4	D	77	A	C5-C6-N6	-5.87	119.00	123.70
6	F	1655	C	N3-C4-N4	5.86	122.10	118.00
6	F	1662	A	C5-C6-N6	-5.85	119.02	123.70
4	D	54	A	O4'-C1'-N9	5.85	112.88	108.20
6	F	1656	A	O4'-C1'-N9	5.85	112.88	108.20
4	D	76	C	N3-C4-N4	5.84	122.09	118.00
4	D	97	A	C5-C6-N1	-5.84	114.78	117.70
4	D	43	A	O4'-C1'-N9	5.84	112.87	108.20
1	A	449	LYS	N-CA-CB	5.83	121.10	110.60
4	D	66	A	C5-C6-N1	-5.83	114.78	117.70
5	E	549	A	C5-C6-N6	-5.83	119.03	123.70
4	D	72	A	C4-C5-C6	5.83	119.91	117.00
5	E	542	A	O4'-C1'-N9	5.82	112.86	108.20
4	D	83	C	C2-N1-C1'	5.82	125.20	118.80
4	D	53	A	C5-C6-N1	-5.81	114.79	117.70
4	D	89	A	C4-C5-C6	5.81	119.91	117.00
4	D	99	C	N3-C4-N4	5.81	122.07	118.00
7	G	1927	G	O4'-C1'-N9	5.80	112.84	108.20
7	G	1917	C	N3-C4-N4	5.80	122.06	118.00
5	E	530	A	C4-C5-C6	5.80	119.90	117.00
8	H	90	PHE	CB-CG-CD2	5.79	124.86	120.80
1	A	277	ALA	N-CA-CB	5.79	118.21	110.10
5	E	535	A	C5-C6-N6	-5.79	119.07	123.70
4	D	71	A	C5-C6-N1	-5.79	114.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	86	U	O4'-C1'-N1	5.78	112.83	108.20
5	E	534	G	O4'-C1'-N9	5.77	112.82	108.20
5	E	545	A	C5-C6-N6	-5.77	119.09	123.70
9	I	39	TRP	N-CA-CB	5.76	120.97	110.60
5	E	546	G	O4'-C1'-N9	5.75	112.80	108.20
6	F	1656	A	C4-C5-C6	5.75	119.88	117.00
9	I	56	ARG	CB-CA-C	5.75	121.91	110.40
4	D	96	A	O4'-C1'-N9	5.75	112.80	108.20
7	G	1925	C	N3-C4-N4	5.75	122.02	118.00
6	F	1662	A	C5-C6-N1	-5.74	114.83	117.70
4	D	77	A	C5-C6-N1	-5.74	114.83	117.70
7	G	1928	G	O4'-C1'-N9	5.74	112.79	108.20
13	M	77	ARG	C-N-CA	5.74	136.05	121.70
14	N	67	ARG	N-CA-CB	-5.74	100.27	110.60
5	E	537	C	N3-C4-N4	5.73	122.01	118.00
4	D	42	G	O4'-C1'-N9	5.73	112.78	108.20
4	D	80	A	C5-C6-N6	-5.73	119.12	123.70
5	E	554	A	C5-C6-N6	-5.73	119.12	123.70
5	E	560	A	C4-C5-C6	5.73	119.86	117.00
4	D	79	A	C5-C6-N6	-5.72	119.12	123.70
4	D	72	A	C5-C6-N6	-5.72	119.13	123.70
6	F	1663	C	N3-C4-N4	5.71	122.00	118.00
4	D	76	C	N3-C4-C5	-5.71	119.62	121.90
4	D	92	A	C4-C5-C6	5.71	119.85	117.00
8	H	209	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	24	PHE	CB-CG-CD1	-5.70	116.81	120.80
5	E	547	A	C5-C6-N1	-5.69	114.85	117.70
7	G	1913	C	N3-C4-N4	5.69	121.98	118.00
7	G	1929	C	N3-C4-N4	5.69	121.98	118.00
6	F	1667	A	C5-C6-N6	-5.68	119.15	123.70
5	E	561	C	N3-C4-N4	5.67	121.97	118.00
8	H	212	ASP	C-N-CA	5.66	135.85	121.70
5	E	545	A	C5-C6-N1	-5.65	114.87	117.70
4	D	65	A	C5-C6-N1	-5.64	114.88	117.70
8	H	57	GLY	C-N-CA	5.64	135.81	121.70
5	E	530	A	C5-C6-N6	-5.64	119.19	123.70
4	D	79	A	C5-C6-N1	-5.63	114.89	117.70
14	N	36	LEU	C-N-CA	5.63	135.78	121.70
4	D	94	C	N3-C4-N4	5.63	121.94	118.00
6	F	1657	C	N3-C4-N4	5.63	121.94	118.00
7	G	1916	G	O4'-C1'-N9	5.63	112.70	108.20
4	D	43	A	C5-C6-N1	-5.63	114.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1912	G	O4'-C1'-N9	5.62	112.70	108.20
1	A	408	MET	C-N-CA	5.62	134.09	122.30
5	E	537	C	N3-C4-C5	-5.62	119.65	121.90
5	E	556	A	C5-C6-N6	-5.61	119.21	123.70
4	D	44	A	O4'-C1'-N9	5.61	112.69	108.20
5	E	541	G	O4'-C1'-N9	5.61	112.69	108.20
4	D	96	A	C5-C6-N1	-5.60	114.90	117.70
4	D	84	C	N3-C4-N4	5.59	121.92	118.00
5	E	530	A	O4'-C1'-N9	5.59	112.67	108.20
5	E	543	A	C5-C6-N6	-5.58	119.23	123.70
4	D	61	A	C5-C6-N1	-5.58	114.91	117.70
5	E	544	A	O4'-C1'-N9	5.58	112.67	108.20
5	E	536	A	C4-C5-C6	5.57	119.78	117.00
6	F	1661	A	C5-C6-N1	-5.56	114.92	117.70
6	F	1674	C	N3-C4-N4	5.56	121.89	118.00
8	H	212	ASP	CB-CA-C	5.56	121.53	110.40
4	D	89	A	C5-C6-N6	-5.55	119.26	123.70
5	E	529	G	O4'-C1'-N9	5.55	112.64	108.20
4	D	45	C	N3-C4-N4	5.55	121.89	118.00
5	E	557	A	C5-C6-N1	-5.55	114.92	117.70
7	G	1915	A	O4'-C1'-N9	5.55	112.64	108.20
4	D	50	C	N3-C4-C5	-5.54	119.69	121.90
8	H	209	TYR	CB-CG-CD2	-5.53	117.68	121.00
5	E	552	G	O4'-C1'-N9	5.53	112.62	108.20
5	E	544	A	C5-C6-N1	-5.53	114.94	117.70
8	H	28	ALA	N-CA-CB	5.52	117.82	110.10
4	D	97	A	C5-C6-N6	-5.50	119.30	123.70
4	D	43	A	C5-C6-N6	-5.50	119.30	123.70
13	M	25	PHE	CB-CG-CD2	5.50	124.65	120.80
4	D	96	A	C5-C6-N6	-5.49	119.31	123.70
6	F	1666	C	N3-C4-N4	5.49	121.84	118.00
8	H	264	SER	N-CA-CB	5.49	118.73	110.50
4	D	45	C	N3-C4-C5	-5.48	119.71	121.90
4	D	48	A	C5-C6-N6	-5.48	119.32	123.70
5	E	531	A	C5-C6-N6	-5.48	119.32	123.70
4	D	57	C	N3-C4-N4	5.47	121.83	118.00
6	F	1663	C	N3-C4-C5	-5.47	119.71	121.90
7	G	1924	G	O4'-C1'-N9	5.47	112.57	108.20
5	E	531	A	C5-C6-N1	-5.46	114.97	117.70
14	N	39	PRO	CA-C-N	5.46	129.21	117.20
4	D	54	A	C5-C6-N1	-5.46	114.97	117.70
4	D	66	A	O4'-C1'-N9	5.46	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	97	A	O4'-C1'-N9	5.46	112.56	108.20
7	G	1915	A	C5-C6-N1	-5.46	114.97	117.70
4	D	94	C	O4'-C1'-N1	5.46	112.56	108.20
5	E	557	A	O4'-C1'-N9	5.46	112.56	108.20
6	F	1664	A	C4-C5-C6	5.45	119.73	117.00
6	F	1667	A	C5-C6-N1	-5.45	114.97	117.70
6	F	1664	A	O4'-C1'-N9	5.45	112.56	108.20
7	G	1919	C	N3-C4-N4	5.45	121.81	118.00
4	D	52	A	O4'-C1'-N9	5.44	112.55	108.20
5	E	532	A	C4-C5-C6	5.44	119.72	117.00
5	E	549	A	O4'-C1'-N9	5.44	112.55	108.20
4	D	71	A	C5-C6-N6	-5.43	119.36	123.70
4	D	92	A	C5-C6-N1	-5.42	114.99	117.70
9	I	90	PHE	CB-CG-CD1	5.41	124.59	120.80
4	D	57	C	N3-C4-C5	-5.41	119.73	121.90
5	E	554	A	C5-C6-N1	-5.41	114.99	117.70
4	D	65	A	O4'-C1'-N9	5.40	112.52	108.20
4	D	91	C	N3-C4-N4	5.39	121.78	118.00
6	F	1657	C	N3-C4-C5	-5.39	119.74	121.90
4	D	58	G	O4'-C1'-N9	5.39	112.51	108.20
4	D	80	A	C4-C5-C6	5.39	119.69	117.00
6	F	1660	C	N3-C4-N4	5.39	121.77	118.00
6	F	1674	C	N3-C4-C5	-5.39	119.74	121.90
4	D	59	A	C5-C6-N1	-5.39	115.01	117.70
9	I	90	PHE	CB-CG-CD2	-5.38	117.03	120.80
5	E	547	A	C5-C6-N6	-5.38	119.39	123.70
6	F	1662	A	O4'-C1'-N9	5.38	112.50	108.20
4	D	79	A	O4'-C1'-N9	5.38	112.50	108.20
5	E	543	A	C5-C6-N1	-5.37	115.01	117.70
4	D	52	A	C5-C6-N6	-5.37	119.41	123.70
4	D	83	C	O4'-C1'-N1	5.37	112.49	108.20
7	G	1918	A	C5-C6-N1	-5.37	115.02	117.70
4	D	61	A	C5-C6-N6	-5.36	119.41	123.70
6	F	1664	A	C5-C6-N1	-5.36	115.02	117.70
14	N	67	ARG	CA-CB-CG	5.35	125.17	113.40
6	F	1656	A	C5-C6-N1	-5.35	115.03	117.70
15	O	5	LYS	CB-CA-C	5.35	121.09	110.40
4	D	80	A	C5-C6-N1	-5.34	115.03	117.70
4	D	84	C	N3-C4-C5	-5.34	119.76	121.90
5	E	553	A	C5-C6-N6	-5.34	119.43	123.70
8	H	253	ALA	N-CA-CB	5.34	117.57	110.10
4	D	48	A	C5-C6-N1	-5.33	115.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1654	C	N3-C4-C5	-5.33	119.77	121.90
5	E	557	A	C5-C6-N6	-5.33	119.43	123.70
7	G	1914	C	N3-C4-C5	-5.33	119.77	121.90
7	G	1915	A	C5-C6-N6	-5.33	119.44	123.70
7	G	1914	C	N3-C4-N4	5.32	121.73	118.00
1	A	175	PHE	CB-CG-CD2	5.32	124.53	120.80
4	D	88	A	C5-C6-N1	-5.32	115.04	117.70
7	G	1918	A	C5-C6-N6	-5.32	119.44	123.70
7	G	1919	C	N3-C4-C5	-5.32	119.77	121.90
7	G	1925	C	N3-C4-C5	-5.32	119.77	121.90
5	E	535	A	C5-C6-N1	-5.31	115.05	117.70
6	F	1660	C	N3-C4-C5	-5.31	119.78	121.90
6	F	1655	C	N3-C4-C5	-5.30	119.78	121.90
5	E	550	G	O4'-C1'-N9	5.30	112.44	108.20
6	F	1666	C	N3-C4-C5	-5.30	119.78	121.90
7	G	1920	C	N3-C4-C5	-5.30	119.78	121.90
5	E	556	A	C5-C6-N1	-5.30	115.05	117.70
5	E	542	A	C5-C6-N1	-5.29	115.05	117.70
8	H	64	SER	N-CA-CB	5.29	118.44	110.50
5	E	554	A	O4'-C1'-N9	5.29	112.43	108.20
4	D	50	C	N3-C4-N4	5.29	121.70	118.00
4	D	103	G	O4'-C1'-N9	5.29	112.43	108.20
14	N	69	LEU	CA-C-O	-5.29	109.00	120.10
14	N	14	LYS	N-CA-CB	5.28	120.09	110.60
5	E	553	A	O4'-C1'-N9	5.27	112.42	108.20
5	E	560	A	C5-C6-N6	-5.26	119.49	123.70
4	D	49	G	O4'-C1'-N9	5.26	112.41	108.20
4	D	85	G	O4'-C1'-N9	5.26	112.41	108.20
6	F	1669	U	O4'-C1'-N1	5.26	112.41	108.20
13	M	78	LYS	N-CA-CB	5.26	120.06	110.60
4	D	62	C	C2-N1-C1'	5.25	124.58	118.80
7	G	1918	A	O4'-C1'-N9	5.25	112.40	108.20
6	F	1673	A	C5-C6-N1	-5.25	115.08	117.70
5	E	535	A	O4'-C1'-N9	5.25	112.40	108.20
4	D	84	C	O4'-C1'-N1	5.24	112.39	108.20
5	E	543	A	O4'-C1'-N9	5.23	112.39	108.20
7	G	1920	C	N3-C4-N4	5.23	121.66	118.00
8	H	247	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	A	412	GLU	C-N-CA	5.21	134.73	121.70
6	F	1678	G	O4'-C1'-N9	5.20	112.36	108.20
8	H	102	PRO	N-CA-C	5.20	125.61	112.10
4	D	47	C	N3-C4-N4	5.19	121.63	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	544	A	C5-C6-N6	-5.19	119.55	123.70
6	F	1664	A	C5-C6-N6	-5.19	119.55	123.70
4	D	47	C	N3-C4-C5	-5.17	119.83	121.90
5	E	547	A	O4'-C1'-N9	5.16	112.33	108.20
5	E	561	C	N3-C4-C5	-5.16	119.83	121.90
7	G	1929	C	N3-C4-C5	-5.16	119.83	121.90
7	G	1917	C	N3-C4-C5	-5.16	119.83	121.90
5	E	560	A	C5-C6-N1	-5.16	115.12	117.70
5	E	553	A	C5-C6-N1	-5.16	115.12	117.70
4	D	59	A	C5-C6-N6	-5.15	119.58	123.70
4	D	94	C	N3-C4-C5	-5.15	119.84	121.90
1	A	410	ARG	NE-CZ-NH2	-5.15	117.73	120.30
5	E	545	A	O4'-C1'-N9	5.14	112.31	108.20
8	H	185	LYS	N-CA-C	5.12	124.83	111.00
4	D	99	C	N3-C4-C5	-5.12	119.85	121.90
7	G	1913	C	N3-C4-C5	-5.11	119.86	121.90
4	D	46	G	O4'-C1'-N9	5.10	112.28	108.20
12	L	85	VAL	C-N-CA	5.10	134.46	121.70
4	D	89	A	C5-C6-N1	-5.10	115.15	117.70
15	O	22	PRO	N-CA-C	5.08	125.32	112.10
4	D	70	G	O4'-C1'-N9	5.07	112.26	108.20
4	D	66	A	C5-C6-N6	-5.07	119.64	123.70
4	D	63	G	O4'-C1'-N9	5.05	112.24	108.20
4	D	53	A	O4'-C1'-N9	5.04	112.23	108.20
9	I	56	ARG	CA-C-N	5.04	128.30	117.20
4	D	92	A	C5-C6-N6	-5.04	119.67	123.70
4	D	52	A	C5-C6-N1	-5.04	115.18	117.70
5	E	532	A	C5-C6-N1	-5.03	115.18	117.70
8	H	105	THR	C-N-CA	5.03	134.28	121.70
4	D	41	A	C5-C6-N1	-5.03	115.19	117.70
5	E	549	A	C5-C6-N1	-5.02	115.19	117.70
9	I	66	SER	C-N-CA	5.02	134.24	121.70
5	E	530	A	C5-C6-N1	-5.01	115.19	117.70
4	D	83	C	C6-N1-C1'	-5.01	114.79	120.80
4	D	72	A	C5-C6-N1	-5.01	115.19	117.70
15	O	31	THR	C-N-CA	5.01	134.22	121.70
4	D	72	A	O4'-C1'-N9	5.01	112.20	108.20
13	M	25	PHE	CB-CG-CD1	-5.00	117.30	120.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	LEU	Peptide
1	A	262	TYR	Sidechain
1	A	407	LEU	Peptide
4	D	55	U	Sidechain
4	D	60	U	Sidechain
8	H	209	TYR	Sidechain
8	H	92	ASN	Peptide
9	I	122	ALA	Peptide
12	L	94	SER	Peptide
14	N	38	ARG	Peptide
14	N	40	SER	Peptide
15	O	23	LEU	Peptide
15	O	24	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3770	0	3941	4	0
2	B	472	0	519	1	0
3	C	162	0	177	0	0
4	D	1347	0	678	0	0
5	E	740	0	369	1	0
6	F	536	0	272	0	0
7	G	379	0	195	0	0
8	H	2039	0	2106	7	0
9	I	1212	0	1231	2	0
10	J	410	0	452	0	0
11	K	663	0	699	0	0
12	L	1002	0	1093	2	0
13	M	706	0	741	0	0
14	N	547	0	613	2	0
15	O	316	0	349	0	0
All	All	14301	0	13435	19	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 1.

All (19) 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)
5:E:539:U:H3	5:E:546:G:H1	1.46	0.61
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.86	0.57
8:H:74:ILE:H	8:H:75:PRO:HA	1.76	0.50
1:A:410:ARG:HH22	1:A:412:GLU:HG3	1.79	0.48
2:B:76:ARG:HA	2:B:76:ARG:HE	1.81	0.46
8:H:55:LYS:HD3	8:H:55:LYS:H	1.80	0.45
8:H:57:GLY:HA3	8:H:58:HIS:HB2	1.99	0.44
14:N:39:PRO:HB2	14:N:40:SER:C	2.38	0.44
9:I:66:SER:HA	9:I:67:ILE:HG22	1.99	0.44
8:H:87:GLN:HA	8:H:87:GLN:HE21	1.83	0.43
9:I:56:ARG:HB3	9:I:57:ALA:HB3	2.01	0.43
1:A:65:ILE:HD12	1:A:68:LEU:HD12	2.01	0.42
1:A:22:LEU:HB2	1:A:23:PRO:HD2	2.01	0.42
8:H:58:HIS:CG	8:H:58:HIS:O	2.73	0.42
8:H:83:GLY:HA3	8:H:84:ARG:HB2	2.01	0.41
12:L:56:VAL:HG22	12:L:106:ILE:HG22	2.01	0.41
12:L:57:LEU:HD12	12:L:107:THR:HG23	2.02	0.41
1:A:342:VAL:HB	1:A:343:PRO:HD2	2.03	0.40
14:N:37:SER:N	14:N:38:ARG:HA	2.36	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 PDB entries followed by that with respect to all EM entries.

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	
1	A	488/490 (100%)	434 (89%)	37 (8%)	17 (4%)	4	39
2	B	58/80 (72%)	55 (95%)	3 (5%)	0	100	100
3	C	19/87 (22%)	17 (90%)	1 (5%)	1 (5%)	2	29
8	H	267/362 (74%)	187 (70%)	47 (18%)	33 (12%)	0	8
9	I	151/184 (82%)	114 (76%)	27 (18%)	10 (7%)	1	24
10	J	51/189 (27%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	81/142 (57%)	72 (89%)	6 (7%)	3 (4%)	4	38
12	L	125/127 (98%)	101 (81%)	12 (10%)	12 (10%)	1	15
13	M	82/113 (73%)	65 (79%)	11 (13%)	6 (7%)	1	21
14	N	67/120 (56%)	61 (91%)	2 (3%)	4 (6%)	2	26
15	O	35/51 (69%)	25 (71%)	5 (14%)	5 (14%)	0	6
All	All	1424/1945 (73%)	1180 (83%)	153 (11%)	91 (6%)	3	25

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	148	VAL
1	A	277	ALA
1	A	411	ARG
1	A	413	GLN
1	A	449	LYS
8	H	3	ARG
8	H	28	ALA
8	H	55	LYS
8	H	58	HIS
8	H	60	THR
8	H	64	SER
8	H	74	ILE
8	H	102	PRO
8	H	146	PRO
8	H	199	TRP
8	H	215	ILE
8	H	222	VAL
8	H	244	LEU
9	I	67	ILE
9	I	123	PRO
12	L	23	PRO
12	L	24	SER
12	L	85	VAL
13	M	24	SER
13	M	26	LYS
13	M	79	ARG
14	N	14	LYS
14	N	39	PRO
15	O	22	PRO

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Mol	Chain	Res	Type
15	O	23	LEU
1	A	24	PHE
1	A	61	VAL
1	A	67	PHE
1	A	276	ARG
1	A	446	LEU
8	H	89	ALA
8	H	98	ARG
8	H	103	THR
8	H	107	ARG
8	H	110	ASN
8	H	132	ALA
8	H	173	GLY
8	H	264	SER
9	I	25	SER
9	I	37	ASN
9	I	54	HIS
9	I	113	TYR
11	K	62	VAL
12	L	6	LEU
12	L	11	ASP
12	L	45	ILE
12	L	87	LYS
12	L	96	PRO
13	M	78	LYS
14	N	4	VAL
14	N	37	SER
15	O	35	ILE
1	A	101	LYS
1	A	226	SER
1	A	487	PRO
1	A	489	ALA
3	C	60	ASP
8	H	54	GLU
8	H	70	ALA
8	H	96	GLY
8	H	187	LEU
8	H	253	ALA
9	I	71	ALA
9	I	107	LEU
12	L	36	SER
12	L	46	LYS

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Mol	Chain	Res	Type
12	L	86	THR
13	M	25	PHE
13	M	90	PHE
15	O	6	SER
15	O	34	THR
1	A	410	ARG
8	H	101	ALA
8	H	131	VAL
8	H	200	THR
8	H	262	TRP
9	I	143	PRO
11	K	109	LYS
1	A	346	PRO
11	K	131	ASP
12	L	97	ILE
8	H	196	ASN
8	H	212	ASP
9	I	39	TRP
8	H	86	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	412/412 (100%)	388 (94%)	24 (6%)	25	61
2	B	50/67 (75%)	48 (96%)	2 (4%)	38	71
3	C	19/73 (26%)	18 (95%)	1 (5%)	28	64
8	H	209/288 (73%)	188 (90%)	21 (10%)	9	38
9	I	124/146 (85%)	113 (91%)	11 (9%)	12	44
10	J	44/154 (29%)	42 (96%)	2 (4%)	34	69
11	K	74/118 (63%)	71 (96%)	3 (4%)	37	71
12	L	110/110 (100%)	100 (91%)	10 (9%)	12	43
13	M	74/97 (76%)	67 (90%)	7 (10%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	62/105 (59%)	57 (92%)	5 (8%)	15	50
15	O	33/46 (72%)	30 (91%)	3 (9%)	12	43
All	All	1211/1616 (75%)	1122 (93%)	89 (7%)	22	54

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	24	PHE
1	A	26	LYS
1	A	47	GLN
1	A	75	GLU
1	A	80	LEU
1	A	121	LYS
1	A	128	TYR
1	A	148	VAL
1	A	154	ASN
1	A	175	PHE
1	A	188	VAL
1	A	194	VAL
1	A	268	VAL
1	A	305	TYR
1	A	309	PHE
1	A	403	GLN
1	A	410	ARG
1	A	412	GLU
1	A	413	GLN
1	A	414	ASN
1	A	449	LYS
1	A	480	LEU
1	A	484	LEU
2	B	52	LYS
2	B	76	ARG
3	C	64	VAL
8	H	35	VAL
8	H	43	ASN
8	H	46	LYS
8	H	48	GLN
8	H	90	PHE
8	H	98	ARG
8	H	102	PRO

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Mol	Chain	Res	Type
8	H	103	THR
8	H	112	LYS
8	H	119	ARG
8	H	140	HIS
8	H	145	ILE
8	H	159	ILE
8	H	161	LYS
8	H	164	GLU
8	H	170	LYS
8	H	193	LYS
8	H	201	GLN
8	H	233	LEU
8	H	243	HIS
8	H	244	LEU
9	I	3	ARG
9	I	36	ILE
9	I	67	ILE
9	I	72	GLN
9	I	79	THR
9	I	80	LYS
9	I	94	LEU
9	I	105	LYS
9	I	108	ASP
9	I	112	LEU
9	I	144	SER
10	J	1	MET
10	J	53	LYS
11	K	65	GLN
11	K	74	LYS
11	K	100	LYS
12	L	37	LYS
12	L	52	ARG
12	L	57	LEU
12	L	64	LYS
12	L	78	PHE
12	L	86	THR
12	L	87	LYS
12	L	88	GLU
12	L	122	LYS
12	L	125	LYS
13	M	28	ARG
13	M	38	LYS

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Mol	Chain	Res	Type
13	M	47	ASP
13	M	62	ARG
13	M	77	ARG
13	M	82	GLU
13	M	86	LYS
14	N	5	LYS
14	N	9	LEU
14	N	23	ASP
14	N	34	GLN
14	N	63	ARG
15	O	17	LYS
15	O	22	PRO
15	O	26	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	403	GLN
1	A	414	ASN
8	H	87	GLN
11	K	111	ASN
11	K	117	ASN
12	L	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63 (98%)	22 (35%)	9 (14%)
5	E	33/34 (97%)	7 (21%)	2 (6%)
6	F	24/25 (96%)	0	0
7	G	17/18 (94%)	1 (5%)	0
All	All	136/140 (97%)	30 (22%)	11 (8%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	49	G
4	D	56	G
4	D	59	A

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Mol	Chain	Res	Type
4	D	62	C
4	D	63	G
4	D	64	U
4	D	66	A
4	D	68	G
4	D	70	G
4	D	82	U
4	D	83	C
4	D	84	C
4	D	85	G
4	D	86	U
4	D	87	G
4	D	88	A
4	D	90	U
4	D	91	C
4	D	92	A
4	D	94	C
4	D	97	A
4	D	98	U
5	E	533	A
5	E	534	G
5	E	556	A
5	E	557	A
5	E	558	G
5	E	560	A
5	E	561	C
7	G	1922	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	55	U
4	D	63	G
4	D	65	A
4	D	69	U
4	D	89	A
4	D	90	U
4	D	93	U
4	D	96	A
5	E	532	A
5	E	560	A

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](#)

There are no ligands in this entry.

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.