wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:43 PM BST

PDB ID	:	2WW9
EMDB ID:	:	EMD-1651
Title	:	Cryo-EM structure of the active 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	:	8.60 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

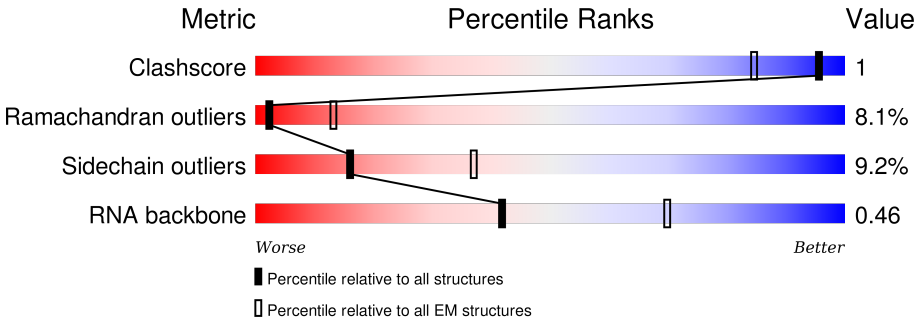
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 8.60 Å.

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



Metric	Whole archive (#Entries)	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	490	86% 11% •
2	B	80	68% 5% • 25%
3	C	87	22% •• 76%
4	D	63	• 43% 48% 8%
5	E	34	65% 35%
6	F	25	92% 8%
7	G	18	94% 6%
8	H	362	50% 16% 7% • 26%

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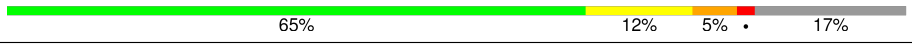
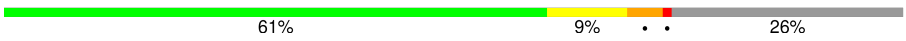
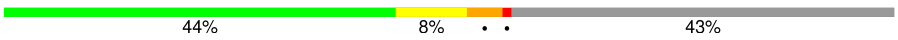
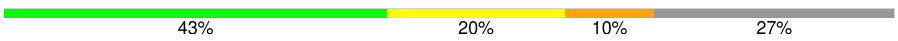
Mol	Chain	Length	Quality of chain
9	I	184	
10	J	189	
11	K	142	
12	L	127	
13	M	113	
14	N	120	
15	O	51	

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
			Total	C	N	O	S		
1	A	490	3770	2487	603	671	9	0	0

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

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

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

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

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

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

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

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

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

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

- 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.

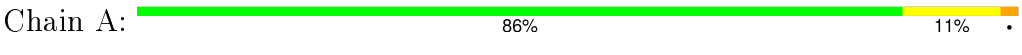
Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	37	Total	C	N	O	S	0	0
			316	200	66	48	2		

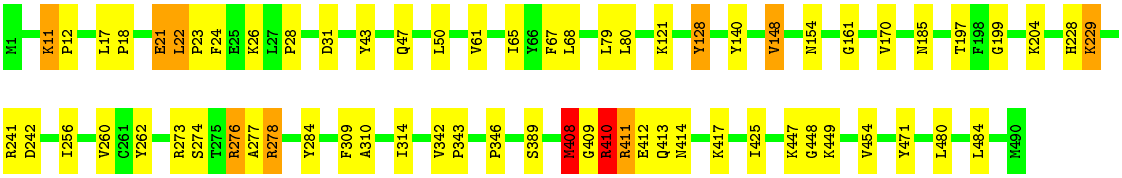
3 Residue-property plots (i)

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

Chain A:



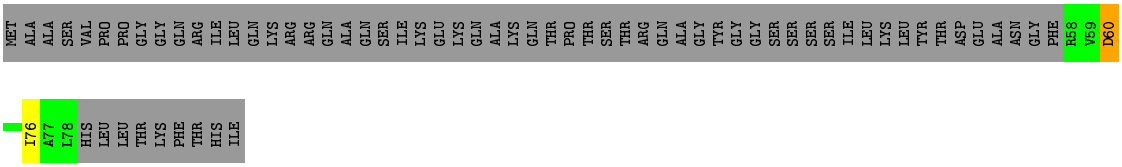


- Molecule 2: PROTEIN TRANSPORT PROTEIN SSS1

Chain B:

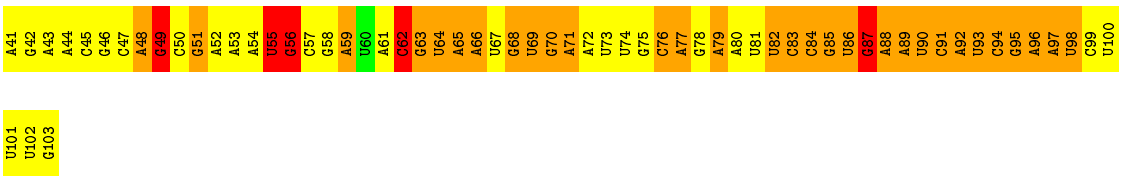
- Molecule 3: PROTEIN TRANSPORT PROTEIN SEB2

Chain C:



- Molecule 4: 25S RRNA

Chain D:

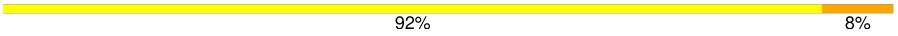


- Molecule 5: 25S RRNA

Chain E:

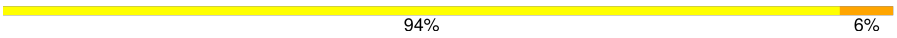
- Molecule 6: 25S RRNA

Chain F:



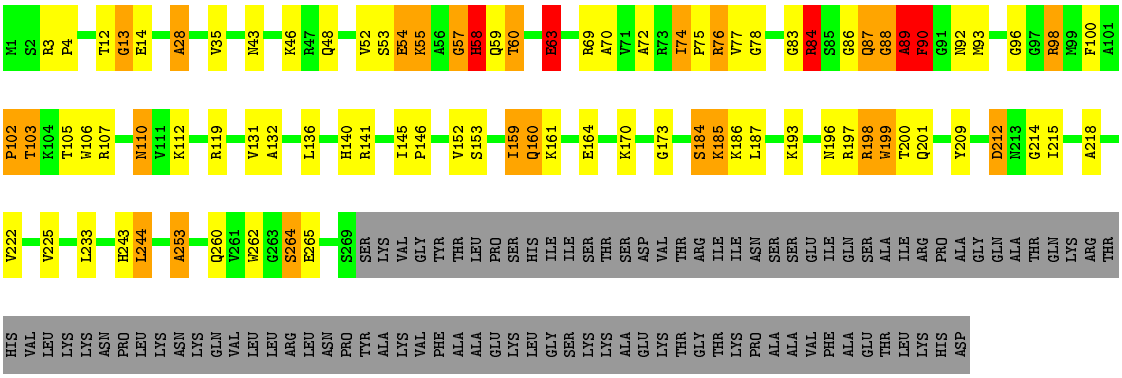
- Molecule 7: 25S RRNA

Chain G:



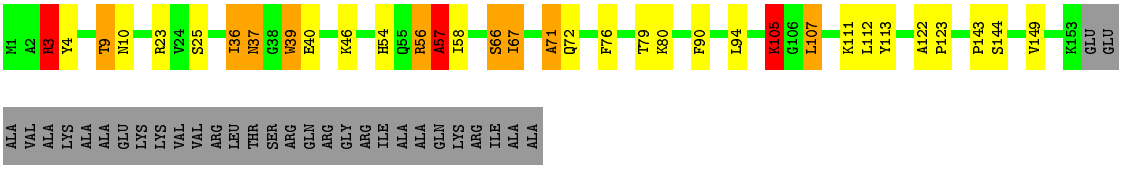
- Molecule 8: 60S RIBOSOMAL PROTEIN L4-B

Chain H:



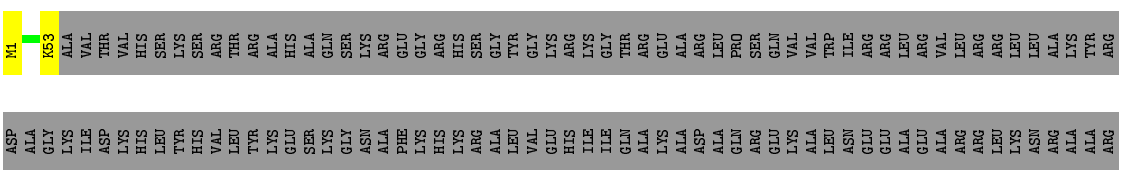
- Molecule 9: 60S RIBOSOMAL PROTEIN L17-A

Chain I:



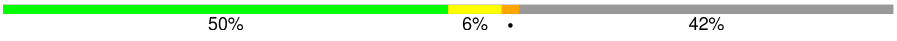
- Molecule 10: 60S RIBOSOMAL PROTEIN L19

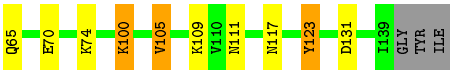
Chain J:



- Molecule 11: 60S RIBOSOMAL PROTEIN L25

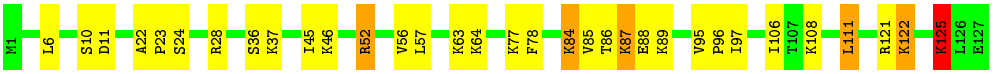
Chain K:





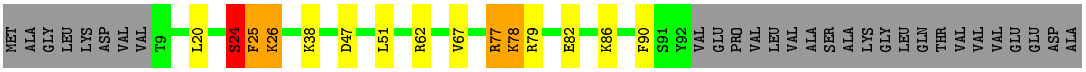
- Molecule 12: 60S RIBOSOMAL PROTEIN L26-A

Chain L:



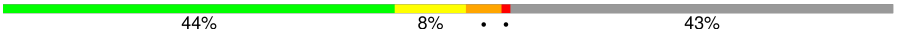
- Molecule 13: 60S RIBOSOMAL PROTEIN L31-A

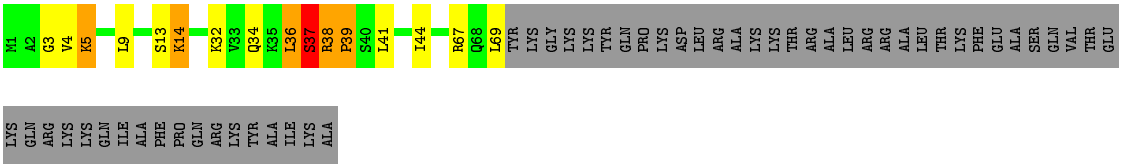
Chain M:



- Molecule 14: 60S RIBOSOMAL PROTEIN L35

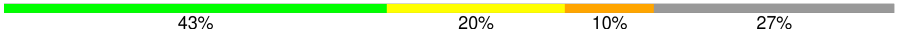
Chain N:





- Molecule 15: 60S RIBOSOMAL PROTEIN L39

Chain O:



4 Experimental information (i)

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 ($e^-/Å^2$)	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	1.07	8/5234 (0.2%)
10	J	1.02	0/412	0.95	0/551
11	K	0.91	0/670	1.08	2/903 (0.2%)
12	L	1.01	0/1013	1.25	3/1351 (0.2%)
13	M	1.11	0/719	1.26	7/959 (0.7%)
14	N	1.07	1/549 (0.2%)	1.40	9/733 (1.2%)
15	O	1.11	0/321	1.41	4/426 (0.9%)
2	B	0.89	0/481	1.00	2/648 (0.3%)
3	C	0.95	0/164	0.88	0/222
4	D	1.62	0/1508	2.62	185/2348 (7.9%)
5	E	1.59	0/833	2.65	109/1298 (8.4%)
6	F	1.60	0/599	2.43	71/932 (7.6%)
7	G	1.54	0/421	2.30	50/653 (7.7%)
8	H	0.99	0/2079	1.39	30/2817 (1.1%)
9	I	1.04	0/1235	1.37	17/1662 (1.0%)
All	All	1.15	1/14852 (0.0%)	1.66	497/20737 (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	9
11	K	0	2
12	L	0	6
14	N	0	3
15	O	0	5
2	B	0	1
4	D	0	7
5	E	0	2
6	F	0	1
8	H	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	2
All	All	0	45

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	69	LEU	C-O	-12.03	1.00	1.23

All (497) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	532	A	P-O3'-C3'	18.10	141.42	119.70
4	D	69	U	P-O3'-C3'	14.78	137.43	119.70
6	F	1661	A	N1-C6-N6	14.08	127.05	118.60
4	D	53	A	N1-C6-N6	14.06	127.04	118.60
4	D	93	U	P-O3'-C3'	13.80	136.26	119.70
4	D	66	A	N1-C6-N6	13.74	126.84	118.60
5	E	557	A	N1-C6-N6	13.50	126.70	118.60
4	D	90	U	P-O3'-C3'	13.23	135.58	119.70
5	E	544	A	N1-C6-N6	13.13	126.48	118.60
5	E	533	A	N1-C6-N6	13.11	126.46	118.60
4	D	55	U	P-O3'-C3'	12.99	135.29	119.70
4	D	54	A	N1-C6-N6	12.93	126.36	118.60
6	F	1662	A	N1-C6-N6	12.92	126.35	118.60
5	E	555	A	N1-C6-N6	12.91	126.35	118.60
4	D	71	A	N1-C6-N6	12.90	126.34	118.60
5	E	554	A	N1-C6-N6	12.76	126.26	118.60
7	G	915	A	N1-C6-N6	12.68	126.21	118.60
4	D	41	A	N1-C6-N6	12.55	126.13	118.60
4	D	52	A	N1-C6-N6	12.53	126.12	118.60
4	D	97	A	N1-C6-N6	12.52	126.11	118.60
6	F	1656	A	N1-C6-N6	12.40	126.04	118.60
5	E	531	A	N1-C6-N6	12.30	125.98	118.60
4	D	65	A	P-O3'-C3'	12.25	134.40	119.70
5	E	553	A	N1-C6-N6	12.21	125.92	118.60
5	E	536	A	N1-C6-N6	12.20	125.92	118.60
6	F	1667	A	N1-C6-N6	12.18	125.91	118.60
4	D	88	A	N1-C6-N6	12.18	125.91	118.60
4	D	79	A	N1-C6-N6	12.17	125.90	118.60
4	D	96	A	P-O3'-C3'	12.14	134.27	119.70
5	E	535	A	N1-C6-N6	12.01	125.81	118.60
5	E	530	A	N1-C6-N6	11.96	125.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	44	A	N1-C6-N6	11.94	125.77	118.60
5	E	542	A	N1-C6-N6	11.87	125.72	118.60
4	D	48	A	N1-C6-N6	11.84	125.71	118.60
5	E	556	A	N1-C6-N6	11.84	125.70	118.60
5	E	547	A	N1-C6-N6	11.82	125.69	118.60
4	D	92	A	N1-C6-N6	11.82	125.69	118.60
5	E	560	A	N1-C6-N6	11.79	125.67	118.60
7	G	918	A	N1-C6-N6	11.77	125.66	118.60
4	D	61	A	N1-C6-N6	11.77	125.66	118.60
5	E	543	A	N1-C6-N6	11.70	125.62	118.60
4	D	59	A	N1-C6-N6	11.62	125.57	118.60
6	F	1664	A	N1-C6-N6	11.51	125.50	118.60
5	E	549	A	N1-C6-N6	11.49	125.49	118.60
5	E	545	A	N1-C6-N6	11.41	125.45	118.60
4	D	96	A	N1-C6-N6	11.35	125.41	118.60
4	D	65	A	N1-C6-N6	11.21	125.33	118.60
4	D	89	A	N1-C6-N6	11.18	125.31	118.60
4	D	43	A	N1-C6-N6	10.98	125.19	118.60
4	D	72	A	N1-C6-N6	10.73	125.04	118.60
4	D	80	A	N1-C6-N6	10.61	124.97	118.60
5	E	560	A	P-O3'-C3'	10.55	132.36	119.70
4	D	63	G	P-O3'-C3'	10.49	132.29	119.70
6	F	1667	A	P-O3'-C3'	10.38	132.15	119.70
4	D	89	A	P-O3'-C3'	10.35	132.12	119.70
5	E	532	A	N1-C6-N6	10.15	124.69	118.60
6	F	1673	A	N1-C6-N6	9.58	124.35	118.60
6	F	1668	G	N1-C6-O6	9.55	125.63	119.90
4	D	56	G	N1-C6-O6	9.53	125.62	119.90
4	D	46	G	N1-C6-O6	9.48	125.59	119.90
5	E	534	G	N1-C6-O6	9.30	125.48	119.90
5	E	546	G	N1-C6-O6	9.21	125.43	119.90
6	F	1678	G	N1-C6-O6	9.18	125.41	119.90
4	D	70	G	N1-C6-O6	9.11	125.37	119.90
5	E	558	G	N1-C6-O6	9.10	125.36	119.90
4	D	68	G	N1-C6-O6	9.09	125.35	119.90
4	D	85	G	N1-C6-O6	9.05	125.33	119.90
7	G	912	G	N1-C6-O6	9.04	125.33	119.90
7	G	928	G	N1-C6-O6	9.04	125.32	119.90
4	D	58	G	N1-C6-O6	9.04	125.32	119.90
4	D	63	G	N1-C6-O6	9.03	125.32	119.90
9	I	56	ARG	C-N-CA	8.95	144.07	121.70
7	G	927	G	N1-C6-O6	8.91	125.24	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	49	G	N1-C6-O6	8.85	125.21	119.90
4	D	92	A	O4'-C1'-N9	8.85	115.28	108.20
7	G	924	G	N1-C6-O6	8.84	125.20	119.90
5	E	548	G	N1-C6-O6	8.83	125.20	119.90
5	E	529	G	N1-C6-O6	8.81	125.19	119.90
7	G	916	G	N1-C6-O6	8.79	125.18	119.90
5	E	552	G	N1-C6-O6	8.77	125.16	119.90
8	H	89	ALA	N-CA-CB	8.76	122.36	110.10
6	F	1658	G	N1-C6-O6	8.75	125.15	119.90
6	F	1677	G	N1-C6-O6	8.66	125.09	119.90
5	E	541	G	N1-C6-O6	8.65	125.09	119.90
5	E	550	G	N1-C6-O6	8.65	125.09	119.90
6	F	1672	G	N1-C6-O6	8.65	125.09	119.90
4	D	90	U	O4'-C1'-N1	8.63	115.11	108.20
8	H	184	SER	C-N-CA	8.62	143.25	121.70
4	D	87	G	N1-C6-O6	8.56	125.03	119.90
4	D	78	G	N1-C6-O6	8.52	125.01	119.90
6	F	1665	G	N1-C6-O6	8.51	125.00	119.90
4	D	42	G	N1-C6-O6	8.45	124.97	119.90
6	F	1675	G	N1-C6-O6	8.40	124.94	119.90
4	D	45	C	O4'-C1'-N1	8.39	114.91	108.20
4	D	103	G	N1-C6-O6	8.36	124.92	119.90
4	D	50	C	O4'-C1'-N1	8.33	114.86	108.20
4	D	57	C	O4'-C1'-N1	8.18	114.74	108.20
4	D	77	A	N1-C6-N6	8.16	123.50	118.60
4	D	95	G	N1-C6-O6	8.12	124.77	119.90
4	D	51	G	N1-C6-O6	8.12	124.77	119.90
6	F	1657	C	O4'-C1'-N1	8.07	114.66	108.20
6	F	1671	G	N1-C6-O6	8.07	124.75	119.90
4	D	69	U	O4'-C1'-N1	7.96	114.57	108.20
6	F	1668	G	C5-C6-O6	-7.89	123.86	128.60
8	H	75	PRO	C-N-CA	7.79	141.17	121.70
7	G	925	C	O4'-C1'-N1	7.76	114.41	108.20
4	D	55	U	O4'-C1'-N1	7.73	114.38	108.20
6	F	1670	U	O4'-C1'-N1	7.72	114.38	108.20
7	G	920	C	O4'-C1'-N1	7.71	114.37	108.20
5	E	558	G	C5-C6-O6	-7.69	123.98	128.60
4	D	75	G	N1-C6-O6	7.65	124.49	119.90
4	D	46	G	C5-C6-O6	-7.61	124.04	128.60
7	G	913	C	O4'-C1'-N1	7.61	114.28	108.20
7	G	914	C	O4'-C1'-N1	7.60	114.28	108.20
4	D	67	U	O4'-C1'-N1	7.57	114.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	102	U	O4'-C1'-N1	7.57	114.25	108.20
4	D	70	G	C5-C6-O6	-7.54	124.07	128.60
4	D	63	G	C5-C6-O6	-7.54	124.08	128.60
4	D	62	C	O4'-C1'-N1	7.49	114.19	108.20
5	E	534	G	C5-C6-O6	-7.49	124.11	128.60
6	F	1666	C	O4'-C1'-N1	7.48	114.18	108.20
5	E	537	C	O4'-C1'-N1	7.33	114.06	108.20
7	G	917	C	O4'-C1'-N1	7.31	114.05	108.20
7	G	919	C	O4'-C1'-N1	7.30	114.04	108.20
4	D	68	G	C5-C6-O6	-7.30	124.22	128.60
7	G	929	C	O4'-C1'-N1	7.30	114.04	108.20
4	D	80	A	O4'-C1'-N9	7.26	114.00	108.20
6	F	1674	C	O4'-C1'-N1	7.25	114.00	108.20
6	F	1661	A	C5-C6-N6	-7.25	117.90	123.70
4	D	53	A	C4-C5-C6	7.21	120.60	117.00
4	D	64	U	O4'-C1'-N1	7.18	113.95	108.20
4	D	56	G	C5-C6-O6	-7.18	124.29	128.60
4	D	65	A	O4'-C1'-N9	7.17	113.94	108.20
4	D	101	U	O4'-C1'-N1	7.15	113.92	108.20
6	F	1663	C	O4'-C1'-N1	7.15	113.92	108.20
7	G	928	G	C5-C6-O6	-7.12	124.33	128.60
4	D	96	A	O4'-C1'-N9	7.11	113.89	108.20
5	E	546	G	C5-C6-O6	-7.10	124.34	128.60
9	I	36	ILE	C-N-CA	7.08	139.40	121.70
14	N	67	ARG	NE-CZ-NH2	7.07	123.84	120.30
8	H	54	GLU	C-N-CA	7.05	139.33	121.70
13	M	25	PHE	CB-CG-CD2	7.04	125.72	120.80
14	N	39	PRO	C-N-CA	7.03	139.26	121.70
6	F	1678	G	C5-C6-O6	-7.01	124.39	128.60
4	D	58	G	C5-C6-O6	-7.01	124.39	128.60
7	G	912	G	C5-C6-O6	-7.00	124.40	128.60
4	D	93	U	O4'-C1'-N1	7.00	113.80	108.20
4	D	98	U	O4'-C1'-N1	6.99	113.79	108.20
5	E	540	U	O4'-C1'-N1	6.99	113.79	108.20
4	D	100	U	O4'-C1'-N1	6.98	113.79	108.20
4	D	53	A	C5-C6-N6	-6.98	118.12	123.70
5	E	536	A	C5-C6-N6	-6.96	118.13	123.70
9	I	56	ARG	CB-CA-C	6.96	124.32	110.40
7	G	924	G	C5-C6-O6	-6.96	124.43	128.60
7	G	926	U	O4'-C1'-N1	6.95	113.76	108.20
4	D	66	A	C5-C6-N6	-6.94	118.15	123.70
11	K	123	TYR	CB-CG-CD1	-6.94	116.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	552	G	C5-C6-O6	-6.94	124.44	128.60
4	D	56	G	O4'-C1'-N9	6.92	113.74	108.20
4	D	81	U	O4'-C1'-N1	6.92	113.74	108.20
5	E	544	A	C4-C5-C6	6.91	120.46	117.00
7	G	927	G	C5-C6-O6	-6.89	124.46	128.60
8	H	90	PHE	CB-CG-CD2	6.89	125.62	120.80
5	E	551	U	O4'-C1'-N1	6.85	113.68	108.20
5	E	528	U	O4'-C1'-N1	6.84	113.67	108.20
7	G	916	G	C5-C6-O6	-6.83	124.50	128.60
4	D	62	C	C6-N1-C1'	-6.83	112.60	120.80
6	F	1658	G	C5-C6-O6	-6.81	124.51	128.60
5	E	529	G	C5-C6-O6	-6.81	124.51	128.60
4	D	62	C	C2-N1-C1'	6.76	126.23	118.80
12	L	84	LYS	C-N-CA	6.74	138.54	121.70
4	D	47	C	O4'-C1'-N1	6.73	113.58	108.20
6	F	1659	U	O4'-C1'-N1	6.72	113.58	108.20
5	E	548	G	C5-C6-O6	-6.71	124.58	128.60
4	D	49	G	C5-C6-O6	-6.70	124.58	128.60
2	B	77	TYR	CB-CG-CD1	-6.70	116.98	121.00
6	F	1655	C	O4'-C1'-N1	6.69	113.56	108.20
5	E	555	A	C5-C6-N6	-6.69	118.35	123.70
6	F	1672	G	C5-C6-O6	-6.68	124.59	128.60
8	H	75	PRO	CA-C-N	6.66	131.86	117.20
6	F	1654	C	N3-C4-N4	6.63	122.64	118.00
9	I	37	ASN	N-CA-CB	6.63	122.53	110.60
4	D	78	G	C5-C6-O6	-6.62	124.63	128.60
6	F	1671	G	O4'-C1'-N9	6.61	113.49	108.20
7	G	923	U	O4'-C1'-N1	6.61	113.49	108.20
5	E	557	A	C5-C6-N6	-6.61	118.41	123.70
6	F	1654	C	O4'-C1'-N1	6.61	113.48	108.20
5	E	541	G	C5-C6-O6	-6.60	124.64	128.60
5	E	538	U	O4'-C1'-N1	6.59	113.47	108.20
5	E	539	U	O4'-C1'-N1	6.58	113.47	108.20
6	F	1661	A	C4-C5-C6	6.58	120.29	117.00
12	L	10	SER	C-N-CA	6.58	138.15	121.70
8	H	60	THR	N-CA-CB	6.56	122.77	110.30
4	D	51	G	C5-C6-O6	-6.56	124.66	128.60
5	E	550	G	C5-C6-O6	-6.56	124.67	128.60
4	D	41	A	C4-C5-C6	6.54	120.27	117.00
4	D	42	G	C5-C6-O6	-6.53	124.68	128.60
4	D	103	G	C5-C6-O6	-6.49	124.71	128.60
4	D	91	C	O4'-C1'-N1	6.48	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	59	A	C4-C5-C6	6.48	120.24	117.00
4	D	85	G	C5-C6-O6	-6.46	124.72	128.60
6	F	1665	G	C5-C6-O6	-6.46	124.72	128.60
6	F	1671	G	C5-C6-O6	-6.45	124.73	128.60
13	M	25	PHE	CB-CG-CD1	-6.45	116.29	120.80
5	E	537	C	N3-C4-C5	-6.42	119.33	121.90
4	D	76	C	O4'-C1'-N1	6.42	113.34	108.20
4	D	76	C	N3-C4-N4	6.41	122.49	118.00
6	F	1676	U	O4'-C1'-N1	6.40	113.32	108.20
2	B	77	TYR	CB-CG-CD2	6.40	124.84	121.00
1	A	411	ARG	N-CA-CB	6.39	122.10	110.60
9	I	90	PHE	CB-CG-CD1	6.37	125.26	120.80
8	H	58	HIS	N-CA-CB	6.36	122.05	110.60
4	D	87	G	C5-C6-O6	-6.36	124.78	128.60
4	D	61	A	C4-C5-C6	6.36	120.18	117.00
8	H	214	GLY	C-N-CA	6.36	137.59	121.70
7	G	917	C	N3-C4-N4	6.35	122.45	118.00
4	D	72	A	C4-C5-C6	6.35	120.17	117.00
8	H	185	LYS	N-CA-C	6.34	128.12	111.00
4	D	99	C	N3-C4-N4	6.34	122.44	118.00
5	E	554	A	C5-C6-N6	-6.33	118.64	123.70
7	G	922	U	O4'-C1'-N1	6.32	113.26	108.20
6	F	1677	G	C5-C6-O6	-6.32	124.81	128.60
5	E	561	C	O4'-C1'-N1	6.31	113.25	108.20
6	F	1675	G	C5-C6-O6	-6.29	124.82	128.60
5	E	544	A	C5-C6-N6	-6.28	118.67	123.70
4	D	91	C	N3-C4-C5	-6.28	119.39	121.90
9	I	39	TRP	N-CA-CB	6.27	121.89	110.60
7	G	913	C	N3-C4-N4	6.27	122.39	118.00
8	H	55	LYS	N-CA-C	6.27	127.93	111.00
5	E	533	A	C5-C6-N6	-6.27	118.69	123.70
5	E	533	A	C4-C5-C6	6.26	120.13	117.00
11	K	123	TYR	CB-CG-CD2	6.26	124.76	121.00
4	D	95	G	C5-C6-O6	-6.25	124.85	128.60
6	F	1662	A	C5-C6-N1	-6.25	114.58	117.70
4	D	83	C	C2-N1-C1'	6.24	125.66	118.80
4	D	52	A	C4-C5-C6	6.23	120.11	117.00
4	D	52	A	C5-C6-N6	-6.22	118.73	123.70
5	E	548	G	O4'-C1'-N9	6.21	113.17	108.20
4	D	73	U	O4'-C1'-N1	6.21	113.17	108.20
4	D	41	A	C5-C6-N6	-6.20	118.74	123.70
6	F	1667	A	C4-C5-C6	6.18	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	915	A	C5-C6-N6	-6.16	118.77	123.70
7	G	920	C	N3-C4-N4	6.15	122.31	118.00
4	D	54	A	C5-C6-N6	-6.15	118.78	123.70
5	E	543	A	C4-C5-C6	6.13	120.07	117.00
4	D	47	C	N3-C4-C5	-6.13	119.45	121.90
4	D	71	A	C5-C6-N6	-6.12	118.80	123.70
4	D	79	A	C4-C5-C6	6.12	120.06	117.00
5	E	557	A	C4-C5-C6	6.11	120.06	117.00
13	M	77	ARG	C-N-CA	6.09	136.93	121.70
4	D	75	G	C4-N9-C1'	6.09	134.41	126.50
5	E	549	A	C4-C5-C6	6.08	120.04	117.00
4	D	91	C	N3-C4-N4	6.08	122.25	118.00
6	F	1660	C	O4'-C1'-N1	6.08	113.06	108.20
5	E	531	A	C4-C5-C6	6.07	120.03	117.00
4	D	94	C	O4'-C1'-N1	6.07	113.05	108.20
4	D	45	C	N3-C4-N4	6.06	122.25	118.00
5	E	556	A	C4-C5-C6	6.06	120.03	117.00
5	E	553	A	C4-C5-C6	6.06	120.03	117.00
9	I	90	PHE	CB-CG-CD2	-6.06	116.56	120.80
5	E	530	A	C5-C6-N6	-6.03	118.87	123.70
4	D	44	A	C4-C5-C6	6.03	120.02	117.00
7	G	919	C	N3-C4-C5	-6.03	119.49	121.90
8	H	57	GLY	C-N-CA	6.02	136.75	121.70
4	D	66	A	O4'-C1'-N9	6.01	113.00	108.20
8	H	159	ILE	C-N-CA	5.99	136.68	121.70
1	A	408	MET	N-CA-CB	5.99	121.38	110.60
4	D	50	C	N3-C4-C5	-5.99	119.51	121.90
4	D	54	A	O4'-C1'-N9	5.97	112.98	108.20
5	E	542	A	C4-C5-C6	5.97	119.98	117.00
4	D	97	A	C5-C6-N6	-5.96	118.93	123.70
5	E	553	A	C5-C6-N6	-5.96	118.93	123.70
4	D	78	G	O4'-C1'-N9	5.94	112.95	108.20
8	H	84	ARG	N-CA-CB	5.94	121.30	110.60
4	D	44	A	C5-C6-N6	-5.94	118.95	123.70
6	F	1656	A	C5-C6-N6	-5.94	118.95	123.70
7	G	915	A	C4-C5-C6	5.94	119.97	117.00
4	D	63	G	O4'-C1'-N9	5.94	112.95	108.20
6	F	1658	G	O4'-C1'-N9	5.93	112.94	108.20
7	G	929	C	N3-C4-N4	5.93	122.15	118.00
4	D	43	A	C4-C5-C6	5.92	119.96	117.00
4	D	61	A	C5-C6-N1	-5.92	114.74	117.70
9	I	71	ALA	N-CA-CB	5.92	118.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	86	U	O4'-C1'-N1	5.92	112.93	108.20
5	E	534	G	O4'-C1'-N9	5.92	112.93	108.20
14	N	67	ARG	N-CA-CB	-5.91	99.95	110.60
4	D	57	C	N3-C4-N4	5.90	122.13	118.00
5	E	546	G	O4'-C1'-N9	5.90	112.92	108.20
4	D	75	G	C5-C6-O6	-5.90	125.06	128.60
8	H	86	GLY	C-N-CA	5.89	136.43	121.70
4	D	47	C	N3-C4-N4	5.89	122.12	118.00
4	D	65	A	C4-C5-C6	5.88	119.94	117.00
6	F	1673	A	C4-C5-C6	5.88	119.94	117.00
7	G	924	G	O4'-C1'-N9	5.88	112.90	108.20
4	D	97	A	C4-C5-C6	5.87	119.93	117.00
4	D	45	C	N3-C4-C5	-5.86	119.56	121.90
5	E	545	A	C4-C5-C6	5.86	119.93	117.00
6	F	1674	C	N3-C4-C5	-5.85	119.56	121.90
7	G	927	G	O4'-C1'-N9	5.85	112.88	108.20
8	H	102	PRO	N-CA-C	5.85	127.31	112.10
6	F	1657	C	N3-C4-C5	-5.85	119.56	121.90
4	D	99	C	O4'-C1'-N1	5.84	112.88	108.20
4	D	88	A	C5-C6-N6	-5.84	119.03	123.70
14	N	39	PRO	CA-C-N	5.84	130.05	117.20
4	D	79	A	C5-C6-N6	-5.84	119.03	123.70
5	E	554	A	C4-C5-C6	5.83	119.92	117.00
5	E	560	A	O4'-C1'-N9	5.83	112.86	108.20
4	D	77	A	C5-C6-N1	-5.82	114.79	117.70
4	D	50	C	P-O3'-C3'	5.82	126.68	119.70
5	E	560	A	C4-C5-C6	5.81	119.91	117.00
4	D	71	A	C4-C5-C6	5.81	119.90	117.00
5	E	531	A	C5-C6-N1	-5.81	114.80	117.70
4	D	42	G	O4'-C1'-N9	5.80	112.84	108.20
4	D	89	A	C4-C5-C6	5.80	119.90	117.00
8	H	253	ALA	N-CA-CB	5.80	118.22	110.10
5	E	530	A	C4-C5-C6	5.80	119.90	117.00
5	E	547	A	C4-C5-C6	5.80	119.90	117.00
5	E	535	A	C5-C6-N6	-5.79	119.07	123.70
6	F	1662	A	C5-C6-N6	-5.79	119.07	123.70
5	E	535	A	C4-C5-C6	5.79	119.89	117.00
7	G	920	C	N3-C4-C5	-5.78	119.59	121.90
4	D	96	A	C4-C5-C6	5.78	119.89	117.00
4	D	57	C	N3-C4-C5	-5.78	119.59	121.90
5	E	541	G	O4'-C1'-N9	5.78	112.82	108.20
4	D	54	A	C4-C5-C6	5.77	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1654	C	N3-C4-C5	-5.77	119.59	121.90
4	D	84	C	N3-C4-N4	5.76	122.03	118.00
7	G	914	C	N3-C4-C5	-5.76	119.59	121.90
4	D	89	A	O4'-C1'-N9	5.76	112.81	108.20
5	E	561	C	N3-C4-C5	-5.75	119.60	121.90
6	F	1660	C	N3-C4-C5	-5.74	119.60	121.90
14	N	3	GLY	C-N-CA	5.74	136.05	121.70
14	N	14	LYS	N-CA-CB	5.74	120.93	110.60
5	E	529	G	O4'-C1'-N9	5.73	112.78	108.20
4	D	66	A	C4-C5-C6	5.72	119.86	117.00
4	D	92	A	C5'-C4'-O4'	5.72	115.97	109.10
4	D	49	G	N3-C2-N2	5.72	123.90	119.90
4	D	53	A	C5-C6-N1	-5.72	114.84	117.70
5	E	542	A	C5-C6-N6	-5.71	119.13	123.70
5	E	560	A	C5-C6-N6	-5.71	119.13	123.70
6	F	1663	C	N3-C4-N4	5.71	122.00	118.00
6	F	1674	C	N3-C4-N4	5.71	122.00	118.00
9	I	56	ARG	CA-C-N	5.71	129.75	117.20
5	E	533	A	C5-C6-N1	-5.70	114.85	117.70
5	E	544	A	C5-C6-N1	-5.70	114.85	117.70
4	D	72	A	C5-C6-N1	-5.70	114.85	117.70
6	F	1669	U	O4'-C1'-N1	5.69	112.75	108.20
4	D	92	A	C5-C6-N6	-5.69	119.15	123.70
15	O	7	PHE	CB-CG-CD1	5.69	124.78	120.80
6	F	1675	G	O4'-C1'-N9	5.69	112.75	108.20
4	D	71	A	C5-C6-N1	-5.68	114.86	117.70
4	D	92	A	C4-C5-C6	5.68	119.84	117.00
4	D	83	C	O4'-C1'-N1	5.68	112.74	108.20
1	A	410	ARG	N-CA-CB	5.68	120.82	110.60
4	D	54	A	C5-C6-N1	-5.67	114.86	117.70
4	D	82	U	O4'-C1'-N1	5.67	112.73	108.20
6	F	1666	C	N3-C4-C5	-5.66	119.64	121.90
1	A	276	ARG	N-CA-CB	5.66	120.79	110.60
7	G	925	C	N3-C4-N4	5.66	121.96	118.00
4	D	44	A	O4'-C1'-N9	5.65	112.72	108.20
4	D	48	A	C5-C6-N1	-5.64	114.88	117.70
5	E	537	C	N3-C4-N4	5.64	121.95	118.00
5	E	559	U	O4'-C1'-N1	5.64	112.71	108.20
4	D	74	U	O4'-C1'-N1	5.63	112.71	108.20
4	D	43	A	O4'-C1'-N9	5.63	112.70	108.20
4	D	85	G	O4'-C1'-N9	5.63	112.71	108.20
4	D	88	A	C4-C5-C6	5.63	119.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	65	A	C5-C6-N1	-5.63	114.89	117.70
6	F	1667	A	C5-C6-N1	-5.63	114.89	117.70
4	D	48	A	C4-C5-C6	5.62	119.81	117.00
5	E	557	A	C5-C6-N1	-5.62	114.89	117.70
13	M	24	SER	N-CA-CB	5.62	118.94	110.50
6	F	1667	A	C5-C6-N6	-5.62	119.20	123.70
5	E	531	A	C5-C6-N6	-5.61	119.21	123.70
6	F	1664	A	C5-C6-N6	-5.61	119.21	123.70
5	E	545	A	C5-C6-N1	-5.60	114.90	117.70
5	E	547	A	C5-C6-N1	-5.60	114.90	117.70
4	D	83	C	N3-C4-C5	-5.60	119.66	121.90
5	E	556	A	C5-C6-N6	-5.60	119.22	123.70
15	O	5	LYS	CB-CA-C	5.60	121.60	110.40
5	E	555	A	C4-C5-C6	5.59	119.79	117.00
4	D	94	C	N3-C4-C5	-5.59	119.67	121.90
4	D	43	A	C5-C6-N1	-5.58	114.91	117.70
1	A	413	GLN	CB-CA-C	5.58	121.56	110.40
1	A	471	TYR	CB-CG-CD2	-5.58	117.65	121.00
6	F	1656	A	C4-C5-C6	5.58	119.79	117.00
5	E	543	A	C5-C6-N1	-5.55	114.93	117.70
9	I	57	ALA	N-CA-C	5.53	125.92	111.00
6	F	1662	A	C4-C5-C6	5.52	119.76	117.00
6	F	1663	C	N3-C4-C5	-5.51	119.69	121.90
7	G	915	A	O4'-C1'-N9	5.51	112.61	108.20
7	G	918	A	C5-C6-N6	-5.50	119.30	123.70
7	G	929	C	N3-C4-C5	-5.50	119.70	121.90
8	H	88	GLY	C-N-CA	5.50	135.44	121.70
7	G	914	C	N3-C4-N4	5.49	121.84	118.00
4	D	97	A	C5-C6-N1	-5.48	114.96	117.70
7	G	917	C	N3-C4-C5	-5.48	119.71	121.90
6	F	1655	C	N3-C4-N4	5.47	121.83	118.00
9	I	105	LYS	C-N-CA	5.47	133.79	122.30
7	G	928	G	O4'-C1'-N9	5.47	112.58	108.20
6	F	1655	C	N3-C4-C5	-5.46	119.71	121.90
8	H	28	ALA	N-CA-CB	5.46	117.75	110.10
4	D	83	C	C6-N1-C1'	-5.46	114.25	120.80
5	E	549	A	C5-C6-N6	-5.45	119.34	123.70
7	G	918	A	C4-C5-C6	5.44	119.72	117.00
4	D	79	A	O4'-C1'-N9	5.43	112.55	108.20
4	D	66	A	C5-C6-N1	-5.42	114.99	117.70
8	H	100	PHE	CB-CG-CD1	5.42	124.59	120.80
7	G	913	C	N3-C4-C5	-5.42	119.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	921	U	O4'-C1'-N1	5.42	112.53	108.20
6	F	1662	A	O4'-C1'-N9	5.42	112.53	108.20
12	L	84	LYS	N-CA-CB	5.41	120.34	110.60
5	E	547	A	O4'-C1'-N9	5.41	112.53	108.20
8	H	212	ASP	C-N-CA	5.41	135.22	121.70
4	D	94	C	N3-C4-N4	5.40	121.78	118.00
4	D	59	A	C5-C6-N1	-5.39	115.00	117.70
4	D	89	A	C5-C6-N6	-5.38	119.39	123.70
8	H	12	THR	C-N-CA	5.38	133.59	122.30
5	E	536	A	O4'-C1'-N9	5.37	112.50	108.20
5	E	547	A	C5-C6-N6	-5.37	119.40	123.70
6	F	1656	A	C5-C6-N1	-5.37	115.02	117.70
4	D	103	G	O4'-C1'-N9	5.36	112.49	108.20
4	D	48	A	C5-C6-N6	-5.36	119.42	123.70
4	D	59	A	C5-C6-N6	-5.35	119.42	123.70
7	G	915	A	C5-C6-N1	-5.35	115.02	117.70
14	N	13	SER	C-N-CA	5.35	135.08	121.70
7	G	925	C	N3-C4-C5	-5.35	119.76	121.90
13	M	26	LYS	N-CA-CB	5.35	120.23	110.60
5	E	543	A	C5-C6-N6	-5.35	119.42	123.70
7	G	918	A	C5-C6-N1	-5.33	115.03	117.70
9	I	105	LYS	CA-C-N	5.33	126.86	116.20
4	D	96	A	C5-C6-N6	-5.33	119.44	123.70
9	I	56	ARG	N-CA-CB	5.33	120.18	110.60
1	A	471	TYR	CB-CG-CD1	5.32	124.19	121.00
7	G	916	G	O4'-C1'-N9	5.32	112.46	108.20
6	F	1661	A	C5-C6-N1	-5.31	115.04	117.70
8	H	90	PHE	CB-CG-CD1	-5.31	117.08	120.80
6	F	1673	A	C5-C6-N1	-5.31	115.05	117.70
8	H	60	THR	N-CA-C	-5.30	96.69	111.00
6	F	1666	C	N3-C4-N4	5.29	121.70	118.00
14	N	69	LEU	CA-C-O	-5.29	109.00	120.10
6	F	1656	A	O4'-C1'-N9	5.28	112.42	108.20
9	I	66	SER	C-N-CA	5.28	134.90	121.70
15	O	7	PHE	CB-CG-CD2	-5.28	117.11	120.80
4	D	62	C	N3-C4-C5	-5.28	119.79	121.90
4	D	88	A	C5-C6-N1	-5.27	115.06	117.70
4	D	41	A	C5-C6-N1	-5.26	115.07	117.70
4	D	79	A	C5-C6-N1	-5.26	115.07	117.70
5	E	556	A	C5-C6-N1	-5.25	115.08	117.70
4	D	49	G	O4'-C1'-N9	5.24	112.39	108.20
1	A	278	ARG	N-CA-C	-5.23	96.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	919	C	N3-C4-N4	5.23	121.66	118.00
14	N	37	SER	N-CA-CB	5.22	118.33	110.50
5	E	554	A	C5-C6-N1	-5.20	115.10	117.70
5	E	553	A	O4'-C1'-N9	5.20	112.36	108.20
13	M	25	PHE	N-CA-CB	5.20	119.95	110.60
4	D	51	G	N3-C2-N2	5.19	123.54	119.90
5	E	542	A	O4'-C1'-N9	5.19	112.35	108.20
7	G	912	G	O4'-C1'-N9	5.19	112.35	108.20
6	F	1668	G	O4'-C1'-N9	5.19	112.35	108.20
5	E	561	C	N3-C4-N4	5.17	121.62	118.00
4	D	52	A	C5-C6-N1	-5.17	115.11	117.70
8	H	264	SER	N-CA-CB	5.17	118.26	110.50
6	F	1657	C	N3-C4-N4	5.17	121.62	118.00
6	F	1677	G	O4'-C1'-N9	5.17	112.33	108.20
8	H	212	ASP	CB-CA-C	5.16	120.73	110.40
5	E	535	A	C5-C6-N1	-5.15	115.13	117.70
5	E	557	A	O4'-C1'-N9	5.13	112.31	108.20
8	H	199	TRP	N-CA-CB	5.13	119.83	110.60
5	E	553	A	C5-C6-N1	-5.13	115.14	117.70
4	D	61	A	C5-C6-N6	-5.13	119.60	123.70
4	D	84	C	N3-C4-C5	-5.12	119.85	121.90
8	H	105	THR	C-N-CA	5.12	134.50	121.70
7	G	918	A	O4'-C1'-N9	5.12	112.30	108.20
4	D	46	G	O4'-C1'-N9	5.12	112.29	108.20
5	E	542	A	C5-C6-N1	-5.10	115.15	117.70
4	D	96	A	C5-C6-N1	-5.09	115.15	117.70
9	I	9	THR	C-N-CA	5.09	134.43	121.70
4	D	92	A	C5-C6-N1	-5.08	115.16	117.70
5	E	536	A	C4-C5-C6	5.08	119.54	117.00
5	E	549	A	C5-C6-N1	-5.07	115.16	117.70
4	D	99	C	N3-C4-C5	-5.07	119.87	121.90
8	H	12	THR	CA-C-N	5.07	126.33	116.20
5	E	554	A	O4'-C1'-N9	5.06	112.25	108.20
5	E	545	A	C5-C6-N6	-5.06	119.65	123.70
5	E	552	G	O4'-C1'-N9	5.06	112.25	108.20
4	D	80	A	C4-C5-C6	5.05	119.53	117.00
15	O	31	THR	C-N-CA	5.04	134.31	121.70
9	I	37	ASN	N-CA-C	-5.04	97.40	111.00
13	M	78	LYS	N-CA-CB	5.04	119.67	110.60
6	F	1664	A	O4'-C1'-N9	5.03	112.22	108.20
6	F	1664	A	C5-C6-N1	-5.03	115.19	117.70
4	D	97	A	O4'-C1'-N9	5.02	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	560	A	C5-C6-N1	-5.02	115.19	117.70
4	D	77	A	O4'-C1'-N9	5.01	112.21	108.20
8	H	63	GLU	N-CA-C	-5.01	97.47	111.00
9	I	3	ARG	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	TYR	Sidechain
1	A	17	LEU	Peptide
1	A	21	GLU	Peptide
1	A	262	TYR	Sidechain
1	A	273	ARG	Sidechain
1	A	408	MET	Peptide
1	A	409	GLY	Peptide
1	A	412	GLU	Peptide
1	A	43	TYR	Sidechain
2	B	30	ARG	Sidechain
4	D	49	G	Sidechain
4	D	55	U	Sidechain
4	D	56	G	Sidechain
4	D	62	C	Sidechain
4	D	76	C	Sidechain
4	D	77	A	Sidechain
4	D	87	G	Sidechain
5	E	536	A	Sidechain
5	E	543	A	Sidechain
6	F	1667	A	Sidechain
8	H	110	ASN	Peptide
8	H	197	ARG	Peptide
8	H	209	TYR	Sidechain
8	H	59	GLN	Peptide
8	H	74	ILE	Peptide
8	H	76	ARG	Peptide
8	H	92	ASN	Peptide
9	I	122	ALA	Peptide
9	I	23	ARG	Sidechain
11	K	105	VAL	Peptide
11	K	57	LEU	Peptide
12	L	111	LEU	Peptide
12	L	121	ARG	Peptide

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Mol	Chain	Res	Type	Group
12	L	125	LYS	Peptide
12	L	52	ARG	Sidechain
12	L	63	LYS	Peptide
12	L	89	LYS	Peptide
14	N	32	LYS	Peptide
14	N	36	LEU	Peptide
14	N	38	ARG	Peptide
15	O	23	LEU	Peptide
15	O	24	PRO	Peptide
15	O	31	THR	Peptide
15	O	32	ASN	Peptide
15	O	36	ARG	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	3770	0	3941	11	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	13	0
9	I	1212	0	1231	5	0
10	J	410	0	452	0	0
11	K	663	0	699	1	0
12	L	1002	0	1093	1	0
13	M	706	0	741	0	0
14	N	547	0	613	4	0
15	O	316	0	349	0	0
All	All	14301	0	13435	37	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 (37) 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)
11:K:100:LYS:HA	11:K:105:VAL:HG22	1.81	0.63
5:E:539:U:H3	5:E:546:G:H1	1.51	0.57
1:A:228:HIS:CG	1:A:229:LYS:H	2.23	0.57
1:A:65:ILE:HD12	1:A:68:LEU:HD12	1.88	0.54
12:L:56:VAL:HG22	12:L:106:ILE:HG22	1.89	0.53
8:H:184:SER:HA	8:H:186:LYS:H	1.73	0.52
9:I:3:ARG:HB2	9:I:4:TYR:HA	1.93	0.51
9:I:9:THR:HG23	9:I:10:ASN:HA	1.93	0.50
1:A:447:LYS:HG2	1:A:448:GLY:H	1.77	0.50
1:A:310:ALA:H	1:A:314:ILE:HD12	1.77	0.50
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.93	0.49
14:N:41:LEU:H	14:N:44:ILE:HD12	1.77	0.49
8:H:77:VAL:HG12	8:H:87:GLN:HA	1.93	0.48
1:A:11:LYS:H	1:A:12:PRO:HD2	1.78	0.47
8:H:83:GLY:HA3	8:H:84:ARG:HB2	1.98	0.45
8:H:184:SER:HA	8:H:186:LYS:N	2.31	0.45
8:H:57:GLY:HA3	8:H:58:HIS:HB2	1.98	0.45
1:A:342:VAL:HB	1:A:343:PRO:HD2	1.98	0.45
1:A:79:LEU:H	1:A:79:LEU:HD22	1.81	0.44
8:H:77:VAL:HG21	8:H:90:PHE:CD1	2.53	0.44
8:H:77:VAL:HG13	8:H:78:GLY:H	1.83	0.44
8:H:52:VAL:HG22	8:H:53:SER:H	1.83	0.44
8:H:77:VAL:HG13	8:H:78:GLY:N	2.33	0.43
1:A:260:VAL:HG11	1:A:454:VAL:HG12	2.01	0.43
14:N:37:SER:N	14:N:38:ARG:HA	2.34	0.43
8:H:152:VAL:HG12	8:H:153:SER:H	1.84	0.42
1:A:22:LEU:HB2	1:A:23:PRO:CD	2.50	0.42
9:I:57:ALA:HB1	9:I:58:ILE:H	1.58	0.42
1:A:128:TYR:CZ	1:A:161:GLY:HA3	2.55	0.42
2:B:57:GLY:O	2:B:61:VAL:HG23	2.19	0.42
8:H:13:GLY:H	8:H:14:GLU:HB2	1.85	0.41
1:A:256:ILE:O	1:A:260:VAL:HG12	2.20	0.41
9:I:105:LYS:HD3	9:I:105:LYS:H	1.86	0.41
8:H:160:GLN:H	8:H:218:ALA:HB3	1.86	0.41
14:N:34:GLN:CA	14:N:36:LEU:H	2.33	0.41
9:I:107:LEU:HD12	9:I:107:LEU:H	1.86	0.40
14:N:34:GLN:HA	14:N:36:LEU:H	1.87	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%)	428 (88%)	41 (8%)	19 (4%)	4 36
2	B	58/80 (72%)	57 (98%)	1 (2%)	0	100 100
3	C	19/87 (22%)	17 (90%)	1 (5%)	1 (5%)	2 29
8	H	267/362 (74%)	186 (70%)	38 (14%)	43 (16%)	0 5
9	I	151/184 (82%)	113 (75%)	24 (16%)	14 (9%)	1 16
10	J	51/189 (27%)	46 (90%)	5 (10%)	0	100 100
11	K	81/142 (57%)	71 (88%)	7 (9%)	3 (4%)	4 38
12	L	125/127 (98%)	101 (81%)	8 (6%)	16 (13%)	0 8
13	M	82/113 (73%)	64 (78%)	11 (13%)	7 (8%)	1 18
14	N	67/120 (56%)	60 (90%)	2 (3%)	5 (8%)	1 21
15	O	35/51 (69%)	25 (71%)	2 (6%)	8 (23%)	0 2
All	All	1424/1945 (73%)	1168 (82%)	140 (10%)	116 (8%)	2 19

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	148	VAL
1	A	274	SER
1	A	276	ARG
1	A	410	ARG
1	A	449	LYS
8	H	3	ARG
8	H	28	ALA
8	H	55	LYS
8	H	58	HIS
8	H	70	ALA
8	H	87	GLN
8	H	89	ALA

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Mol	Chain	Res	Type
8	H	98	ARG
8	H	102	PRO
8	H	103	THR
8	H	146	PRO
8	H	185	LYS
8	H	199	TRP
8	H	212	ASP
8	H	215	ILE
8	H	222	VAL
8	H	244	LEU
9	I	37	ASN
9	I	56	ARG
9	I	57	ALA
9	I	67	ILE
9	I	107	LEU
9	I	113	TYR
9	I	123	PRO
9	I	143	PRO
12	L	23	PRO
12	L	24	SER
12	L	85	VAL
13	M	26	LYS
13	M	78	LYS
13	M	79	ARG
14	N	4	VAL
14	N	14	LYS
14	N	39	PRO
15	O	22	PRO
15	O	23	LEU
15	O	24	PRO
1	A	61	VAL
1	A	277	ALA
1	A	389	SER
1	A	484	LEU
3	C	60	ASP
8	H	13	GLY
8	H	72	ALA
8	H	93	MET
8	H	107	ARG
8	H	160	GLN
8	H	173	GLY
8	H	187	LEU

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Mol	Chain	Res	Type
8	H	200	THR
8	H	262	TRP
8	H	264	SER
9	I	71	ALA
9	I	111	LYS
11	K	62	VAL
12	L	11	ASP
12	L	45	ILE
12	L	46	LYS
12	L	96	PRO
12	L	122	LYS
13	M	25	PHE
13	M	90	PHE
14	N	5	LYS
14	N	37	SER
15	O	6	SER
15	O	20	ASN
1	A	67	PHE
1	A	278	ARG
1	A	408	MET
1	A	411	ARG
8	H	54	GLU
8	H	60	THR
8	H	63	GLU
8	H	69	ARG
8	H	76	ARG
9	I	3	ARG
9	I	25	SER
9	I	54	HIS
12	L	36	SER
12	L	87	LYS
12	L	125	LYS
13	M	24	SER
1	A	11	LYS
8	H	74	ILE
8	H	84	ARG
8	H	106	TRP
8	H	110	ASN
8	H	132	ALA
8	H	253	ALA
8	H	265	GLU
9	I	39	TRP

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Mol	Chain	Res	Type
11	K	109	LYS
12	L	6	LEU
12	L	86	THR
15	O	34	THR
1	A	28	PRO
1	A	346	PRO
8	H	131	VAL
8	H	196	ASN
8	H	198	ARG
11	K	131	ASP
12	L	84	LYS
12	L	97	ILE
13	M	51	LEU
15	O	25	GLN
1	A	284	TYR
12	L	22	ALA
15	O	5	LYS
1	A	199	GLY
8	H	96	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	387 (94%)	25 (6%)	23 60
2	B	50/67 (75%)	46 (92%)	4 (8%)	15 50
3	C	19/73 (26%)	17 (90%)	2 (10%)	8 36
8	H	209/288 (73%)	182 (87%)	27 (13%)	5 28
9	I	124/146 (85%)	109 (88%)	15 (12%)	6 31
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%)	96 (87%)	14 (13%)	5 29
13	M	74/97 (76%)	65 (88%)	9 (12%)	6 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	62/105 (59%)	59 (95%)	3 (5%)	31 67
15	O	33/46 (72%)	29 (88%)	4 (12%)	6 31
All	All	1211/1616 (75%)	1099 (91%)	112 (9%)	16 43

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	22	LEU
1	A	24	PHE
1	A	26	LYS
1	A	31	ASP
1	A	47	GLN
1	A	50	LEU
1	A	80	LEU
1	A	121	LYS
1	A	128	TYR
1	A	148	VAL
1	A	154	ASN
1	A	170	VAL
1	A	185	ASN
1	A	197	THR
1	A	204	LYS
1	A	229	LYS
1	A	241	ARG
1	A	242	ASP
1	A	309	PHE
1	A	410	ARG
1	A	414	ASN
1	A	417	LYS
1	A	425	ILE
1	A	480	LEU
2	B	30	ARG
2	B	35	PHE
2	B	52	LYS
2	B	77	TYR
3	C	60	ASP
3	C	76	ILE
8	H	4	PRO
8	H	35	VAL
8	H	43	ASN

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Mol	Chain	Res	Type
8	H	46	LYS
8	H	48	GLN
8	H	63	GLU
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
8	H	159	ILE
8	H	161	LYS
8	H	164	GLU
8	H	170	LYS
8	H	193	LYS
8	H	198	ARG
8	H	201	GLN
8	H	225	VAL
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	46	LYS
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	112	LEU
9	I	144	SER
9	I	149	VAL
10	J	1	MET
10	J	53	LYS
11	K	65	GLN

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Mol	Chain	Res	Type
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
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	88	GLU
12	L	95	VAL
12	L	108	LYS
12	L	111	LEU
12	L	122	LYS
12	L	125	LYS
13	M	20	LEU
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	82	GLU
13	M	86	LYS
14	N	5	LYS
14	N	9	LEU
14	N	37	SER
15	O	17	LYS
15	O	18	LYS
15	O	22	PRO
15	O	26	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	386	GLN

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Mol	Chain	Res	Type
1	A	403	GLN
1	A	414	ASN
8	H	43	ASN
8	H	213	ASN
11	K	111	ASN
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%)	7 (21%)	2 (6%)
6	F	24/25 (96%)	1 (4%)	0
7	G	17/18 (94%)	1 (5%)	0
All	All	136/140 (97%)	36 (26%)	12 (8%)

All (36) 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

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Mol	Chain	Res	Type
4	D	92	A
4	D	94	C
4	D	95	G
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
6	F	1668	G
7	G	922	U

All (12) 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	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.