



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:39 AM UTC

PDB ID : 4V7F / pdb_00004v7f
EMDB ID : EMD-2528
Title : Arx1 pre-60S particle.
Authors : Leidig, C.; Thoms, M.; Holdermann, I.; Bradatsch, B.; Berninghausen, O.;
Bange, G.; Sinning, I.; Hurt, E.; Beckmann, R.
Deposited on : 2013-12-10
Resolution : 8.70 Å(reported)
Based on initial model : 3U5D

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

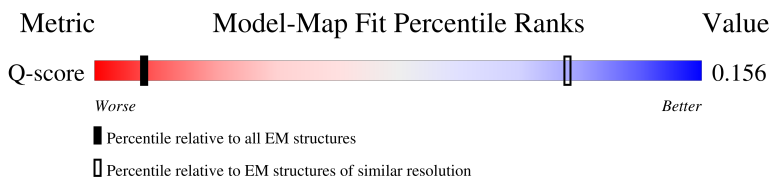
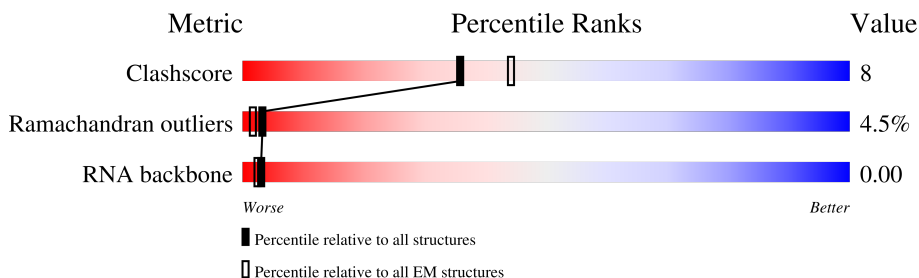
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 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.



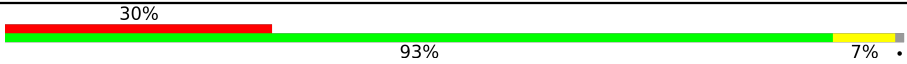
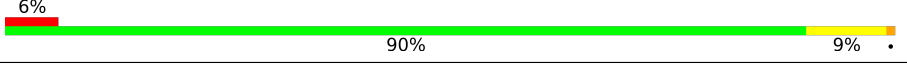
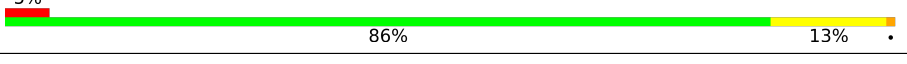
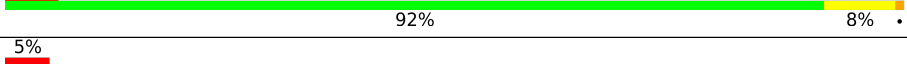
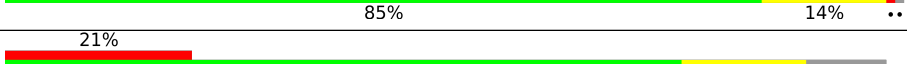
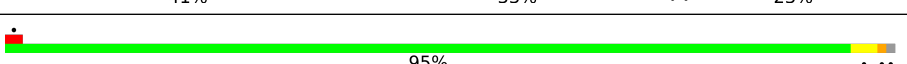
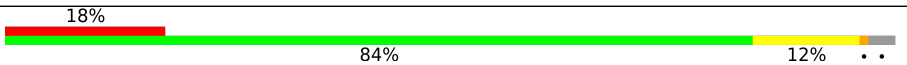
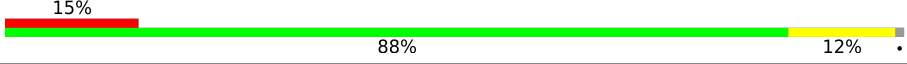
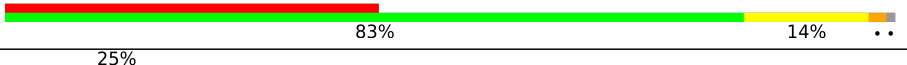
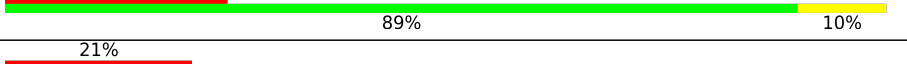
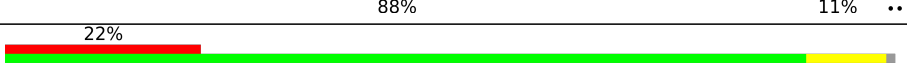
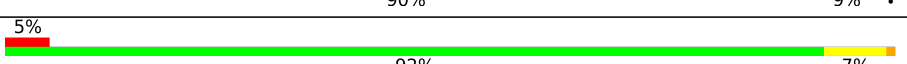
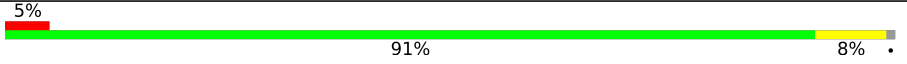
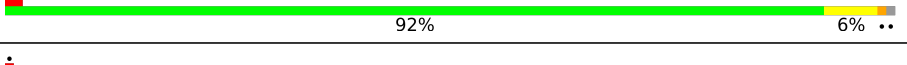
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
RNA backbone	8273	3508	-
Q-score	-	25397	282 (8.20 - 9.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	13% 91% 9%
2	2	158	98% .
3	3	121	91% 9%
4	A	217	98% 69% 29% .

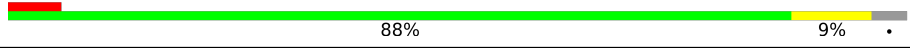
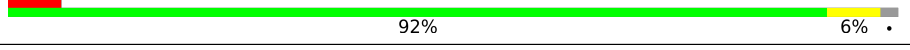
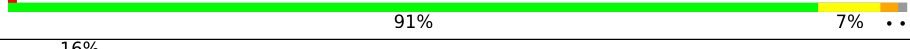
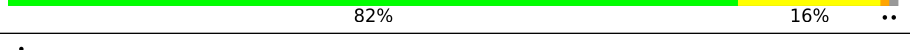
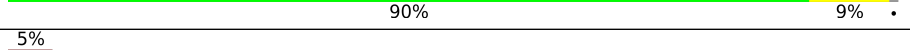
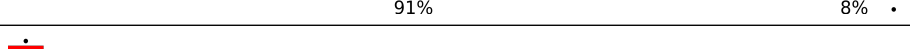
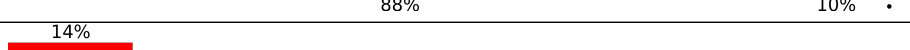
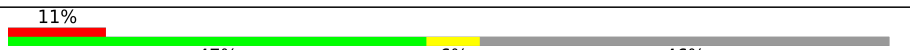
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Mol	Chain	Length	Quality of chain
5	B	254	
6	C	387	
7	D	362	
8	E	174	
9	F	191	
10	G	176	
11	H	256	
12	I	165	
13	J	199	
14	K	199	
15	L	137	
16	M	138	
17	N	149	
18	O	204	
19	P	297	
20	Q	186	
21	R	189	
22	S	172	
23	T	160	
24	U	184	
25	V	121	
26	W	142	
27	X	127	
28	Y	136	
29	Z	120	

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Mol	Chain	Length	Quality of chain
30	a	244	
31	b	105	
32	c	113	
33	d	130	
34	e	107	
35	f	121	
36	g	100	
37	h	88	
38	i	78	
39	j	51	
40	k	92	
41	l	593	
42	m	245	
43	n	236	
44	o	647	
45	p	199	
46	q	515	
47	r	322	
47	s	322	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 47221 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 RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	3394	Total	C	O	P	0	0
			20363	10182	6788	3393		

- Molecule 2 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	158	Total	C	O	P	0	0
			948	474	316	158		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	121	Total	C	O	P	0	0
			725	363	242	120		

- Molecule 4 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms			AltConf	Trace
4	A	217	Total	C	N	0	0
			651	434	217		

- Molecule 5 is a protein called 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms			AltConf	Trace
5	B	252	Total	C	N	0	0
			756	504	252		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	C	386	Total	C	N	0	0
			1158	772	386		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	D	361	Total	C	N	0	0
			1083	722	361		

- Molecule 8 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms			AltConf	Trace
8	E	169	Total	C	N	0	0
			507	338	169		

- Molecule 9 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms			AltConf	Trace
9	F	191	Total	C	N	0	0
			573	382	191		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms			AltConf	Trace
10	G	175	Total	C	N	0	0
			525	350	175		

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms			AltConf	Trace
11	H	233	Total	C	N	0	0
			699	466	233		

- Molecule 12 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms			AltConf	Trace
12	I	127	Total	C	N	0	0
			381	254	127		

- Molecule 13 is a protein called 60S ribosomal protein L16.

Mol	Chain	Residues	Atoms			AltConf	Trace
13	J	197	Total	C	N	0	0
			591	394	197		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms			AltConf	Trace
14	K	193	Total	C	N	0	0
			579	386	193		

- Molecule 15 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms			AltConf	Trace
15	L	136	Total	C	N	0	0
			408	272	136		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms			AltConf	Trace
16	M	136	Total	C	N	0	0
			408	272	136		

- Molecule 17 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms			AltConf	Trace
17	N	148	Total	C	N	0	0
			444	296	148		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms			AltConf	Trace
18	O	203	Total	C	N	0	0
			609	406	203		

- Molecule 19 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms			AltConf	Trace
19	P	269	Total	C	N	0	0
			807	538	269		

- Molecule 20 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms			AltConf	Trace
20	Q	185	Total	C	N	0	0
			555	370	185		

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms			AltConf	Trace
21	R	188	Total	C	N	0	0
			564	376	188		

- Molecule 22 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms			AltConf	Trace
22	S	172	Total	C	N	0	0
			516	344	172		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms			AltConf	Trace
23	T	159	Total	C	N	0	0
			477	318	159		

- Molecule 24 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms			AltConf	Trace
24	U	183	Total	C	N	0	0
			549	366	183		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms			AltConf	Trace
25	V	100	Total	C	N	0	0
			300	200	100		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms			AltConf	Trace
26	W	121	Total	C	N	0	0
			363	242	121		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms			AltConf	Trace
27	X	126	Total	C	N	0	0
			378	252	126		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms			AltConf	Trace
28	Y	135	Total	C	N	0	0
			405	270	135		

- Molecule 29 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms			AltConf	Trace
29	Z	119	Total	C	N	0	0
			357	238	119		

- Molecule 30 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms			AltConf	Trace
30	a	222	Total	C	N	0	0
			666	444	222		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms			AltConf	Trace
31	b	97	Total	C	N	0	0
			291	194	97		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms			AltConf	Trace
32	c	109	Total	C	N	0	0
			327	218	109		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms			AltConf	Trace
33	d	127	Total	C	N	0	0
			381	254	127		

- Molecule 34 is a protein called 60S ribosomal protein L33.

Mol	Chain	Residues	Atoms			AltConf	Trace
34	e	106	Total	C	N	0	0
			318	212	106		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms			AltConf	Trace
35	f	112	Total	C	N	0	0
			336	224	112		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms			AltConf	Trace
36	g	99	Total	C	N	0	0
			297	198	99		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms			AltConf	Trace
37	h	87	Total	C	N	0	0
			261	174	87		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms			AltConf	Trace
38	i	77	Total	C	N	0	0
			231	154	77		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms			AltConf	Trace
39	j	50	Total	C	N	0	0
			150	100	50		

- Molecule 40 is a protein called 60S ribosomal protein L43.

Mol	Chain	Residues	Atoms			AltConf	Trace
40	k	91	Total	C	N	0	0
			273	182	91		

- Molecule 41 is a protein called metalloprotease ARX1.

Mol	Chain	Residues	Atoms			AltConf	Trace
41	l	380	Total	C	N	0	0
			1140	760	380		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms			AltConf	Trace
42	m	224	Total	C	N	0	0
			672	448	224		

- Molecule 43 is a protein called mRNA turnover protein 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
43	n	236	Total	C	N	0	0
			708	472	236		

- Molecule 44 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms			AltConf	Trace
44	o	347	Total	C	N	0	0
			1041	694	347		

- Molecule 45 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms			AltConf	Trace
45	p	63	Total	C	N	0	0
			189	126	63		

- Molecule 46 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms			AltConf	Trace
46	q	443	Total	C	N	0	0
			1329	886	443		

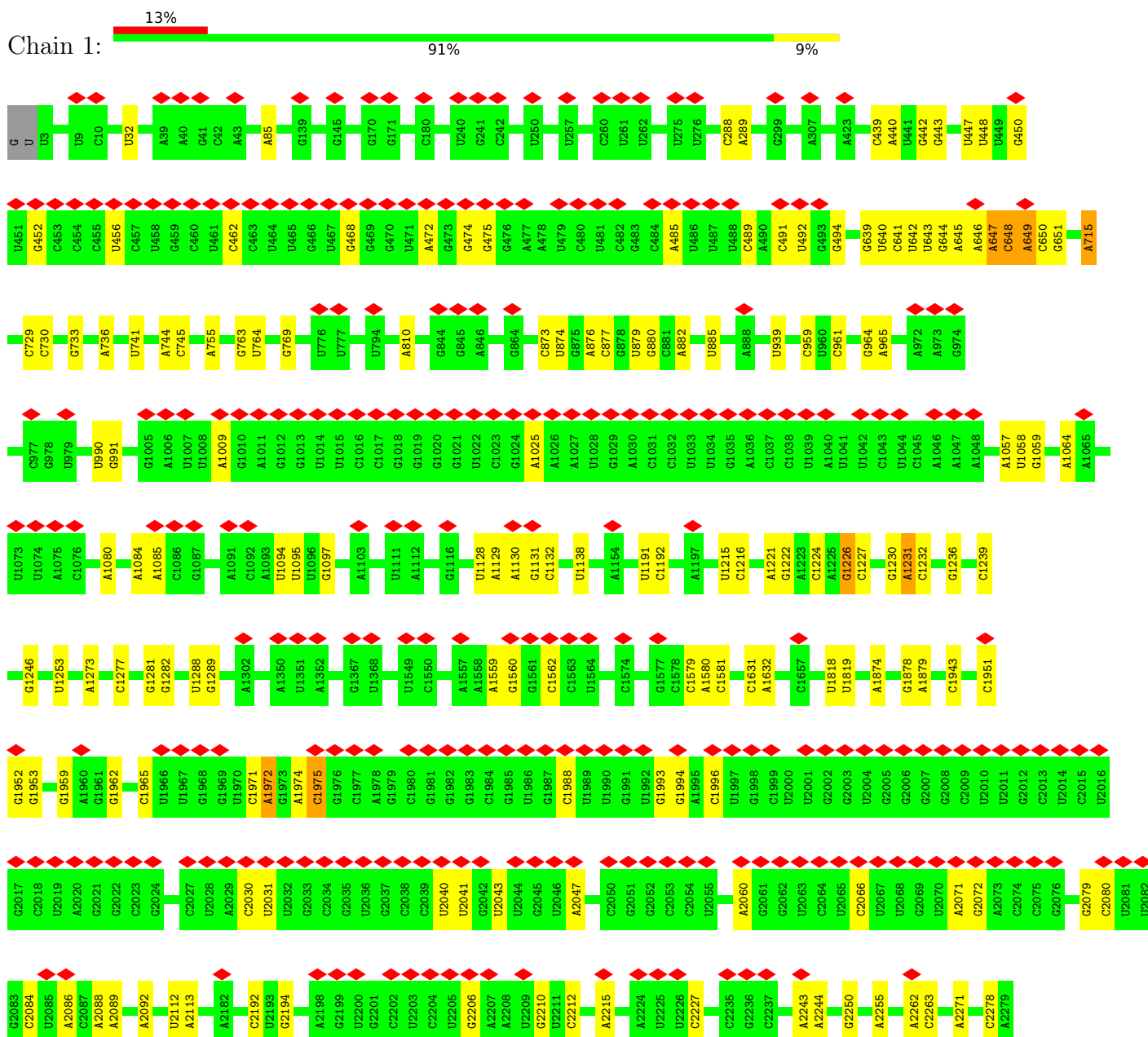
- Molecule 47 is a protein called Ribosome biogenesis protein RLP7.

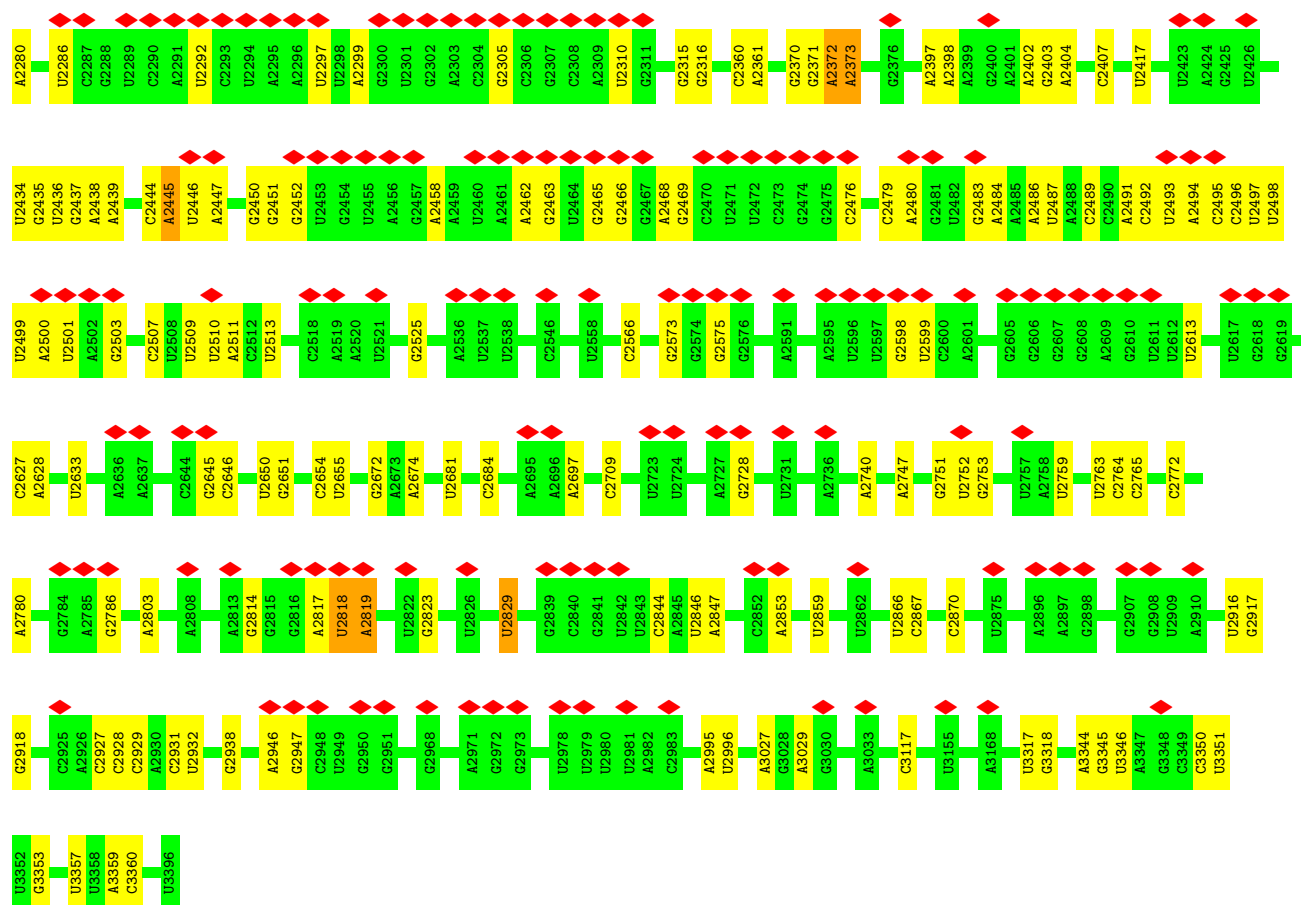
Mol	Chain	Residues	Atoms			AltConf	Trace
47	r	322	Total	C	N	0	0
			966	644	322		
47	s	322	Total	C	N	0	0
			966	644	322		

3 Residue-property plots

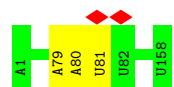
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 25S ribosomal RNA

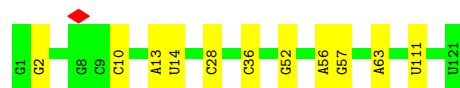
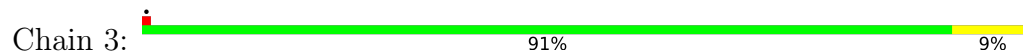




• Molecule 2: 5.8S ribosomal RNA

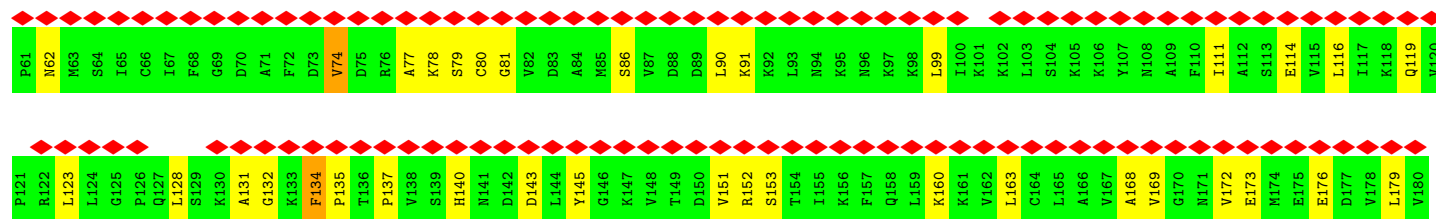


• Molecule 3: 5S ribosomal RNA

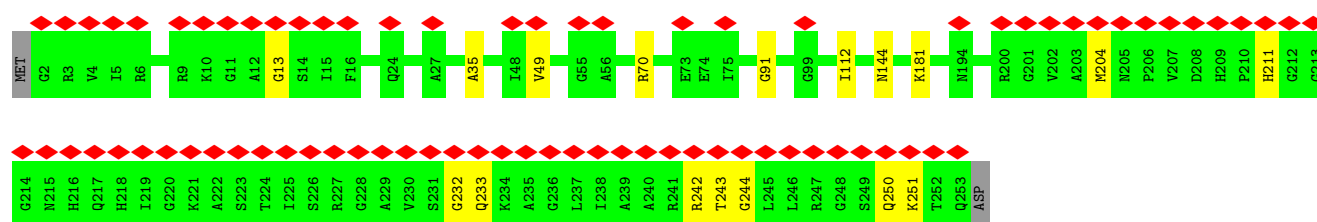
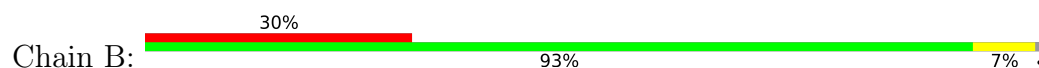


• Molecule 4: 60S ribosomal protein L1

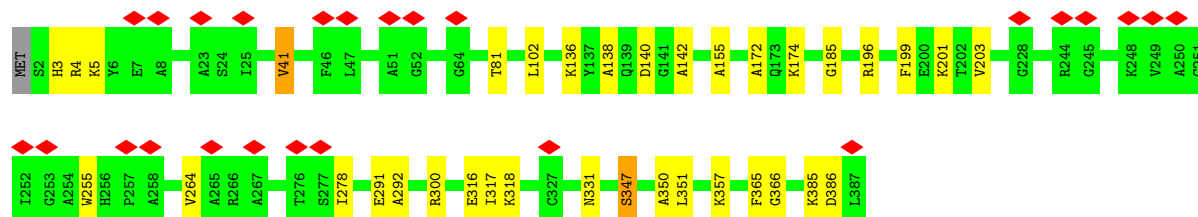
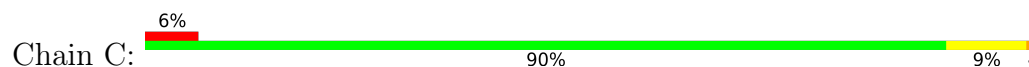




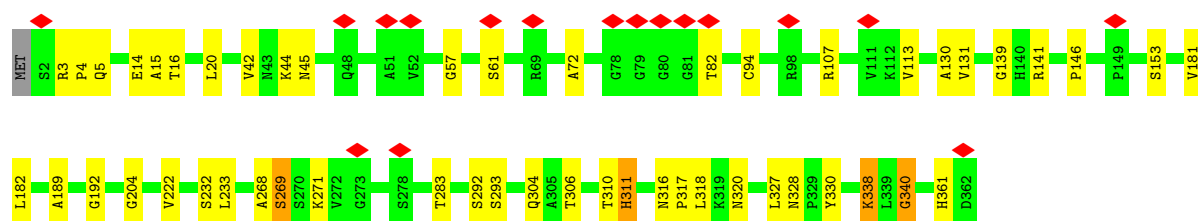
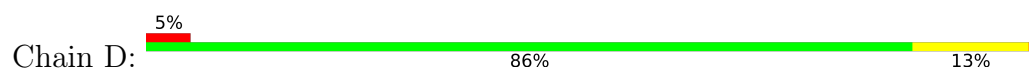
• Molecule 5: 60S ribosomal protein L2



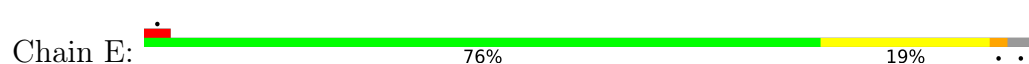
• Molecule 6: 60S ribosomal protein L3

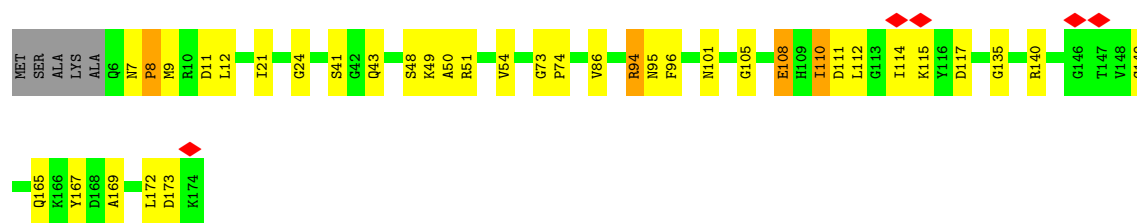


• Molecule 7: 60S ribosomal protein L4

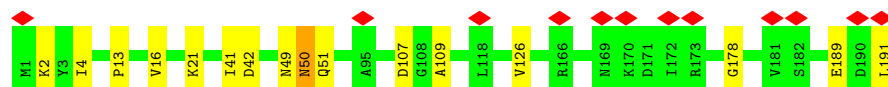
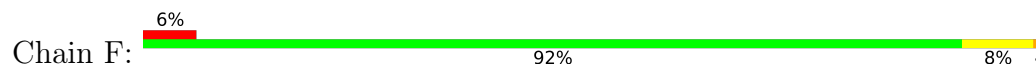


• Molecule 8: 60S ribosomal protein L11

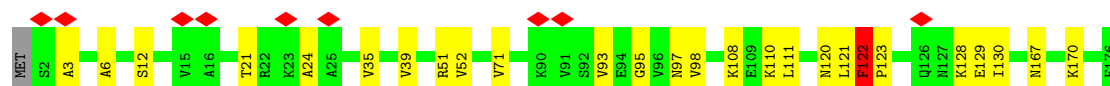
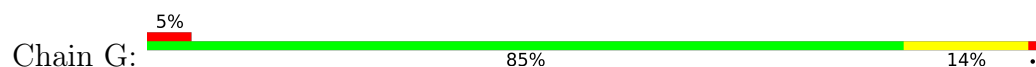




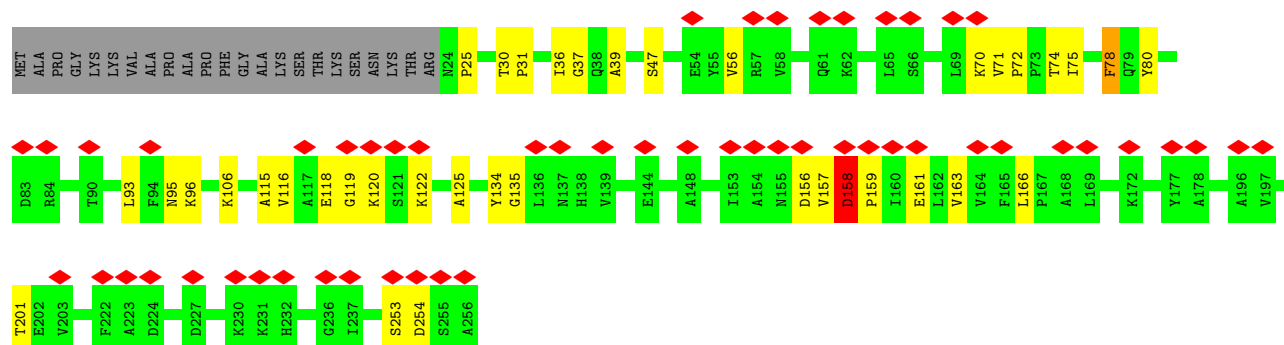
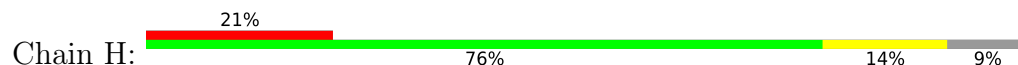
- Molecule 9: 60S ribosomal protein L9



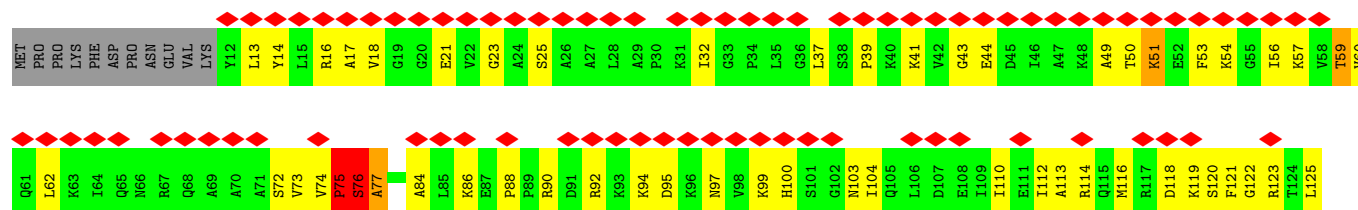
- Molecule 10: 60S ribosomal protein L6

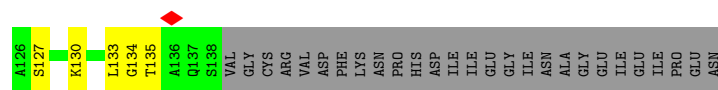


- Molecule 11: 60S ribosomal protein L8



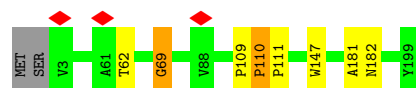
- Molecule 12: 60S ribosomal protein L12





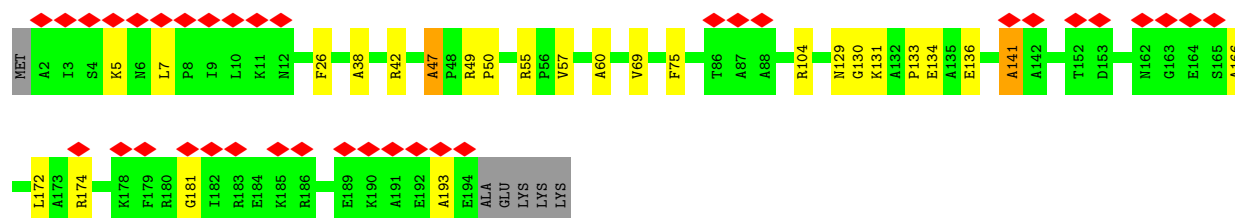
- Molecule 13: 60S ribosomal protein L16

Chain J: 95%



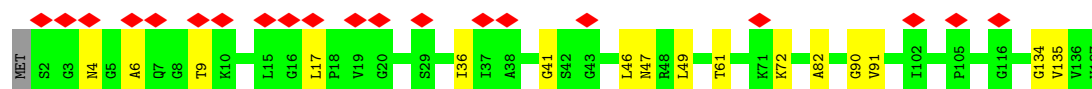
- Molecule 14: 60S ribosomal protein L13

Chain K: 18% 84% 12%



- Molecule 15: 60S ribosomal protein L23

Chain L: 15% 88% 12%



- Molecule 16: 60S ribosomal protein L14

Chain M: 86% 13%

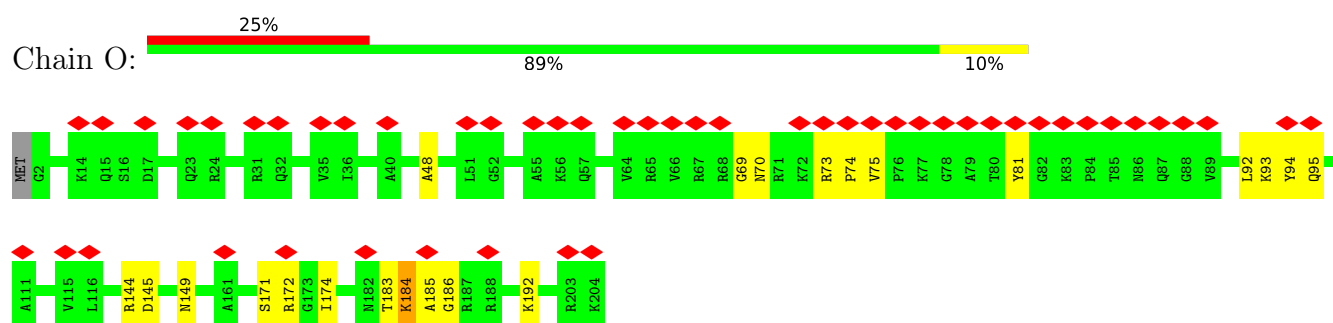


- Molecule 17: 60S ribosomal protein L28

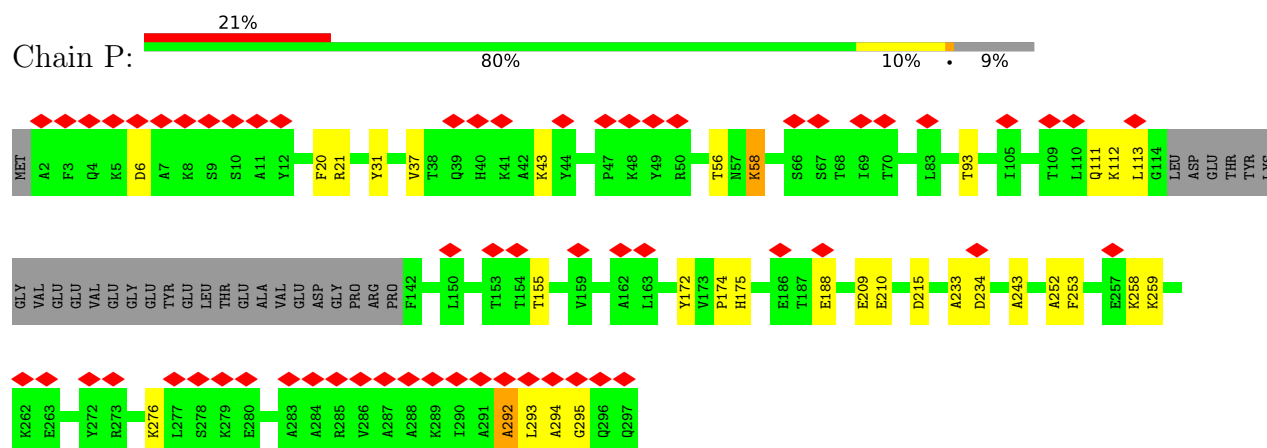
Chain N: 42% 83% 14%



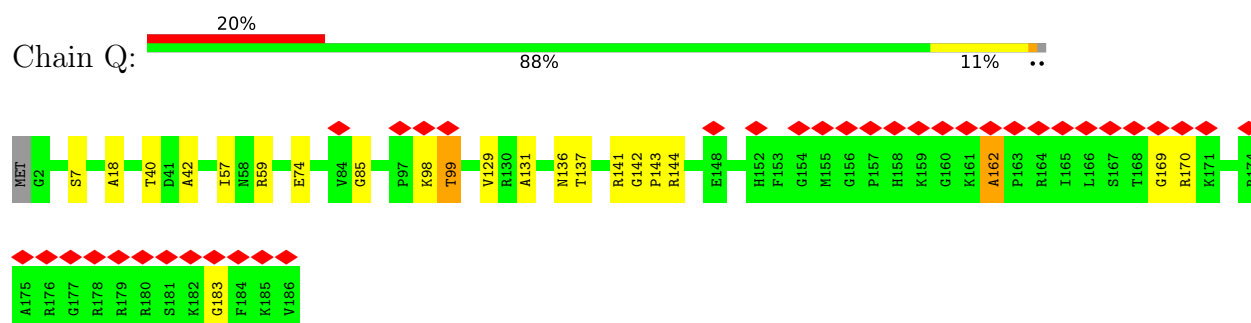
- Molecule 18: 60S ribosomal protein L15



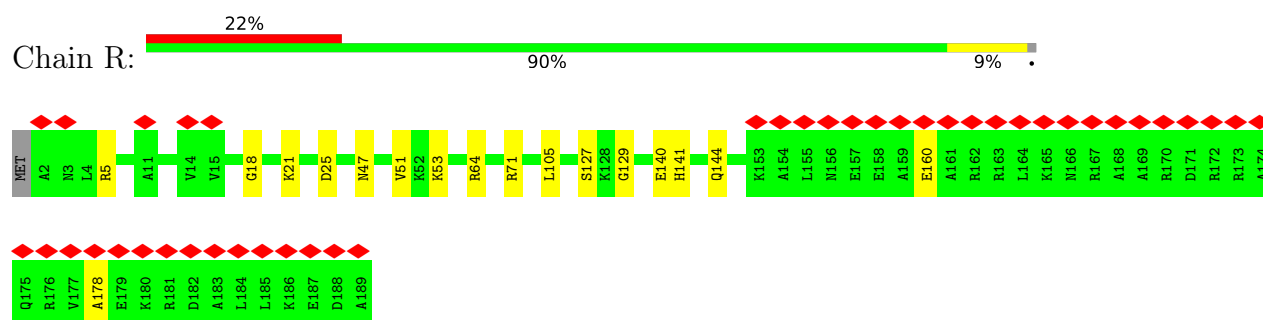
• Molecule 19: 60S ribosomal protein L5



• Molecule 20: 60S ribosomal protein L18

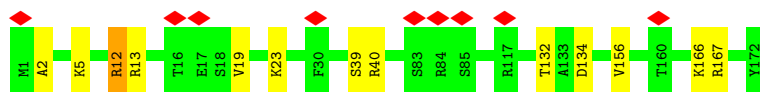


• Molecule 21: 60S ribosomal protein L19

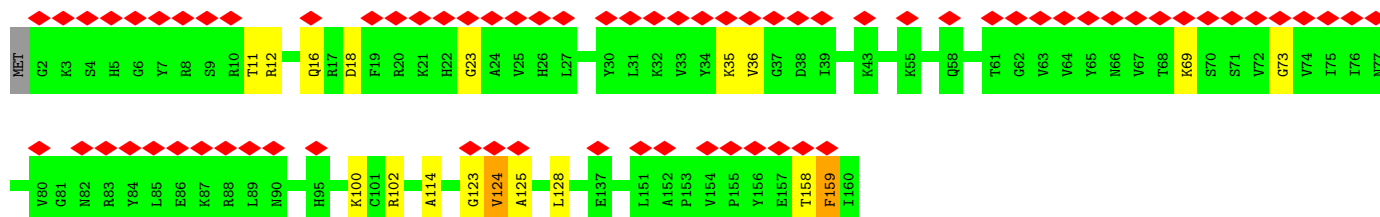
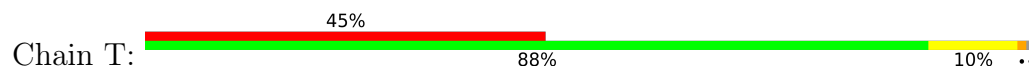


• Molecule 22: 60S ribosomal protein L20

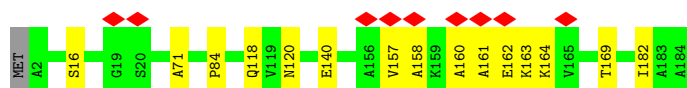
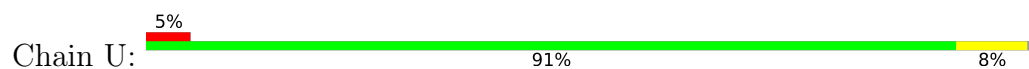




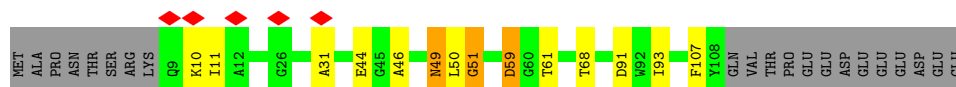
- Molecule 23: 60S ribosomal protein L21



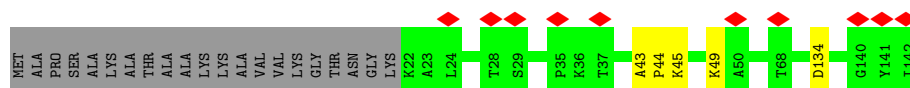
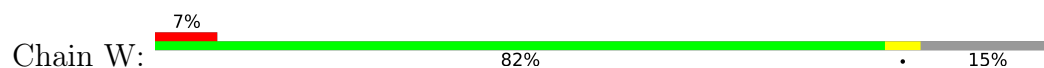
- Molecule 24: 60S ribosomal protein L17



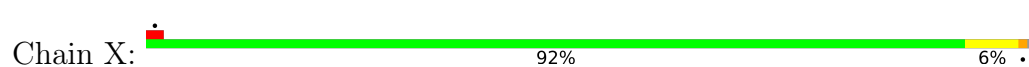
- Molecule 25: 60S ribosomal protein L22



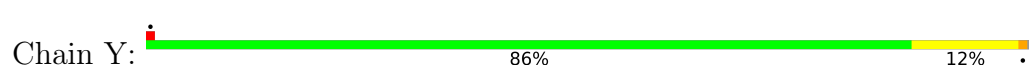
- Molecule 26: 60S ribosomal protein L25



- Molecule 27: 60S ribosomal protein L26

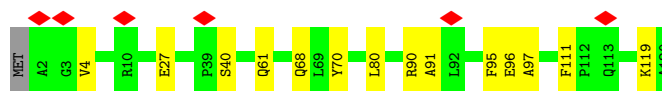
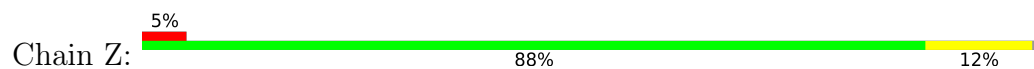


- Molecule 28: 60S ribosomal protein L27

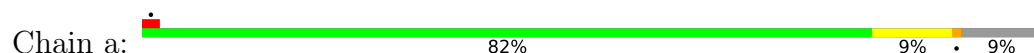




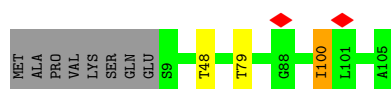
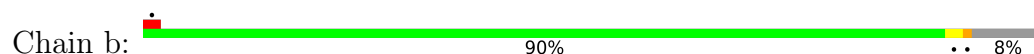
- Molecule 29: 60S ribosomal protein L35



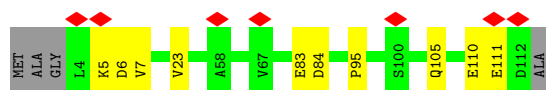
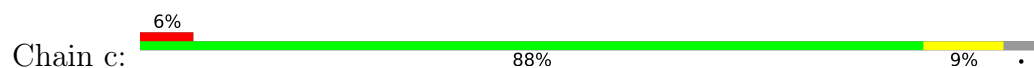
- Molecule 30: 60S ribosomal protein L7



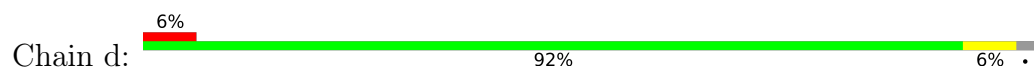
- Molecule 31: 60S ribosomal protein L30



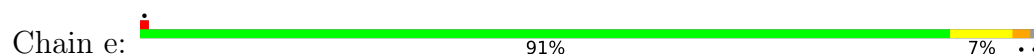
- Molecule 32: 60S ribosomal protein L31

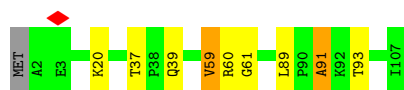


- Molecule 33: 60S ribosomal protein L32

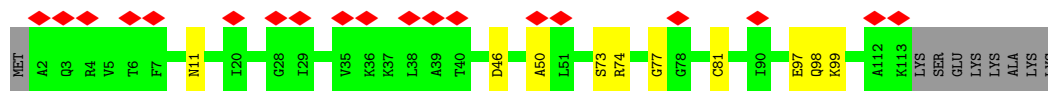
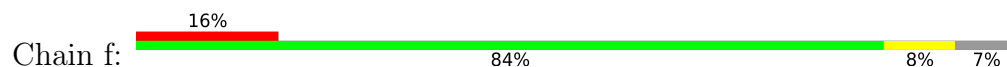


- Molecule 34: 60S ribosomal protein L33

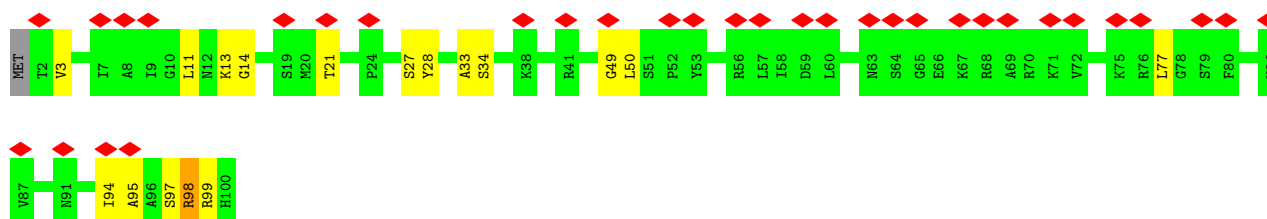
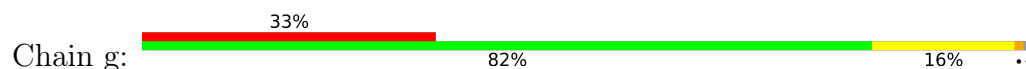




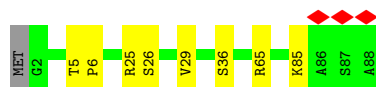
- Molecule 35: 60S ribosomal protein L34



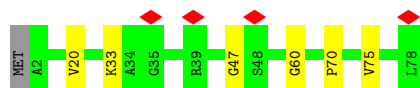
- Molecule 36: 60S ribosomal protein L36



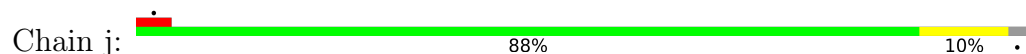
- Molecule 37: 60S ribosomal protein L37



- Molecule 38: 60S ribosomal protein L38



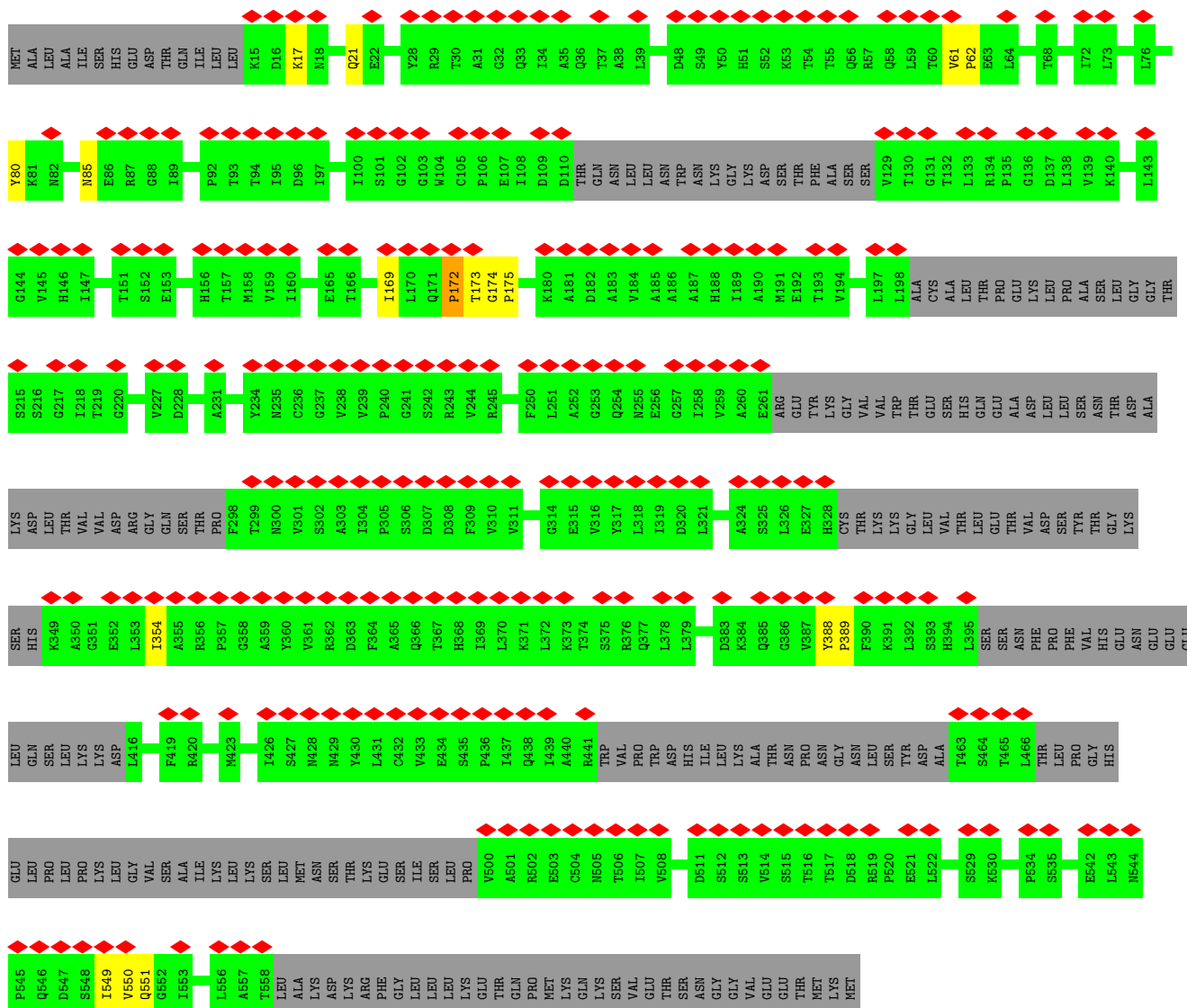
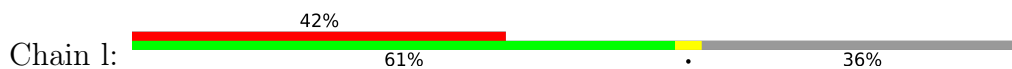
- Molecule 39: 60S ribosomal protein L39



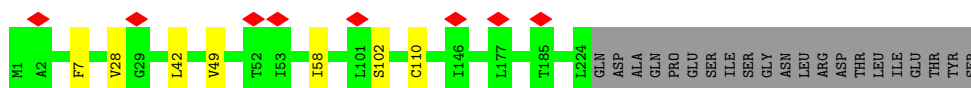
- Molecule 40: 60S ribosomal protein L43



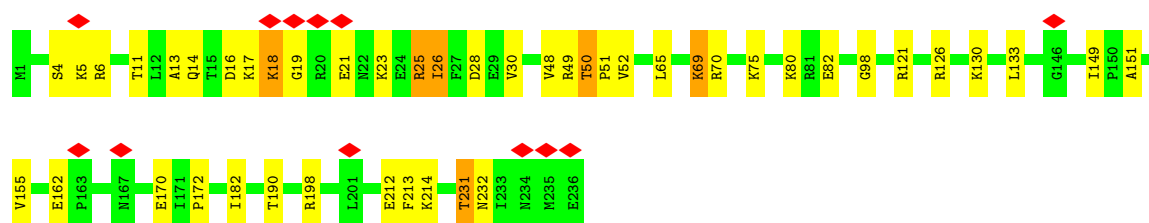
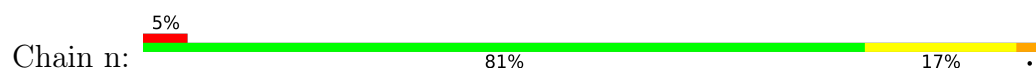
- Molecule 41: metalloprotease ARX1



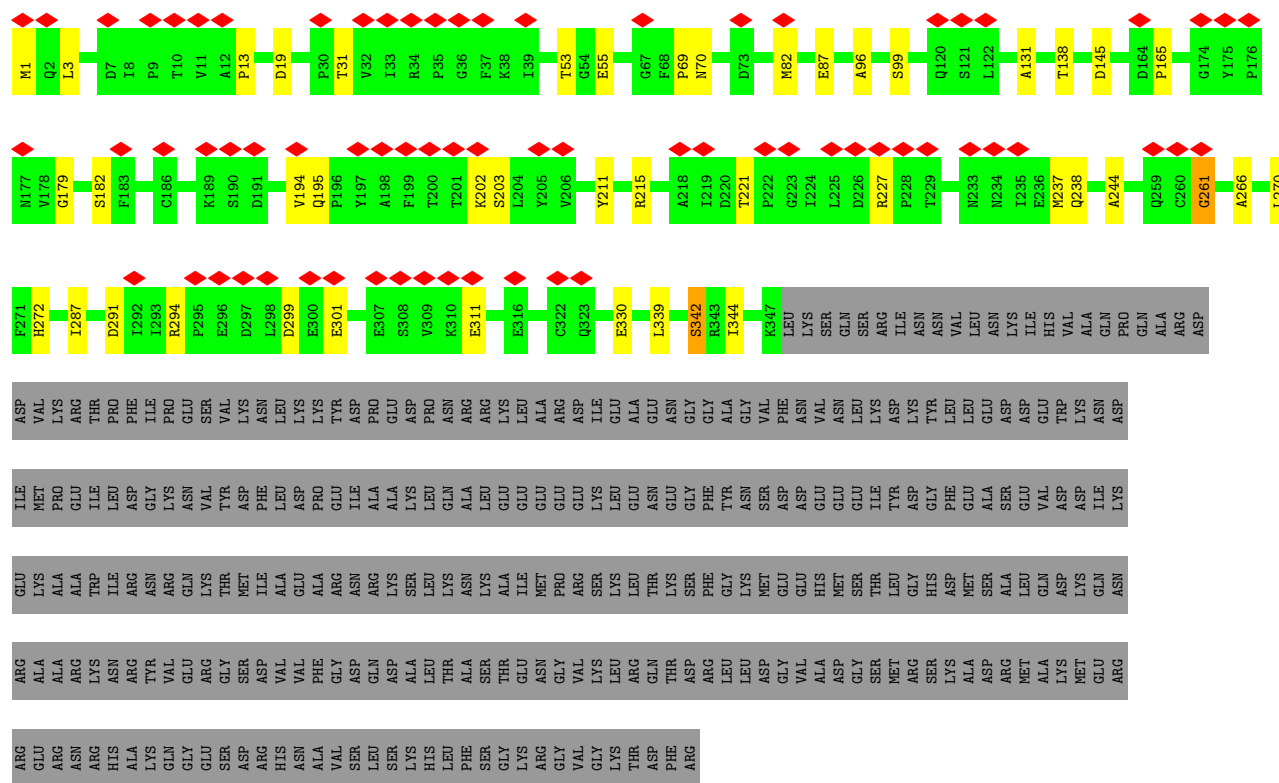
- Molecule 42: Eukaryotic translation initiation factor 6



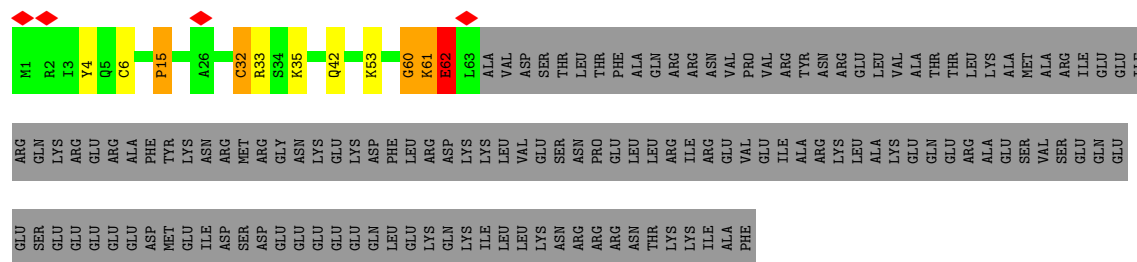
- Molecule 43: mRNA turnover protein 4



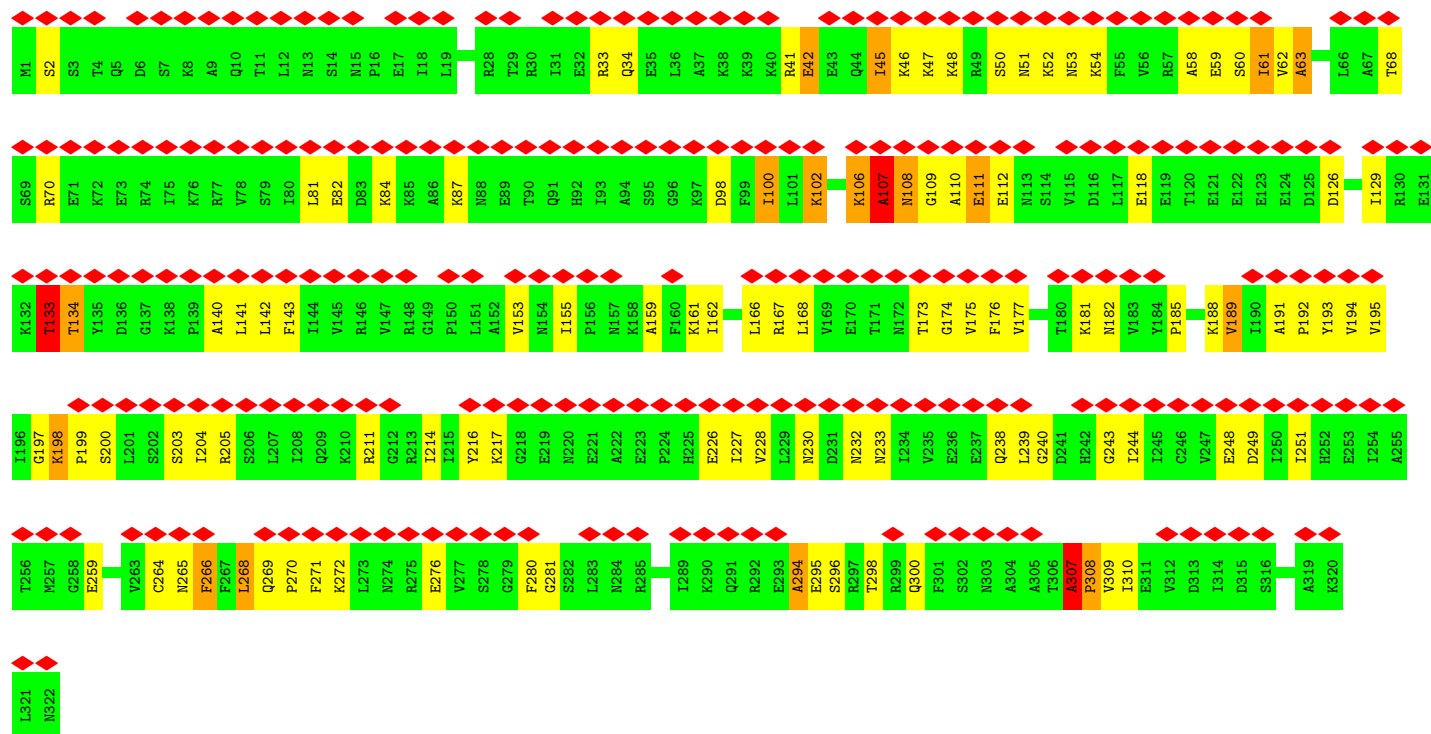
• Molecule 44: Nucleolar GTP-binding protein 1



• Molecule 45: Ribosome biogenesis protein RLP24



• Molecule 46: Ribosome assembly protein 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75887	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	2.010	Depositor
Minimum map value	-0.822	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	439.047, 439.047, 439.047	wwPDB
Map dimensions	414, 414, 414	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0605, 1.0605, 1.0605	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 > 5$	RMSZ	# $ Z > 5$
1	1	1.08	31/20361 (0.2%)	1.80	334/20359 (1.6%)
2	2	0.86	0/947	0.93	0/946
3	3	1.29	1/724 (0.1%)	1.66	4/723 (0.6%)
4	A	2.36	22/650 (3.4%)	3.29	78/649 (12.0%)
5	B	0.98	0/755	1.89	11/754 (1.5%)
6	C	1.14	0/1157	1.98	21/1156 (1.8%)
7	D	1.16	2/1082 (0.2%)	2.10	31/1081 (2.9%)
8	E	0.94	0/506	1.87	6/505 (1.2%)
9	F	0.97	0/572	1.76	7/571 (1.2%)
10	G	1.21	1/524 (0.2%)	1.95	20/523 (3.8%)
11	H	0.85	0/698	1.83	17/697 (2.4%)
12	I	3.02	35/380 (9.2%)	3.54	60/379 (15.8%)
13	J	0.80	0/590	1.68	5/589 (0.8%)
14	K	1.11	1/578 (0.2%)	2.17	19/577 (3.3%)
15	L	1.02	0/407	1.92	11/406 (2.7%)
16	M	1.10	0/407	1.99	11/406 (2.7%)
17	N	1.28	3/443 (0.7%)	2.15	14/442 (3.2%)
18	O	1.14	0/608	1.98	11/607 (1.8%)
19	P	0.93	0/805	1.72	6/803 (0.7%)
20	Q	1.21	0/554	2.20	18/553 (3.3%)
21	R	0.97	1/563 (0.2%)	1.76	9/562 (1.6%)
22	S	1.25	1/515 (0.2%)	1.96	10/514 (1.9%)
23	T	1.10	0/476	1.83	7/475 (1.5%)
24	U	1.14	0/548	1.90	7/547 (1.3%)
25	V	0.77	0/299	1.63	4/298 (1.3%)
26	W	0.91	0/362	1.84	4/361 (1.1%)
27	X	1.04	0/377	1.86	5/376 (1.3%)
28	Y	0.76	0/404	1.75	6/403 (1.5%)
29	Z	1.00	0/356	1.85	6/355 (1.7%)
30	a	1.18	0/665	2.02	19/664 (2.9%)
31	b	0.71	0/290	1.67	4/289 (1.4%)
32	c	1.01	0/326	1.82	6/325 (1.8%)
33	d	1.17	0/380	1.89	5/379 (1.3%)
34	e	1.32	0/317	2.04	8/316 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	f	0.96	0/335	1.83	6/334 (1.8%)
36	g	1.07	1/296 (0.3%)	1.89	4/295 (1.4%)
37	h	1.23	1/260 (0.4%)	2.19	6/259 (2.3%)
38	i	0.79	0/230	1.81	5/229 (2.2%)
39	j	1.00	0/149	1.95	4/148 (2.7%)
40	k	1.03	0/272	1.83	3/271 (1.1%)
41	l	0.84	3/1138 (0.3%)	1.28	8/1136 (0.7%)
42	m	0.42	0/671	1.48	5/670 (0.7%)
43	n	2.01	6/707 (0.8%)	2.70	49/706 (6.9%)
44	o	1.91	4/1040 (0.4%)	2.60	57/1039 (5.5%)
45	p	2.74	3/188 (1.6%)	2.93	10/187 (5.3%)
46	q	1.96	9/1327 (0.7%)	2.54	63/1325 (4.8%)
47	r	1.93	2/965 (0.2%)	2.43	46/964 (4.8%)
47	s	1.93	2/965 (0.2%)	2.43	46/964 (4.8%)
All	All	1.25	129/47169 (0.3%)	1.96	1096/47117 (2.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	2
6	C	0	1
7	D	0	1
8	E	0	1
9	F	0	1
10	G	0	1
11	H	0	3
12	I	0	5
13	J	0	1
23	T	0	1
30	a	0	1
32	c	0	1
43	n	0	2
45	p	0	1
46	q	0	7
47	r	0	1
47	s	0	1
All	All	0	31

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	p	61	LYS	C-N	23.23	1.66	1.33
1	1	648	C	O5'-C5'	20.94	2.05	1.42
1	1	2819	A	C5'-C4'	15.12	1.82	1.52
12	I	76	SER	N-CA	13.81	1.64	1.46
1	1	648	C	P-O5'	-13.35	1.33	1.60
1	1	2818	U	O3'-P	-11.52	1.43	1.61
1	1	648	C	O3'-P	-10.71	1.45	1.61
1	1	439	C	O3'-P	10.46	1.76	1.61
12	I	57	LYS	CA-C	-10.29	1.39	1.52
1	1	651	G	C5'-C4'	10.20	1.72	1.52
10	G	128	LYS	CA-C	10.18	1.63	1.53
12	I	97	ASN	N-CA	-9.97	1.34	1.46
1	1	651	G	C4'-C3'	9.36	1.71	1.52
1	1	2370	G	O3'-P	-9.33	1.47	1.61
12	I	77	ALA	N-CA	9.29	1.58	1.46
1	1	2373	A	O3'-P	-8.76	1.48	1.61
1	1	642	U	O3'-P	-8.63	1.48	1.61
46	q	482	LEU	CA-C	8.48	1.61	1.52
45	p	62	GLU	N-CA	8.42	1.57	1.46
12	I	123	ARG	CA-C	-8.25	1.42	1.52
1	1	650	C	C4'-C3'	8.21	1.69	1.52
12	I	75	PRO	C-N	8.00	1.44	1.33
45	p	32	CYS	C-N	7.72	1.44	1.33
12	I	75	PRO	N-CA	7.72	1.57	1.47
12	I	73	VAL	CA-C	-7.66	1.43	1.52
12	I	56	ILE	CA-C	-7.60	1.44	1.52
46	q	482	LEU	C-N	7.53	1.51	1.33
1	1	2372	A	P-O5'	-7.45	1.45	1.60
12	I	77	ALA	CA-C	7.44	1.62	1.52
12	I	119	LYS	N-CA	-7.44	1.37	1.46
4	A	172	VAL	C-N	7.29	1.43	1.33
12	I	18	VAL	N-CA	-7.25	1.37	1.46
12	I	17	ALA	CA-C	-7.21	1.43	1.52
12	I	92	ARG	N-CA	-7.10	1.37	1.46
1	1	644	G	C4'-C3'	-7.09	1.38	1.52
4	A	43	PRO	N-CA	-6.92	1.38	1.47
4	A	5	THR	C-N	6.85	1.42	1.33
12	I	76	SER	C-N	6.74	1.43	1.33
4	A	74	VAL	N-CA	6.70	1.54	1.46
12	I	135	THR	C-N	6.64	1.43	1.33
4	A	116	LEU	N-CA	-6.58	1.38	1.46
12	I	122	GLY	C-N	6.53	1.42	1.33
12	I	17	ALA	N-CA	-6.43	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	n	213	PHE	N-CA	-6.41	1.38	1.46
1	1	644	G	O3'-P	-6.39	1.51	1.61
12	I	16	ARG	C-N	6.38	1.41	1.33
4	A	24	LYS	CA-C	-6.36	1.43	1.52
1	1	2819	A	O5'-C5'	6.29	1.61	1.42
1	1	643	U	P-O5'	-6.27	1.47	1.59
4	A	91	LYS	C-N	6.26	1.42	1.33
41	l	85	ASN	C-N	-6.26	1.24	1.33
43	n	6	ARG	CA-C	-6.26	1.45	1.52
4	A	54	LYS	CA-C	-6.26	1.44	1.52
41	l	21	GLN	C-N	-6.22	1.25	1.33
12	I	84	ALA	C-N	6.19	1.42	1.33
1	1	2417	U	O3'-P	-6.19	1.51	1.61
47	s	198	LYS	C-N	-6.18	1.26	1.33
47	r	198	LYS	C-N	-6.16	1.26	1.33
4	A	179	LEU	N-CA	-6.13	1.39	1.46
44	o	3	LEU	CA-C	-6.12	1.45	1.52
12	I	120	SER	CA-C	-6.11	1.44	1.53
44	o	202	LYS	C-N	6.08	1.42	1.33
12	I	44	GLU	C-N	6.08	1.42	1.33
17	N	47	LYS	N-CA	6.08	1.54	1.46
1	1	642	U	C4'-C3'	-6.05	1.40	1.52
43	n	214	LYS	CA-C	-6.00	1.45	1.52
43	n	65	LEU	CA-C	-5.98	1.45	1.52
12	I	50	THR	C-N	5.97	1.42	1.33
12	I	130	LYS	CA-C	-5.93	1.45	1.52
12	I	25	SER	CA-C	-5.87	1.45	1.52
1	1	2503	G	O3'-P	-5.83	1.52	1.61
7	D	316	ASN	CA-C	-5.82	1.47	1.53
46	q	84	GLN	CA-C	-5.80	1.45	1.52
1	1	1988	C	O3'-P	-5.74	1.52	1.61
36	g	77	LEU	CA-C	-5.73	1.47	1.53
12	I	54	LYS	C-N	5.71	1.41	1.33
46	q	121	TYR	CA-C	-5.68	1.45	1.52
17	N	66	ALA	CA-C	-5.66	1.45	1.52
12	I	62	LEU	N-CA	-5.66	1.39	1.46
46	q	98	THR	CA-C	-5.64	1.45	1.52
4	A	185	MET	CA-C	-5.62	1.45	1.52
12	I	72	SER	CA-C	-5.62	1.45	1.52
14	K	57	VAL	CA-C	-5.60	1.46	1.52
12	I	86	LYS	C-N	5.58	1.40	1.33
17	N	46	ASP	CA-C	-5.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2497	U	O3'-P	-5.54	1.52	1.61
12	I	14	TYR	CA-C	-5.54	1.46	1.52
21	R	25	ASP	CA-C	-5.54	1.46	1.52
4	A	205	VAL	C-N	5.48	1.41	1.33
1	1	640	U	C5'-C4'	5.46	1.61	1.51
1	1	440	A	C5'-C4'	5.46	1.63	1.52
4	A	163	LEU	CA-C	-5.44	1.45	1.52
4	A	111	ILE	C-N	5.40	1.41	1.34
41	l	551	GLN	C-N	5.40	1.41	1.33
1	1	2305	G	O3'-P	-5.39	1.53	1.61
1	1	2271	A	O3'-P	-5.38	1.53	1.61
12	I	104	ILE	CA-C	-5.37	1.46	1.52
4	A	153	SER	C-N	5.34	1.40	1.33
1	1	2299	A	O3'-P	-5.31	1.53	1.61
1	1	650	C	C5'-C4'	5.31	1.62	1.52
46	q	64	LEU	CA-C	-5.30	1.46	1.52
4	A	190	PHE	N-CA	-5.28	1.40	1.46
4	A	119	GLN	N-CA	-5.27	1.39	1.46
44	o	211	TYR	CA-C	-5.24	1.46	1.52
7	D	141	ARG	CA-C	-5.24	1.47	1.53
12	I	56	ILE	N-CA	-5.24	1.40	1.46
4	A	128	LEU	C-N	5.24	1.40	1.33
4	A	77	ALA	CA-C	-5.23	1.46	1.52
46	q	118	THR	C-N	5.22	1.41	1.33
4	A	198	TRP	C-N	5.22	1.41	1.33
47	r	133	THR	C-N	5.19	1.41	1.33
12	I	39	PRO	CA-C	-5.16	1.46	1.52
4	A	11	GLU	N-CA	-5.15	1.39	1.46
43	n	98	GLY	C-N	5.13	1.39	1.33
47	s	133	THR	C-N	5.13	1.40	1.33
37	h	36	SER	CA-C	-5.13	1.47	1.52
22	S	166	LYS	CA-C	-5.12	1.49	1.52
3	3	111	U	O3'-P	-5.11	1.53	1.61
4	A	160	LYS	C-N	5.09	1.40	1.33
43	n	130	LYS	CA-C	-5.07	1.46	1.52
12	I	21	GLU	N-CA	-5.07	1.39	1.45
46	q	466	THR	CA-C	-5.07	1.46	1.53
1	1	468	G	O3'-P	-5.06	1.53	1.61
46	q	123	PRO	C-N	5.04	1.40	1.33
1	1	2509	U	O3'-P	-5.04	1.53	1.61
4	A	8	GLN	N-CA	-5.03	1.40	1.46
12	I	90	ARG	CA-C	-5.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	85	A	O3'-P	-5.02	1.53	1.61
44	o	291	ASP	C-N	5.01	1.40	1.33

All (1096) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	885	U	P-O3'-C3'	35.13	172.90	120.20
1	1	649	A	P-O5'-C5'	33.74	170.61	120.00
1	1	2819	A	O5'-C5'-C4'	33.06	160.39	110.80
1	1	648	C	P-O5'-C5'	-30.57	74.15	120.00
1	1	647	A	O3'-P-O5'	-24.75	66.87	104.00
1	1	2370	G	P-O3'-C3'	21.73	152.80	120.20
1	1	648	C	O3'-P-O5'	-21.56	71.66	104.00
1	1	2509	U	P-O3'-C3'	21.39	152.28	120.20
1	1	440	A	C5'-C4'-C3'	21.37	146.95	114.90
1	1	651	G	C5'-C4'-C3'	21.28	146.82	114.90
1	1	2497	U	P-O3'-C3'	20.70	151.24	120.20
1	1	2507	C	P-O3'-C3'	19.81	149.92	120.20
1	1	2372	A	P-O5'-C5'	19.70	149.56	120.00
1	1	991	G	P-O5'-C5'	19.63	149.45	120.00
1	1	647	A	C5'-C4'-C3'	-17.79	88.22	114.90
1	1	876	A	C5'-C4'-C3'	17.56	141.24	114.90
1	1	2503	G	P-O3'-C3'	17.46	146.39	120.20
1	1	2462	A	P-O3'-C3'	17.05	145.78	120.20
1	1	1138	U	P-O3'-C3'	16.64	145.16	120.20
1	1	2041	U	P-O3'-C3'	16.49	144.93	120.20
1	1	2500	A	P-O3'-C3'	16.47	144.90	120.20
1	1	651	G	P-O5'-C5'	16.17	144.25	120.00
12	I	76	SER	N-CA-C	-15.89	76.96	110.80
1	1	645	A	O3'-P-O5'	-15.30	81.05	104.00
1	1	2030	C	P-O3'-C3'	15.25	143.08	120.20
4	A	22	GLU	N-CA-C	15.24	127.60	111.14
12	I	77	ALA	CA-C-N	15.06	140.46	120.28
12	I	77	ALA	C-N-CA	15.06	140.46	120.28
1	1	650	C	C5'-C4'-C3'	15.04	137.46	114.90
1	1	2310	U	P-O3'-C3'	14.87	142.50	120.20
1	1	2489	C	P-O3'-C3'	14.84	142.46	120.20
1	1	2818	U	P-O3'-C3'	14.40	141.80	120.20
46	q	123	PRO	CA-C-N	14.40	147.62	121.70
46	q	123	PRO	C-N-CA	14.40	147.62	121.70
1	1	2819	A	P-O5'-C5'	14.38	141.58	120.00
1	1	1288	U	P-O3'-C3'	14.38	141.76	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1965	C	P-O3'-C3'	14.29	141.64	120.20
1	1	2439	A	P-O3'-C3'	14.07	141.30	120.20
1	1	456	U	P-O3'-C3'	14.05	141.28	120.20
1	1	2468	A	P-O3'-C3'	14.05	141.28	120.20
1	1	2194	G	P-O3'-C3'	14.05	141.27	120.20
1	1	650	C	O3'-P-O5'	13.87	124.80	104.00
1	1	2697	A	P-O3'-C3'	13.86	140.99	120.20
1	1	2079	G	P-O3'-C3'	13.73	140.79	120.20
1	1	468	G	P-O3'-C3'	13.72	140.78	120.20
20	Q	18	ALA	CA-C-N	-13.35	107.23	120.31
20	Q	18	ALA	C-N-CA	-13.35	107.23	120.31
1	1	651	G	O5'-C5'-C4'	13.21	130.61	110.80
1	1	649	A	O5'-C5'-C4'	13.18	130.57	110.80
1	1	2080	C	P-O3'-C3'	13.04	139.76	120.20
1	1	2192	C	P-O3'-C3'	12.94	139.61	120.20
1	1	2436	U	O3'-P-O5'	-12.59	85.11	104.00
1	1	2483	G	P-O3'-C3'	12.59	139.09	120.20
1	1	880	G	P-O3'-C3'	12.47	138.91	120.20
45	p	61	LYS	CA-C-N	-12.40	97.86	121.54
45	p	61	LYS	C-N-CA	-12.40	97.86	121.54
1	1	2480	A	P-O3'-C3'	12.09	138.33	120.20
1	1	1580	A	P-O3'-C3'	12.07	138.31	120.20
1	1	494	G	P-O3'-C3'	12.05	138.28	120.20
1	1	2446	U	P-O3'-C3'	12.04	138.25	120.20
1	1	2511	A	P-O5'-C5'	12.01	138.01	120.00
1	1	879	U	P-O3'-C3'	11.95	138.12	120.20
45	p	62	GLU	N-CA-C	11.92	136.19	110.80
1	1	2445	A	P-O5'-C5'	11.89	137.83	120.00
1	1	494	G	O3'-P-O5'	11.88	121.82	104.00
14	K	49	ARG	CA-C-N	-11.83	105.05	119.84
14	K	49	ARG	C-N-CA	-11.83	105.05	119.84
1	1	2086	A	P-O3'-C3'	11.82	137.92	120.20
1	1	2434	U	P-O3'-C3'	11.80	137.89	120.20
1	1	2450	G	P-O3'-C3'	11.71	137.76	120.20
1	1	639	G	C5'-C4'-C3'	11.69	132.44	114.90
46	q	222	GLY	N-CA-C	-11.63	99.27	115.32
1	1	1064	A	P-O3'-C3'	11.61	137.61	120.20
1	1	2297	U	P-O3'-C3'	11.55	137.53	120.20
1	1	2031	U	P-O3'-C3'	11.52	137.47	120.20
1	1	2654	C	P-O3'-C3'	11.51	137.47	120.20
1	1	2043	U	P-O3'-C3'	11.41	137.32	120.20
1	1	2509	U	O3'-P-O5'	-11.31	87.03	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2803	A	P-O3'-C3'	11.26	137.09	120.20
1	1	1132	C	C5'-C4'-C3'	11.16	131.64	114.90
46	q	146	ILE	CA-C-N	10.98	142.50	121.54
46	q	146	ILE	C-N-CA	10.98	142.50	121.54
8	E	54	VAL	N-CA-C	10.96	120.28	111.62
1	1	491	C	P-O3'-C3'	10.94	136.61	120.20
1	1	2316	G	P-O3'-C3'	10.84	136.46	120.20
1	1	2445	A	P-O3'-C3'	10.81	136.42	120.20
1	1	2463	G	P-O3'-C3'	10.80	136.40	120.20
45	p	60	GLY	N-CA-C	-10.79	100.89	114.92
1	1	2451	G	P-O5'-C5'	10.78	136.17	120.00
1	1	959	C	P-O3'-C3'	10.77	136.36	120.20
1	1	2501	U	P-O3'-C3'	10.64	136.16	120.20
1	1	472	A	P-O3'-C3'	10.55	136.03	120.20
1	1	2492	C	P-O3'-C3'	10.55	136.02	120.20
1	1	1058	U	P-O3'-C3'	10.53	136.00	120.20
47	r	308	PRO	N-CA-C	10.52	134.15	112.47
47	s	308	PRO	N-CA-C	10.52	134.13	112.47
1	1	2655	U	P-O3'-C3'	10.51	135.97	120.20
1	1	2469	G	C5'-C4'-C3'	10.47	130.60	114.90
1	1	2370	G	O3'-P-O5'	-10.40	88.40	104.00
1	1	645	A	C4'-C3'-O3'	10.37	125.55	110.00
6	C	316	GLU	N-CA-C	10.37	126.06	113.41
1	1	647	A	C4'-C3'-O3'	10.36	125.54	110.00
1	1	2403	G	P-O3'-C3'	10.35	135.72	120.20
1	1	2751	G	P-O3'-C3'	10.23	135.55	120.20
17	N	46	ASP	N-CA-C	-10.23	94.06	110.32
8	E	7	ASN	CA-C-N	10.19	132.58	119.84
8	E	7	ASN	C-N-CA	10.19	132.58	119.84
1	1	3350	C	P-O3'-C3'	10.13	135.40	120.20
1	1	2060	A	P-O3'-C3'	10.10	135.34	120.20
1	1	2071	A	P-O3'-C3'	10.08	135.33	120.20
1	1	2484	A	P-O3'-C3'	10.03	135.24	120.20
1	1	1221	A	P-O3'-C3'	10.02	135.22	120.20
1	1	2927	C	P-O3'-C3'	-10.01	105.18	120.20
26	W	43	ALA	CA-C-N	9.94	132.26	119.84
26	W	43	ALA	C-N-CA	9.94	132.26	119.84
37	h	5	THR	CA-C-N	-9.90	109.46	119.56
37	h	5	THR	C-N-CA	-9.90	109.46	119.56
46	q	147	LEU	N-CA-C	9.88	131.84	110.80
1	1	2437	G	P-O3'-C3'	9.82	134.93	120.20
1	1	442	G	P-O3'-C3'	9.82	134.92	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2819	A	C5'-C4'-C3'	9.82	129.63	114.90
1	1	877	C	P-O5'-C5'	-9.80	105.29	120.00
1	1	763	G	P-O3'-C3'	9.78	134.88	120.20
1	1	2495	C	P-O3'-C3'	9.76	134.84	120.20
1	1	1972	A	P-O3'-C3'	9.73	134.79	120.20
1	1	2372	A	O5'-C5'-C4'	-9.72	96.22	110.80
33	d	42	VAL	N-CA-C	-9.71	102.42	111.45
1	1	650	C	C4'-C3'-O3'	9.69	124.54	110.00
1	1	639	G	O3'-P-O5'	9.69	118.54	104.00
1	1	2373	A	P-O3'-C3'	9.65	134.68	120.20
13	J	69	GLY	CA-C-N	9.65	129.70	119.76
13	J	69	GLY	C-N-CA	9.65	129.70	119.76
1	1	715	A	P-O3'-C3'	9.62	134.64	120.20
1	1	2633	U	P-O3'-C3'	9.62	134.64	120.20
46	q	287	GLY	N-CA-C	-9.52	102.84	115.21
1	1	1975	C	P-O5'-C5'	9.47	134.21	120.00
1	1	439	C	P-O3'-C3'	-9.43	106.05	120.20
22	S	40	ARG	N-CA-C	-9.41	101.10	111.36
1	1	1094	U	P-O3'-C3'	9.39	134.28	120.20
1	1	2250	G	P-O5'-C5'	9.37	134.05	120.00
45	p	15	PRO	N-CA-C	9.34	131.71	112.47
13	J	109	PRO	CA-C-N	9.34	130.00	120.38
13	J	109	PRO	C-N-CA	9.34	130.00	120.38
36	g	27	SER	N-CA-C	-9.33	96.06	109.96
14	K	57	VAL	N-CA-C	-9.29	96.54	109.45
1	1	2829	U	P-O3'-C3'	9.25	134.08	120.20
30	a	216	VAL	N-CA-C	9.23	128.82	108.88
1	1	990	U	O3'-P-O5'	-9.22	90.17	104.00
1	1	448	U	P-O3'-C3'	9.20	134.00	120.20
14	K	47	ALA	CA-C-N	-9.10	110.45	121.00
14	K	47	ALA	C-N-CA	-9.10	110.45	121.00
7	D	192	GLY	N-CA-C	-9.08	101.20	113.37
14	K	174	ARG	N-CA-C	-9.08	101.39	111.28
1	1	1972	A	C5'-C4'-C3'	9.02	128.44	114.90
1	1	1059	G	P-O3'-C3'	9.00	133.70	120.20
1	1	639	G	C4'-C3'-O3'	8.96	123.44	110.00
18	O	185	ALA	N-CA-C	-8.96	102.27	113.02
14	K	38	ALA	N-CA-C	-8.93	101.20	112.90
1	1	2492	C	O5'-C5'-C4'	8.92	124.18	110.80
47	s	70	ARG	CA-C-N	8.91	133.12	120.28
47	s	70	ARG	C-N-CA	8.91	133.12	120.28
31	b	48	THR	CA-C-N	8.91	128.99	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	48	THR	C-N-CA	8.91	128.99	119.90
1	1	2494	A	P-O3'-C3'	8.90	133.55	120.20
47	r	70	ARG	CA-C-N	8.90	133.09	120.28
47	r	70	ARG	C-N-CA	8.90	133.09	120.28
1	1	2823	G	P-O3'-C3'	8.86	133.49	120.20
1	1	645	A	C5'-C4'-C3'	-8.85	101.62	114.90
1	1	764	U	P-O3'-C3'	8.80	133.40	120.20
1	1	961	C	P-O3'-C3'	8.78	133.36	120.20
1	1	2040	U	P-O3'-C3'	8.77	133.36	120.20
1	1	2438	A	C5'-C4'-C3'	8.75	128.03	114.90
7	D	327	LEU	N-CA-C	-8.72	98.78	110.55
1	1	1988	C	P-O3'-C3'	8.71	133.27	120.20
1	1	1273	A	P-O3'-C3'	8.63	133.15	120.20
1	1	644	G	O3'-P-O5'	-8.61	91.09	104.00
14	K	75	PHE	N-CA-C	8.61	123.78	113.28
1	1	646	A	P-O3'-C3'	8.58	133.07	120.20
1	1	1562	C	P-O3'-C3'	8.57	133.06	120.20
16	M	53	VAL	N-CA-C	8.56	116.41	107.76
1	1	646	A	O5'-C5'-C4'	-8.55	97.97	110.80
1	1	2469	G	O3'-P-O5'	-8.55	91.18	104.00
4	A	176	GLU	CA-C-N	8.54	132.42	120.29
4	A	176	GLU	C-N-CA	8.54	132.42	120.29
7	D	3	ARG	CA-C-N	8.50	130.46	119.84
7	D	3	ARG	C-N-CA	8.50	130.46	119.84
1	1	647	A	O5'-C5'-C4'	8.48	123.52	110.80
11	H	71	VAL	CA-C-N	8.47	125.85	119.66
11	H	71	VAL	C-N-CA	8.47	125.85	119.66
7	D	204	GLY	CA-C-N	-8.46	112.02	120.31
7	D	204	GLY	C-N-CA	-8.46	112.02	120.31
1	1	474	G	P-O3'-C3'	8.43	132.85	120.20
1	1	1095	U	P-O3'-C3'	8.42	132.83	120.20
12	I	133	LEU	CA-C-N	8.41	129.31	119.98
12	I	133	LEU	C-N-CA	8.41	129.31	119.98
1	1	1131	G	C5'-C4'-C3'	8.40	127.50	114.90
43	n	232	ASN	N-CA-C	8.39	120.42	111.28
1	1	2372	A	P-O3'-C3'	-8.34	107.69	120.20
47	r	70	ARG	N-CA-C	-8.32	101.75	112.23
1	1	2072	G	P-O3'-C3'	8.31	132.67	120.20
1	1	2575	G	P-O5'-C5'	8.31	132.47	120.00
47	s	70	ARG	N-CA-C	-8.31	101.76	112.23
1	1	2493	U	P-O3'-C3'	8.30	132.66	120.20
1	1	644	G	O5'-C5'-C4'	8.21	123.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2227	C	P-O3'-C3'	8.18	132.47	120.20
46	q	138	ALA	CA-C-N	-8.16	112.24	123.10
46	q	138	ALA	C-N-CA	-8.16	112.24	123.10
1	1	2753	G	P-O3'-C3'	8.16	132.44	120.20
1	1	2088	A	C5'-C4'-C3'	8.14	127.12	114.90
1	1	2499	U	P-O5'-C5'	8.12	145.26	120.90
20	Q	59	ARG	CA-C-N	-8.11	112.03	120.38
20	Q	59	ARG	C-N-CA	-8.11	112.03	120.38
18	O	93	LYS	N-CA-C	8.10	124.33	113.97
4	A	123	LEU	N-CA-C	8.09	120.17	111.36
4	A	132	GLY	CA-C-N	8.07	130.93	120.44
4	A	132	GLY	C-N-CA	8.07	130.93	120.44
1	1	1129	A	O5'-C5'-C4'	8.07	122.91	110.80
4	A	74	VAL	CA-C-N	8.07	131.90	120.28
4	A	74	VAL	C-N-CA	8.07	131.90	120.28
1	1	2066	C	P-O3'-C3'	8.05	132.28	120.20
7	D	316	ASN	CA-C-N	-8.04	109.79	119.84
7	D	316	ASN	C-N-CA	-8.04	109.79	119.84
11	H	158	ASP	N-CA-C	8.02	127.53	109.81
7	D	330	TYR	N-CA-C	-7.99	102.98	112.89
20	Q	99	THR	N-CA-C	7.96	127.76	110.80
43	n	69	LYS	CA-C-N	7.94	130.92	120.28
43	n	69	LYS	C-N-CA	7.94	130.92	120.28
22	S	23	LYS	N-CA-C	7.94	120.84	111.71
1	1	1131	G	P-O5'-C5'	7.91	131.87	120.00
1	1	2763	U	P-O3'-C3'	7.90	132.06	120.20
1	1	2870	C	P-O3'-C3'	7.90	132.06	120.20
46	q	95	ILE	CA-C-N	7.89	132.03	120.90
46	q	95	ILE	C-N-CA	7.89	132.03	120.90
1	1	2210	G	P-O5'-C5'	7.87	131.80	120.00
34	e	37	THR	CA-C-N	-7.87	111.70	119.64
34	e	37	THR	C-N-CA	-7.87	111.70	119.64
14	K	42	ARG	N-CA-C	-7.85	102.80	111.36
32	c	111	GLU	N-CA-C	7.84	120.76	109.71
30	a	215	GLY	N-CA-C	-7.82	98.61	112.22
1	1	2462	A	O3'-P-O5'	-7.82	92.27	104.00
1	1	2404	A	P-O3'-C3'	7.79	131.88	120.20
47	s	217	LYS	N-CA-C	-7.76	103.76	113.23
1	1	1560	G	P-O5'-C5'	7.75	131.63	120.00
1	1	2818	U	O3'-P-O5'	7.75	115.63	104.00
1	1	1057	A	P-O5'-C5'	7.75	131.62	120.00
47	r	217	LYS	N-CA-C	-7.74	103.79	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	80	CYS	CA-C-N	7.72	129.80	120.14
4	A	80	CYS	C-N-CA	7.72	129.80	120.14
6	C	291	GLU	N-CA-C	-7.72	100.34	110.53
21	R	71	ARG	N-CA-C	-7.72	103.31	112.89
16	M	30	GLY	N-CA-C	-7.71	105.18	115.21
20	Q	57	ILE	N-CA-C	-7.71	102.94	110.72
47	r	281	GLY	N-CA-C	-7.71	104.23	114.25
47	s	281	GLY	N-CA-C	-7.70	104.24	114.25
12	I	127	SER	CA-C-N	7.69	131.00	120.46
12	I	127	SER	C-N-CA	7.69	131.00	120.46
4	A	58	CYS	CA-C-N	7.68	127.58	119.05
4	A	58	CYS	C-N-CA	7.68	127.58	119.05
1	1	2931	C	P-O5'-C5'	7.68	131.53	120.00
30	a	138	TYR	CA-C-N	-7.68	111.70	119.99
30	a	138	TYR	C-N-CA	-7.68	111.70	119.99
21	R	160	GLU	N-CA-C	-7.63	102.62	112.23
1	1	2262	A	O3'-P-O5'	-7.63	92.56	104.00
16	M	113	THR	N-CA-C	-7.63	98.32	110.14
14	K	26	PHE	N-CA-C	-7.62	103.87	113.01
1	1	440	A	P-O5'-C5'	7.61	131.41	120.00
1	1	2928	C	P-O3'-C3'	-7.59	108.82	120.20
47	r	280	PHE	N-CA-C	-7.59	99.80	110.50
47	s	280	PHE	N-CA-C	-7.58	99.82	110.50
11	H	158	ASP	CA-C-N	7.57	129.30	119.84
11	H	158	ASP	C-N-CA	7.57	129.30	119.84
1	1	1953	G	P-O3'-C3'	7.55	131.53	120.20
17	N	66	ALA	N-CA-C	-7.55	94.71	110.80
46	q	147	LEU	CA-C-N	-7.55	110.12	122.81
46	q	147	LEU	C-N-CA	-7.55	110.12	122.81
47	r	106	LYS	N-CA-C	-7.55	98.76	110.17
47	s	106	LYS	N-CA-C	-7.54	98.79	110.17
7	D	82	THR	CA-C-N	-7.52	111.51	123.31
7	D	82	THR	C-N-CA	-7.52	111.51	123.31
4	A	78	LYS	CA-C-N	7.51	130.35	120.28
4	A	78	LYS	C-N-CA	7.51	130.35	120.28
4	A	211	GLY	CA-C-N	7.51	127.42	120.21
4	A	211	GLY	C-N-CA	7.51	127.42	120.21
1	1	1277	C	P-O3'-C3'	7.49	131.44	120.20
44	o	13	PRO	CA-C-N	7.46	130.28	120.28
44	o	13	PRO	C-N-CA	7.46	130.28	120.28
1	1	1216	C	P-O3'-C3'	7.46	131.38	120.20
7	D	139	GLY	N-CA-C	-7.45	98.66	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	885	U	O3'-P-O5'	-7.44	92.83	104.00
4	A	23	THR	CA-C-N	7.44	133.15	120.72
4	A	23	THR	C-N-CA	7.44	133.15	120.72
43	n	25	ARG	CA-C-N	7.44	132.23	120.47
43	n	25	ARG	C-N-CA	7.44	132.23	120.47
46	q	388	PRO	CA-C-N	7.44	131.24	120.38
46	q	388	PRO	C-N-CA	7.44	131.24	120.38
15	L	9	THR	N-CA-C	-7.42	99.24	110.14
4	A	169	VAL	N-CA-C	-7.41	97.63	108.89
1	1	1994	G	P-O3'-C3'	7.41	131.31	120.20
1	1	645	A	P-O3'-C3'	7.40	131.30	120.20
14	K	141	ALA	N-CA-C	-7.40	95.04	110.80
46	q	197	ASP	N-CA-C	-7.38	103.24	111.28
23	T	11	THR	N-CA-C	7.37	121.99	112.92
1	1	2510	U	P-O5'-C5'	7.34	142.92	120.90
1	1	2927	C	O3'-P-O5'	-7.34	92.99	104.00
4	A	143	ASP	CA-C-N	7.33	130.71	120.29
4	A	143	ASP	C-N-CA	7.33	130.71	120.29
1	1	2628	A	C5'-C4'-C3'	7.33	125.89	114.90
47	s	228	VAL	CA-C-N	7.33	132.96	120.72
47	s	228	VAL	C-N-CA	7.33	132.96	120.72
47	r	244	ILE	CA-C-N	7.33	130.82	120.42
47	r	244	ILE	C-N-CA	7.33	130.82	120.42
41	l	388	TYR	CA-C-N	-7.33	110.68	119.84
41	l	388	TYR	C-N-CA	-7.33	110.68	119.84
1	1	2513	U	P-O3'-C3'	7.32	131.18	120.20
47	s	244	ILE	CA-C-N	7.32	130.81	120.42
47	s	244	ILE	C-N-CA	7.32	130.81	120.42
1	1	876	A	O3'-P-O5'	-7.31	93.04	104.00
1	1	651	G	C4'-C3'-O3'	7.30	120.96	110.00
47	r	228	VAL	CA-C-N	7.30	132.91	120.72
47	r	228	VAL	C-N-CA	7.30	132.91	120.72
4	A	184	LEU	CA-C-N	7.29	129.92	120.44
4	A	184	LEU	C-N-CA	7.29	129.92	120.44
36	g	14	GLY	N-CA-C	7.27	119.42	112.08
15	L	91	VAL	N-CA-C	7.26	119.53	108.71
12	I	60	VAL	CA-C-N	7.26	133.83	122.94
12	I	60	VAL	C-N-CA	7.26	133.83	122.94
1	1	2447	A	P-O3'-C3'	7.23	131.05	120.20
12	I	59	THR	CA-C-N	-7.23	110.52	122.67
12	I	59	THR	C-N-CA	-7.23	110.52	122.67
46	q	466	THR	CA-C-N	-7.23	112.09	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	q	466	THR	C-N-CA	-7.23	112.09	122.94
46	q	288	GLY	N-CA-C	-7.23	103.77	113.24
1	l	2444	C	P-O3'-C3'	-7.23	109.36	120.20
47	s	45	ILE	CA-C-N	7.23	130.69	120.28
47	s	45	ILE	C-N-CA	7.23	130.69	120.28
43	n	80	LYS	CA-C-N	7.23	129.96	120.28
43	n	80	LYS	C-N-CA	7.23	129.96	120.28
47	r	45	ILE	CA-C-N	7.22	130.68	120.28
47	r	45	ILE	C-N-CA	7.22	130.68	120.28
3	3	52	G	P-O3'-C3'	7.21	131.01	120.20
1	l	2263	C	C5'-C4'-C3'	7.20	125.70	114.90
40	k	59	CYS	N-CA-C	-7.19	100.84	110.55
16	M	4	ASP	N-CA-C	-7.19	99.57	110.14
4	A	86	SER	CA-C-N	7.18	130.18	120.63
4	A	86	SER	C-N-CA	7.18	130.18	120.63
1	l	2206	G	P-O5'-C5'	7.17	130.75	120.00
1	l	2927	C	P-O5'-C5'	7.17	130.75	120.00
4	A	77	ALA	CA-C-N	7.15	129.86	120.28
4	A	77	ALA	C-N-CA	7.15	129.86	120.28
6	C	357	LYS	N-CA-C	-7.12	105.12	113.88
7	D	181	VAL	N-CA-C	-7.12	99.41	110.09
1	l	2371	G	P-O5'-C5'	7.10	130.66	120.00
46	q	482	LEU	N-CA-C	7.10	121.83	112.17
1	l	644	G	C4'-C3'-O3'	-7.10	99.35	110.00
1	l	2503	G	O3'-P-O5'	-7.10	93.35	104.00
24	U	140	GLU	N-CA-C	7.08	121.00	109.59
4	A	30	GLU	N-CA-C	7.07	119.43	110.24
1	l	1097	G	P-O3'-C3'	7.07	130.80	120.20
15	L	49	LEU	CA-C-N	-7.06	112.72	119.85
15	L	49	LEU	C-N-CA	-7.06	112.72	119.85
30	a	89	ILE	N-CA-C	-7.04	106.63	113.53
12	I	43	GLY	CA-C-N	7.04	130.01	120.44
12	I	43	GLY	C-N-CA	7.04	130.01	120.44
4	A	42	ASP	N-CA-C	-7.03	98.15	109.40
24	U	118	GLN	CA-C-N	-7.02	114.49	123.19
24	U	118	GLN	C-N-CA	-7.02	114.49	123.19
10	G	21	THR	N-CA-C	6.99	120.14	110.35
20	Q	162	ALA	CA-C-N	6.98	127.02	119.90
20	Q	162	ALA	C-N-CA	6.98	127.02	119.90
42	m	28	VAL	N-CA-C	6.97	117.73	110.62
47	r	63	ALA	N-CA-C	-6.96	103.70	111.28
47	r	280	PHE	CA-C-N	-6.95	112.40	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	r	280	PHE	C-N-CA	-6.95	112.40	123.31
47	s	280	PHE	CA-C-N	-6.95	112.40	123.31
47	s	280	PHE	C-N-CA	-6.95	112.40	123.31
1	1	2450	G	O3'-P-O5'	-6.93	93.61	104.00
47	s	63	ALA	N-CA-C	-6.93	103.73	111.28
11	H	72	PRO	CA-C-N	6.92	128.50	119.84
11	H	72	PRO	C-N-CA	6.92	128.50	119.84
35	f	11	ASN	CA-C-N	6.92	127.88	120.47
35	f	11	ASN	C-N-CA	6.92	127.88	120.47
1	1	2250	G	O5'-C5'-C4'	6.91	121.16	110.80
47	r	118	GLU	CA-C-N	-6.91	112.92	123.14
47	r	118	GLU	C-N-CA	-6.91	112.92	123.14
8	E	101	ASN	N-CA-C	-6.90	99.75	109.69
47	s	118	GLU	CA-C-N	-6.90	112.93	123.14
47	s	118	GLU	C-N-CA	-6.90	112.93	123.14
1	1	1128	U	O3'-P-O5'	6.90	114.35	104.00
12	I	118	ASP	N-CA-C	6.87	118.85	111.36
44	o	238	GLN	CA-C-N	6.87	129.49	120.28
44	o	238	GLN	C-N-CA	6.87	129.49	120.28
1	1	1226	G	P-O5'-C5'	6.86	130.30	120.00
22	S	134	ASP	N-CA-C	-6.86	104.80	113.72
1	1	2435	G	P-O3'-C3'	6.84	130.47	120.20
1	1	2613	U	P-O3'-C3'	6.84	130.46	120.20
37	h	29	VAL	N-CA-C	6.84	116.93	110.30
14	K	7	LEU	CA-C-N	-6.83	112.95	119.85
14	K	7	LEU	C-N-CA	-6.83	112.95	119.85
28	Y	75	VAL	N-CA-C	6.83	117.63	108.27
34	e	89	LEU	CA-C-N	6.83	126.51	119.82
34	e	89	LEU	C-N-CA	6.83	126.51	119.82
43	n	28	ASP	CA-C-N	6.83	129.43	120.28
43	n	28	ASP	C-N-CA	6.83	129.43	120.28
8	E	21	ILE	N-CA-C	6.82	117.57	106.72
43	n	231	THR	CA-C-N	6.82	129.42	120.28
43	n	231	THR	C-N-CA	6.82	129.42	120.28
1	1	1952	G	P-O3'-C3'	6.82	130.43	120.20
11	H	106	LYS	N-CA-C	-6.81	103.78	111.07
41	l	549	ILE	N-CA-C	6.81	121.85	113.00
16	M	78	THR	N-CA-C	6.80	119.27	111.11
1	1	2192	C	P-O5'-C5'	6.79	130.19	120.00
4	A	199	GLN	CA-C-N	6.79	129.38	120.28
4	A	199	GLN	C-N-CA	6.79	129.38	120.28
1	1	1215	U	P-O3'-C3'	6.78	130.38	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2765	C	P-O5'-C5'	6.75	130.12	120.00
4	A	183	ILE	CA-C-N	6.75	129.22	120.44
4	A	183	ILE	C-N-CA	6.75	129.22	120.44
44	o	301	GLU	CA-C-N	6.74	129.32	120.28
44	o	301	GLU	C-N-CA	6.74	129.32	120.28
7	D	328	ASN	N-CA-C	6.74	124.70	109.81
44	o	342	SER	CA-C-N	6.73	129.60	120.38
44	o	342	SER	C-N-CA	6.73	129.60	120.38
12	I	122	GLY	CA-C-N	-6.73	111.29	120.44
12	I	122	GLY	C-N-CA	-6.73	111.29	120.44
43	n	30	VAL	CA-C-N	6.73	129.30	120.28
43	n	30	VAL	C-N-CA	6.73	129.30	120.28
1	1	442	G	P-O5'-C5'	-6.73	109.91	120.00
14	K	69	VAL	N-CA-C	-6.73	97.85	108.95
1	1	2496	C	O3'-P-O5'	-6.70	93.95	104.00
1	1	991	G	C5'-C4'-C3'	6.69	124.93	114.90
44	o	244	ALA	N-CA-C	6.69	118.57	111.28
1	1	2486	A	P-O3'-C3'	6.69	130.23	120.20
46	q	389	LEU	CA-C-N	-6.68	113.58	123.00
46	q	389	LEU	C-N-CA	-6.68	113.58	123.00
6	C	142	ALA	N-CA-C	6.67	119.37	111.71
11	H	70	LYS	CA-C-N	-6.67	116.91	123.04
11	H	70	LYS	C-N-CA	-6.67	116.91	123.04
1	1	644	G	P-O3'-C3'	-6.66	110.21	120.20
1	1	640	U	P-O5'-C5'	6.64	140.81	120.90
11	H	56	VAL	N-CA-C	-6.63	104.39	110.82
12	I	73	VAL	N-CA-C	-6.63	95.55	109.34
17	N	70	LYS	CA-C-N	-6.63	112.94	119.76
17	N	70	LYS	C-N-CA	-6.63	112.94	119.76
4	A	134	PHE	CA-C-N	6.61	128.10	119.84
4	A	134	PHE	C-N-CA	6.61	128.10	119.84
18	O	172	ARG	N-CA-C	-6.60	105.20	113.18
44	o	211	TYR	N-CA-C	-6.58	97.64	108.76
47	s	268	LEU	N-CA-C	-6.56	104.13	111.28
6	C	102	LEU	N-CA-C	6.56	121.41	113.41
21	R	105	LEU	N-CA-C	-6.55	104.22	111.36
41	l	85	ASN	CA-C-N	6.55	132.77	122.94
41	l	85	ASN	C-N-CA	6.55	132.77	122.94
47	r	268	LEU	N-CA-C	-6.55	104.14	111.28
1	1	2772	C	P-O3'-C3'	6.55	130.02	120.20
35	f	73	SER	N-CA-C	6.55	119.42	111.82
10	G	35	VAL	CA-C-N	-6.53	113.25	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	35	VAL	C-N-CA	-6.53	113.25	119.85
22	S	12	ARG	N-CA-C	6.52	124.69	110.80
32	c	23	VAL	N-CA-C	6.51	118.82	109.51
46	q	87	LYS	N-CA-C	-6.51	99.00	107.73
43	n	50	THR	CA-C-N	6.51	126.09	119.19
43	n	50	THR	C-N-CA	6.51	126.09	119.19
38	i	75	VAL	N-CA-C	6.51	117.72	108.93
12	I	114	ARG	CA-C-N	6.51	131.71	120.58
12	I	114	ARG	C-N-CA	6.51	131.71	120.58
1	1	2479	C	C5'-C4'-C3'	6.49	124.63	114.90
46	q	51	VAL	N-CA-C	-6.49	101.68	109.01
6	C	81	THR	CA-C-N	-6.48	114.99	119.66
6	C	81	THR	C-N-CA	-6.48	114.99	119.66
21	R	21	LYS	N-CA-C	6.47	121.22	112.88
46	q	481	ASP	CA-C-N	6.46	127.01	119.83
46	q	481	ASP	C-N-CA	6.46	127.01	119.83
1	1	2466	G	C5'-C4'-C3'	6.44	124.56	114.90
44	o	287	ILE	N-CA-C	-6.43	97.72	106.85
10	G	71	VAL	N-CA-C	6.43	116.54	110.30
20	Q	7	SER	N-CA-C	-6.42	98.75	108.52
44	o	294	ARG	CA-C-N	6.42	126.11	119.56
44	o	294	ARG	C-N-CA	6.42	126.11	119.56
43	n	126	ARG	N-CA-C	-6.42	100.75	110.50
42	m	7	PHE	N-CA-C	-6.41	97.24	108.20
1	1	2500	A	O3'-P-O5'	-6.41	94.39	104.00
27	X	125	LYS	N-CA-C	6.41	120.76	111.02
1	1	1129	A	P-O5'-C5'	-6.41	110.39	120.00
1	1	2402	A	P-O3'-C3'	6.39	129.78	120.20
24	U	71	ALA	N-CA-C	-6.39	105.45	113.18
1	1	2491	A	C4'-C3'-O3'	6.38	119.56	110.00
1	1	1581	C	P-O3'-C3'	6.37	129.76	120.20
46	q	456	CYS	N-CA-C	-6.37	104.34	111.28
12	I	21	GLU	CA-C-N	6.37	131.69	121.95
12	I	21	GLU	C-N-CA	6.37	131.69	121.95
46	q	483	PRO	N-CA-C	6.36	125.56	112.47
1	1	2372	A	C4'-C3'-O3'	6.35	119.53	110.00
1	1	3351	U	P-O3'-C3'	6.33	129.70	120.20
12	I	75	PRO	N-CA-C	-6.32	99.44	112.47
1	1	645	A	O5'-C5'-C4'	-6.29	101.36	110.80
1	1	450	G	P-O3'-C3'	6.29	129.63	120.20
4	A	131	ALA	CA-C-N	6.29	128.00	120.14
4	A	131	ALA	C-N-CA	6.29	128.00	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	22	ILE	N-CA-C	6.28	116.32	110.42
1	1	494	G	O5'-C5'-C4'	6.27	120.20	110.80
12	I	49	ALA	N-CA-C	6.27	119.09	111.82
6	C	203	VAL	N-CA-C	6.26	116.87	108.11
43	n	75	LYS	CA-C-N	6.25	128.66	120.28
43	n	75	LYS	C-N-CA	6.25	128.66	120.28
7	D	57	GLY	N-CA-C	-6.25	105.89	114.64
18	O	73	ARG	CA-C-N	6.25	127.65	119.84
18	O	73	ARG	C-N-CA	6.25	127.65	119.84
1	1	2292	U	P-O3'-C3'	6.25	129.57	120.20
4	A	81	GLY	CA-C-N	6.23	128.41	120.56
4	A	81	GLY	C-N-CA	6.23	128.41	120.56
47	s	68	THR	CA-C-N	-6.23	113.72	123.13
47	s	68	THR	C-N-CA	-6.23	113.72	123.13
1	1	991	G	P-O3'-C3'	-6.23	110.86	120.20
44	o	19	ASP	CA-C-N	6.23	129.27	120.42
44	o	19	ASP	C-N-CA	6.23	129.27	120.42
9	F	4	ILE	N-CA-C	6.23	116.40	110.42
1	1	2476	C	C5'-C4'-C3'	6.22	124.23	114.90
47	r	68	THR	CA-C-N	-6.22	113.74	123.13
47	r	68	THR	C-N-CA	-6.22	113.74	123.13
47	s	195	VAL	N-CA-C	-6.21	99.41	108.11
47	r	195	VAL	N-CA-C	-6.20	99.42	108.11
6	C	264	VAL	N-CA-C	6.20	118.58	108.97
43	n	149	ILE	CA-C-N	6.19	126.16	119.78
43	n	149	ILE	C-N-CA	6.19	126.16	119.78
1	1	2466	G	O3'-P-O5'	6.19	113.28	104.00
4	A	194	LEU	CA-C-N	6.18	129.18	120.28
4	A	194	LEU	C-N-CA	6.18	129.18	120.28
1	1	733	G	P-O5'-C5'	6.18	129.26	120.00
1	1	1224	C	P-O5'-C5'	6.17	129.26	120.00
21	R	178	ALA	N-CA-C	-6.17	106.72	114.56
1	1	2764	C	P-O3'-C3'	-6.17	110.94	120.20
1	1	2373	A	C5'-C4'-C3'	6.17	124.15	114.90
1	1	2434	U	O3'-P-O5'	6.16	113.24	104.00
12	I	88	PRO	CA-C-N	6.16	127.54	119.84
12	I	88	PRO	C-N-CA	6.16	127.54	119.84
1	1	475	G	P-O3'-C3'	6.16	129.44	120.20
1	1	641	C	C4'-C3'-O3'	6.16	119.24	110.00
10	G	3	ALA	N-CA-C	-6.15	105.91	113.41
1	1	2684	C	P-O3'-C3'	-6.15	110.98	120.20
1	1	462	C	O3'-P-O5'	-6.14	94.78	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2494	A	O3'-P-O5'	-6.14	94.79	104.00
1	1	1288	U	O3'-P-O5'	-6.14	94.79	104.00
17	N	125	VAL	N-CA-C	6.13	116.45	107.37
23	T	158	THR	N-CA-C	6.13	120.79	113.12
7	D	222	VAL	CA-C-N	6.13	127.50	119.84
7	D	222	VAL	C-N-CA	6.13	127.50	119.84
12	I	53	PHE	N-CA-C	6.13	118.21	110.24
40	k	90	VAL	N-CA-C	6.12	116.86	110.62
1	1	2492	C	C5'-C4'-C3'	6.12	124.08	114.90
24	U	120	ASN	N-CA-C	6.11	117.85	109.18
24	U	16	SER	N-CA-C	6.10	117.16	108.74
1	1	2672	G	O3'-P-O5'	-6.09	94.86	104.00
38	i	20	VAL	N-CA-C	6.09	112.72	106.21
12	I	54	LYS	N-CA-C	6.08	117.58	111.07
1	1	650	C	O5'-C5'-C4'	6.08	119.92	110.80
20	Q	170	ARG	CA-C-N	-6.07	114.35	125.02
20	Q	170	ARG	C-N-CA	-6.07	114.35	125.02
39	j	35	ILE	N-CA-C	6.07	116.25	108.12
44	o	165	PRO	CA-C-N	6.06	128.69	120.44
44	o	165	PRO	C-N-CA	6.06	128.69	120.44
1	1	2262	A	C4'-C3'-O3'	6.06	119.09	110.00
25	V	46	ALA	N-CA-C	6.06	117.40	108.86
46	q	246	GLY	N-CA-C	-6.06	105.46	112.73
43	n	121	ARG	N-CA-C	-6.05	99.53	108.79
1	1	2645	G	C5'-C4'-C3'	-6.05	105.83	114.90
47	r	102	LYS	CA-C-N	-6.04	111.09	121.97
47	r	102	LYS	C-N-CA	-6.04	111.09	121.97
3	3	10	C	P-O5'-C5'	6.04	129.06	120.00
19	P	31	TYR	N-CA-C	-6.04	104.62	111.14
1	1	2846	U	P-O3'-C3'	-6.03	111.15	120.20
46	q	131	PRO	N-CA-C	6.03	121.91	113.53
47	s	102	LYS	CA-C-N	-6.02	111.13	121.97
47	s	102	LYS	C-N-CA	-6.02	111.13	121.97
1	1	1959	G	C5'-C4'-C3'	6.02	123.92	114.90
1	1	2451	G	P-O3'-C3'	6.01	129.22	120.20
35	f	81	CYS	N-CA-C	6.01	119.36	112.57
44	o	96	ALA	CA-C-N	6.01	128.33	120.28
44	o	96	ALA	C-N-CA	6.01	128.33	120.28
44	o	53	THR	CA-C-N	6.00	126.60	120.00
44	o	53	THR	C-N-CA	6.00	126.60	120.00
18	O	174	ILE	N-CA-C	6.00	115.25	106.55
7	D	310	THR	N-CA-C	-6.00	101.58	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	30	GLU	CA-C-N	5.99	128.31	120.28
4	A	30	GLU	C-N-CA	5.99	128.31	120.28
44	o	99	SER	CA-C-N	5.99	128.31	120.28
44	o	99	SER	C-N-CA	5.99	128.31	120.28
18	O	48	ALA	N-CA-C	-5.99	104.84	111.36
47	r	266	PHE	N-CA-C	-5.98	96.14	108.53
47	s	266	PHE	N-CA-C	-5.98	96.14	108.53
20	Q	85	GLY	CA-C-N	-5.98	113.24	122.87
20	Q	85	GLY	C-N-CA	-5.98	113.24	122.87
1	1	2278	C	C5'-C4'-C3'	5.98	123.87	114.90
22	S	39	SER	N-CA-C	-5.98	104.84	111.36
30	a	203	TRP	CA-C-N	-5.98	113.60	119.76
30	a	203	TRP	C-N-CA	-5.98	113.60	119.76
1	1	2525	G	C4'-C3'-O3'	5.97	118.95	110.00
34	e	60	ARG	N-CA-C	-5.97	105.08	113.20
17	N	52	TYR	N-CA-C	5.97	118.30	111.02
10	G	110	LYS	N-CA-C	5.96	116.15	108.34
28	Y	90	GLU	N-CA-C	5.96	117.47	110.97
1	1	2047	A	P-O3'-C3'	5.95	129.12	120.20
11	H	201	THR	N-CA-C	-5.94	106.36	113.97
1	1	489	C	P-O5'-C5'	5.94	128.91	120.00
1	1	1289	G	P-O5'-C5'	5.94	128.90	120.00
44	o	179	GLY	CA-C-N	5.93	128.23	120.28
44	o	179	GLY	C-N-CA	5.93	128.23	120.28
46	q	391	SER	CA-C-N	5.93	131.28	122.74
46	q	391	SER	C-N-CA	5.93	131.28	122.74
43	n	155	VAL	N-CA-C	-5.93	101.33	108.45
45	p	53	LYS	N-CA-C	-5.93	104.94	111.82
43	n	198	ARG	CA-C-N	5.93	128.22	120.28
43	n	198	ARG	C-N-CA	5.93	128.22	120.28
36	g	11	LEU	CA-C-N	-5.92	114.35	123.17
36	g	11	LEU	C-N-CA	-5.92	114.35	123.17
1	1	2866	U	P-O3'-C3'	5.92	129.08	120.20
11	H	96	LYS	N-CA-C	-5.91	104.91	111.36
6	C	331	ASN	N-CA-C	5.91	118.20	109.69
46	q	221	LEU	N-CA-C	-5.91	105.18	112.38
12	I	76	SER	CA-C-N	-5.90	110.28	121.54
12	I	76	SER	C-N-CA	-5.90	110.28	121.54
12	I	113	ALA	CA-C-N	5.89	128.18	120.28
12	I	113	ALA	C-N-CA	5.89	128.18	120.28
46	q	80	SER	N-CA-C	-5.89	100.45	109.41
7	D	189	ALA	CA-C-N	-5.89	109.87	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	189	ALA	C-N-CA	-5.89	109.87	121.41
44	o	138	THR	CA-C-N	5.89	128.53	120.46
44	o	138	THR	C-N-CA	5.89	128.53	120.46
4	A	209	SER	N-CA-C	5.87	118.56	111.40
14	K	60	ALA	CA-C-N	5.87	126.69	120.11
14	K	60	ALA	C-N-CA	5.87	126.69	120.11
1	1	1058	U	O3'-P-O5'	-5.87	95.20	104.00
7	D	130	ALA	N-CA-C	-5.87	100.62	109.60
15	L	61	THR	N-CA-C	-5.87	100.43	109.52
23	T	128	LEU	N-CA-C	5.87	117.94	110.61
13	J	147	TRP	N-CA-C	-5.86	101.61	110.28
45	p	6	CYS	N-CA-C	-5.86	101.23	109.96
1	1	2465	G	C5'-C4'-C3'	5.86	123.69	114.90
12	I	100	HIS	N-CA-C	-5.86	102.64	110.55
15	L	90	GLY	CA-C-N	-5.86	114.54	122.91
15	L	90	GLY	C-N-CA	-5.86	114.54	122.91
44	o	215	ARG	N-CA-C	-5.86	100.35	109.72
44	o	182	SER	CA-C-N	5.85	128.12	120.28
44	o	182	SER	C-N-CA	5.85	128.12	120.28
6	C	278	ILE	N-CA-C	5.85	117.27	108.96
46	q	75	VAL	CA-C-N	5.85	125.54	119.05
46	q	75	VAL	C-N-CA	5.85	125.54	119.05
37	h	26	SER	N-CA-C	-5.85	103.85	113.50
1	1	2030	C	O3'-P-O5'	-5.85	95.23	104.00
27	X	112	ASP	N-CA-C	-5.83	100.55	109.41
1	1	2853	A	P-O5'-C5'	5.83	128.74	120.00
1	1	2494	A	P-O5'-C5'	5.82	128.73	120.00
1	1	3359	A	P-O3'-C3'	-5.82	111.47	120.20
29	Z	80	LEU	N-CA-C	-5.80	104.72	113.89
1	1	2859	U	P-O3'-C3'	5.80	128.90	120.20
17	N	115	LYS	CA-C-N	-5.79	110.05	121.41
17	N	115	LYS	C-N-CA	-5.79	110.05	121.41
1	1	1131	G	O5'-C5'-C4'	-5.79	102.11	110.80
10	G	24	ALA	N-CA-C	5.79	118.72	110.10
11	H	134	TYR	N-CA-C	5.79	115.74	108.45
8	E	110	ILE	N-CA-C	-5.79	104.88	113.39
46	q	456	CYS	CA-C-N	5.79	128.03	120.28
46	q	456	CYS	C-N-CA	5.79	128.03	120.28
4	A	195	LYS	CA-C-N	5.78	129.32	120.82
4	A	195	LYS	C-N-CA	5.78	129.32	120.82
1	1	2407	C	C5'-C4'-C3'	5.78	123.57	114.90
44	o	70	ASN	CA-C-N	5.78	128.38	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	o	70	ASN	C-N-CA	5.78	128.38	120.46
23	T	73	GLY	CA-C-N	-5.78	115.57	123.14
23	T	73	GLY	C-N-CA	-5.78	115.57	123.14
43	n	182	ILE	CA-C-N	5.77	127.95	120.44
43	n	182	ILE	C-N-CA	5.77	127.95	120.44
47	r	107	ALA	CA-C-N	5.76	132.53	121.54
47	r	107	ALA	C-N-CA	5.76	132.53	121.54
1	1	1579	C	C5'-C4'-C3'	5.75	123.52	114.90
12	I	112	ILE	CA-C-N	5.74	127.97	120.28
12	I	112	ILE	C-N-CA	5.74	127.97	120.28
47	r	111	GLU	N-CA-C	5.74	116.98	108.60
47	s	111	GLU	N-CA-C	5.74	116.98	108.60
29	Z	111	PHE	CA-C-N	-5.74	114.66	120.85
29	Z	111	PHE	C-N-CA	-5.74	114.66	120.85
47	s	107	ALA	CA-C-N	5.73	132.49	121.54
47	s	107	ALA	C-N-CA	5.73	132.49	121.54
42	m	42	LEU	N-CA-C	-5.73	106.63	113.97
1	1	2371	G	C4'-C3'-O3'	5.73	118.60	110.00
45	p	42	GLN	N-CA-C	-5.73	105.39	112.38
1	1	1009	A	C5'-C4'-C3'	5.73	123.49	114.90
1	1	2373	A	P-O5'-C5'	-5.73	111.41	120.00
9	F	16	VAL	N-CA-C	5.73	118.20	108.86
43	n	82	GLU	CA-C-N	5.72	127.95	120.28
43	n	82	GLU	C-N-CA	5.72	127.95	120.28
43	n	11	THR	CA-C-N	5.72	127.95	120.28
43	n	11	THR	C-N-CA	5.72	127.95	120.28
46	q	198	GLY	N-CA-C	-5.72	107.77	115.21
44	o	82	MET	CA-C-N	5.72	127.94	120.28
44	o	82	MET	C-N-CA	5.72	127.94	120.28
1	1	2752	U	P-O3'-C3'	5.72	128.78	120.20
5	B	181	LYS	N-CA-C	5.72	117.66	109.14
11	H	125	ALA	N-CA-C	-5.72	104.71	112.26
44	o	202	LYS	CA-C-N	5.72	132.46	121.54
44	o	202	LYS	C-N-CA	5.72	132.46	121.54
12	I	14	TYR	CA-C-N	5.71	131.50	122.36
12	I	14	TYR	C-N-CA	5.71	131.50	122.36
1	1	2371	G	O3'-P-O5'	5.71	112.56	104.00
1	1	447	U	P-O3'-C3'	5.70	128.75	120.20
15	L	36	ILE	N-CA-C	5.70	116.36	108.84
30	a	177	GLY	N-CA-C	-5.70	100.48	112.45
1	1	755	A	P-O5'-C5'	-5.70	111.46	120.00
1	1	650	C	P-O3'-C3'	5.69	128.74	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	k	16	VAL	N-CA-C	-5.69	106.76	113.42
1	1	2465	G	P-O5'-C5'	-5.69	111.47	120.00
19	P	93	THR	N-CA-C	-5.68	104.13	113.50
1	1	2510	U	O3'-P-O5'	5.68	112.52	104.00
45	p	35	LYS	N-CA-C	-5.67	105.10	111.28
1	1	2299	A	P-O3'-C3'	5.67	128.70	120.20
27	X	111	LEU	N-CA-C	5.67	118.96	109.95
1	1	1951	C	O3'-P-O5'	-5.66	95.50	104.00
9	F	126	VAL	CA-C-N	-5.66	114.10	119.76
9	F	126	VAL	C-N-CA	-5.66	114.10	119.76
9	F	41	ILE	N-CA-C	5.65	121.10	109.34
6	C	347	SER	N-CA-C	5.65	122.84	110.80
6	C	365	PHE	N-CA-C	-5.65	105.59	112.88
17	N	13	GLY	N-CA-C	-5.65	107.76	114.48
1	1	2918	G	P-O3'-C3'	-5.65	111.73	120.20
3	3	2	G	C5'-C4'-C3'	5.65	123.37	114.90
12	I	90	ARG	CA-C-N	5.65	132.33	121.54
12	I	90	ARG	C-N-CA	5.65	132.33	121.54
46	q	151	PHE	CA-C-N	-5.65	113.76	121.61
46	q	151	PHE	C-N-CA	-5.65	113.76	121.61
30	a	220	PHE	N-CA-C	5.64	118.52	110.68
1	1	2438	A	P-O5'-C5'	-5.63	111.55	120.00
44	o	339	LEU	N-CA-C	-5.63	106.45	113.55
47	r	193	TYR	N-CA-C	-5.63	100.11	109.46
47	s	61	ILE	N-CA-C	5.63	116.41	110.72
1	1	448	U	O3'-P-O5'	5.63	112.44	104.00
1	1	2280	A	P-O5'-C5'	-5.63	111.56	120.00
47	s	193	TYR	N-CA-C	-5.62	100.12	109.46
12	I	57	LYS	N-CA-C	5.62	118.60	110.28
10	G	12	SER	N-CA-C	-5.62	103.11	110.53
7	D	153	SER	N-CA-C	5.62	117.54	110.24
46	q	468	LEU	N-CA-C	-5.62	99.26	108.41
1	1	2498	U	O3'-P-O5'	5.61	112.42	104.00
47	r	61	ILE	N-CA-C	5.61	116.39	110.72
1	1	2709	C	P-O5'-C5'	5.61	128.41	120.00
30	a	145	ARG	N-CA-C	-5.61	105.25	111.36
6	C	350	ALA	N-CA-C	-5.60	101.35	110.20
33	d	62	LYS	N-CA-C	5.60	117.47	111.36
6	C	41	VAL	N-CA-C	5.60	116.93	109.37
6	C	318	LYS	N-CA-C	-5.60	104.69	112.30
1	1	492	U	P-O3'-C3'	5.59	128.58	120.20
22	S	132	THR	N-CA-C	-5.59	103.11	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1236	G	P-O5'-C5'	5.58	128.38	120.00
16	M	80	THR	N-CA-C	-5.58	104.82	111.69
16	M	48	GLY	CA-C-N	5.58	125.05	119.24
16	M	48	GLY	C-N-CA	5.58	125.05	119.24
1	1	1222	G	O3'-P-O5'	-5.58	95.63	104.00
1	1	2627	C	C5'-C4'-C3'	5.58	123.27	114.90
4	A	45	ARG	N-CA-C	-5.57	101.28	109.81
10	G	93	VAL	N-CA-C	-5.57	105.97	111.88
34	e	39	GLN	N-CA-C	-5.57	105.13	111.14
1	1	1216	C	C4'-C3'-O3'	5.57	118.35	110.00
1	1	2215	A	P-O5'-C5'	5.56	128.35	120.00
12	I	134	GLY	CA-C-N	5.56	128.19	120.29
12	I	134	GLY	C-N-CA	5.56	128.19	120.29
1	1	646	A	C4'-C3'-O3'	5.56	118.34	110.00
5	B	232	GLY	N-CA-C	-5.56	107.43	115.27
7	D	45	ASN	N-CA-C	5.56	120.06	113.16
1	1	2438	A	O3'-P-O5'	-5.56	95.66	104.00
4	A	17	LEU	N-CA-C	-5.55	102.26	110.48
1	1	1951	C	P-O3'-C3'	5.55	128.53	120.20
1	1	2479	C	P-O3'-C3'	-5.55	111.87	120.20
1	1	3344	A	P-O3'-C3'	5.55	128.53	120.20
12	I	88	PRO	N-CA-C	5.55	117.47	110.70
4	A	13	VAL	CA-C-N	5.55	127.71	120.28
4	A	13	VAL	C-N-CA	5.55	127.71	120.28
16	M	52	GLY	CA-C-N	-5.55	118.60	122.59
16	M	52	GLY	C-N-CA	-5.55	118.60	122.59
21	R	129	GLY	N-CA-C	-5.54	102.05	112.64
5	B	91	GLY	N-CA-C	5.54	117.55	110.96
22	S	19	VAL	CA-C-N	-5.54	114.89	120.21
22	S	19	VAL	C-N-CA	-5.54	114.89	120.21
23	T	69	LYS	N-CA-C	5.54	117.00	111.07
1	1	641	C	O3'-P-O5'	-5.53	95.70	104.00
46	q	122	THR	CA-C-N	5.53	126.75	119.84
46	q	122	THR	C-N-CA	5.53	126.75	119.84
19	P	43	LYS	N-CA-C	-5.53	105.14	112.94
39	j	34	THR	N-CA-C	-5.53	107.79	114.75
42	m	110	CYS	N-CA-C	5.53	117.19	108.96
18	O	183	THR	N-CA-C	-5.52	98.00	107.61
1	1	2740	A	P-O5'-C5'	5.52	128.28	120.00
1	1	2437	G	P-O5'-C5'	5.51	128.27	120.00
17	N	98	THR	N-CA-C	5.51	118.78	107.37
4	A	152	ARG	N-CA-C	-5.51	101.50	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	293	SER	N-CA-C	-5.51	99.07	110.80
10	G	170	LYS	CA-C-N	5.51	126.72	119.84
10	G	170	LYS	C-N-CA	5.51	126.72	119.84
1	1	2435	G	C5'-C4'-C3'	5.50	123.15	114.90
43	n	172	PRO	CA-C-N	5.50	128.90	120.82
43	n	172	PRO	C-N-CA	5.50	128.90	120.82
20	Q	131	ALA	CA-C-N	5.49	126.71	119.84
20	Q	131	ALA	C-N-CA	5.49	126.71	119.84
1	1	2089	A	P-O3'-C3'	5.49	128.44	120.20
1	1	1132	C	P-O3'-C3'	5.48	128.43	120.20
4	A	140	HIS	CA-C-N	5.48	128.07	120.29
4	A	140	HIS	C-N-CA	5.48	128.07	120.29
22	S	156	VAL	N-CA-C	5.48	115.48	107.37
6	C	255	TRP	N-CA-C	-5.48	104.95	111.69
12	I	103	ASN	N-CA-C	-5.47	99.60	108.52
1	1	880	G	C5'-C4'-C3'	5.47	123.10	114.90
44	o	55	GLU	CA-C-N	5.46	126.01	120.00
44	o	55	GLU	C-N-CA	5.46	126.01	120.00
1	1	2086	A	C5'-C4'-C3'	5.46	123.09	114.90
1	1	485	A	P-O3'-C3'	5.46	128.39	120.20
5	B	112	ILE	N-CA-C	5.46	115.72	107.75
1	1	2817	A	O3'-P-O5'	-5.46	95.82	104.00
12	I	60	VAL	N-CA-C	-5.46	100.45	108.85
1	1	1246	G	P-O5'-C5'	5.45	128.17	120.00
1	1	2492	C	P-O5'-C5'	-5.44	111.84	120.00
1	1	2469	G	P-O3'-C3'	5.44	128.36	120.20
1	1	2507	C	C5'-C4'-C3'	-5.44	106.74	114.90
1	1	452	G	P-O5'-C5'	5.44	128.16	120.00
46	q	434	GLY	N-CA-C	-5.44	107.60	115.27
47	r	298	THR	CA-C-N	-5.44	112.84	122.74
47	r	298	THR	C-N-CA	-5.44	112.84	122.74
4	A	202	GLY	N-CA-C	5.43	119.06	112.49
7	D	20	LEU	CA-C-N	5.42	125.34	119.76
7	D	20	LEU	C-N-CA	5.42	125.34	119.76
5	B	233	GLN	CA-C-N	-5.42	114.03	122.16
5	B	233	GLN	C-N-CA	-5.42	114.03	122.16
47	s	298	THR	CA-C-N	-5.42	112.88	122.74
47	s	298	THR	C-N-CA	-5.42	112.88	122.74
46	q	152	ALA	CA-C-N	5.42	125.39	120.03
46	q	152	ALA	C-N-CA	5.42	125.39	120.03
1	1	2286	U	P-O3'-C3'	5.41	128.32	120.20
1	1	2212	C	O3'-P-O5'	-5.41	95.88	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	443	G	C5'-C4'-C3'	-5.41	106.79	114.90
30	a	119	VAL	N-CA-C	5.41	115.42	107.15
1	1	2084	C	O3'-P-O5'	-5.40	95.90	104.00
4	A	116	LEU	CA-C-N	5.39	127.85	120.46
4	A	116	LEU	C-N-CA	5.39	127.85	120.46
1	1	1962	G	O3'-P-O5'	-5.39	95.91	104.00
14	K	104	ARG	N-CA-C	-5.39	106.45	114.64
17	N	114	GLY	CA-C-N	-5.39	113.11	120.44
17	N	114	GLY	C-N-CA	-5.39	113.11	120.44
9	F	50	ASN	N-CA-C	5.38	122.27	110.80
1	1	2487	U	P-O3'-C3'	-5.38	112.12	120.20
1	1	3360	C	P-O3'-C3'	5.38	128.27	120.20
43	n	52	VAL	CA-C-N	5.38	127.48	120.28
43	n	52	VAL	C-N-CA	5.38	127.48	120.28
44	o	330	GLU	N-CA-C	-5.38	104.84	111.40
9	F	178	GLY	N-CA-C	5.37	118.83	110.88
30	a	229	PHE	N-CA-C	5.37	118.38	110.59
1	1	736	A	P-O5'-C5'	5.37	128.05	120.00
1	1	1231	A	P-O5'-C5'	5.36	128.05	120.00
30	a	159	GLN	N-CA-C	5.36	122.23	110.80
1	1	2491	A	C5'-C4'-C3'	5.36	122.94	114.90
7	D	340	GLY	N-CA-C	-5.36	106.46	115.62
4	A	173	GLU	CA-C-N	5.35	127.44	120.28
4	A	173	GLU	C-N-CA	5.35	127.44	120.28
1	1	1559	A	P-O3'-C3'	5.34	128.21	120.20
1	1	1993	G	C5'-C4'-C3'	5.34	122.91	114.90
7	D	311	HIS	N-CA-C	5.34	122.18	110.80
43	n	190	THR	N-CA-C	-5.34	101.17	109.72
1	1	2255	A	C5'-C4'-C3'	5.34	122.90	114.90
26	W	49	LYS	N-CA-C	5.34	120.60	112.54
41	l	17	LYS	N-CA-C	-5.34	99.71	108.41
18	O	92	LEU	CA-C-N	-5.33	113.37	122.11
18	O	92	LEU	C-N-CA	-5.33	113.37	122.11
1	1	2315	G	C5'-C4'-C3'	5.33	122.89	114.90
1	1	2452	G	P-O3'-C3'	5.32	128.18	120.20
1	1	3345	G	P-O5'-C5'	5.32	127.97	120.00
47	r	211	ARG	N-CA-C	5.32	117.98	111.82
6	C	292	ALA	CA-C-N	5.31	127.34	120.44
6	C	292	ALA	C-N-CA	5.31	127.34	120.44
28	Y	43	VAL	N-CA-C	5.31	115.36	108.35
10	G	39	VAL	N-CA-C	5.31	115.94	109.30
28	Y	34	LYS	N-CA-C	-5.30	105.58	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	o	227	ARG	CA-C-N	5.30	125.56	119.83
44	o	227	ARG	C-N-CA	5.30	125.56	119.83
27	X	124	GLY	CA-C-N	-5.30	116.13	122.44
27	X	124	GLY	C-N-CA	-5.30	116.13	122.44
12	I	110	ILE	CA-C-N	5.30	127.81	120.29
12	I	110	ILE	C-N-CA	5.30	127.81	120.29
20	Q	170	ARG	N-CA-C	-5.30	103.49	110.33
1	1	1277	C	P-O5'-C5'	5.30	127.94	120.00
39	j	3	ALA	CA-C-N	5.30	128.75	121.33
39	j	3	ALA	C-N-CA	5.30	128.75	121.33
47	s	211	ARG	N-CA-C	5.30	117.97	111.82
29	Z	40	SER	CA-C-N	-5.29	117.03	122.85
29	Z	40	SER	C-N-CA	-5.29	117.03	122.85
44	o	261	GLY	N-CA-C	-5.29	107.91	115.64
1	1	2646	C	P-O3'-C3'	-5.29	112.26	120.20
43	n	162	GLU	CA-C-N	5.29	124.62	118.85
43	n	162	GLU	C-N-CA	5.29	124.62	118.85
1	1	2371	G	C5'-C4'-C3'	5.29	122.84	114.90
10	G	111	LEU	N-CA-C	5.29	115.01	108.19
21	R	127	SER	CA-C-N	5.29	128.10	120.38
21	R	127	SER	C-N-CA	5.29	128.10	120.38
5	B	204	MET	N-CA-C	5.28	118.25	110.59
31	b	79	THR	N-CA-C	-5.28	105.58	112.23
12	I	41	LYS	N-CA-C	-5.27	103.49	111.56
5	B	242	ARG	N-CA-C	-5.27	101.46	108.74
1	1	1974	A	P-O3'-C3'	5.27	128.11	120.20
47	s	100	ILE	N-CA-C	-5.27	98.90	107.28
46	q	93	LYS	CA-C-N	5.27	127.77	120.29
46	q	93	LYS	C-N-CA	5.27	127.77	120.29
47	r	226	GLU	N-CA-C	-5.26	105.72	111.82
12	I	120	SER	N-CA-C	-5.26	102.74	110.52
47	r	100	ILE	N-CA-C	-5.25	98.93	107.28
12	I	51	LYS	CA-C-N	5.25	131.74	121.66
12	I	51	LYS	C-N-CA	5.25	131.74	121.66
1	1	882	A	P-O5'-C5'	5.25	127.87	120.00
47	s	2	SER	N-CA-C	-5.25	105.46	111.07
47	s	226	GLU	N-CA-C	-5.24	105.74	111.82
44	o	69	PRO	CA-C-N	5.24	129.17	120.94
44	o	69	PRO	C-N-CA	5.24	129.17	120.94
1	1	2243	A	P-O5'-C5'	-5.24	112.14	120.00
12	I	16	ARG	N-CA-C	-5.24	101.40	109.52
47	s	129	ILE	N-CA-C	-5.24	101.93	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1130	A	P-O3'-C3'	5.24	128.05	120.20
44	o	266	ALA	CA-C-N	5.24	127.30	120.28
44	o	266	ALA	C-N-CA	5.24	127.30	120.28
43	n	162	GLU	N-CA-C	5.23	120.05	113.25
46	q	412	PRO	N-CA-C	-5.23	107.92	114.20
45	p	4	TYR	N-CA-C	-5.23	101.18	109.96
47	r	129	ILE	N-CA-C	-5.23	101.94	108.84
1	1	2927	C	C4'-C3'-O3'	5.22	117.84	110.00
31	b	100	ILE	N-CA-C	5.22	120.21	109.34
1	1	1580	A	C5'-C4'-C3'	-5.22	107.07	114.90
1	1	2929	C	C5'-C4'-C3'	5.22	122.73	114.90
1	1	1080	A	P-O5'-C5'	-5.22	112.18	120.00
12	I	13	LEU	CA-C-N	-5.22	113.74	122.92
12	I	13	LEU	C-N-CA	-5.22	113.74	122.92
43	n	4	SER	CA-C-N	5.22	131.50	121.54
43	n	4	SER	C-N-CA	5.22	131.50	121.54
1	1	462	C	P-O5'-C5'	5.21	127.82	120.00
11	H	166	LEU	CA-C-N	-5.21	113.55	118.97
11	H	166	LEU	C-N-CA	-5.21	113.55	118.97
47	r	2	SER	N-CA-C	-5.21	105.49	111.07
43	n	212	GLU	CA-C-N	5.21	128.95	121.50
43	n	212	GLU	C-N-CA	5.21	128.95	121.50
12	I	53	PHE	CA-C-N	5.21	127.21	120.44
12	I	53	PHE	C-N-CA	5.21	127.21	120.44
32	c	95	PRO	CA-C-N	-5.21	116.73	123.19
32	c	95	PRO	C-N-CA	-5.21	116.73	123.19
30	a	88	ARG	CA-C-N	5.21	127.96	121.71
30	a	88	ARG	C-N-CA	5.21	127.96	121.71
19	P	37	VAL	N-CA-C	5.20	116.29	111.45
17	N	120	ASN	N-CA-C	5.20	117.03	111.36
4	A	8	GLN	CA-C-N	5.20	127.80	120.42
4	A	8	GLN	C-N-CA	5.20	127.80	120.42
20	Q	169	GLY	N-CA-C	-5.20	103.00	110.38
37	h	6	PRO	CA-C-N	-5.20	112.52	121.66
37	h	6	PRO	C-N-CA	-5.20	112.52	121.66
4	A	193	LEU	CA-C-N	5.19	127.67	120.29
4	A	193	LEU	C-N-CA	5.19	127.67	120.29
1	1	644	G	P-O5'-C5'	-5.19	112.21	120.00
44	o	272	HIS	CA-C-N	5.19	127.66	120.29
44	o	272	HIS	C-N-CA	5.19	127.66	120.29
46	q	218	GLY	N-CA-C	-5.19	105.93	114.76
16	M	5	SER	N-CA-C	5.19	118.07	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	79	SER	N-CA-C	-5.19	105.62	111.28
35	f	50	ALA	CA-C-N	-5.18	115.30	122.30
35	f	50	ALA	C-N-CA	-5.18	115.30	122.30
4	A	145	TYR	CA-C-N	5.18	125.73	119.98
4	A	145	TYR	C-N-CA	5.18	125.73	119.98
5	B	211	HIS	N-CA-C	-5.18	106.80	113.23
44	o	299	ASP	CA-C-N	5.18	127.22	120.28
44	o	299	ASP	C-N-CA	5.18	127.22	120.28
10	G	122	PHE	CA-C-N	-5.18	113.36	119.84
10	G	122	PHE	C-N-CA	-5.18	113.36	119.84
12	I	116	MET	CA-C-N	5.18	127.74	120.28
12	I	116	MET	C-N-CA	5.18	127.74	120.28
44	o	145	ASP	CA-C-N	5.18	124.98	119.28
44	o	145	ASP	C-N-CA	5.18	124.98	119.28
38	i	70	PRO	CA-C-N	5.18	127.01	121.00
38	i	70	PRO	C-N-CA	5.18	127.01	121.00
12	I	125	LEU	CA-C-N	5.17	127.73	120.28
12	I	125	LEU	C-N-CA	5.17	127.73	120.28
4	A	208	SER	CA-C-N	-5.17	112.07	120.71
4	A	208	SER	C-N-CA	-5.17	112.07	120.71
42	m	49	VAL	N-CA-C	5.17	116.13	108.23
28	Y	18	TYR	N-CA-C	-5.16	106.57	112.92
1	1	2867	C	C5'-C4'-C3'	5.16	122.64	114.90
1	1	1130	A	P-O5'-C5'	-5.15	112.28	120.00
43	n	151	ALA	CA-C-N	5.15	127.18	120.28
43	n	151	ALA	C-N-CA	5.15	127.18	120.28
4	A	62	ASN	CA-C-N	5.15	129.45	122.19
4	A	62	ASN	C-N-CA	5.15	129.45	122.19
28	Y	4	PHE	N-CA-C	5.15	119.43	113.20
15	L	17	LEU	CA-C-N	-5.14	115.43	120.52
15	L	17	LEU	C-N-CA	-5.14	115.43	120.52
24	U	169	THR	N-CA-C	5.14	116.97	110.33
1	1	2847	A	P-O5'-C5'	-5.14	112.29	120.00
4	A	114	GLU	CA-C-N	5.14	128.74	120.30
4	A	114	GLU	C-N-CA	5.14	128.74	120.30
43	n	26	ILE	CA-C-N	5.14	127.12	120.44
43	n	26	ILE	C-N-CA	5.14	127.12	120.44
4	A	209	SER	CA-C-N	5.14	129.37	120.58
4	A	209	SER	C-N-CA	5.14	129.37	120.58
6	C	196	ARG	N-CA-C	-5.14	105.57	111.07
10	G	52	VAL	CA-C-N	-5.14	116.45	122.93
10	G	52	VAL	C-N-CA	-5.14	116.45	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	93	ASN	N-CA-C	5.14	118.11	110.14
34	e	20	LYS	CA-C-N	-5.14	114.27	122.29
34	e	20	LYS	C-N-CA	-5.14	114.27	122.29
4	A	90	LEU	CA-C-N	5.14	127.16	120.28
4	A	90	LEU	C-N-CA	5.14	127.16	120.28
1	1	3353	G	P-O3'-C3'	5.13	127.90	120.20
38	i	47	GLY	N-CA-C	-5.13	104.75	112.60
1	1	2759	U	P-O3'-C3'	5.13	127.89	120.20
25	V	59	ASP	N-CA-C	-5.13	107.19	112.93
30	a	164	SER	N-CA-C	5.13	121.72	110.80
32	c	105	GLN	CA-C-N	-5.13	114.09	121.42
32	c	105	GLN	C-N-CA	-5.13	114.09	121.42
1	1	2728	G	P-O5'-C5'	5.12	127.69	120.00
4	A	190	PHE	N-CA-C	5.12	116.86	111.28
26	W	134	ASP	N-CA-C	-5.12	105.59	111.07
14	K	55	ARG	CA-C-N	5.12	125.10	120.03
14	K	55	ARG	C-N-CA	5.12	125.10	120.03
41	l	172	PRO	CA-C-N	-5.12	111.77	121.54
41	l	172	PRO	C-N-CA	-5.12	111.77	121.54
1	1	1239	C	P-O3'-C3'	-5.12	112.53	120.20
10	G	167	ASN	N-CA-C	-5.11	102.48	110.10
47	s	42	GLU	N-CA-C	-5.11	105.62	111.14
1	1	1975	C	P-O3'-C3'	5.11	127.87	120.20
1	1	2458	A	P-O3'-C3'	5.11	127.86	120.20
3	3	63	A	P-O5'-C5'	-5.11	112.34	120.00
7	D	61	SER	N-CA-C	-5.10	106.36	112.59
15	L	72	LYS	N-CA-C	5.10	116.83	109.07
30	a	192	GLY	CA-C-N	5.10	126.22	119.84
30	a	192	GLY	C-N-CA	5.10	126.22	119.84
47	s	61	ILE	CA-C-N	5.10	128.53	120.47
47	s	61	ILE	C-N-CA	5.10	128.53	120.47
1	1	2566	C	P-O3'-C3'	-5.10	112.55	120.20
33	d	28	VAL	N-CA-C	5.10	115.10	107.51
4	A	36	VAL	CA-C-N	5.10	126.30	121.46
4	A	36	VAL	C-N-CA	5.10	126.30	121.46
47	r	42	GLU	N-CA-C	-5.09	105.64	111.14
1	1	2786	G	C5'-C4'-C3'	5.09	122.54	114.90
47	r	307	ALA	CA-C-N	5.09	126.20	119.84
47	r	307	ALA	C-N-CA	5.09	126.20	119.84
23	T	124	VAL	N-CA-C	5.09	119.92	109.34
20	Q	129	VAL	N-CA-C	5.09	115.81	110.62
5	B	243	THR	N-CA-C	-5.08	100.59	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	q	400	GLY	CA-C-N	-5.08	112.96	121.39
46	q	400	GLY	C-N-CA	-5.08	112.96	121.39
43	n	65	LEU	N-CA-C	-5.08	100.90	109.07
29	Z	61	GLN	N-CA-C	5.08	116.50	111.07
46	q	224	ALA	CA-C-N	-5.08	115.94	123.05
46	q	224	ALA	C-N-CA	-5.08	115.94	123.05
1	l	2650	U	O3'-P-O5'	-5.07	96.39	104.00
25	V	93	ILE	N-CA-C	5.07	115.21	108.11
46	q	232	ILE	CA-C-N	5.07	127.49	120.29
46	q	232	ILE	C-N-CA	5.07	127.49	120.29
6	C	366	GLY	N-CA-C	-5.07	103.32	111.59
10	G	128	LYS	CA-C-N	5.07	130.82	121.70
10	G	128	LYS	C-N-CA	5.07	130.82	121.70
47	r	61	ILE	CA-C-N	5.07	128.48	120.47
47	r	61	ILE	C-N-CA	5.07	128.48	120.47
19	P	243	ALA	N-CA-C	-5.07	105.76	111.28
46	q	52	PRO	CA-C-N	5.06	126.47	120.14
46	q	52	PRO	C-N-CA	5.06	126.47	120.14
47	s	300	GLN	N-CA-C	-5.06	102.97	110.46
47	s	307	ALA	CA-C-N	5.06	126.17	119.84
47	s	307	ALA	C-N-CA	5.06	126.17	119.84
43	n	14	GLN	CA-C-N	5.06	127.06	120.28
43	n	14	GLN	C-N-CA	5.06	127.06	120.28
25	V	68	THR	N-CA-C	-5.06	107.14	113.72
7	D	94	CYS	N-CA-C	5.06	117.86	109.46
47	r	300	GLN	N-CA-C	-5.05	102.98	110.46
7	D	113	VAL	N-CA-C	-5.05	100.98	108.45
18	O	192	LYS	N-CA-C	-5.04	105.86	111.36
21	R	51	VAL	N-CA-C	5.04	116.61	108.85
44	o	270	LEU	CA-C-N	5.04	127.03	120.28
44	o	270	LEU	C-N-CA	5.04	127.03	120.28
1	l	1132	C	P-O5'-C5'	5.03	127.55	120.00
46	q	164	GLY	N-CA-C	-5.03	108.07	114.16
47	r	189	VAL	CA-C-N	5.03	128.41	120.47
47	r	189	VAL	C-N-CA	5.03	128.41	120.47
46	q	382	THR	N-CA-C	-5.03	101.65	109.24
33	d	6	HIS	CA-C-N	-5.02	115.06	120.03
33	d	6	HIS	C-N-CA	-5.02	115.06	120.03
1	l	1227	C	O3'-P-O5'	-5.02	96.47	104.00
1	l	3357	U	P-O3'-C3'	-5.02	112.67	120.20
12	I	72	SER	N-CA-C	-5.02	100.33	108.52
22	S	5	LYS	N-CA-C	-5.02	102.13	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2194	G	C5'-C4'-C3'	5.02	122.43	114.90
19	P	21	ARG	N-CA-C	-5.01	100.12	110.80
44	o	237	MET	CA-C-N	5.01	127.41	120.29
44	o	237	MET	C-N-CA	5.01	127.41	120.29
47	s	189	VAL	CA-C-N	5.01	128.39	120.47
47	s	189	VAL	C-N-CA	5.01	128.39	120.47
46	q	82	THR	CA-C-N	5.01	130.99	121.97
46	q	82	THR	C-N-CA	5.01	130.99	121.97
5	B	49	VAL	N-CA-C	5.00	114.95	108.35
1	1	1025	A	P-O5'-C5'	5.00	127.50	120.00

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	19	TYR	Peptide
4	A	210	MET	Peptide
6	C	172	ALA	Peptide
7	D	318	LEU	Peptide
8	E	8	PRO	Peptide
9	F	21	LYS	Peptide
10	G	51	ARG	Peptide
11	H	158	ASP	Peptide
11	H	30	THR	Peptide
11	H	74	THR	Peptide
12	I	121	PHE	Peptide
12	I	59	THR	Peptide
12	I	74	VAL	Peptide
12	I	75	PRO	Peptide
12	I	76	SER	Peptide
13	J	110	PRO	Peptide
23	T	16	GLN	Peptide
30	a	157	ASN	Peptide
32	c	110	GLU	Peptide
43	n	231	THR	Peptide
43	n	26	ILE	Peptide
45	p	32	CYS	Peptide
46	q	123	PRO	Peptide
46	q	124	ARG	Peptide
46	q	133	THR	Peptide
46	q	146	ILE	Peptide
46	q	81	CYS	Peptide

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Mol	Chain	Res	Type	Group
46	q	85	GLY	Peptide
46	q	94	THR	Peptide
47	r	307	ALA	Peptide
47	s	307	ALA	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	1	20363	0	6792	187	0
2	2	948	0	317	2	0
3	3	725	0	244	8	0
4	A	651	0	230	0	0
5	B	756	0	310	3	0
6	C	1158	0	433	2	0
7	D	1083	0	399	4	0
8	E	507	0	193	26	0
9	F	573	0	215	2	0
10	G	525	0	179	2	0
11	H	699	0	242	5	0
12	I	381	0	140	7	0
13	J	591	0	214	1	0
14	K	579	0	199	3	0
15	L	408	0	162	13	0
16	M	408	0	145	0	0
17	N	444	0	176	11	0
18	O	609	0	221	11	0
19	P	807	0	293	14	0
20	Q	555	0	204	23	0
21	R	564	0	202	6	0
22	S	516	0	175	0	0
23	T	477	0	175	9	0
24	U	549	0	196	0	0
25	V	300	0	109	2	0
26	W	363	0	121	0	0
27	X	378	0	134	2	0
28	Y	405	0	142	3	0
29	Z	357	0	118	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	666	0	241	0	0
31	b	291	0	113	0	0
32	c	327	0	114	0	0
33	d	381	0	135	0	0
34	e	318	0	117	4	0
35	f	336	0	121	1	0
36	g	297	0	109	2	0
37	h	261	0	104	0	0
38	i	231	0	79	1	0
39	j	150	0	47	1	0
40	k	273	0	108	0	0
41	l	1140	0	412	6	0
42	m	672	0	257	2	0
43	n	708	0	251	30	0
44	o	1041	0	359	19	0
45	p	189	0	68	2	0
46	q	1329	0	491	13	0
47	r	966	0	321	209	0
47	s	966	0	316	212	0
All	All	47221	0	16443	498	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 8.

All (498) 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)
1:1:3027:A:H5'	44:o:194:VAL:C	1.16	1.58
47:r:50:SER:H	47:s:61:ILE:C	1.11	1.57
1:1:2819:A:C5'	1:1:2819:A:C4'	1.82	1.51
1:1:3027:A:C5'	44:o:194:VAL:C	1.86	1.48
47:r:199:PRO:CA	47:s:177:VAL:CA	1.90	1.47
47:r:116:ASP:C	47:s:233:ASN:CA	1.83	1.46
47:r:69:SER:CA	47:s:189:VAL:C	1.88	1.46
43:n:13:ALA:CA	43:n:18:LYS:H	1.26	1.45
47:r:40:LYS:C	47:s:60:SER:N	1.75	1.45
47:r:202:SER:CA	47:s:199:PRO:CA	1.94	1.45
47:r:199:PRO:CA	47:s:177:VAL:N	1.78	1.44
1:1:1996:C:H5'	41:l:80:TYR:N	1.18	1.43
47:r:199:PRO:N	47:s:177:VAL:CA	1.83	1.42
1:1:1996:C:C5'	41:l:80:TYR:H	1.33	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:115:VAL:C	47:s:233:ASN:C	1.89	1.39
47:r:235:VAL:CA	47:s:52:LYS:N	1.83	1.39
1:1:648:C:P	1:1:648:C:C5'	2.12	1.37
47:r:116:ASP:N	47:s:233:ASN:CA	1.80	1.37
47:r:255:ALA:CA	47:s:140:ALA:C	1.94	1.36
47:r:113:ASN:CA	47:s:239:LEU:H	1.22	1.35
47:r:201:LEU:C	47:s:199:PRO:N	1.83	1.34
12:I:99:LYS:CA	46:q:227:GLY:C	2.01	1.34
47:r:69:SER:C	47:s:189:VAL:C	1.95	1.33
1:1:1230:G:C4'	43:n:49:ARG:CA	2.05	1.33
1:1:1230:G:C5'	43:n:49:ARG:CA	2.07	1.33
47:r:205:ARG:C	47:s:204:ILE:CA	2.03	1.32
47:r:224:PRO:CA	47:s:34:GLN:C	2.03	1.32
1:1:1281:G:H5'	43:n:69:LYS:CA	1.60	1.31
12:I:99:LYS:C	46:q:227:GLY:C	1.97	1.31
1:1:730:C:P	20:Q:136:ASN:N	2.04	1.30
47:r:202:SER:N	47:s:199:PRO:N	1.79	1.30
1:1:715:A:P	17:N:114:GLY:H	1.54	1.29
47:r:47:LYS:H	47:s:59:GLU:C	1.20	1.28
47:r:134:THR:H	47:s:142:LEU:C	1.34	1.27
47:r:233:ASN:CA	47:s:42:GLU:CA	2.13	1.27
1:1:1943:C:C5'	1:1:3346:U:H5'	1.64	1.26
47:r:116:ASP:CA	47:s:233:ASN:N	1.95	1.26
47:r:224:PRO:N	47:s:34:GLN:CA	1.98	1.25
12:I:99:LYS:C	46:q:227:GLY:CA	2.10	1.25
43:n:13:ALA:CA	43:n:18:LYS:N	1.98	1.25
47:r:50:SER:N	47:s:61:ILE:C	1.94	1.24
1:1:1943:C:C4'	1:1:3346:U:H5'	1.65	1.23
47:r:134:THR:N	47:s:142:LEU:C	1.83	1.22
47:r:69:SER:CA	47:s:189:VAL:CA	2.15	1.22
47:r:235:VAL:CA	47:s:52:LYS:CA	2.18	1.22
1:1:2573:G:P	28:Y:57:HIS:CA	2.28	1.21
19:P:172:TYR:CA	46:q:133:THR:H	1.52	1.21
1:1:3027:A:C4'	44:o:194:VAL:C	2.13	1.20
1:1:1230:G:H5''	43:n:49:ARG:CA	1.70	1.20
47:r:317:LEU:C	47:s:270:PRO:CA	2.15	1.19
47:r:116:ASP:CA	47:s:233:ASN:C	2.17	1.16
47:r:174:GLY:HA3	47:s:266:PHE:N	1.59	1.15
47:r:113:ASN:CA	47:s:239:LEU:N	2.06	1.15
47:r:109:GLY:C	47:s:265:ASN:CA	2.14	1.14
1:1:1226:G:C4'	1:1:3117:C:C4'	2.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:99:LYS:C	46:q:227:GLY:HA2	1.72	1.13
47:r:40:LYS:C	47:s:59:GLU:C	2.01	1.13
47:r:201:LEU:CA	47:s:198:LYS:CA	2.28	1.12
47:r:47:LYS:N	47:s:59:GLU:C	2.06	1.11
1:1:965:A:H5'	17:N:41:HIS:CA	1.81	1.10
1:1:1281:G:C5'	43:n:69:LYS:CA	2.30	1.10
1:1:1996:C:H5'	41:l:80:TYR:CA	1.79	1.10
47:r:269:GLN:CA	47:s:243:GLY:HA3	1.81	1.10
47:r:206:SER:CA	47:s:204:ILE:CA	2.30	1.10
47:r:314:ILE:C	47:s:175:VAL:CA	2.25	1.09
47:r:269:GLN:CA	47:s:243:GLY:CA	2.30	1.09
47:r:320:LYS:N	47:s:111:GLU:C	2.11	1.08
1:1:2829:U:H5'	44:o:131:ALA:CA	1.84	1.08
1:1:1281:G:H5'	43:n:69:LYS:N	1.68	1.08
15:L:134:GLY:C	42:m:102:SER:CA	2.26	1.07
47:r:132:LYS:CA	47:s:109:GLY:CA	1.84	1.07
47:r:202:SER:CA	47:s:199:PRO:N	2.12	1.06
43:n:13:ALA:C	43:n:17:LYS:CA	2.28	1.06
1:1:1996:C:C5'	41:l:80:TYR:N	2.03	1.05
47:r:201:LEU:H	47:s:197:GLY:C	1.64	1.05
1:1:648:C:C5'	1:1:648:C:O5'	2.05	1.03
47:r:174:GLY:HA3	47:s:266:PHE:H	1.13	1.02
47:r:145:VAL:CA	47:s:266:PHE:CA	2.36	1.02
47:r:116:ASP:C	47:s:233:ASN:N	2.14	1.02
47:r:245:ILE:N	47:s:53:ASN:CA	2.20	1.02
1:1:647:A:O3'	1:1:648:C:C5'	2.09	1.01
47:r:206:SER:N	47:s:133:THR:C	2.18	1.01
1:1:2681:U:H5''	8:E:49:LYS:N	1.76	1.01
1:1:2844:C:H5''	23:T:159:PHE:C	1.86	1.01
47:r:115:VAL:C	47:s:233:ASN:CA	2.28	1.01
47:r:317:LEU:N	47:s:174:GLY:C	2.16	1.00
47:r:201:LEU:N	47:s:197:GLY:C	2.20	0.99
1:1:2599:U:P	18:O:70:ASN:H	1.86	0.99
47:r:208:ILE:C	47:s:251:ILE:CA	2.36	0.98
1:1:1943:C:H5'	1:1:3346:U:H5'	1.41	0.98
1:1:3027:A:H5'	44:o:194:VAL:CA	1.92	0.98
1:1:2092:A:P	21:R:140:GLU:C	2.47	0.97
1:1:2092:A:O5'	21:R:144:GLN:N	1.86	0.97
1:1:715:A:P	17:N:114:GLY:N	2.37	0.97
47:r:255:ALA:CA	47:s:141:LEU:N	2.26	0.97
47:r:318:LEU:H	47:s:175:VAL:CA	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2681:U:H5''	8:E:48:SER:C	1.90	0.96
1:1:744:A:C4'	20:Q:142:GLY:C	2.39	0.95
1:1:1943:C:C5'	1:1:3346:U:C5'	2.43	0.95
47:r:40:LYS:C	47:s:60:SER:H	1.51	0.95
1:1:729:C:C4'	20:Q:137:THR:C	2.41	0.94
1:1:729:C:O3'	20:Q:136:ASN:N	2.00	0.94
47:r:206:SER:N	47:s:204:ILE:CA	2.31	0.93
19:P:172:TYR:CA	46:q:133:THR:N	2.30	0.93
47:r:47:LYS:CA	47:s:58:ALA:C	2.41	0.93
47:r:174:GLY:CA	47:s:266:PHE:N	2.31	0.93
1:1:1943:C:H5'	1:1:3346:U:C5'	1.98	0.92
47:r:174:GLY:CA	47:s:266:PHE:CA	2.47	0.92
1:1:2844:C:C4'	23:T:159:PHE:C	2.43	0.92
47:r:132:LYS:H	47:s:110:ALA:CA	1.80	0.92
1:1:2747:A:H5'	19:P:175:HIS:CA	2.00	0.92
47:r:199:PRO:CA	47:s:177:VAL:H	1.83	0.91
1:1:1231:A:H5'	43:n:50:THR:CA	2.00	0.91
47:r:117:LEU:N	47:s:233:ASN:CA	2.33	0.91
47:r:201:LEU:C	47:s:107:ALA:CA	2.46	0.89
47:r:174:GLY:HA3	47:s:266:PHE:CA	2.03	0.88
47:r:235:VAL:CA	47:s:52:LYS:H	1.85	0.88
47:r:237:GLU:CA	47:s:46:LYS:C	2.46	0.88
1:1:729:C:O3'	20:Q:136:ASN:CA	2.23	0.87
47:r:125:ASP:CA	47:s:126:ASP:CA	2.53	0.87
47:r:116:ASP:CA	47:s:233:ASN:CA	0.86	0.86
1:1:2651:G:H5''	23:T:23:GLY:HA2	1.57	0.85
1:1:2844:C:C5'	23:T:159:PHE:C	2.49	0.85
47:r:201:LEU:C	47:s:198:LYS:CA	2.49	0.85
1:1:964:G:C4'	17:N:40:HIS:CA	2.54	0.85
1:1:648:C:P	1:1:648:C:H5''	2.17	0.84
1:1:1230:G:C4'	43:n:49:ARG:C	2.47	0.84
47:r:134:THR:N	47:s:177:VAL:H	1.74	0.84
1:1:964:G:C3'	17:N:40:HIS:C	2.50	0.84
1:1:288:C:H5''	18:O:171:SER:CA	2.08	0.84
47:r:246:CYS:CA	47:s:52:LYS:C	2.49	0.84
1:1:2917:G:H5''	15:L:47:ASN:N	1.93	0.84
1:1:2829:U:C5'	44:o:131:ALA:CA	2.55	0.84
47:r:224:PRO:CA	47:s:34:GLN:CA	2.46	0.84
1:1:2917:G:H5''	15:L:47:ASN:H	1.44	0.83
1:1:1226:G:C5'	1:1:3117:C:C4'	2.56	0.83
1:1:1281:G:H5'	43:n:69:LYS:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:40:LYS:CA	47:s:60:SER:N	2.43	0.82
1:1:1281:G:C5'	43:n:69:LYS:N	2.42	0.82
1:1:3027:A:H5''	44:o:194:VAL:H	1.42	0.82
1:1:3027:A:C5'	44:o:194:VAL:N	2.44	0.81
47:r:201:LEU:CA	47:s:197:GLY:C	2.54	0.81
47:r:318:LEU:N	47:s:174:GLY:C	2.40	0.80
1:1:730:C:P	20:Q:136:ASN:CA	2.68	0.80
47:r:174:GLY:HA2	47:s:266:PHE:CA	2.11	0.80
47:r:132:LYS:N	47:s:110:ALA:CA	2.17	0.80
47:r:315:ASP:CA	47:s:175:VAL:C	2.55	0.80
47:r:318:LEU:H	47:s:174:GLY:C	1.88	0.79
47:r:40:LYS:CA	47:s:60:SER:H	1.95	0.79
47:r:235:VAL:C	47:s:52:LYS:N	2.41	0.79
47:r:105:GLU:N	47:s:182:ASN:C	2.41	0.79
47:r:201:LEU:CA	47:s:107:ALA:CA	2.60	0.79
1:1:965:A:C5'	17:N:41:HIS:CA	2.61	0.79
47:r:73:GLU:H	47:s:159:ALA:CA	1.95	0.79
47:r:269:GLN:CA	47:s:243:GLY:N	2.45	0.78
47:r:205:ARG:C	47:s:133:THR:C	2.47	0.77
47:r:203:SER:CA	47:s:143:PHE:CA	2.63	0.77
47:r:132:LYS:N	47:s:110:ALA:C	2.43	0.77
47:r:235:VAL:CA	47:s:51:ASN:C	2.57	0.76
1:1:769:G:H5''	14:K:172:LEU:CA	2.14	0.76
1:1:2916:U:O3'	15:L:46:LEU:CA	2.33	0.76
47:r:230:ASN:H	47:s:248:GLU:CA	1.99	0.76
1:1:2829:U:C4'	44:o:131:ALA:CA	2.63	0.76
47:r:238:GLN:CA	47:s:50:SER:CA	2.64	0.75
47:r:249:ASP:H	47:s:54:LYS:C	1.95	0.75
47:r:235:VAL:C	47:s:52:LYS:H	1.93	0.75
47:r:268:LEU:C	47:s:243:GLY:HA3	2.11	0.75
1:1:2681:U:C5'	8:E:48:SER:C	2.59	0.75
47:r:132:LYS:H	47:s:110:ALA:C	1.93	0.75
47:r:206:SER:H	47:s:133:THR:C	1.93	0.75
47:r:233:ASN:CA	47:s:42:GLU:C	2.59	0.75
1:1:2938:G:C4'	44:o:31:THR:C	2.60	0.74
47:r:132:LYS:CA	47:s:109:GLY:HA3	2.14	0.74
1:1:1226:G:H5''	1:1:3117:C:C4'	2.17	0.74
1:1:744:A:C4'	20:Q:142:GLY:CA	2.65	0.74
47:r:230:ASN:N	47:s:248:GLU:CA	2.50	0.74
47:r:104:THR:C	47:s:182:ASN:C	2.55	0.74
1:1:1281:G:C4'	43:n:69:LYS:CA	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2917:G:C5'	15:L:47:ASN:H	2.01	0.74
47:r:236:GLU:N	47:s:48:LYS:C	2.46	0.74
1:1:3027:A:C5'	44:o:194:VAL:H	2.00	0.73
47:r:200:SER:N	47:s:143:PHE:C	2.37	0.73
1:1:2829:U:H5'	44:o:131:ALA:C	2.13	0.73
45:p:60:GLY:C	45:p:62:GLU:N	2.46	0.73
3:3:56:A:O3'	8:E:149:GLY:N	2.22	0.72
47:r:235:VAL:C	47:s:52:LYS:CA	2.62	0.72
1:1:1943:C:O5'	1:1:3346:U:C4'	2.38	0.72
47:r:245:ILE:N	47:s:53:ASN:C	2.44	0.72
1:1:1282:G:P	43:n:70:ARG:H	2.12	0.71
1:1:3027:A:C5'	44:o:194:VAL:CA	2.63	0.71
47:r:133:THR:C	47:s:108:ASN:CA	2.64	0.71
47:r:228:VAL:CA	47:s:249:ASP:H	2.02	0.71
47:r:73:GLU:CA	47:s:162:ILE:H	2.04	0.71
6:C:41:VAL:CA	6:C:185:GLY:HA3	2.21	0.70
47:r:117:LEU:N	47:s:232:ASN:C	2.49	0.70
47:r:132:LYS:CA	47:s:109:GLY:HA2	2.15	0.70
1:1:2932:U:P	15:L:41:GLY:H	2.14	0.70
1:1:647:A:O3'	1:1:648:C:H5'	1.89	0.70
47:r:116:ASP:N	47:s:233:ASN:C	2.26	0.70
47:r:208:ILE:CA	47:s:251:ILE:CA	2.69	0.70
47:r:73:GLU:N	47:s:159:ALA:CA	2.55	0.70
1:1:1943:C:C5'	1:1:3346:U:C4'	2.70	0.69
47:r:245:ILE:H	47:s:53:ASN:CA	2.01	0.69
1:1:729:C:C4'	20:Q:137:THR:N	2.55	0.69
47:r:46:LYS:C	47:s:61:ILE:C	2.60	0.69
1:1:1943:C:H5'	1:1:3346:U:C4'	2.23	0.69
47:r:275:ARG:N	47:s:214:ILE:N	2.40	0.69
1:1:2819:A:C4'	1:1:2819:A:H5'	2.15	0.68
47:r:224:PRO:N	47:s:33:ARG:C	2.51	0.68
47:r:275:ARG:N	47:s:214:ILE:C	2.51	0.68
1:1:1084:A:O3'	23:T:35:LYS:CA	2.42	0.68
47:r:201:LEU:CA	47:s:106:LYS:C	2.66	0.68
47:r:133:THR:C	47:s:177:VAL:H	2.02	0.68
1:1:2917:G:P	15:L:47:ASN:H	2.17	0.67
1:1:2681:U:C5'	8:E:49:LYS:C	2.68	0.67
1:1:2946:A:H5''	1:1:2947:G:H5'	1.75	0.67
47:r:228:VAL:CA	47:s:249:ASP:N	2.53	0.67
1:1:744:A:C3'	20:Q:142:GLY:C	2.68	0.67
1:1:2397:A:O5'	1:1:2398:A:H5'	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:301:PHE:C	47:s:161:LYS:CA	2.69	0.66
47:r:209:GLN:CA	47:s:205:ARG:CA	2.73	0.66
47:r:314:ILE:C	47:s:175:VAL:N	2.53	0.66
1:1:1231:A:C5'	43:n:50:THR:CA	2.73	0.66
47:r:314:ILE:N	47:s:166:LEU:C	2.54	0.66
47:r:199:PRO:CA	47:s:176:PHE:C	2.68	0.65
1:1:1943:C:C4'	1:1:3346:U:C5'	2.60	0.65
1:1:964:G:C3'	17:N:40:HIS:CA	2.75	0.65
1:1:2917:G:H5''	15:L:47:ASN:CA	2.27	0.65
47:r:51:ASN:H	47:s:62:VAL:CA	2.09	0.65
47:r:318:LEU:C	47:s:271:PHE:N	2.55	0.65
1:1:648:C:H5''	1:1:649:A:H5''	1.77	0.65
1:1:741:U:C4'	20:Q:74:GLU:CA	2.75	0.65
47:r:138:LYS:C	47:s:181:LYS:CA	2.70	0.64
47:r:134:THR:H	47:r:200:SER:N	1.96	0.64
47:r:67:ALA:CA	47:s:192:PRO:N	2.60	0.64
47:r:50:SER:CA	47:s:61:ILE:C	2.70	0.64
47:r:133:THR:C	47:s:177:VAL:N	2.54	0.64
1:1:741:U:C4'	20:Q:74:GLU:C	2.71	0.64
47:s:134:THR:H	47:s:200:SER:N	1.96	0.64
1:1:744:A:C4'	20:Q:142:GLY:HA2	2.28	0.63
47:r:275:ARG:H	47:s:214:ILE:N	1.95	0.63
47:r:269:GLN:CA	47:s:243:GLY:C	2.71	0.63
1:1:1818:U:C3'	1:1:1819:U:H5''	2.30	0.62
1:1:2819:A:C4'	1:1:2819:A:H5''	2.15	0.62
47:r:73:GLU:CA	47:s:159:ALA:CA	2.74	0.62
1:1:1230:G:H5'	43:n:48:VAL:C	2.25	0.62
1:1:965:A:O3'	17:N:44:ASN:N	2.32	0.61
47:r:104:THR:CA	47:s:182:ASN:C	2.74	0.61
47:r:314:ILE:N	47:s:166:LEU:CA	2.64	0.61
1:1:1281:G:C4'	43:n:69:LYS:N	2.64	0.61
1:1:2372:A:C3'	1:1:2373:A:H5'	2.29	0.61
47:r:117:LEU:N	47:s:233:ASN:N	2.47	0.61
45:p:60:GLY:C	45:p:62:GLU:H	2.09	0.60
47:r:237:GLU:C	47:s:47:LYS:C	2.70	0.60
1:1:2818:U:C4'	1:1:2819:A:H5'	2.32	0.60
47:r:100:ILE:CA	47:s:185:PRO:CA	2.80	0.60
47:r:318:LEU:N	47:s:175:VAL:CA	2.56	0.59
8:E:94:ARG:C	8:E:96:PHE:H	2.09	0.59
1:1:2674:A:P	8:E:105:GLY:N	2.75	0.59
47:r:40:LYS:C	47:s:59:GLU:N	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:q:464:LYS:C	46:q:466:THR:H	2.11	0.59
1:1:3029:A:H5''	44:o:1:MET:N	2.17	0.59
1:1:2445:A:C3'	36:g:98:ARG:CA	2.80	0.59
47:r:175:VAL:N	47:s:265:ASN:N	2.51	0.58
1:1:2244:A:P	5:B:244:GLY:HA2	2.43	0.58
47:r:201:LEU:C	47:s:198:LYS:C	2.66	0.58
1:1:2780:A:O3'	14:K:181:GLY:HA3	2.02	0.58
47:r:57:ARG:CA	47:s:102:LYS:C	2.77	0.58
1:1:729:C:C4'	20:Q:137:THR:H	2.16	0.58
3:3:28:C:C4'	8:E:135:GLY:HA2	2.33	0.58
1:1:810:A:H5''	18:O:81:TYR:C	2.28	0.58
47:r:201:LEU:CA	47:s:198:LYS:N	2.66	0.57
1:1:729:C:C4'	20:Q:137:THR:CA	2.83	0.57
47:s:133:THR:H	47:s:203:SER:C	2.12	0.57
3:3:56:A:O3'	8:E:149:GLY:CA	2.53	0.57
47:r:133:THR:C	47:s:109:GLY:H	2.12	0.57
1:1:1253:U:P	12:I:94:LYS:C	2.88	0.57
19:P:111:GLN:C	19:P:113:LEU:H	2.12	0.56
1:1:2244:A:P	5:B:244:GLY:CA	2.94	0.56
1:1:2747:A:C4'	19:P:174:PRO:C	2.78	0.56
47:r:250:ILE:H	47:s:54:LYS:CA	2.18	0.56
43:n:13:ALA:C	43:n:18:LYS:H	2.08	0.56
29:Z:68:GLN:C	29:Z:70:TYR:H	2.13	0.56
1:1:2681:U:H5'	8:E:49:LYS:C	2.31	0.55
47:r:237:GLU:C	47:s:46:LYS:C	2.74	0.55
47:r:174:GLY:HA3	47:s:266:PHE:C	2.31	0.55
47:r:318:LEU:CA	47:s:110:ALA:CA	2.85	0.55
1:1:2681:U:O3'	8:E:48:SER:CA	2.55	0.55
15:L:135:VAL:N	42:m:102:SER:CA	2.69	0.55
1:1:1230:G:H5'	43:n:49:ARG:CA	2.28	0.55
10:G:120:ASN:C	10:G:122:PHE:H	2.15	0.55
47:r:224:PRO:N	47:s:34:GLN:N	2.54	0.55
1:1:741:U:O3'	20:Q:74:GLU:N	2.40	0.55
1:1:741:U:C4'	20:Q:74:GLU:N	2.69	0.55
1:1:1226:G:C4'	1:1:3117:C:C5'	2.85	0.54
47:r:314:ILE:CA	47:s:166:LEU:C	2.80	0.54
1:1:2995:A:C3'	1:1:2996:U:H5''	2.37	0.54
13:J:62:THR:H	13:J:69:GLY:HA3	1.72	0.54
1:1:1191:U:C4'	1:1:1192:C:H5'	2.38	0.54
47:r:275:ARG:H	47:s:214:ILE:H	1.55	0.54
47:r:111:GLU:N	47:r:174:GLY:HA3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:338:LYS:C	7:D:340:GLY:H	2.16	0.53
47:s:111:GLU:N	47:s:174:GLY:HA3	2.23	0.53
36:g:97:SER:C	36:g:99:ARG:H	2.17	0.53
1:1:289:A:H5'	18:O:95:GLN:C	2.34	0.53
1:1:965:A:C4'	17:N:41:HIS:CA	2.87	0.53
1:1:3027:A:C4'	44:o:195:GLN:N	2.70	0.53
47:r:70:ARG:C	47:s:159:ALA:CA	2.82	0.52
47:r:317:LEU:CA	47:s:270:PRO:CA	2.87	0.52
47:r:203:SER:H	47:s:143:PHE:CA	2.22	0.52
1:1:1631:C:H5''	1:1:1632:A:H5''	1.91	0.52
1:1:2598:G:O3'	18:O:69:GLY:HA3	2.09	0.52
1:1:2747:A:H5'	19:P:175:HIS:N	2.25	0.52
47:r:273:LEU:CA	47:s:268:LEU:H	2.23	0.52
47:s:111:GLU:C	47:s:174:GLY:N	2.68	0.52
47:r:111:GLU:C	47:r:174:GLY:N	2.68	0.52
1:1:2818:U:C4'	1:1:2819:A:C5'	2.88	0.52
27:X:90:VAL:C	27:X:92:GLY:H	2.18	0.51
1:1:2917:G:C5'	15:L:47:ASN:N	2.64	0.51
47:r:135:TYR:CA	47:s:141:LEU:C	2.84	0.51
47:r:249:ASP:N	47:s:54:LYS:C	2.66	0.51
12:I:23:GLY:HA2	44:o:261:GLY:C	2.36	0.51
3:3:56:A:O3'	8:E:149:GLY:HA3	2.09	0.51
47:r:313:ASP:CA	47:s:168:LEU:N	2.73	0.51
47:r:65:THR:CA	47:s:188:LYS:CA	2.89	0.51
47:r:319:ALA:N	47:s:271:PHE:N	2.55	0.51
1:1:2747:A:C5'	19:P:174:PRO:C	2.84	0.51
9:F:49:ASN:C	9:F:51:GLN:H	2.19	0.51
1:1:2372:A:H5''	1:1:2373:A:H5''	1.92	0.51
43:n:16:ASP:H	43:n:17:LYS:CA	2.23	0.51
47:r:223:GLU:C	47:s:34:GLN:CA	2.81	0.51
6:C:199:PHE:C	6:C:201:LYS:H	2.19	0.50
47:r:203:SER:N	47:s:143:PHE:CA	2.74	0.50
11:H:78:PHE:C	11:H:80:TYR:H	2.20	0.50
47:r:244:ILE:C	47:s:53:ASN:C	2.80	0.50
1:1:965:A:C3'	17:N:44:ASN:H	2.25	0.50
47:r:318:LEU:H	47:s:175:VAL:N	2.07	0.50
1:1:2598:G:O3'	18:O:69:GLY:CA	2.60	0.49
43:n:16:ASP:N	43:n:17:LYS:CA	2.75	0.49
46:q:379:ASP:C	46:q:381:TYR:H	2.18	0.49
1:1:2681:U:C4'	8:E:48:SER:CA	2.91	0.49
47:r:111:GLU:CA	47:r:174:GLY:HA3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:s:82:GLU:C	47:s:84:LYS:H	2.20	0.49
47:s:111:GLU:CA	47:s:174:GLY:HA3	2.43	0.49
1:1:2651:G:H5''	23:T:23:GLY:CA	2.37	0.49
1:1:744:A:C4'	20:Q:143:PRO:N	2.75	0.49
34:e:59:VAL:C	34:e:61:GLY:H	2.21	0.49
7:D:269:SER:C	7:D:271:LYS:H	2.20	0.49
1:1:288:C:C5'	18:O:171:SER:C	2.86	0.49
47:r:67:ALA:CA	47:s:192:PRO:CA	2.91	0.49
1:1:1085:A:H5'	23:T:36:VAL:N	2.28	0.48
8:E:110:ILE:C	8:E:112:LEU:H	2.21	0.48
9:F:189:GLU:C	9:F:191:LEU:H	2.21	0.48
43:n:13:ALA:CA	43:n:17:LYS:C	2.79	0.48
47:r:82:GLU:C	47:r:84:LYS:H	2.20	0.48
1:1:873:C:H5''	1:1:874:U:O5'	2.13	0.48
47:r:234:ILE:C	47:s:48:LYS:C	2.81	0.48
1:1:1874:A:H5''	21:R:18:GLY:HA3	1.95	0.48
1:1:1191:U:C5'	1:1:1192:C:H5'	2.43	0.48
47:s:111:GLU:N	47:s:174:GLY:C	2.72	0.48
41:l:172:PRO:C	41:l:174:GLY:H	2.22	0.48
1:1:2681:U:H5''	8:E:49:LYS:C	2.38	0.48
47:r:135:TYR:N	47:s:141:LEU:C	2.41	0.48
1:1:2092:A:H5''	21:R:140:GLU:C	2.39	0.48
47:s:111:GLU:N	47:s:174:GLY:CA	2.78	0.47
47:r:111:GLU:N	47:r:174:GLY:CA	2.77	0.47
47:s:112:GLU:CA	47:s:173:THR:CA	2.92	0.47
27:X:91:ASN:C	27:X:93:ALA:H	2.22	0.47
1:1:288:C:H5''	18:O:171:SER:C	2.39	0.47
19:P:56:THR:C	19:P:58:LYS:H	2.22	0.47
47:s:134:THR:H	47:s:200:SER:H	1.62	0.47
47:r:73:GLU:CA	47:s:159:ALA:C	2.87	0.47
47:r:316:SER:C	47:s:111:GLU:C	2.81	0.47
1:1:730:C:C5'	20:Q:136:ASN:CA	2.92	0.47
1:1:741:U:C5'	20:Q:74:GLU:CA	2.93	0.47
23:T:100:LYS:C	23:T:102:ARG:H	2.22	0.47
47:r:134:THR:N	47:s:108:ASN:CA	2.78	0.47
47:r:112:GLU:CA	47:r:173:THR:CA	2.92	0.47
47:r:269:GLN:CA	47:s:243:GLY:H	2.27	0.47
1:1:2917:G:P	15:L:46:LEU:CA	3.03	0.47
1:1:2681:U:P	8:E:51:ARG:N	2.88	0.46
11:H:118:GLU:C	11:H:120:LYS:H	2.22	0.46
47:r:133:THR:C	47:s:109:GLY:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:r:201:LEU:C	47:s:199:PRO:CA	2.79	0.46
1:1:2946:A:C5'	1:1:2947:G:H5'	2.44	0.46
10:G:120:ASN:C	10:G:122:PHE:N	2.74	0.46
47:r:134:THR:H	47:r:200:SER:H	1.62	0.46
34:e:91:ALA:C	34:e:93:THR:H	2.24	0.46
1:1:3027:A:C4'	44:o:194:VAL:N	2.76	0.46
47:r:313:ASP:C	47:s:168:LEU:N	2.73	0.46
1:1:2674:A:P	8:E:105:GLY:CA	3.04	0.46
8:E:41:SER:C	8:E:43:GLN:H	2.24	0.46
47:r:106:LYS:CA	47:r:140:ALA:CA	2.94	0.45
47:s:133:THR:N	47:s:203:SER:C	2.74	0.45
47:r:238:GLN:N	47:s:46:LYS:C	2.75	0.45
1:1:1975:C:P	38:i:60:GLY:HA2	2.56	0.45
34:e:91:ALA:C	34:e:93:THR:N	2.73	0.45
47:s:112:GLU:N	47:s:173:THR:CA	2.80	0.45
47:r:112:GLU:N	47:r:173:THR:CA	2.80	0.45
1:1:2681:U:C4'	8:E:48:SER:C	2.90	0.45
47:r:65:THR:C	47:s:191:ALA:N	2.57	0.45
2:2:80:A:H5'	2:2:81:U:P	2.57	0.45
47:r:155:ILE:N	47:r:294:ALA:CA	2.80	0.45
47:r:274:ASN:C	47:s:214:ILE:C	2.84	0.45
1:1:744:A:C4'	20:Q:141:ARG:C	2.89	0.45
47:r:313:ASP:C	47:s:166:LEU:C	2.85	0.45
46:q:411:SER:C	46:q:413:ASP:H	2.24	0.44
43:n:13:ALA:CA	43:n:17:LYS:CA	2.94	0.44
47:s:106:LYS:CA	47:s:140:ALA:CA	2.94	0.44
46:q:286:TRP:C	46:q:288:GLY:H	2.22	0.44
47:s:155:ILE:N	47:s:294:ALA:CA	2.80	0.44
1:1:288:C:C5'	18:O:171:SER:CA	2.88	0.44
1:1:648:C:C5'	1:1:649:A:H5''	2.44	0.44
8:E:94:ARG:C	8:E:96:PHE:N	2.75	0.44
1:1:32:U:P	18:O:95:GLN:H	2.41	0.44
1:1:965:A:C4'	17:N:41:HIS:C	2.91	0.44
1:1:2747:A:H5'	19:P:174:PRO:C	2.42	0.44
19:P:172:TYR:N	46:q:133:THR:H	2.08	0.44
47:s:112:GLU:C	47:s:272:LYS:CA	2.91	0.44
7:D:42:VAL:C	7:D:44:LYS:H	2.25	0.44
47:r:134:THR:H	47:s:143:PHE:N	2.04	0.44
1:1:1281:G:O3'	43:n:69:LYS:CA	2.66	0.44
47:r:112:GLU:C	47:r:272:LYS:CA	2.91	0.44
47:r:313:ASP:CA	47:s:168:LEU:CA	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:78:PHE:C	11:H:80:TYR:N	2.75	0.43
43:n:19:GLY:C	43:n:21:GLU:N	2.74	0.43
47:r:227:ILE:CA	47:s:41:ARG:CA	2.96	0.43
1:1:1878:G:C3'	1:1:1879:A:H5'	2.48	0.43
1:1:2092:A:P	21:R:141:HIS:C	3.01	0.43
1:1:3027:A:H5''	44:o:194:VAL:N	2.11	0.43
47:r:132:LYS:C	47:s:175:VAL:C	2.85	0.43
1:1:769:G:C5'	14:K:172:LEU:CA	2.90	0.43
1:1:2674:A:C4'	8:E:105:GLY:HA3	2.49	0.43
25:V:49:ASN:C	25:V:51:GLY:H	2.26	0.43
41:l:172:PRO:C	41:l:174:GLY:N	2.77	0.43
1:1:2397:A:P	1:1:2398:A:H5'	2.59	0.43
47:s:42:GLU:CA	47:s:48:LYS:N	2.82	0.43
11:H:93:LEU:C	11:H:95:ASN:H	2.27	0.43
19:P:292:ALA:C	19:P:294:ALA:H	2.26	0.43
47:r:98:ASP:C	47:r:100:ILE:H	2.27	0.43
1:1:730:C:H5'	20:Q:136:ASN:CA	2.49	0.43
1:1:2112:U:C4'	1:1:2113:A:H5'	2.49	0.43
3:3:36:C:H5'	19:P:155:THR:C	2.44	0.43
47:s:98:ASP:C	47:s:100:ILE:H	2.27	0.43
1:1:1191:U:H5''	1:1:1192:C:H5'	2.00	0.42
19:P:111:GLN:C	19:P:113:LEU:N	2.75	0.42
47:r:144:ILE:C	47:s:266:PHE:CA	2.92	0.42
47:r:322:ASN:H	47:s:271:PHE:CA	2.32	0.42
1:1:939:U:H5'	1:1:2814:G:O3'	2.19	0.42
3:3:13:A:C3'	3:3:14:U:H5'	2.50	0.42
47:r:42:GLU:CA	47:r:48:LYS:N	2.82	0.42
11:H:161:GLU:C	11:H:163:VAL:H	2.27	0.42
35:f:97:GLU:C	35:f:99:LYS:N	2.78	0.42
1:1:1971:C:C3'	1:1:1972:A:H5'	2.50	0.42
47:r:46:LYS:N	47:s:60:SER:CA	2.82	0.42
47:r:117:LEU:H	47:s:233:ASN:CA	2.25	0.42
47:r:174:GLY:CA	47:s:264:CYS:C	2.90	0.42
1:1:2244:A:P	5:B:244:GLY:HA3	2.59	0.42
15:L:4:ASN:C	15:L:6:ALA:H	2.27	0.42
47:r:174:GLY:HA3	47:s:264:CYS:C	2.45	0.42
25:V:59:ASP:C	25:V:61:THR:H	2.28	0.42
1:1:1226:G:O3'	1:1:3117:C:C4'	2.68	0.41
1:1:2681:U:P	8:E:50:ALA:CA	3.08	0.41
7:D:304:GLN:C	7:D:306:THR:H	2.29	0.41
1:1:1232:C:C4'	43:n:51:PRO:CA	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:G:P	8:E:149:GLY:HA3	2.61	0.41
1:1:1226:G:H5''	1:1:3117:C:C3'	2.49	0.41
1:1:3029:A:H5''	44:o:1:MET:H3	1.84	0.41
34:e:59:VAL:C	34:e:61:GLY:N	2.79	0.41
46:q:464:LYS:C	46:q:466:THR:N	2.78	0.41
47:r:63:ALA:N	47:s:309:VAL:H	2.18	0.41
1:1:1943:C:C3'	1:1:3346:U:H5'	2.40	0.41
1:1:2674:A:P	8:E:105:GLY:HA3	2.60	0.41
1:1:1253:U:P	12:I:94:LYS:CA	3.08	0.41
47:s:134:THR:C	47:s:200:SER:C	2.89	0.41
1:1:2917:G:H5''	15:L:47:ASN:C	2.45	0.41
18:O:184:LYS:H	18:O:186:GLY:H	1.68	0.41
43:n:13:ALA:C	43:n:18:LYS:N	2.68	0.41
43:n:17:LYS:C	43:n:19:GLY:N	2.78	0.41
47:r:202:SER:N	47:s:198:LYS:C	2.65	0.41
1:1:2092:A:C5'	21:R:144:GLN:N	2.80	0.41
8:E:108:GLU:C	8:E:110:ILE:H	2.29	0.41
19:P:172:TYR:N	46:q:132:VAL:CA	2.84	0.41
39:j:27:ILE:C	39:j:29:LEU:H	2.28	0.41
47:r:46:LYS:C	47:s:63:ALA:H	2.29	0.41
47:r:113:ASN:H	47:s:240:GLY:H	1.69	0.41
1:1:745:C:H5'	20:Q:144:ARG:H	1.86	0.40
1:1:1085:A:H5'	23:T:36:VAL:CA	2.51	0.40
1:1:2360:C:H5''	1:1:2361:A:P	2.61	0.40
3:3:28:C:O3'	8:E:135:GLY:HA2	2.22	0.40
29:Z:68:GLN:C	29:Z:70:TYR:N	2.79	0.40
1:1:1281:G:C5'	43:n:69:LYS:H	2.20	0.40
1:1:3317:U:C4'	1:1:3318:G:O5'	2.69	0.40
28:Y:16:GLY:C	28:Y:18:TYR:H	2.29	0.40
1:1:2573:G:P	28:Y:56:LYS:C	3.05	0.40
2:2:79:A:O3'	2:2:80:A:C4'	2.70	0.40
20:Q:40:THR:C	20:Q:42:ALA:H	2.29	0.40
47:r:111:GLU:C	47:r:271:PHE:C	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	A	215/217 (99%)	194 (90%)	11 (5%)	10 (5%)	2	16
5	B	250/254 (98%)	230 (92%)	14 (6%)	6 (2%)	4	27
6	C	384/387 (99%)	333 (87%)	37 (10%)	14 (4%)	2	20
7	D	359/362 (99%)	304 (85%)	34 (10%)	21 (6%)	1	14
8	E	167/174 (96%)	120 (72%)	26 (16%)	21 (13%)	0	4
9	F	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	3	21
10	G	173/176 (98%)	147 (85%)	16 (9%)	10 (6%)	1	14
11	H	231/256 (90%)	186 (80%)	26 (11%)	19 (8%)	0	9
12	I	125/165 (76%)	107 (86%)	11 (9%)	7 (6%)	1	14
13	J	195/199 (98%)	180 (92%)	11 (6%)	4 (2%)	5	30
14	K	191/199 (96%)	161 (84%)	18 (9%)	12 (6%)	1	13
15	L	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	18	56
16	M	134/138 (97%)	117 (87%)	8 (6%)	9 (7%)	1	12
17	N	146/149 (98%)	120 (82%)	15 (10%)	11 (8%)	1	10
18	O	201/204 (98%)	184 (92%)	10 (5%)	7 (4%)	3	20
19	P	265/297 (89%)	220 (83%)	27 (10%)	18 (7%)	1	11
20	Q	183/186 (98%)	163 (89%)	16 (9%)	4 (2%)	5	29
21	R	186/189 (98%)	170 (91%)	12 (6%)	4 (2%)	5	29
22	S	170/172 (99%)	154 (91%)	12 (7%)	4 (2%)	4	27
23	T	157/160 (98%)	140 (89%)	10 (6%)	7 (4%)	2	17
24	U	181/184 (98%)	155 (86%)	17 (9%)	9 (5%)	1	16
25	V	98/121 (81%)	75 (76%)	14 (14%)	9 (9%)	0	8
26	W	119/142 (84%)	106 (89%)	11 (9%)	2 (2%)	7	36
27	X	124/127 (98%)	107 (86%)	15 (12%)	2 (2%)	7	38
28	Y	133/136 (98%)	114 (86%)	9 (7%)	10 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	117/120 (98%)	99 (85%)	10 (8%)	8 (7%)	1	11
30	a	220/244 (90%)	200 (91%)	11 (5%)	9 (4%)	2	18
31	b	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	11	46
32	c	107/113 (95%)	94 (88%)	8 (8%)	5 (5%)	2	16
33	d	125/130 (96%)	111 (89%)	10 (8%)	4 (3%)	3	21
34	e	104/107 (97%)	100 (96%)	2 (2%)	2 (2%)	6	32
35	f	110/121 (91%)	97 (88%)	9 (8%)	4 (4%)	2	20
36	g	97/100 (97%)	75 (77%)	11 (11%)	11 (11%)	0	5
37	h	85/88 (97%)	71 (84%)	11 (13%)	3 (4%)	3	20
38	i	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	9	42
39	j	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
40	k	89/92 (97%)	77 (86%)	9 (10%)	3 (3%)	3	21
41	l	376/593 (63%)	354 (94%)	14 (4%)	8 (2%)	5	30
42	m	222/245 (91%)	208 (94%)	13 (6%)	1 (0%)	24	63
43	n	234/236 (99%)	219 (94%)	9 (4%)	6 (3%)	4	25
44	o	345/647 (53%)	330 (96%)	9 (3%)	6 (2%)	7	36
45	p	61/199 (31%)	53 (87%)	4 (7%)	4 (7%)	1	12
46	q	439/515 (85%)	377 (86%)	40 (9%)	22 (5%)	1	16
47	r	320/322 (99%)	266 (83%)	31 (10%)	23 (7%)	1	11
47	s	320/322 (99%)	266 (83%)	31 (10%)	23 (7%)	1	11
All	All	8299/9350 (89%)	7270 (88%)	658 (8%)	371 (4%)	3	17

All (371) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	21	ASN
4	A	74	VAL
4	A	135	PRO
4	A	151	VAL
5	B	144	ASN
6	C	3	HIS
6	C	5	LYS
6	C	140	ASP
6	C	174	LYS
6	C	300	ARG

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Mol	Chain	Res	Type
6	C	347	SER
6	C	351	LEU
6	C	385	LYS
7	D	4	PRO
7	D	268	ALA
7	D	269	SER
7	D	283	THR
7	D	292	SER
7	D	320	ASN
7	D	338	LYS
7	D	361	HIS
8	E	8	PRO
8	E	11	ASP
8	E	12	LEU
8	E	74	PRO
8	E	94	ARG
8	E	165	GLN
9	F	50	ASN
9	F	109	ALA
10	G	6	ALA
10	G	98	VAL
10	G	121	LEU
10	G	122	PHE
11	H	25	PRO
11	H	31	PRO
11	H	36	ILE
11	H	37	GLY
11	H	156	ASP
12	I	37	LEU
12	I	51	LYS
12	I	75	PRO
12	I	76	SER
13	J	110	PRO
13	J	111	PRO
13	J	182	ASN
14	K	5	LYS
14	K	47	ALA
14	K	50	PRO
14	K	129	ASN
14	K	131	LYS
14	K	193	ALA
16	M	8	LYS

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Mol	Chain	Res	Type
16	M	9	ALA
16	M	135	LEU
16	M	136	ALA
17	N	66	ALA
17	N	76	ASP
18	O	74	PRO
18	O	75	VAL
19	P	20	PHE
19	P	58	LYS
19	P	210	GLU
19	P	233	ALA
19	P	234	ASP
19	P	258	LYS
19	P	276	LYS
19	P	293	LEU
19	P	295	GLY
20	Q	99	THR
21	R	5	ARG
21	R	47	ASN
22	S	167	ARG
23	T	124	VAL
23	T	159	PHE
24	U	157	VAL
24	U	182	ILE
25	V	107	PHE
26	W	44	PRO
27	X	84	LYS
28	Y	17	ARG
28	Y	59	ALA
28	Y	125	GLY
28	Y	128	GLN
28	Y	129	TRP
29	Z	97	ALA
29	Z	119	LYS
30	a	25	GLN
30	a	26	VAL
30	a	216	VAL
31	b	100	ILE
32	c	5	LYS
32	c	6	ASP
32	c	7	VAL
32	c	83	GLU

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Mol	Chain	Res	Type
32	c	84	ASP
33	d	12	LYS
33	d	27	ARG
33	d	123	LYS
36	g	13	LYS
36	g	33	ALA
37	h	85	LYS
41	l	62	PRO
41	l	169	ILE
43	n	18	LYS
43	n	25	ARG
43	n	133	LEU
44	o	203	SER
45	p	15	PRO
45	p	33	ARG
46	q	77	TYR
46	q	83	ILE
46	q	84	GLN
46	q	91	PRO
46	q	107	LYS
46	q	124	ARG
46	q	132	VAL
46	q	133	THR
46	q	391	SER
46	q	455	ASP
47	r	81	LEU
47	r	107	ALA
47	r	133	THR
47	r	134	THR
47	r	153	VAL
47	r	194	VAL
47	r	216	TYR
47	r	227	ILE
47	r	238	GLN
47	r	269	GLN
47	r	294	ALA
47	r	296	SER
47	r	308	PRO
47	s	81	LEU
47	s	107	ALA
47	s	133	THR
47	s	134	THR

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Mol	Chain	Res	Type
47	s	153	VAL
47	s	194	VAL
47	s	216	TYR
47	s	227	ILE
47	s	238	GLN
47	s	269	GLN
47	s	294	ALA
47	s	296	SER
47	s	308	PRO
4	A	99	LEU
4	A	168	ALA
4	A	198	TRP
4	A	199	GLN
5	B	13	GLY
5	B	70	ARG
6	C	136	LYS
6	C	138	ALA
7	D	15	ALA
7	D	107	ARG
7	D	182	LEU
7	D	232	SER
7	D	311	HIS
7	D	317	PRO
8	E	9	MET
8	E	73	GLY
8	E	86	VAL
8	E	115	LYS
8	E	167	TYR
10	G	97	ASN
10	G	123	PRO
11	H	39	ALA
11	H	115	ALA
11	H	159	PRO
11	H	254	ASP
12	I	32	ILE
12	I	77	ALA
14	K	136	GLU
14	K	141	ALA
15	L	82	ALA
16	M	10	SER
17	N	47	LYS
17	N	57	GLY

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Mol	Chain	Res	Type
17	N	121	VAL
18	O	144	ARG
18	O	184	LYS
19	P	188	GLU
19	P	209	GLU
19	P	215	ASP
19	P	292	ALA
20	Q	98	LYS
20	Q	183	GLY
22	S	2	ALA
22	S	12	ARG
22	S	13	ARG
23	T	125	ALA
24	U	164	LYS
25	V	11	ILE
25	V	50	LEU
25	V	51	GLY
25	V	91	ASP
26	W	45	LYS
27	X	92	GLY
29	Z	90	ARG
29	Z	95	PHE
29	Z	96	GLU
30	a	24	GLU
30	a	175	LYS
35	f	74	ARG
35	f	77	GLY
36	g	28	TYR
36	g	49	GLY
36	g	50	LEU
37	h	65	ARG
40	k	60	CYS
41	l	61	VAL
41	l	354	ILE
43	n	170	GLU
44	o	87	GLU
45	p	62	GLU
46	q	106	ILE
46	q	129	VAL
46	q	146	ILE
46	q	154	HIS
46	q	308	SER

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Mol	Chain	Res	Type
46	q	309	GLN
46	q	318	SER
47	r	45	ILE
47	r	108	ASN
47	r	230	ASN
47	r	276	GLU
47	s	45	ILE
47	s	108	ASN
47	s	230	ASN
47	s	276	GLU
4	A	137	PRO
5	B	250	GLN
6	C	4	ARG
7	D	14	GLU
7	D	16	THR
8	E	140	ARG
8	E	169	ALA
8	E	173	ASP
9	F	42	ASP
11	H	78	PHE
11	H	122	LYS
14	K	134	GLU
14	K	166	ALA
16	M	28	SER
16	M	95	ALA
17	N	93	SER
18	O	145	ASP
19	P	112	LYS
21	R	53	LYS
21	R	64	ARG
23	T	114	ALA
24	U	160	ALA
25	V	10	LYS
25	V	44	GLU
28	Y	16	GLY
28	Y	35	SER
28	Y	102	GLU
29	Z	4	VAL
29	Z	91	ALA
35	f	46	ASP
35	f	98	GLN
36	g	34	SER

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Mol	Chain	Res	Type
36	g	95	ALA
36	g	98	ARG
40	k	58	SER
41	l	173	THR
41	l	175	PRO
43	n	5	LYS
43	n	23	LYS
44	o	311	GLU
44	o	342	SER
45	p	61	LYS
46	q	486	LYS
47	r	259	GLU
47	s	259	GLU
6	C	386	ASP
7	D	146	PRO
7	D	233	LEU
8	E	95	ASN
8	E	108	GLU
8	E	114	ILE
8	E	117	ASP
9	F	13	PRO
10	G	95	GLY
10	G	129	GLU
11	H	157	VAL
11	H	253	SER
13	J	181	ALA
17	N	96	LYS
18	O	94	TYR
18	O	149	ASN
19	P	6	ASP
19	P	252	ALA
19	P	253	PHE
20	Q	162	ALA
23	T	12	ARG
24	U	158	ALA
24	U	161	ALA
24	U	163	LYS
25	V	31	ALA
25	V	49	ASN
28	Y	103	GLN
29	Z	27	GLU
30	a	160	ARG

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Mol	Chain	Res	Type
33	d	40	SER
37	h	25	ARG
38	i	33	LYS
40	k	51	ALA
46	q	49	LEU
47	r	87	LYS
47	r	307	ALA
47	r	310	ILE
47	s	87	LYS
47	s	307	ALA
47	s	310	ILE
5	B	35	ALA
5	B	251	LYS
7	D	5	GLN
8	E	24	GLY
8	E	111	ASP
8	E	172	LEU
9	F	2	LYS
9	F	107	ASP
10	G	108	LYS
11	H	47	SER
12	I	95	ASP
14	K	130	GLY
14	K	133	PRO
16	M	6	ILE
16	M	36	VAL
17	N	56	VAL
17	N	117	ARG
23	T	18	ASP
30	a	178	ILE
34	e	59	VAL
36	g	3	VAL
47	r	167	ARG
47	r	295	GLU
47	s	167	ARG
47	s	295	GLU
4	A	134	PHE
6	C	155	ALA
6	C	317	ILE
7	D	72	ALA
10	G	130	ILE
11	H	75	ILE

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Mol	Chain	Res	Type
17	N	91	LEU
19	P	259	LYS
24	U	162	GLU
30	a	164	SER
34	e	91	ALA
36	g	21	THR
36	g	94	ILE
44	o	221	THR
17	N	29	PRO
41	l	389	PRO
11	H	158	ASP
30	a	91	GLY
41	l	550	VAL
44	o	344	ILE
46	q	73	ASP
11	H	116	VAL
11	H	119	GLY
11	H	135	GLY
28	Y	36	HIS
7	D	131	VAL
24	U	84	PRO
42	m	58	ILE
46	q	387	ASN
46	q	483	PRO
23	T	123	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	0/3396	-	-
2	2	0/158	-	-
3	3	0/121	-	-
All	All	0/3675	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1
45	p	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	439:C	O3'	440:A	P	1.76
1	p	61:LYS	C	62:GLU	N	1.66

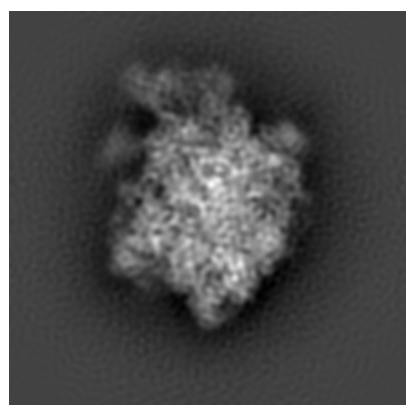
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2528. These allow visual inspection of the internal detail of the map and identification of artifacts.

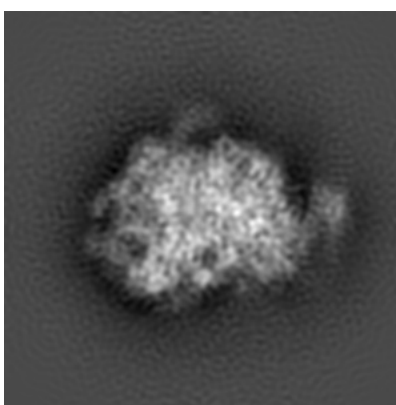
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

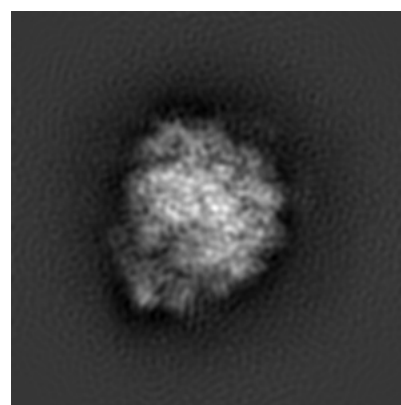
6.1.1 Primary map



X



Y

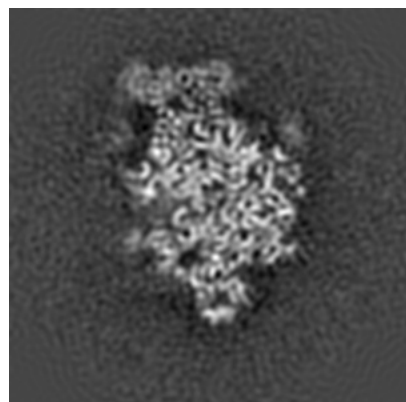


Z

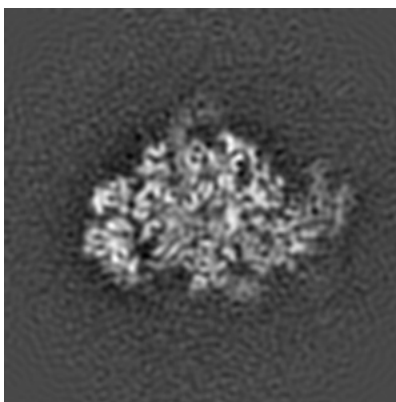
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

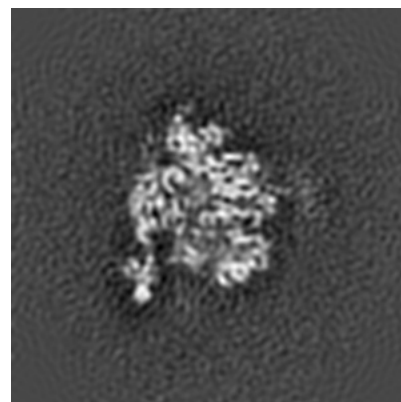
6.2.1 Primary map



X Index: 207



Y Index: 207

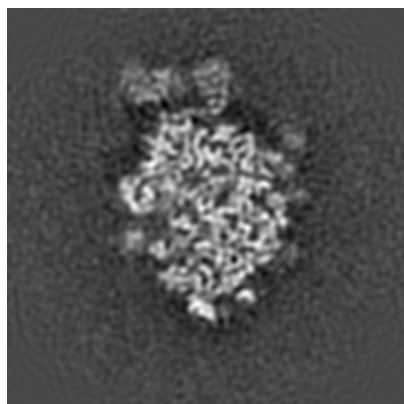


Z Index: 207

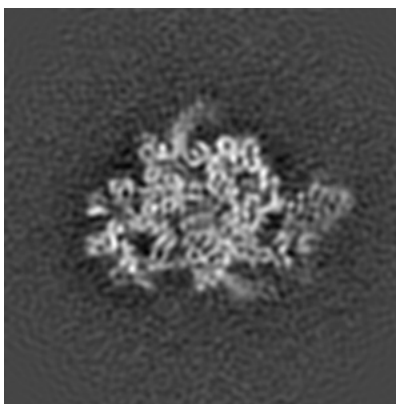
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

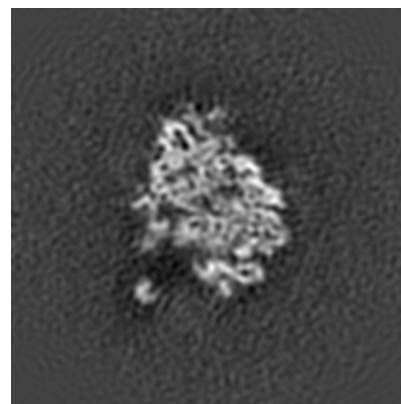
6.3.1 Primary map



X Index: 218



Y Index: 215

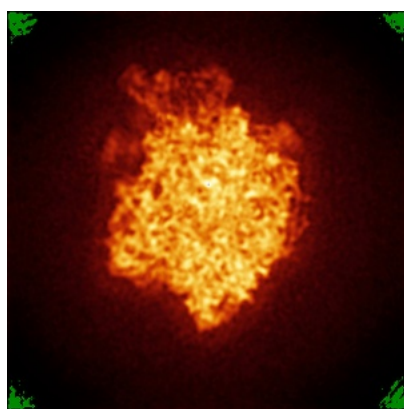


Z Index: 223

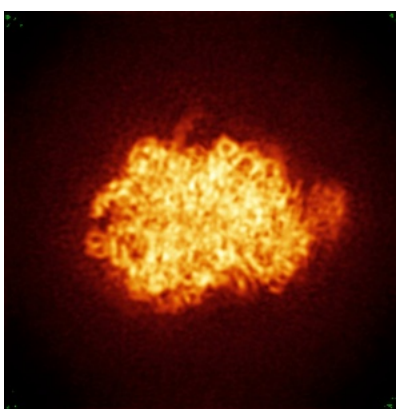
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

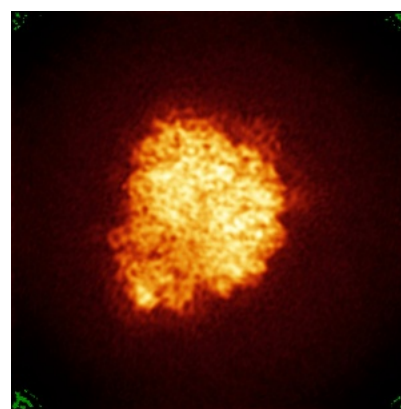
6.4.1 Primary map



X



Y

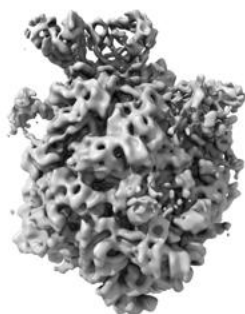


Z

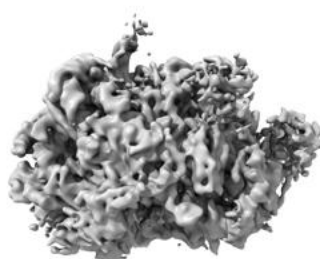
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

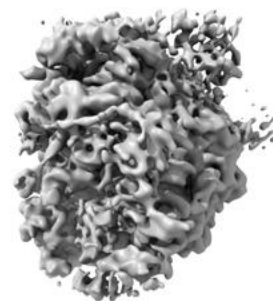
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

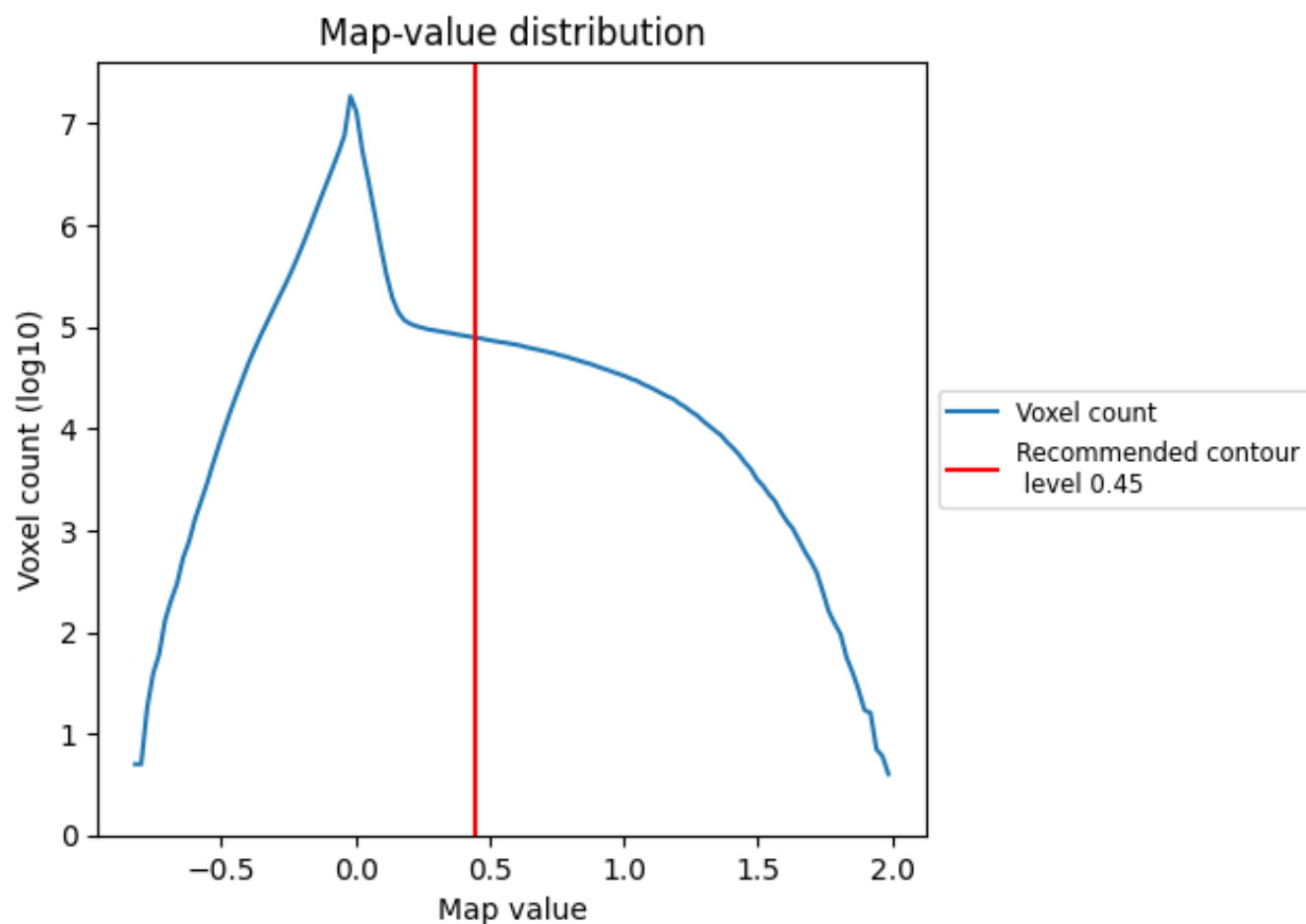
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

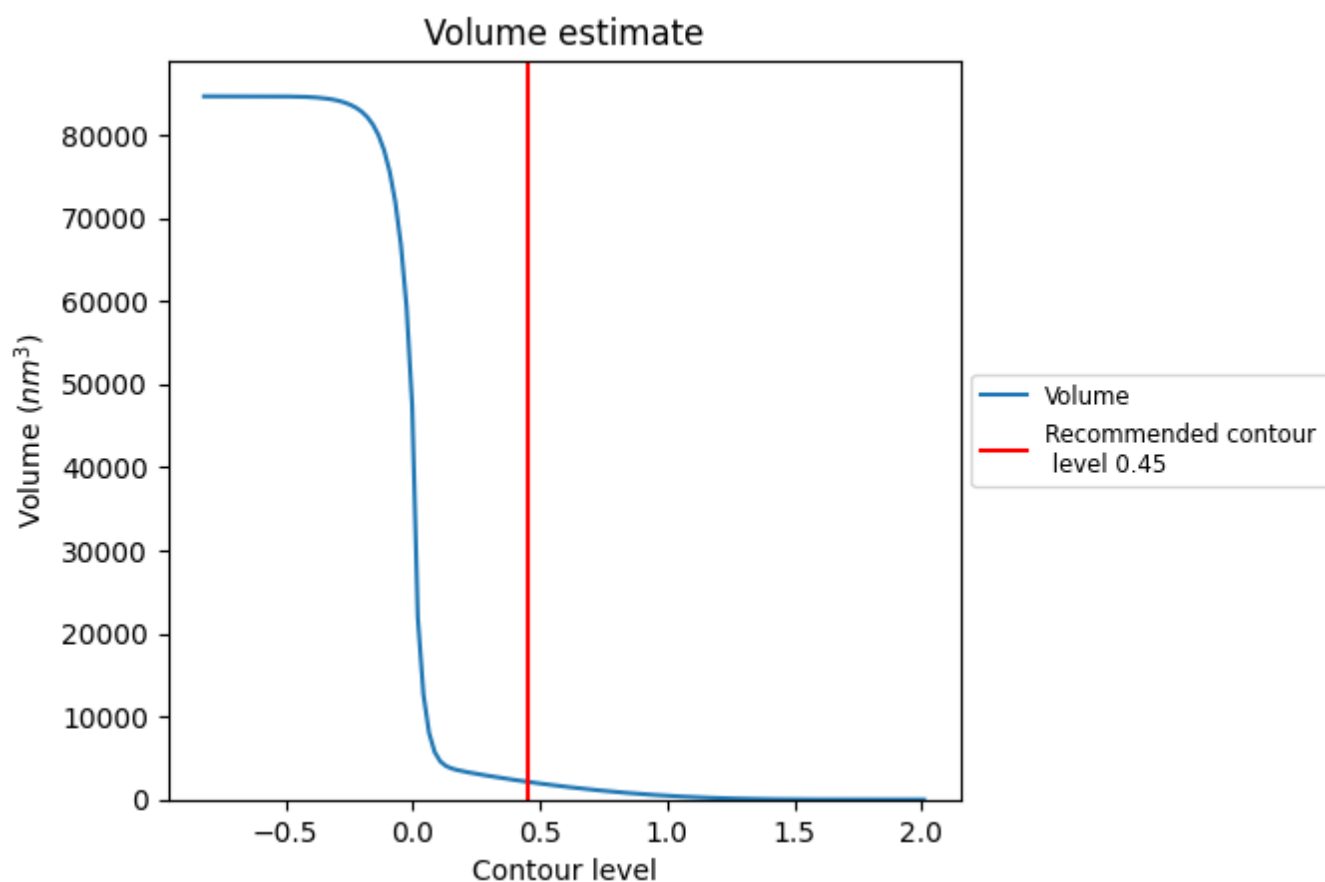
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

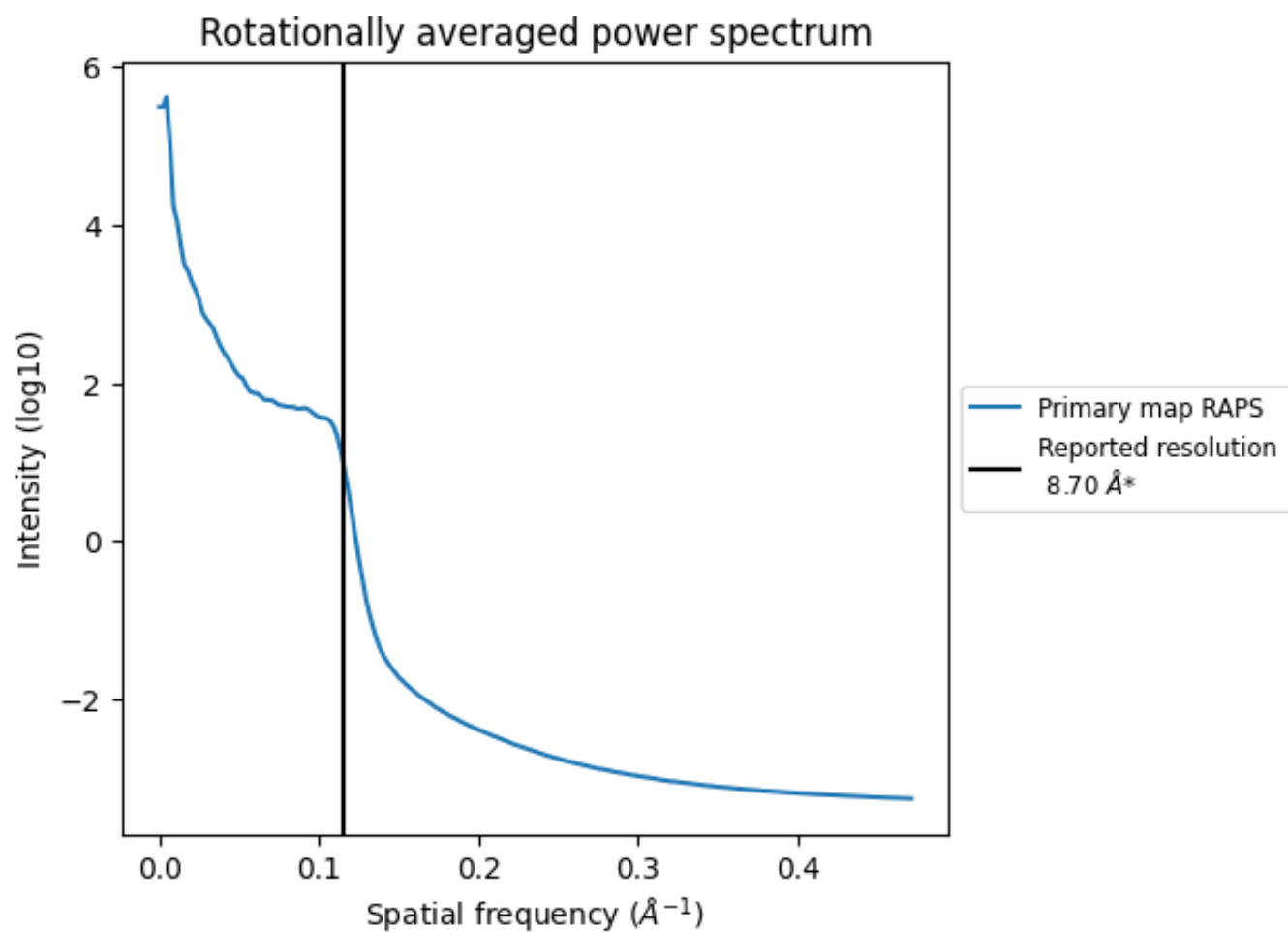
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2140 nm³; this corresponds to an approximate mass of 1933 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.115 $\text{\AA}^{-1}$

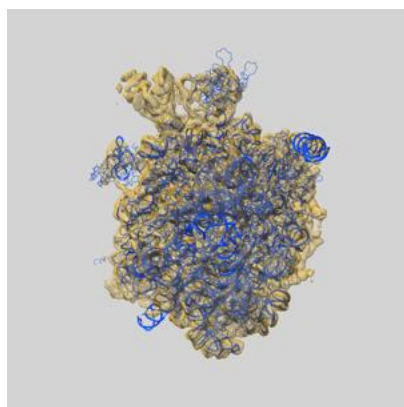
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

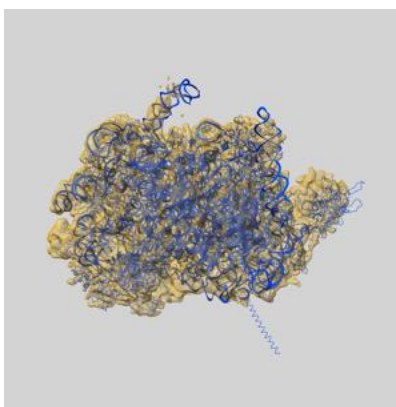
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2528 and PDB model 4V7F. Per-residue inclusion information can be found in section [3](#) on page [12](#).

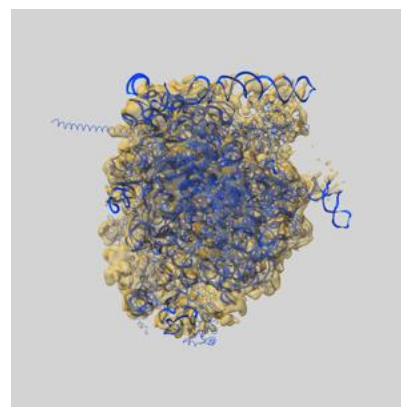
9.1 Map-model overlay [i](#)



X



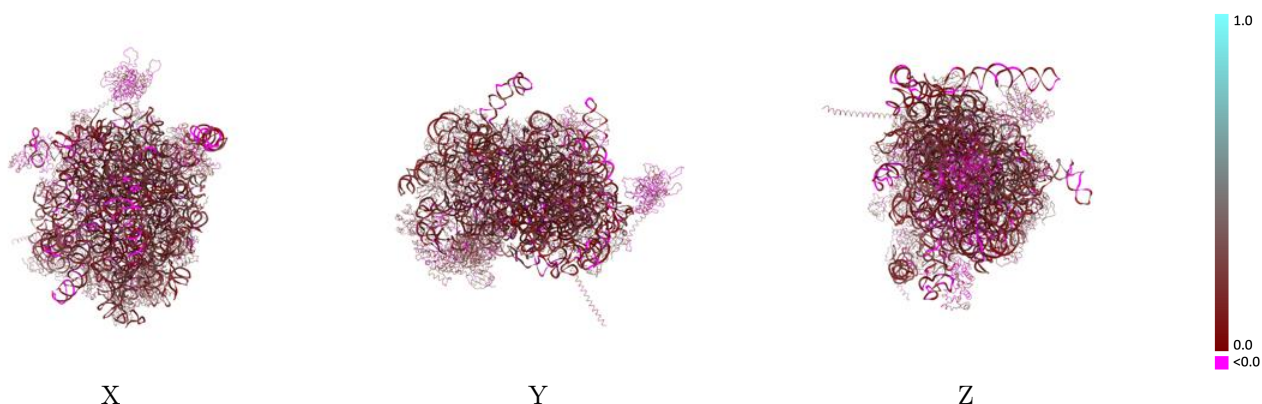
Y



Z

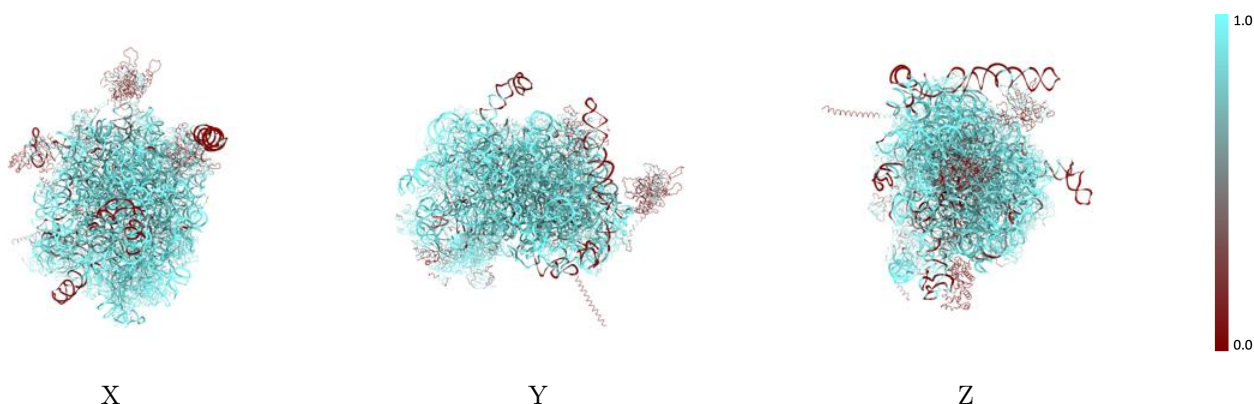
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



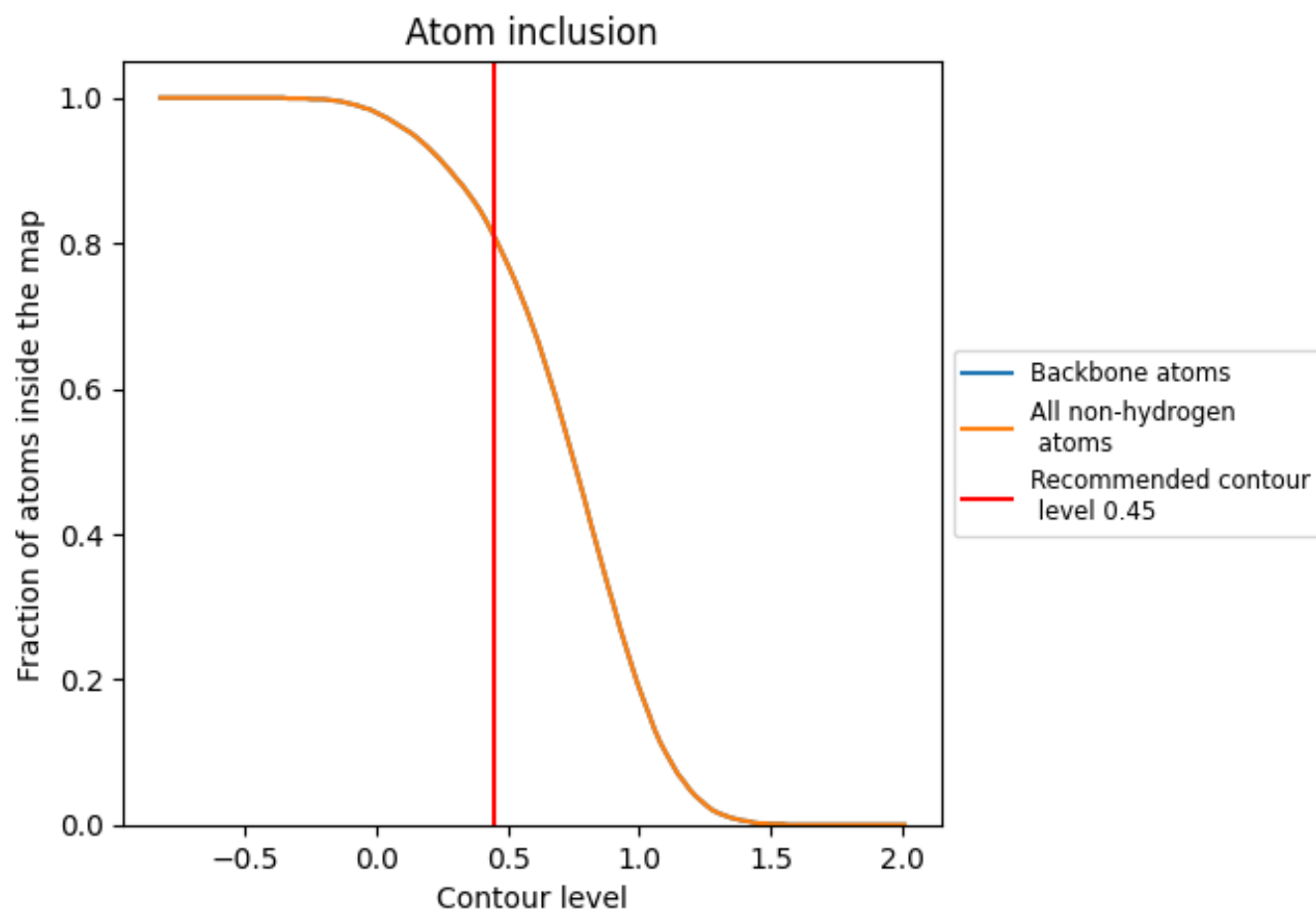
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.1560
1	 0.8440	 0.1400
2	 0.9670	 0.1700
3	 0.9720	 0.1540
A	 0.0250	 0.0170
B	 0.6840	 0.1120
C	 0.9380	 0.1990
D	 0.9400	 0.2090
E	 0.9650	 0.1880
F	 0.9280	 0.2120
G	 0.9520	 0.2310
H	 0.7670	 0.1650
I	 0.3600	 0.0670
J	 0.9800	 0.2570
K	 0.8120	 0.1400
L	 0.8580	 0.1920
M	 0.9800	 0.2690
N	 0.5810	 0.0550
O	 0.7590	 0.1340
P	 0.7810	 0.1580
Q	 0.7870	 0.1820
R	 0.7730	 0.2020
S	 0.9420	 0.2150
T	 0.5410	 0.0560
U	 0.9490	 0.2170
V	 0.9400	 0.2290
W	 0.9010	 0.2300
X	 0.9820	 0.2090
Y	 0.9850	 0.2490
Z	 0.9610	 0.2350
a	 0.9760	 0.2420
b	 0.9830	 0.2430
c	 0.9360	 0.2360
d	 0.9260	 0.2230
e	 0.9840	 0.1910



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Chain	Atom inclusion	Q-score
f	 0.8270	 0.1640
g	 0.6700	 0.1370
h	 0.9430	 0.1650
i	 0.9570	 0.2660
j	 0.9670	 0.2530
k	 0.8500	 0.1810
l	 0.3630	 0.1410
m	 0.9630	 0.2360
n	 0.9450	 0.1950
o	 0.8010	 0.1900
p	 0.9420	 0.2080
q	 0.8130	 0.1440
r	 0.2470	 0.0310
s	 0.2280	 0.0010