



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 2WWB
EMDB ID: : EMD-1651
Title : CRYO-EM STRUCTURE OF THE MAMMALIAN SEC61 COMPLEX
BOUND TO THE ACTIVELY TRANSLATING WHEAT GERM 80S RI-
BOSOME
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 : 6.48 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>

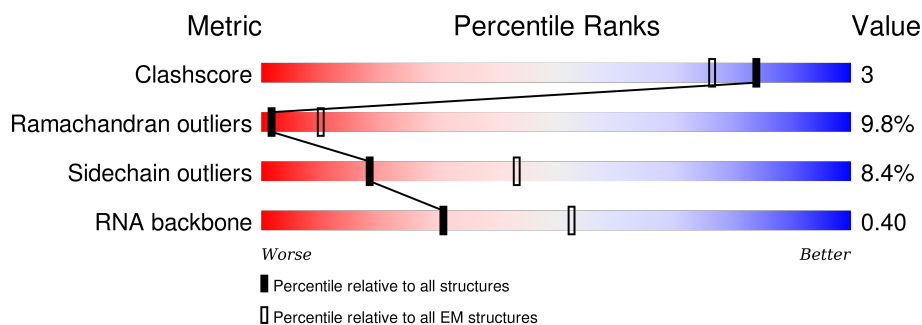
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance

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

The reported resolution of this entry is 6.48 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	476	88% 9% ..
2	B	68	90% 9% .
3	C	96	34% .. 63%
4	D	63	. 38% 51% 10%
5	E	34	53% 44% .
6	F	25	72% 28%
7	G	14	36% 64%
8	H	362	48% 16% 9% . 26%

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Mol	Chain	Length	Quality of chain
9	I	184	<div><div></div><div>57%19%6%17%</div></div>
10	J	189	<div><div></div><div>26%72%</div></div>
11	K	142	<div><div></div><div>47%9%42%</div></div>
12	L	127	<div><div></div><div>74%19%6%</div></div>
13	M	113	<div><div></div><div>58%12%26%</div></div>
14	N	120	<div><div></div><div>44%9%43%</div></div>
15	O	51	<div><div></div><div>33%31%27%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 14313 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 PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3675	2409	591	650	25		

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	68	Total	C	N	O	S	0	0
			543	355	94	89	5		

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	36	Total	C	N	O	S	0	0
			281	188	44	47	2		

- Molecule 4 is a RNA chain called 5.8S 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	14	Total	C	N	O	P	0	0
			296	133	54	96	13		

- 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		

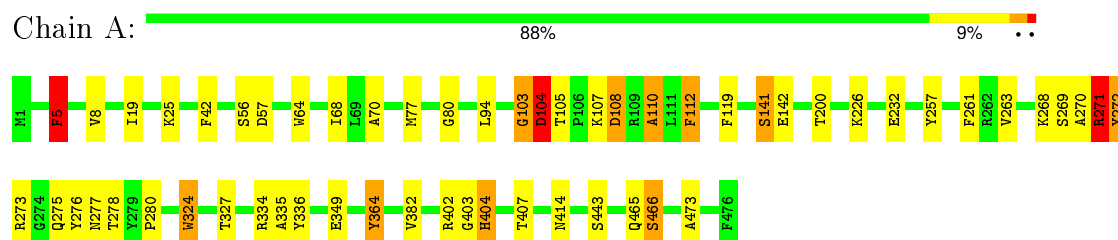
- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

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

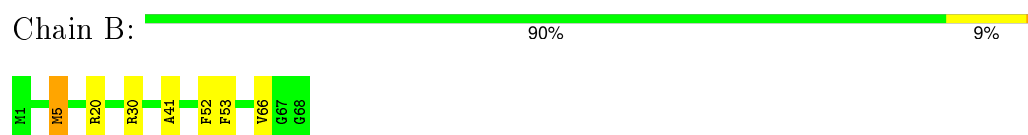
3 Residue-property plots

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.

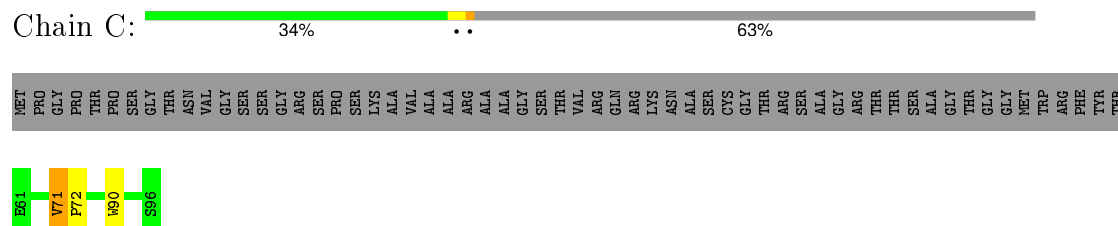
• Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1



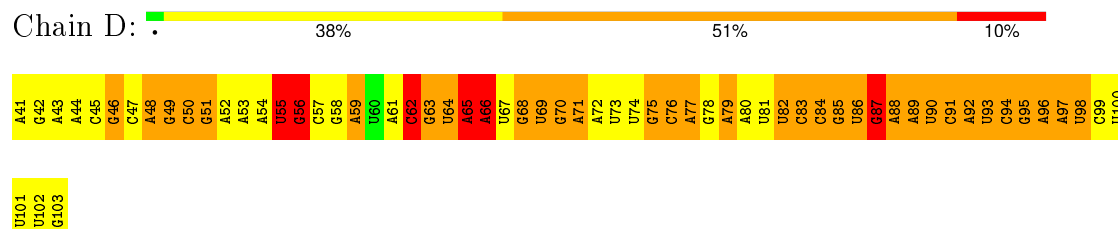
• Molecule 2: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA



• Molecule 3: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA



• Molecule 4: 5.8S RRNA



• Molecule 5: 25S RRNA

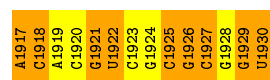




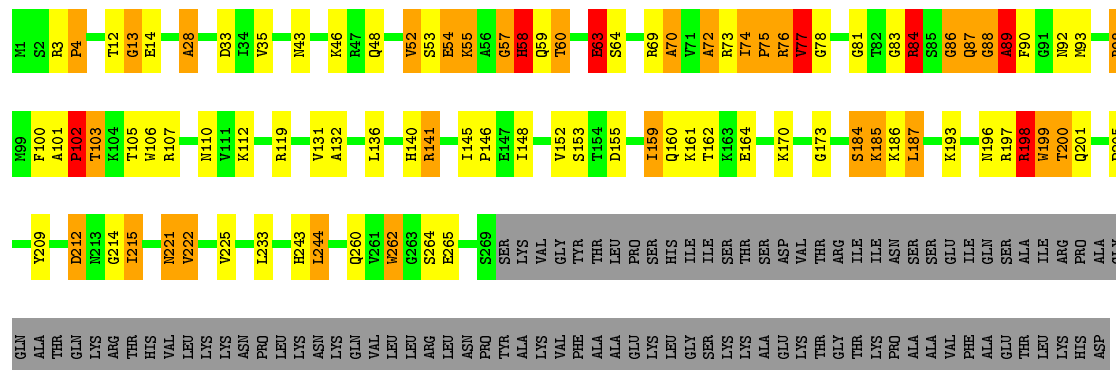
- Molecule 6: 25S RRNA



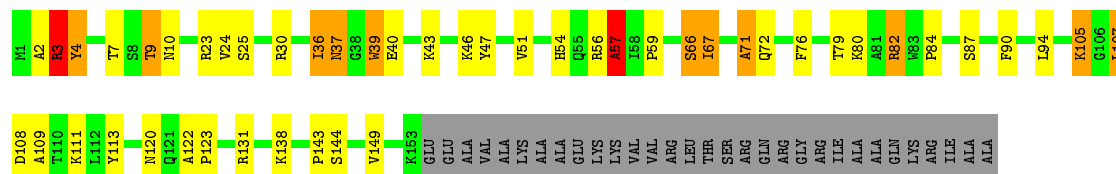
- Molecule 7: 25S RRNA



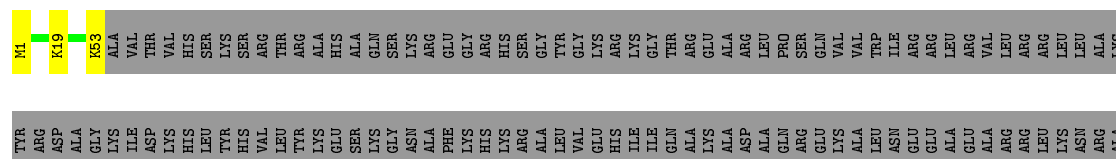
- Molecule 8: 60S RIBOSOMAL PROTEIN L4-B



- Molecule 9: 60S RIBOSOMAL PROTEIN L17-A



- Molecule 10: 60S RIBOSOMAL PROTEIN L19



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

• Molecule 11: 60S RIBOSOMAL PROTEIN L25

Chain K:  47% 9% 42%

MET ALA
ALA PRO
SER SER
LYS ALA
ALA ALA
THR THR
ALA ALA
LYS LYS
LYS LYS
VAL VAL
VAL VAL
LYS LYS
GLY THR
ASN ASN
GLY GLY
LYS LYS
LYS LYS
LEU LEU
LYS LYS
VAL VAL
ARG ARG
THR THR
SER SER
GLY GLY
ALA ALA
PHE PHE
ARG ARG
LEU LEU
PRO PRO
LYS LYS
THR THR
LEU LEU
LYS LYS
ALA ALA
ARG ARG
ALA ALA
PRO PRO
LYS LYS
TYR TYR
ALA ALA
SER SER
LYS LYS
ALA ALA
VAL VAL
PRO PRO
HIS HIS
TYR TYR
ASN ASN
ARG ARG
L57 L57
V60 V60
P61 P61

V62 V62
Q65 Q65
E70 E70
K74 K74
K100 K100
V105 V105
D106 D106
K109 K109
V110 V110
N111 N111
R115 R115
P116 P116
N117 N117
Y123 Y123
D131 D131
M137 M137
R138 R138
I139 I139
GLY GLY
TYR TYR
ILE ILE

• Molecule 12: 60S RIBOSOMAL PROTEIN L26-A

Chain L:  74% 19% 6%

M1 M1
L6 L6
S10 S10
D11 D11
P23 P23
R28 R28
S36 S36
K37 K37
R40 R40
I45 I45
K46 K46
R52 R52
V56 V56
L57 L57
K64 K64
K77 K77
F78 F78
D83 D83
K84 K84
V85 V85
T86 T86
K87 K87
P96 P96
I97 I97
N98 N98
I106 I106
T107 T107
K108 K108
L111 L111
D112 D112
K113 K113
K116 K116
R121 R121
K122 K122
G123 G123
G124 G124
K125 K125
L126 L126
E127 E127

• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A

Chain M:  58% 12% 26%

MET MET
ALA ALA
GLY GLY
LEU LEU
LYS LYS
ASP ASP
VAL VAL
VAL VAL
T9 T9
R10 R10
S24 S24
F25 F25
K26 K26
K38 K38
D47 D47
L51 L51
R62 R62
V64 V64
V67 V67
E68 E68
V69 V69
R74 R74
R77 R77
K78 K78
R79 R79
E82 E82
K86 K86
F90 F90
S91 S91
Y92 Y92
VAL VAL
GLU GLU
PRO PRO
VAL VAL
LEU LEU
ARG ARG
ALA ALA
SER SER
LYS LYS
PHE PHE
GLY GLY
LEU LEU
GLN GLN
THR THR
VAL VAL
VAL VAL
GLU GLU

GLU
ASP
ALA

• Molecule 14: 60S RIBOSOMAL PROTEIN L35

Chain N:  44% 9% 43%

M1 M1
A2 A2
G3 G3
V4 V4
K5 K5
L9 L9
S13 S13
K14 K14
K32 K32
V33 V33
Q34 Q34
S37 S37
R38 R38
P39 P39
S40 S40
L41 L41
I44 I44
R67 R67
Q68 Q68
L69 L69
TYR TYR
LYS LYS
GLY GLY
LYS LYS
LYS LYS
TYR TYR
GLN GLN
PRO PRO
LYS LYS
ASP ASP
LEU LEU
ARG ARG
ALA ALA
LYS LYS
LYS LYS
THR THR
ARG ARG
ALA ALA
LEU LEU
ARG ARG
VAL VAL
ALA ALA
SER SER
LYS LYS
PHE PHE
GLU GLU
ALA ALA
SER SER
GLN GLN
VAL VAL
THR THR
LYS LYS

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

• Molecule 15: 60S RIBOSOMAL PROTEIN L39

Chain O:  33% 31% 27%

M1 M1
Q4 Q4
K5 K5
S6 S6
F7 F7
K17 K17
K18 K18
Q19 Q19
N20 N20
R21 R21
P22 P22
L23 L23
P24 P24
Q25 Q25
V26 V26
I27 I27
R30 R30
T31 T31
N32 N32
H33 H33
T34 T34
I35 I35
R36 R36
Y37 Y37
ASN ASN
ALA ALA
LYS LYS
ARG ARG
ARG ARG
ASN ASN
TRP TRP
ARG ARG
ARG ARG
THR THR
LYS LYS
MET MET
ASN ASN
ILE 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	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	4700	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	1.89	8/3755 (0.2%)	1.10	22/5089 (0.4%)
10	J	1.01	0/412	0.97	0/551
11	K	0.90	0/670	1.17	3/903 (0.3%)
12	L	1.02	0/1013	1.30	6/1351 (0.4%)
13	M	1.10	0/719	1.35	6/959 (0.6%)
14	N	1.05	1/549 (0.2%)	1.42	8/733 (1.1%)
15	O	1.10	0/321	1.45	4/426 (0.9%)
2	B	0.94	0/553	1.12	2/738 (0.3%)
3	C	0.86	0/289	1.10	0/391
4	D	1.62	5/1508 (0.3%)	2.64	188/2348 (8.0%)
5	E	1.67	2/833 (0.2%)	2.72	115/1298 (8.9%)
6	F	1.64	0/599	2.49	73/932 (7.8%)
7	G	1.70	2/330 (0.6%)	2.56	42/513 (8.2%)
8	H	1.00	0/2079	1.46	33/2817 (1.2%)
9	I	1.03	0/1235	1.43	17/1662 (1.0%)
All	All	1.43	18/14865 (0.1%)	1.71	519/20711 (2.5%)

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	5
11	K	0	3
12	L	0	5
13	M	0	2
14	N	0	2
15	O	0	7
3	C	0	1
4	D	0	10
5	E	0	6
6	F	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	12
9	I	0	6
All	All	0	63

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ASP	N-CA	81.65	3.09	1.46
1	A	5	PHE	CG-CD2	29.16	1.82	1.38
1	A	5	PHE	CG-CD1	28.74	1.81	1.38
1	A	5	PHE	CE1-CZ	22.75	1.80	1.37
1	A	5	PHE	CE2-CZ	22.22	1.79	1.37
1	A	5	PHE	CD2-CE2	21.21	1.81	1.39
1	A	5	PHE	CD1-CE1	20.69	1.80	1.39
14	N	69	LEU	C-O	-12.08	1.00	1.23
4	D	53	A	N7-C5	-5.46	1.35	1.39
1	A	104	ASP	CA-CB	5.38	1.65	1.53
5	E	544	A	N7-C5	-5.34	1.36	1.39
4	D	100	U	C2-N3	5.32	1.41	1.37
4	D	75	G	C2-N3	5.26	1.36	1.32
7	G	1928	G	N1-C2	5.21	1.42	1.37
4	D	103	G	C2-N3	5.13	1.36	1.32
7	G	1924	G	N1-C2	5.09	1.41	1.37
4	D	101	U	C2-N3	5.06	1.41	1.37
5	E	548	G	N1-C2	5.04	1.41	1.37

All (519) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	532	A	P-O3'-C3'	17.86	141.14	119.70
4	D	90	U	P-O3'-C3'	14.96	137.65	119.70
4	D	93	U	P-O3'-C3'	14.57	137.18	119.70
4	D	69	U	P-O3'-C3'	14.40	136.98	119.70
4	D	53	A	N1-C6-N6	14.32	127.19	118.60
4	D	65	A	P-O3'-C3'	13.29	135.65	119.70
4	D	96	A	P-O3'-C3'	13.27	135.62	119.70
5	E	557	A	N1-C6-N6	13.12	126.47	118.60
5	E	530	A	N1-C6-N6	13.04	126.43	118.60
4	D	55	U	P-O3'-C3'	13.02	135.32	119.70
4	D	54	A	N1-C6-N6	12.98	126.39	118.60
5	E	543	A	N1-C6-N6	12.94	126.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	544	A	N1-C6-N6	12.91	126.35	118.60
6	F	1661	A	N1-C6-N6	12.83	126.30	118.60
4	D	41	A	N1-C6-N6	12.77	126.26	118.60
4	D	97	A	N1-C6-N6	12.73	126.24	118.60
5	E	533	A	N1-C6-N6	12.66	126.19	118.60
5	E	536	A	N1-C6-N6	12.58	126.15	118.60
6	F	1662	A	N1-C6-N6	12.50	126.10	118.60
4	D	52	A	N1-C6-N6	12.43	126.06	118.60
5	E	555	A	N1-C6-N6	12.43	126.06	118.60
4	D	44	A	N1-C6-N6	12.41	126.04	118.60
4	D	88	A	N1-C6-N6	12.10	125.86	118.60
5	E	549	A	N1-C6-N6	12.07	125.84	118.60
5	E	554	A	N1-C6-N6	12.02	125.81	118.60
6	F	1667	A	N1-C6-N6	11.98	125.79	118.60
5	E	531	A	N1-C6-N6	11.98	125.79	118.60
5	E	545	A	N1-C6-N6	11.96	125.78	118.60
6	F	1673	A	N1-C6-N6	11.92	125.75	118.60
4	D	80	A	N1-C6-N6	11.92	125.75	118.60
4	D	65	A	N1-C6-N6	11.89	125.73	118.60
5	E	556	A	N1-C6-N6	11.88	125.73	118.60
5	E	535	A	N1-C6-N6	11.80	125.68	118.60
5	E	553	A	N1-C6-N6	11.77	125.66	118.60
5	E	560	A	N1-C6-N6	11.73	125.64	118.60
4	D	71	A	N1-C6-N6	11.64	125.58	118.60
4	D	72	A	N1-C6-N6	11.62	125.57	118.60
5	E	542	A	N1-C6-N6	11.62	125.57	118.60
4	D	66	A	N1-C6-N6	11.60	125.56	118.60
7	G	1926	G	P-O3'-C3'	11.54	133.55	119.70
5	E	547	A	N1-C6-N6	11.52	125.51	118.60
4	D	61	A	N1-C6-N6	11.48	125.49	118.60
4	D	89	A	N1-C6-N6	11.40	125.44	118.60
4	D	96	A	N1-C6-N6	11.32	125.39	118.60
4	D	79	A	N1-C6-N6	11.31	125.39	118.60
7	G	1917	A	N1-C6-N6	11.22	125.33	118.60
4	D	43	A	N1-C6-N6	11.07	125.24	118.60
4	D	48	A	N1-C6-N6	11.02	125.21	118.60
6	F	1664	A	N1-C6-N6	11.00	125.20	118.60
7	G	1919	A	N1-C6-N6	10.98	125.19	118.60
6	F	1667	A	P-O3'-C3'	10.89	132.77	119.70
4	D	63	G	P-O3'-C3'	10.81	132.67	119.70
4	D	59	A	N1-C6-N6	10.69	125.02	118.60
4	D	92	A	N1-C6-N6	10.66	124.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	89	A	P-O3'-C3'	10.42	132.21	119.70
6	F	1678	G	N1-C6-O6	10.32	126.09	119.90
5	E	560	A	P-O3'-C3'	10.31	132.08	119.70
4	D	63	G	N1-C6-O6	10.01	125.90	119.90
4	D	77	A	N1-C6-N6	9.95	124.57	118.60
6	F	1677	G	N1-C6-O6	9.93	125.86	119.90
6	F	1656	A	N1-C6-N6	9.88	124.53	118.60
1	A	104	ASP	N-CA-CB	9.83	128.30	110.60
6	F	1668	G	N1-C6-O6	9.82	125.80	119.90
7	G	1928	G	N1-C6-O6	9.80	125.78	119.90
7	G	1917	A	P-O3'-C3'	9.78	131.44	119.70
1	A	103	GLY	C-N-CA	9.68	145.91	121.70
5	E	532	A	N1-C6-N6	9.59	124.35	118.60
7	G	1929	G	N1-C6-O6	9.58	125.65	119.90
5	E	534	G	N1-C6-O6	9.57	125.64	119.90
5	E	558	G	N1-C6-O6	9.54	125.62	119.90
5	E	552	G	N1-C6-O6	9.40	125.54	119.90
4	D	56	G	N1-C6-O6	9.36	125.51	119.90
4	D	49	G	N1-C6-O6	9.34	125.50	119.90
5	E	548	G	N1-C6-O6	9.33	125.50	119.90
7	G	1921	G	N1-C6-O6	9.25	125.45	119.90
4	D	58	G	N1-C6-O6	9.22	125.43	119.90
5	E	546	G	N1-C6-O6	9.19	125.42	119.90
9	I	56	ARG	C-N-CA	9.18	144.64	121.70
4	D	103	G	N1-C6-O6	9.16	125.39	119.90
7	G	1922	U	O4'-C1'-N1	9.15	115.52	108.20
5	E	529	G	N1-C6-O6	9.15	125.39	119.90
6	F	1658	G	N1-C6-O6	9.14	125.38	119.90
6	F	1675	G	N1-C6-O6	9.12	125.38	119.90
6	F	1672	G	N1-C6-O6	9.07	125.34	119.90
5	E	550	G	N1-C6-O6	9.06	125.34	119.90
4	D	78	G	N1-C6-O6	8.92	125.25	119.90
6	F	1665	G	N1-C6-O6	8.78	125.17	119.90
4	D	92	A	O4'-C1'-N9	8.74	115.19	108.20
4	D	42	G	N1-C6-O6	8.73	125.14	119.90
4	D	46	G	N1-C6-O6	8.72	125.13	119.90
4	D	87	G	N1-C6-O6	8.72	125.13	119.90
7	G	1926	G	N1-C6-O6	8.68	125.11	119.90
8	H	184	SER	C-N-CA	8.62	143.25	121.70
4	D	85	G	N1-C6-O6	8.57	125.05	119.90
5	E	541	G	N1-C6-O6	8.57	125.05	119.90
4	D	63	G	C5-C6-O6	-8.55	123.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1671	G	N1-C6-O6	8.54	125.02	119.90
9	I	56	ARG	CB-CA-C	8.48	127.35	110.40
4	D	68	G	N1-C6-O6	8.43	124.96	119.90
4	D	50	C	O4'-C1'-N1	8.39	114.91	108.20
6	F	1668	G	C5-C6-O6	-8.39	123.57	128.60
4	D	70	G	N1-C6-O6	8.34	124.90	119.90
5	E	558	G	C5-C6-O6	-8.34	123.60	128.60
4	D	102	U	O4'-C1'-N1	8.29	114.83	108.20
7	G	1924	G	N1-C6-O6	8.25	124.85	119.90
7	G	1925	C	O4'-C1'-N1	8.25	114.80	108.20
4	D	95	G	N1-C6-O6	8.23	124.84	119.90
4	D	62	C	O4'-C1'-N1	8.16	114.73	108.20
8	H	54	GLU	C-N-CA	8.16	142.09	121.70
6	F	1670	U	O4'-C1'-N1	8.14	114.72	108.20
4	D	69	U	O4'-C1'-N1	8.09	114.67	108.20
8	H	75	PRO	C-N-CA	8.07	141.88	121.70
6	F	1678	G	C5-C6-O6	-8.00	123.80	128.60
8	H	59	GLN	C-N-CA	7.97	141.63	121.70
4	D	45	C	O4'-C1'-N1	7.91	114.52	108.20
11	K	123	TYR	CB-CG-CD1	-7.84	116.30	121.00
4	D	90	U	O4'-C1'-N1	7.80	114.44	108.20
7	G	1928	G	C5-C6-O6	-7.70	123.98	128.60
4	D	51	G	N1-C6-O6	7.67	124.50	119.90
4	D	81	U	O4'-C1'-N1	7.62	114.30	108.20
4	D	101	U	O4'-C1'-N1	7.62	114.29	108.20
8	H	89	ALA	N-CA-CB	7.61	120.76	110.10
4	D	57	C	O4'-C1'-N1	7.59	114.27	108.20
1	A	104	ASP	CB-CA-C	-7.58	95.23	110.40
1	A	257	TYR	CB-CG-CD2	-7.58	116.45	121.00
5	E	534	G	C5-C6-O6	-7.56	124.06	128.60
6	F	1657	C	O4'-C1'-N1	7.48	114.18	108.20
7	G	1927	C	O4'-C1'-N1	7.47	114.17	108.20
8	H	60	THR	N-CA-CB	7.45	124.46	110.30
4	D	67	U	O4'-C1'-N1	7.45	114.16	108.20
6	F	1666	C	O4'-C1'-N1	7.42	114.13	108.20
5	E	536	A	C5-C6-N6	-7.38	117.79	123.70
6	F	1677	G	C5-C6-O6	-7.37	124.18	128.60
9	I	36	ILE	C-N-CA	7.37	140.12	121.70
4	D	56	G	O4'-C1'-N9	7.34	114.07	108.20
6	F	1663	C	O4'-C1'-N1	7.27	114.01	108.20
4	D	96	A	O4'-C1'-N9	7.26	114.01	108.20
5	E	540	U	O4'-C1'-N1	7.25	114.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1923	C	O4'-C1'-N1	7.25	114.00	108.20
4	D	53	A	C5-C6-N6	-7.24	117.91	123.70
6	F	1672	G	C5-C6-O6	-7.24	124.26	128.60
5	E	546	G	C5-C6-O6	-7.18	124.29	128.60
5	E	548	G	C5-C6-O6	-7.18	124.29	128.60
11	K	123	TYR	CB-CG-CD2	7.17	125.30	121.00
5	E	529	G	C5-C6-O6	-7.16	124.31	128.60
5	E	530	A	C5-C6-N6	-7.14	117.99	123.70
5	E	537	C	O4'-C1'-N1	7.14	113.91	108.20
4	D	76	C	N3-C4-N4	7.13	122.99	118.00
7	G	1924	G	C5-C6-O6	-7.12	124.33	128.60
4	D	85	G	C5-C6-O6	-7.12	124.33	128.60
5	E	552	G	C5-C6-O6	-7.12	124.33	128.60
4	D	65	A	O4'-C1'-N9	7.11	113.89	108.20
7	G	1919	A	O4'-C1'-N9	7.10	113.88	108.20
4	D	99	C	O4'-C1'-N1	7.09	113.88	108.20
4	D	98	U	O4'-C1'-N1	7.08	113.87	108.20
4	D	53	A	C4-C5-C6	7.05	120.53	117.00
4	D	91	C	O4'-C1'-N1	7.04	113.83	108.20
13	M	25	PHE	CB-CG-CD2	7.04	125.72	120.80
4	D	103	G	C5-C6-O6	-7.03	124.38	128.60
4	D	46	G	C5-C6-O6	-7.03	124.38	128.60
4	D	47	C	O4'-C1'-N1	7.02	113.81	108.20
6	F	1654	C	O4'-C1'-N1	7.02	113.81	108.20
6	F	1658	G	C5-C6-O6	-7.01	124.40	128.60
4	D	49	G	C5-C6-O6	-7.00	124.40	128.60
6	F	1674	C	O4'-C1'-N1	7.00	113.80	108.20
4	D	55	U	O4'-C1'-N1	6.98	113.78	108.20
7	G	1929	G	O4'-C1'-N9	6.95	113.76	108.20
4	D	93	U	O4'-C1'-N1	6.94	113.75	108.20
6	F	1675	G	C5-C6-O6	-6.94	124.44	128.60
5	E	544	A	C4-C5-C6	6.94	120.47	117.00
4	D	100	U	O4'-C1'-N1	6.94	113.75	108.20
4	D	68	G	C5-C6-O6	-6.92	124.44	128.60
4	D	78	G	C5-C6-O6	-6.90	124.46	128.60
7	G	1930	U	O4'-C1'-N1	6.89	113.72	108.20
5	E	539	U	O4'-C1'-N1	6.86	113.69	108.20
4	D	62	C	C6-N1-C1'	-6.86	112.57	120.80
4	D	62	C	C2-N1-C1'	6.85	126.34	118.80
9	I	71	ALA	N-CA-CB	6.84	119.67	110.10
4	D	91	C	N3-C4-C5	-6.84	119.17	121.90
4	D	64	U	O4'-C1'-N1	6.83	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1659	U	O4'-C1'-N1	6.83	113.66	108.20
8	H	75	PRO	CA-C-N	6.82	132.19	117.20
4	D	87	G	C5-C6-O6	-6.79	124.53	128.60
7	G	1929	G	C5-C6-O6	-6.78	124.53	128.60
1	A	5	PHE	CB-CG-CD1	-6.76	116.07	120.80
6	F	1671	G	C5-C6-O6	-6.75	124.55	128.60
12	L	84	LYS	C-N-CA	6.75	138.56	121.70
8	H	72	ALA	N-CA-CB	6.74	119.54	110.10
7	G	1926	G	C5-C6-O6	-6.74	124.56	128.60
6	F	1656	A	O4'-C1'-N9	6.73	113.58	108.20
5	E	528	U	O4'-C1'-N1	6.72	113.58	108.20
6	F	1661	A	C4-C5-C6	6.72	120.36	117.00
6	F	1655	C	O4'-C1'-N1	6.71	113.57	108.20
5	E	541	G	O4'-C1'-N9	6.71	113.57	108.20
1	A	257	TYR	CB-CG-CD1	6.70	125.02	121.00
4	D	82	U	O4'-C1'-N1	6.70	113.56	108.20
5	E	537	C	N3-C4-C5	-6.68	119.23	121.90
14	N	67	ARG	NE-CZ-NH2	6.68	123.64	120.30
5	E	538	U	O4'-C1'-N1	6.67	113.54	108.20
4	D	58	G	C5-C6-O6	-6.67	124.60	128.60
8	H	86	GLY	C-N-CA	6.66	138.36	121.70
13	M	25	PHE	CB-CG-CD1	-6.66	116.14	120.80
5	E	551	U	O4'-C1'-N1	6.64	113.51	108.20
5	E	548	G	O4'-C1'-N9	6.62	113.50	108.20
4	D	95	G	C5-C6-O6	-6.61	124.63	128.60
5	E	550	G	C5-C6-O6	-6.59	124.64	128.60
7	G	1921	G	C5-C6-O6	-6.59	124.64	128.60
4	D	72	A	C4-C5-C6	6.59	120.30	117.00
5	E	541	G	C5-C6-O6	-6.58	124.65	128.60
5	E	549	A	C4-C5-C6	6.58	120.29	117.00
6	F	1671	G	O4'-C1'-N9	6.57	113.46	108.20
6	F	1665	G	C5-C6-O6	-6.57	124.66	128.60
4	D	41	A	C5-C6-N6	-6.55	118.46	123.70
5	E	531	A	C5-C6-N1	-6.55	114.42	117.70
6	F	1675	G	O4'-C1'-N9	6.46	113.36	108.20
14	N	39	PRO	C-N-CA	6.45	137.82	121.70
5	E	543	A	C4-C5-C6	6.42	120.21	117.00
4	D	70	G	C5-C6-O6	-6.42	124.75	128.60
4	D	42	G	C5-C6-O6	-6.41	124.75	128.60
8	H	87	GLN	N-CA-C	6.40	128.29	111.00
12	L	10	SER	C-N-CA	6.40	137.69	121.70
4	D	44	A	C5-C6-N6	-6.39	118.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	43	A	O4'-C1'-N9	6.37	113.30	108.20
9	I	37	ASN	N-CA-CB	6.37	122.07	110.60
13	M	77	ARG	C-N-CA	6.37	137.61	121.70
6	F	1662	A	C5-C6-N6	-6.36	118.61	123.70
9	I	90	PHE	CB-CG-CD1	6.35	125.25	120.80
7	G	1926	G	O4'-C1'-N9	6.35	113.28	108.20
4	D	52	A	C4-C5-C6	6.35	120.18	117.00
4	D	52	A	C5-C6-N6	-6.35	118.62	123.70
4	D	83	C	C2-N1-C1'	6.34	125.77	118.80
4	D	76	C	O4'-C1'-N1	6.32	113.25	108.20
4	D	56	G	C5-C6-O6	-6.31	124.81	128.60
8	H	84	ARG	N-CA-CB	6.29	121.92	110.60
4	D	72	A	C5-C6-N1	-6.28	114.56	117.70
5	E	542	A	C4-C5-C6	6.28	120.14	117.00
4	D	61	A	C5-C6-N1	-6.28	114.56	117.70
4	D	83	C	O4'-C1'-N1	6.27	113.21	108.20
6	F	1654	C	N3-C4-N4	6.25	122.37	118.00
6	F	1674	C	N3-C4-N4	6.24	122.37	118.00
5	E	553	A	C4-C5-C6	6.24	120.12	117.00
13	M	24	SER	N-CA-CB	6.23	119.85	110.50
8	H	102	PRO	N-CA-C	6.22	128.28	112.10
4	D	73	U	O4'-C1'-N1	6.22	113.17	108.20
1	A	364	TYR	CB-CG-CD2	-6.22	117.27	121.00
9	I	39	TRP	N-CA-CB	6.21	121.78	110.60
4	D	92	A	C4-C5-C6	6.21	120.11	117.00
5	E	533	A	C4-C5-C6	6.20	120.10	117.00
4	D	89	A	C4-C5-C6	6.20	120.10	117.00
8	H	185	LYS	N-CA-C	6.18	127.69	111.00
8	H	63	GLU	N-CA-C	-6.17	94.33	111.00
4	D	79	A	C4-C5-C6	6.17	120.08	117.00
5	E	557	A	C4-C5-C6	6.17	120.08	117.00
4	D	75	G	N1-C6-O6	6.17	123.60	119.90
7	G	1920	C	P-O3'-C3'	6.16	127.09	119.70
4	D	66	A	O4'-C1'-N9	6.15	113.12	108.20
4	D	88	A	C5-C6-N1	-6.15	114.62	117.70
5	E	560	A	C4-C5-C6	6.14	120.07	117.00
5	E	545	A	P-O3'-C3'	6.14	127.07	119.70
6	F	1667	A	C4-C5-C6	6.14	120.07	117.00
8	H	214	GLY	C-N-CA	6.13	137.02	121.70
4	D	41	A	C4-C5-C6	6.11	120.06	117.00
5	E	555	A	C4-C5-C6	6.11	120.06	117.00
5	E	533	A	C5-C6-N1	-6.11	114.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	42	G	O4'-C1'-N9	6.11	113.09	108.20
4	D	65	A	C4-C5-C6	6.10	120.05	117.00
4	D	89	A	O4'-C1'-N9	6.09	113.08	108.20
8	H	58	HIS	N-CA-CB	6.09	121.57	110.60
4	D	54	A	C5-C6-N1	-6.08	114.66	117.70
9	I	56	ARG	CA-C-N	6.08	130.58	117.20
4	D	61	A	C4-C5-C6	6.08	120.04	117.00
5	E	546	G	O4'-C1'-N9	6.08	113.06	108.20
6	F	1676	U	O4'-C1'-N1	6.07	113.06	108.20
4	D	50	C	N3-C4-C5	-6.07	119.47	121.90
5	E	544	A	C5-C6-N6	-6.07	118.85	123.70
9	I	90	PHE	CB-CG-CD2	-6.07	116.55	120.80
5	E	557	A	C5-C6-N1	-6.06	114.67	117.70
5	E	557	A	C5-C6-N6	-6.06	118.85	123.70
6	F	1654	C	N3-C4-C5	-6.05	119.48	121.90
4	D	88	A	C4-C5-C6	6.05	120.03	117.00
5	E	561	C	O4'-C1'-N1	6.05	113.04	108.20
1	A	104	ASP	N-CA-C	6.04	127.31	111.00
8	H	55	LYS	N-CA-C	6.04	127.31	111.00
4	D	49	G	O4'-C1'-N9	6.03	113.03	108.20
4	D	57	C	N3-C4-N4	6.03	122.22	118.00
5	E	556	A	C4-C5-C6	6.02	120.01	117.00
4	D	74	U	O4'-C1'-N1	6.02	113.02	108.20
5	E	534	G	O4'-C1'-N9	6.02	113.01	108.20
5	E	543	A	C5-C6-N1	-6.02	114.69	117.70
5	E	547	A	C5-C6-N1	-6.02	114.69	117.70
6	F	1673	A	C5-C6-N6	-6.02	118.89	123.70
4	D	59	A	C4-C5-C6	6.01	120.01	117.00
4	D	54	A	O4'-C1'-N9	6.01	113.01	108.20
5	E	535	A	C4-C5-C6	6.01	120.00	117.00
9	I	105	LYS	C-N-CA	6.01	134.92	122.30
15	O	7	PHE	CB-CG-CD1	6.01	125.01	120.80
15	O	5	LYS	CB-CA-C	6.00	122.39	110.40
5	E	543	A	C5-C6-N6	-5.99	118.91	123.70
4	D	84	C	N3-C4-N4	5.99	122.19	118.00
5	E	555	A	C5-C6-N6	-5.99	118.91	123.70
1	A	119	PHE	CB-CG-CD1	5.98	124.98	120.80
6	F	1655	C	N3-C4-C5	-5.97	119.51	121.90
5	E	529	G	O4'-C1'-N9	5.97	112.97	108.20
6	F	1661	A	C5-C6-N6	-5.96	118.93	123.70
8	H	159	ILE	C-N-CA	5.96	136.60	121.70
4	D	57	C	N3-C4-C5	-5.96	119.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ALA	N-CA-CB	5.96	118.44	110.10
4	D	54	A	C5-C6-N6	-5.96	118.94	123.70
13	M	26	LYS	N-CA-CB	5.94	121.28	110.60
5	E	532	A	O4'-C1'-N9	5.92	112.94	108.20
5	E	560	A	O4'-C1'-N9	5.92	112.94	108.20
4	D	92	A	C5-C6-N1	-5.92	114.74	117.70
6	F	1658	G	O4'-C1'-N9	5.92	112.94	108.20
4	D	65	A	C5-C6-N1	-5.91	114.74	117.70
4	D	97	A	C5-C6-N1	-5.91	114.74	117.70
7	G	1920	C	N3-C4-C5	-5.90	119.54	121.90
6	F	1663	C	N3-C4-N4	5.90	122.13	118.00
4	D	80	A	O4'-C1'-N9	5.90	112.92	108.20
7	G	1924	G	O4'-C1'-N9	5.89	112.92	108.20
5	E	547	A	C4-C5-C6	5.89	119.94	117.00
4	D	97	A	C5-C6-N6	-5.88	119.00	123.70
4	D	79	A	O4'-C1'-N9	5.87	112.90	108.20
6	F	1661	A	C5-C6-N1	-5.87	114.77	117.70
4	D	91	C	N3-C4-N4	5.85	122.09	118.00
7	G	1927	C	N3-C4-C5	-5.85	119.56	121.90
12	L	84	LYS	N-CA-CB	5.84	121.11	110.60
13	M	25	PHE	N-CA-CB	5.82	121.08	110.60
7	G	1917	A	C5-C6-N1	-5.82	114.79	117.70
4	D	63	G	O4'-C1'-N9	5.81	112.84	108.20
4	D	54	A	C4-C5-C6	5.80	119.90	117.00
5	E	544	A	C5-C6-N1	-5.79	114.80	117.70
4	D	62	C	N3-C4-C5	-5.79	119.58	121.90
7	G	1918	C	O4'-C1'-N1	5.78	112.83	108.20
14	N	3	GLY	C-N-CA	5.78	136.15	121.70
6	F	1656	A	C5-C6-N1	-5.78	114.81	117.70
5	E	554	A	C4-C5-C6	5.78	119.89	117.00
5	E	545	A	C5-C6-N1	-5.77	114.82	117.70
5	E	547	A	O4'-C1'-N9	5.76	112.81	108.20
4	D	47	C	N3-C4-N4	5.76	122.03	118.00
5	E	530	A	C4-C5-C6	5.75	119.88	117.00
4	D	44	A	C4-C5-C6	5.75	119.88	117.00
5	E	561	C	N3-C4-N4	5.75	122.02	118.00
9	I	105	LYS	CA-C-N	5.75	127.69	116.20
6	F	1668	G	O4'-C1'-N9	5.74	112.79	108.20
14	N	14	LYS	N-CA-CB	5.73	120.92	110.60
6	F	1674	C	N3-C4-C5	-5.73	119.61	121.90
4	D	45	C	N3-C4-N4	5.72	122.00	118.00
6	F	1667	A	C5-C6-N1	-5.72	114.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	86	U	O4'-C1'-N1	5.71	112.77	108.20
7	G	1925	C	N3-C4-N4	5.71	122.00	118.00
8	H	88	GLY	C-N-CA	5.71	135.96	121.70
1	A	364	TYR	CB-CG-CD1	5.70	124.42	121.00
7	G	1925	C	N3-C4-C5	-5.70	119.62	121.90
4	D	80	A	C4-C5-C6	5.69	119.85	117.00
4	D	94	C	N3-C4-N4	5.68	121.98	118.00
7	G	1920	C	O4'-C1'-N1	5.68	112.75	108.20
5	E	533	A	C5-C6-N6	-5.68	119.16	123.70
5	E	542	A	C5-C6-N1	-5.68	114.86	117.70
5	E	560	A	C5-C6-N1	-5.67	114.86	117.70
15	O	7	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	A	119	PHE	CB-CG-CD2	-5.66	116.84	120.80
4	D	92	A	C5'-C4'-O4'	5.65	115.88	109.10
5	E	554	A	C5-C6-N6	-5.64	119.18	123.70
4	D	53	A	C5-C6-N1	-5.64	114.88	117.70
5	E	559	U	O4'-C1'-N1	5.64	112.71	108.20
8	H	57	GLY	C-N-CA	5.63	135.78	121.70
7	G	1921	G	O4'-C1'-N9	5.63	112.70	108.20
4	D	70	G	O4'-C1'-N9	5.63	112.70	108.20
5	E	549	A	C5-C6-N6	-5.63	119.20	123.70
4	D	59	A	C5-C6-N1	-5.62	114.89	117.70
5	E	545	A	C4-C5-C6	5.61	119.81	117.00
4	D	71	A	C5-C6-N6	-5.61	119.21	123.70
5	E	531	A	C4-C5-C6	5.61	119.80	117.00
4	D	51	G	C5-C6-O6	-5.60	125.24	128.60
4	D	99	C	N3-C4-N4	5.60	121.92	118.00
8	H	54	GLU	N-CA-CB	5.59	120.67	110.60
8	H	262	TRP	C-N-CA	5.58	134.03	122.30
12	L	125	LYS	N-CA-CB	5.58	120.65	110.60
15	O	31	THR	C-N-CA	5.58	135.66	121.70
4	D	43	A	C4-C5-C6	5.58	119.79	117.00
5	E	561	C	N3-C4-C5	-5.58	119.67	121.90
5	E	557	A	O4'-C1'-N9	5.57	112.66	108.20
4	D	75	G	C4-N9-C1'	5.57	133.74	126.50
14	N	13	SER	C-N-CA	5.55	135.59	121.70
4	D	59	A	O4'-C1'-N9	5.55	112.64	108.20
4	D	79	A	C5-C6-N1	-5.55	114.92	117.70
4	D	83	C	C6-N1-C1'	-5.55	114.14	120.80
7	G	1917	A	C4-C5-C6	5.55	119.77	117.00
7	G	1919	A	C4-C5-C6	5.55	119.78	117.00
6	F	1664	A	C5-C6-N1	-5.54	114.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	66	A	C4-C5-C6	5.54	119.77	117.00
6	F	1673	A	C4-C5-C6	5.54	119.77	117.00
4	D	94	C	N3-C4-C5	-5.54	119.68	121.90
6	F	1660	C	N3-C4-C5	-5.53	119.69	121.90
5	E	549	A	C5-C6-N1	-5.53	114.94	117.70
5	E	553	A	C5-C6-N1	-5.52	114.94	117.70
5	E	556	A	C5-C6-N1	-5.52	114.94	117.70
4	D	80	A	C5-C6-N1	-5.52	114.94	117.70
6	F	1666	C	N3-C4-N4	5.52	121.86	118.00
5	E	549	A	O4'-C1'-N9	5.50	112.60	108.20
6	F	1663	C	N3-C4-C5	-5.50	119.70	121.90
7	G	1923	C	N3-C4-N4	5.50	121.85	118.00
6	F	1660	C	O4'-C1'-N1	5.50	112.60	108.20
1	A	466	SER	N-CA-CB	5.49	118.74	110.50
4	D	80	A	C5-C6-N6	-5.49	119.31	123.70
9	I	3	ARG	C-N-CA	5.49	135.42	121.70
8	H	77	VAL	CA-CB-CG1	5.48	119.12	110.90
5	E	535	A	C5-C6-N6	-5.47	119.32	123.70
8	H	12	THR	C-N-CA	5.47	133.79	122.30
6	F	1655	C	N3-C4-N4	5.46	121.83	118.00
5	E	556	A	C5-C6-N6	-5.46	119.33	123.70
4	D	66	A	C5-C6-N1	-5.46	114.97	117.70
9	I	36	ILE	CA-C-N	5.45	129.19	117.20
4	D	75	G	C5-C6-O6	-5.45	125.33	128.60
9	I	57	ALA	N-CA-C	5.45	125.70	111.00
6	F	1664	A	O4'-C1'-N9	5.44	112.55	108.20
1	A	324	TRP	N-CA-CB	5.44	120.39	110.60
14	N	39	PRO	CA-C-N	5.44	129.17	117.20
4	D	96	A	C4-C5-C6	5.44	119.72	117.00
4	D	96	A	C5-C6-N6	-5.43	119.36	123.70
6	F	1657	C	N3-C4-C5	-5.42	119.73	121.90
4	D	89	A	C5-C6-N6	-5.42	119.36	123.70
5	E	535	A	C5-C6-N1	-5.42	114.99	117.70
1	A	5	PHE	CB-CG-CD2	5.42	124.59	120.80
5	E	554	A	C5-C6-N1	-5.42	114.99	117.70
9	I	3	ARG	CB-CA-C	5.42	121.23	110.40
6	F	1667	A	C5-C6-N6	-5.42	119.37	123.70
5	E	553	A	C5-C6-N6	-5.41	119.38	123.70
4	D	75	G	N3-C2-N2	5.40	123.68	119.90
6	F	1666	C	N3-C4-C5	-5.39	119.74	121.90
6	F	1669	U	O4'-C1'-N1	5.39	112.51	108.20
5	E	545	A	C5-C6-N6	-5.39	119.39	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1918	C	N3-C4-N4	5.39	121.77	118.00
14	N	37	SER	C-N-CA	5.39	135.17	121.70
1	A	141	SER	N-CA-CB	5.38	118.58	110.50
5	E	542	A	O4'-C1'-N9	5.38	112.50	108.20
1	A	276	TYR	CB-CG-CD2	5.38	124.23	121.00
6	F	1664	A	C4-C5-C6	5.38	119.69	117.00
7	G	1928	G	O4'-C1'-N9	5.38	112.50	108.20
2	B	53	PHE	CB-CG-CD2	-5.37	117.04	120.80
4	D	77	A	C4-C5-C6	5.36	119.68	117.00
8	H	28	ALA	N-CA-CB	5.36	117.61	110.10
5	E	537	C	N3-C4-N4	5.35	121.75	118.00
8	H	57	GLY	N-CA-C	-5.35	99.72	113.10
4	D	43	A	C5-C6-N1	-5.35	115.03	117.70
4	D	78	G	O4'-C1'-N9	5.34	112.48	108.20
4	D	99	C	N3-C4-C5	-5.34	119.76	121.90
5	E	555	A	C5-C6-N1	-5.34	115.03	117.70
4	D	46	G	O4'-C1'-N9	5.34	112.47	108.20
4	D	47	C	N3-C4-C5	-5.33	119.77	121.90
4	D	66	A	C5-C6-N6	-5.32	119.44	123.70
7	G	1919	A	C5-C6-N1	-5.30	115.05	117.70
5	E	553	A	O4'-C1'-N9	5.29	112.44	108.20
8	H	105	THR	C-N-CA	5.29	134.93	121.70
14	N	69	LEU	CA-C-O	-5.29	108.99	120.10
4	D	85	G	O4'-C1'-N9	5.28	112.42	108.20
4	D	103	G	O4'-C1'-N9	5.26	112.41	108.20
5	E	536	A	O4'-C1'-N9	5.26	112.41	108.20
4	D	65	A	C5-C6-N6	-5.26	119.49	123.70
4	D	71	A	C4-C5-C6	5.26	119.63	117.00
5	E	560	A	C5-C6-N6	-5.25	119.50	123.70
4	D	88	A	C5-C6-N6	-5.25	119.50	123.70
7	G	1918	C	N3-C4-C5	-5.24	119.81	121.90
5	E	532	A	C4-C5-C6	5.23	119.61	117.00
4	D	77	A	C5-C6-N1	-5.22	115.09	117.70
8	H	100	PHE	CB-CG-CD1	5.22	124.45	120.80
4	D	58	G	O4'-C1'-N9	5.22	112.38	108.20
4	D	77	A	O4'-C1'-N9	5.22	112.38	108.20
4	D	97	A	O4'-C1'-N9	5.22	112.37	108.20
6	F	1656	A	C4-C5-C6	5.21	119.61	117.00
9	I	9	THR	C-N-CA	5.19	134.67	121.70
4	D	44	A	O4'-C1'-N9	5.18	112.35	108.20
6	F	1662	A	O4'-C1'-N9	5.18	112.35	108.20
4	D	45	C	N3-C4-C5	-5.18	119.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	84	C	N3-C4-C5	-5.18	119.83	121.90
7	G	1927	C	N3-C4-N4	5.18	121.63	118.00
6	F	1660	C	N3-C4-N4	5.18	121.62	118.00
6	F	1677	G	O4'-C1'-N9	5.18	112.34	108.20
8	H	12	THR	CA-C-N	5.17	126.55	116.20
5	E	542	A	C5-C6-N6	-5.16	119.57	123.70
1	A	261	PHE	CB-CG-CD1	5.16	124.41	120.80
5	E	531	A	O4'-C1'-N9	5.16	112.33	108.20
12	L	83	ASP	C-N-CA	5.16	134.59	121.70
4	D	51	G	N3-C2-N2	5.15	123.50	119.90
12	L	124	GLY	C-N-CA	5.15	134.57	121.70
8	H	63	GLU	N-CA-CB	5.14	119.86	110.60
2	B	53	PHE	CB-CG-CD1	5.14	124.40	120.80
4	D	48	A	C5-C6-N6	-5.13	119.60	123.70
6	F	1678	G	O4'-C1'-N9	5.13	112.30	108.20
1	A	42	PHE	CB-CG-CD2	5.13	124.39	120.80
7	G	1928	G	P-O3'-C3'	5.12	125.84	119.70
5	E	554	A	O4'-C1'-N9	5.09	112.27	108.20
5	E	543	A	O4'-C1'-N9	5.09	112.27	108.20
7	G	1923	C	N3-C4-C5	-5.09	119.86	121.90
5	E	550	G	O4'-C1'-N9	5.08	112.27	108.20
11	K	115	ARG	NE-CZ-NH1	5.08	122.84	120.30
8	H	70	ALA	N-CA-C	-5.07	97.32	111.00
1	A	271	ARG	N-CA-CB	5.06	119.71	110.60
4	D	71	A	C5-C6-N1	-5.06	115.17	117.70
6	F	1654	C	C6-N1-C2	-5.05	118.28	120.30
4	D	53	A	O4'-C1'-N9	5.05	112.24	108.20
4	D	76	C	C5-C4-N4	-5.04	116.67	120.20
6	F	1657	C	N3-C4-N4	5.04	121.53	118.00
9	I	66	SER	C-N-CA	5.04	134.31	121.70
4	D	68	G	O4'-C1'-N9	5.04	112.23	108.20
4	D	73	U	C5'-C4'-C3'	-5.04	107.94	116.00
8	H	86	GLY	N-CA-C	-5.04	100.51	113.10
5	E	535	A	O4'-C1'-N9	5.03	112.22	108.20
4	D	97	A	C4-C5-C6	5.03	119.52	117.00
1	A	276	TYR	CB-CG-CD1	-5.03	117.98	121.00
6	F	1672	G	O4'-C1'-N9	5.03	112.22	108.20
4	D	49	G	P-O5'-C5'	5.03	128.94	120.90
4	D	48	A	C5-C6-N1	-5.02	115.19	117.70
1	A	278	THR	N-CA-CB	5.02	119.84	110.30
4	D	79	A	C5-C6-N6	-5.02	119.69	123.70
4	D	89	A	C5-C6-N1	-5.02	115.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1664	A	C5-C6-N6	-5.02	119.69	123.70
8	H	221	ASN	N-CA-CB	5.01	119.62	110.60
5	E	545	A	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PHE	Sidechain
1	A	270	ALA	Peptide
1	A	271	ARG	Sidechain
1	A	336	TYR	Peptide
1	A	404	HIS	Sidechain
3	C	71	VAL	Peptide
4	D	46	G	Sidechain
4	D	50	C	Sidechain
4	D	55	U	Sidechain
4	D	56	G	Sidechain
4	D	62	C	Sidechain
4	D	65	A	Sidechain
4	D	66	A	Sidechain
4	D	76	C	Sidechain
4	D	77	A	Sidechain
4	D	87	G	Sidechain
5	E	536	A	Sidechain
5	E	541	G	Sidechain
5	E	543	A	Sidechain
5	E	545	A	Sidechain
5	E	552	G	Sidechain
5	E	558	G	Sidechain
6	F	1662	A	Sidechain
6	F	1667	A	Sidechain
6	F	1673	A	Sidechain
7	G	1925	C	Sidechain
8	H	102	PRO	Peptide
8	H	110	ASN	Peptide
8	H	141	ARG	Sidechain
8	H	148	ILE	Peptide
8	H	187	LEU	Peptide
8	H	197	ARG	Peptide
8	H	209	TYR	Sidechain
8	H	212	ASP	Peptide

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Mol	Chain	Res	Type	Group
8	H	63	GLU	Peptide
8	H	73	ARG	Sidechain
8	H	76	ARG	Peptide
8	H	92	ASN	Peptide
9	I	122	ALA	Peptide
9	I	23	ARG	Sidechain
9	I	30	ARG	Sidechain
9	I	4	TYR	Sidechain
9	I	47	TYR	Sidechain
9	I	82	ARG	Sidechain
11	K	105	VAL	Peptide
11	K	57	LEU	Peptide
11	K	60	TYR	Sidechain
12	L	121	ARG	Peptide
12	L	125	LYS	Peptide
12	L	23	PRO	Peptide
12	L	40	ARG	Sidechain
12	L	52	ARG	Sidechain
13	M	10	ARG	Sidechain
13	M	74	ARG	Sidechain
14	N	32	LYS	Peptide
14	N	38	ARG	Sidechain
15	O	19	GLN	Peptide
15	O	23	LEU	Peptide
15	O	24	PRO	Peptide
15	O	30	ARG	Sidechain
15	O	32	ASN	Peptide
15	O	36	ARG	Peptide
15	O	4	GLN	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	3675	0	3798	44	0
2	B	543	0	577	1	0
3	C	281	0	294	0	0
4	D	1347	0	678	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	740	0	369	1	0
6	F	536	0	272	1	0
7	G	296	0	154	0	0
8	H	2039	0	2106	16	0
9	I	1212	0	1231	8	0
10	J	410	0	452	0	0
11	K	663	0	699	4	0
12	L	1002	0	1093	2	0
13	M	706	0	741	1	0
14	N	547	0	613	8	0
15	O	316	0	349	2	0
All	All	14313	0	13426	81	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 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CE2	1:A:5:PHE:CD2	1.81	1.68
1:A:5:PHE:CE1	1:A:5:PHE:CD1	1.80	1.66
1:A:5:PHE:CE2	1:A:5:PHE:CZ	1.79	1.64
1:A:5:PHE:CG	1:A:5:PHE:CD1	1.81	1.61
1:A:5:PHE:CE1	1:A:5:PHE:CZ	1.80	1.61
1:A:5:PHE:CD2	1:A:5:PHE:CG	1.82	1.59
1:A:5:PHE:CZ	1:A:104:ASP:HA	1.56	1.37
1:A:5:PHE:CE1	1:A:104:ASP:HA	1.82	1.14
1:A:5:PHE:CG	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CD2	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CE1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CD1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CE2	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CZ	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CD1	1:A:104:ASP:N	2.32	0.96
1:A:5:PHE:CD2	1:A:104:ASP:N	2.33	0.96
1:A:5:PHE:CG	1:A:104:ASP:N	2.33	0.95
1:A:5:PHE:CE2	1:A:104:ASP:N	2.35	0.94
1:A:5:PHE:CE1	1:A:104:ASP:N	2.37	0.93
1:A:5:PHE:CZ	1:A:104:ASP:N	2.39	0.90
1:A:5:PHE:CE2	1:A:104:ASP:HA	2.14	0.82
11:K:100:LYS:HA	11:K:105:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:CD1	1:A:104:ASP:C	2.62	0.73
1:A:5:PHE:CD2	1:A:104:ASP:CB	2.72	0.72
1:A:268:LYS:HB2	14:N:38:ARG:HH21	1.65	0.61
1:A:5:PHE:CE2	1:A:104:ASP:HB2	2.36	0.60
5:E:539:U:H3	5:E:546:G:H1	1.50	0.59
1:A:5:PHE:CE2	1:A:104:ASP:CB	2.86	0.58
9:I:57:ALA:HB3	9:I:82:ARG:O	2.06	0.56
1:A:277:ASN:H	14:N:38:ARG:HH22	1.56	0.55
12:L:56:VAL:HG22	12:L:106:ILE:HG22	1.88	0.54
1:A:94:LEU:HB3	1:A:112:PHE:CG	2.42	0.54
1:A:277:ASN:H	14:N:38:ARG:NH2	2.07	0.53
8:H:184:SER:HA	8:H:186:LYS:H	1.73	0.53
1:A:5:PHE:CD2	1:A:103:GLY:C	2.81	0.52
11:K:105:VAL:HG23	11:K:106:ASP:HA	1.91	0.52
1:A:275:GLN:HB3	14:N:38:ARG:CZ	2.40	0.52
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.92	0.52
8:H:58:HIS:O	8:H:58:HIS:CG	2.64	0.51
14:N:41:LEU:H	14:N:44:ILE:HD12	1.75	0.51
8:H:52:VAL:HG22	8:H:53:SER:H	1.76	0.50
8:H:198:ARG:CG	8:H:199:TRP:H	2.24	0.50
1:A:5:PHE:CB	1:A:5:PHE:CD1	2.84	0.50
2:B:20:ARG:HA	11:K:137:ASN:HD21	1.76	0.50
14:N:39:PRO:HB2	14:N:40:SER:C	2.32	0.49
9:I:3:ARG:HB2	9:I:4:TYR:HA	1.95	0.49
1:A:404:HIS:CE1	6:F:1657:C:H1'	2.48	0.49
8:H:184:SER:HA	8:H:186:LYS:N	2.28	0.49
8:H:57:GLY:HA3	8:H:58:HIS:HB2	1.95	0.48
1:A:268:LYS:CB	14:N:38:ARG:HH21	2.27	0.48
1:A:94:LEU:HB3	1:A:112:PHE:CD1	2.49	0.47
8:H:83:GLY:HA3	8:H:84:ARG:HB2	1.96	0.47
14:N:39:PRO:HA	14:N:41:LEU:HD22	1.96	0.47
9:I:9:THR:HG23	9:I:10:ASN:HA	1.98	0.46
1:A:273:ARG:HE	1:A:273:ARG:HA	1.81	0.46
9:I:108:ASP:HB2	9:I:109:ALA:HA	1.97	0.45
1:A:5:PHE:CD2	1:A:103:GLY:O	2.70	0.45
1:A:5:PHE:CD2	1:A:104:ASP:HB2	2.52	0.45
1:A:269:SER:HB2	1:A:403:GLY:H	1.82	0.45
8:H:63:GLU:CD	8:H:64:SER:H	2.20	0.45
8:H:152:VAL:HG12	8:H:153:SER:H	1.83	0.44
9:I:51:VAL:HG13	9:I:57:ALA:H	1.83	0.44
1:A:64:TRP:H	1:A:334:ARG:HE	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HD3	1:A:272:TYR:CE2	2.53	0.44
8:H:77:VAL:HG13	8:H:78:GLY:N	2.32	0.44
8:H:222:VAL:HB	8:H:225:VAL:HG12	1.99	0.43
11:K:105:VAL:HG23	11:K:106:ASP:CA	2.49	0.43
8:H:74:ILE:H	8:H:75:PRO:HA	1.83	0.43
1:A:108:ASP:HB2	1:A:112:PHE:CE1	2.55	0.42
9:I:107:LEU:H	9:I:107:LEU:HD12	1.85	0.42
9:I:24:VAL:HG11	9:I:87:SER:HA	2.02	0.42
12:L:10:SER:N	12:L:11:ASP:HB2	2.35	0.42
8:H:74:ILE:N	8:H:75:PRO:HA	2.35	0.41
13:M:82:GLU:CD	13:M:82:GLU:H	2.22	0.41
8:H:13:GLY:H	8:H:14:GLU:HB2	1.86	0.41
4:D:55:U:C2	4:D:56:G:C8	3.08	0.41
1:A:272:TYR:CE2	15:O:24:PRO:HG3	2.55	0.41
1:A:5:PHE:CG	1:A:104:ASP:C	2.93	0.41
9:I:138:LYS:HD3	9:I:138:LYS:H	1.86	0.41
8:H:199:TRP:HA	8:H:200:THR:HB	2.02	0.41
4:D:75:G:C2	15:O:27:ILE:HD13	2.56	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	474/476 (100%)	402 (85%)	46 (10%)	26 (6%)	2	28
2	B	66/68 (97%)	60 (91%)	2 (3%)	4 (6%)	2	26
3	C	34/96 (35%)	27 (79%)	4 (12%)	3 (9%)	1	17
8	H	267/362 (74%)	181 (68%)	38 (14%)	48 (18%)	0	4
9	I	151/184 (82%)	119 (79%)	15 (10%)	17 (11%)	0	10
10	J	51/189 (27%)	46 (90%)	4 (8%)	1 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	81/142 (57%)	73 (90%)	5 (6%)	3 (4%)	4	37
12	L	125/127 (98%)	101 (81%)	9 (7%)	15 (12%)	0	8
13	M	82/113 (73%)	65 (79%)	8 (10%)	9 (11%)	0	11
14	N	67/120 (56%)	59 (88%)	3 (4%)	5 (8%)	1	21
15	O	35/51 (69%)	26 (74%)	0	9 (26%)	0	1
All	All	1433/1928 (74%)	1159 (81%)	134 (9%)	140 (10%)	2	14

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	104	ASP
1	A	108	ASP
1	A	110	ALA
1	A	142	GLU
1	A	280	PRO
1	A	402	ARG
1	A	466	SER
1	A	473	ALA
2	B	30	ARG
2	B	41	ALA
3	C	71	VAL
3	C	72	PRO
8	H	3	ARG
8	H	28	ALA
8	H	54	GLU
8	H	55	LYS
8	H	58	HIS
8	H	60	THR
8	H	63	GLU
8	H	69	ARG
8	H	70	ALA
8	H	72	ALA
8	H	74	ILE
8	H	76	ARG
8	H	87	GLN
8	H	89	ALA
8	H	98	ARG
8	H	102	PRO
8	H	103	THR

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Mol	Chain	Res	Type
8	H	146	PRO
8	H	185	LYS
8	H	187	LEU
8	H	198	ARG
8	H	199	TRP
8	H	200	THR
8	H	212	ASP
8	H	222	VAL
8	H	244	LEU
8	H	262	TRP
9	I	37	ASN
9	I	57	ALA
9	I	67	ILE
9	I	107	LEU
9	I	111	LYS
9	I	113	TYR
9	I	123	PRO
9	I	143	PRO
12	L	23	PRO
12	L	85	VAL
12	L	125	LYS
13	M	78	LYS
13	M	79	ARG
13	M	90	PHE
14	N	4	VAL
14	N	14	LYS
14	N	39	PRO
15	O	20	ASN
15	O	22	PRO
15	O	23	LEU
1	A	107	LYS
1	A	141	SER
1	A	200	THR
1	A	226	LYS
1	A	324	TRP
2	B	66	VAL
8	H	13	GLY
8	H	81	GLY
8	H	93	MET
8	H	160	GLN
8	H	173	GLY
8	H	264	SER

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Mol	Chain	Res	Type
9	I	7	THR
9	I	71	ALA
11	K	62	VAL
12	L	6	LEU
12	L	11	ASP
12	L	45	ILE
12	L	46	LYS
12	L	87	LYS
12	L	96	PRO
12	L	113	LYS
12	L	122	LYS
13	M	25	PHE
13	M	26	LYS
13	M	69	TYR
14	N	37	SER
15	O	5	LYS
15	O	6	SER
15	O	24	PRO
1	A	57	ASP
1	A	70	ALA
1	A	335	ALA
1	A	349	GLU
2	B	5	MET
8	H	107	ARG
8	H	132	ALA
8	H	221	ASN
8	H	265	GLU
9	I	2	ALA
9	I	3	ARG
9	I	25	SER
9	I	54	HIS
11	K	109	LYS
12	L	36	SER
12	L	84	LYS
14	N	5	LYS
15	O	25	GLN
1	A	105	THR
1	A	272	TYR
3	C	90	TRP
8	H	101	ALA
8	H	131	VAL
8	H	215	ILE

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Mol	Chain	Res	Type
9	I	39	TRP
11	K	131	ASP
12	L	97	ILE
13	M	24	SER
1	A	19	ILE
1	A	77	MET
1	A	443	SER
8	H	52	VAL
8	H	84	ARG
8	H	106	TRP
8	H	196	ASN
9	I	131	ARG
10	J	19	LYS
12	L	86	THR
15	O	34	THR
1	A	382	VAL
8	H	4	PRO
8	H	205	PRO
13	M	51	LEU
13	M	64	VAL
1	A	80	GLY
9	I	84	PRO
15	O	35	ILE
8	H	86	GLY
1	A	8	VAL
8	H	77	VAL

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	398/398 (100%)	388 (98%)	10 (2%)	55	81
2	B	59/59 (100%)	57 (97%)	2 (3%)	44	75
3	C	32/74 (43%)	32 (100%)	0	100	100
8	H	209/288 (73%)	179 (86%)	30 (14%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	124/146 (85%)	107 (86%)	17 (14%)	4	27
10	J	44/154 (29%)	42 (96%)	2 (4%)	34	69
11	K	74/118 (63%)	67 (90%)	7 (10%)	11	41
12	L	110/110 (100%)	95 (86%)	15 (14%)	5	27
13	M	74/97 (76%)	64 (86%)	10 (14%)	5	27
14	N	62/105 (59%)	57 (92%)	5 (8%)	15	50
15	O	33/46 (72%)	28 (85%)	5 (15%)	3	23
All	All	1219/1595 (76%)	1116 (92%)	103 (8%)	18	48

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	25	LYS
1	A	68	ILE
1	A	232	GLU
1	A	263	VAL
1	A	327	THR
1	A	364	TYR
1	A	407	THR
1	A	414	ASN
1	A	465	GLN
2	B	5	MET
2	B	52	PHE
8	H	4	PRO
8	H	33	ASP
8	H	35	VAL
8	H	43	ASN
8	H	46	LYS
8	H	48	GLN
8	H	77	VAL
8	H	90	PHE
8	H	98	ARG
8	H	103	THR
8	H	112	LYS
8	H	119	ARG
8	H	136	LEU
8	H	140	HIS
8	H	141	ARG
8	H	145	ILE

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Mol	Chain	Res	Type
8	H	155	ASP
8	H	159	ILE
8	H	161	LYS
8	H	162	THR
8	H	164	GLU
8	H	170	LYS
8	H	193	LYS
8	H	198	ARG
8	H	201	GLN
8	H	215	ILE
8	H	233	LEU
8	H	243	HIS
8	H	244	LEU
8	H	260	GLN
9	I	3	ARG
9	I	36	ILE
9	I	40	GLU
9	I	43	LYS
9	I	46	LYS
9	I	59	PRO
9	I	66	SER
9	I	67	ILE
9	I	72	GLN
9	I	76	PHE
9	I	79	THR
9	I	80	LYS
9	I	94	LEU
9	I	105	LYS
9	I	120	ASN
9	I	144	SER
9	I	149	VAL
10	J	1	MET
10	J	53	LYS
11	K	65	GLN
11	K	70	GLU
11	K	74	LYS
11	K	100	LYS
11	K	111	ASN
11	K	117	ASN
11	K	123	TYR
12	L	28	ARG
12	L	37	LYS

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Mol	Chain	Res	Type
12	L	52	ARG
12	L	57	LEU
12	L	64	LYS
12	L	77	LYS
12	L	78	PHE
12	L	87	LYS
12	L	98	ASN
12	L	108	LYS
12	L	111	LEU
12	L	113	LYS
12	L	116	LYS
12	L	122	LYS
12	L	125	LYS
13	M	24	SER
13	M	38	LYS
13	M	47	ASP
13	M	62	ARG
13	M	67	VAL
13	M	77	ARG
13	M	79	ARG
13	M	82	GLU
13	M	86	LYS
13	M	92	TYR
14	N	5	LYS
14	N	9	LEU
14	N	34	GLN
14	N	38	ARG
14	N	39	PRO
15	O	17	LYS
15	O	18	LYS
15	O	22	PRO
15	O	23	LEU
15	O	26	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
2	B	58	HIS
8	H	43	ASN
8	H	213	ASN
11	K	111	ASN

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Mol	Chain	Res	Type
12	L	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63 (98%)	27 (43%)	10 (16%)
5	E	33/34 (97%)	9 (27%)	3 (9%)
6	F	24/25 (96%)	3 (12%)	0
7	G	14/14 (100%)	6 (42%)	2 (14%)
All	All	133/136 (97%)	45 (33%)	15 (11%)

All (45) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	49	G
4	D	51	G
4	D	56	G
4	D	59	A
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	71	A
4	D	79	A
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	95	G
4	D	97	A
4	D	98	U

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Mol	Chain	Res	Type
5	E	532	A
5	E	533	A
5	E	534	G
5	E	553	A
5	E	556	A
5	E	557	A
5	E	558	G
5	E	560	A
5	E	561	C
6	F	1665	G
6	F	1666	C
6	F	1668	G
7	G	1918	C
7	G	1921	G
7	G	1922	U
7	G	1927	C
7	G	1929	G
7	G	1930	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	48	A
4	D	51	G
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	558	G
5	E	560	A
7	G	1917	A
7	G	1926	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.