



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:44 AM UTC

PDB ID : 5OPT / pdb_00005opt
EMDB ID : EMD-3844
Title : Structure of KSRP in context of Trypanosoma cruzi 40S
Authors : Brito Querido, J.; Mancera-Martinez, E.; Vicens, Q.; Bochler, A.; Chicher, J.; Simonetti, A.; Hashem, Y.
Deposited on : 2017-08-10
Resolution : 4.00 Å(reported)

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:

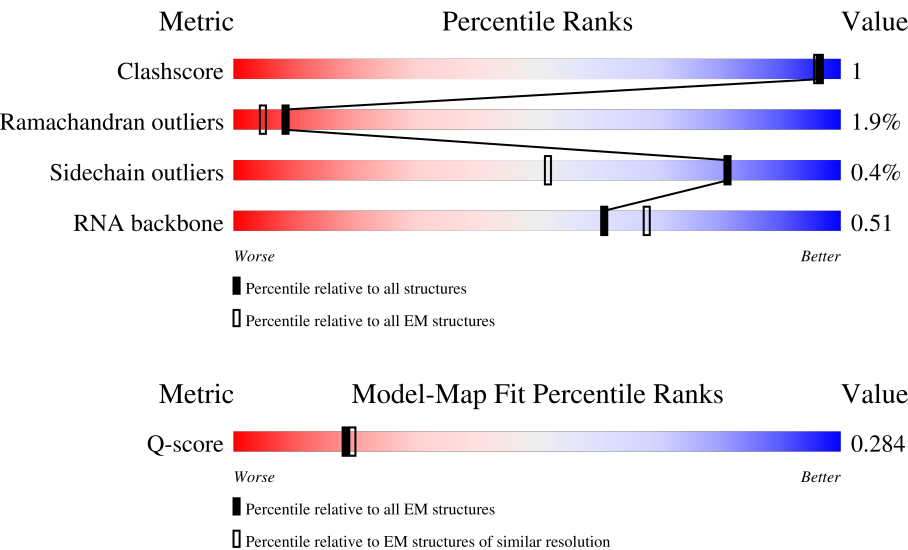
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	p	318	85% 94%
2	q	57	37% 60% 7% 33%
3	r	149	50% 77% 15% 6%

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Mol	Chain	Length	Quality of chain
4	t	152	
5	u	153	
6	L	273	
7	M	143	
8	O	190	
9	Q	211	
10	R	151	
11	S	86	
12	T	112	
13	U	112	
14	V	144	
15	W	261	
16	X	173	
17	Y	137	
18	Z	221	
19	b	190	
20	f	245	
21	d	263	
22	e	130	
23	g	236	
24	a	110	
25	i	141	
26	j	150	
27	P	250	
28	k	196	

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Mol	Chain	Length	Quality of chain
29	l	117	57% 84% 15%
30	m	214	67% 87% 6%7%
31	n	161	41% 54% 42%
32	o	167	44% 75% 8%16%
33	c	66	33% 82% 9%9%
34	h	257	47% 49% 12% 33%
35	E	2319	12% 61% 18% 6% 13%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 82219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Activated protein kinase C receptor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	310	Total	C	N	O	S	0	0
			2405	1505	424	463	13		

- Molecule 2 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	38	Total	C	N	O	S	0	0
			311	191	64	52	4		

- Molecule 3 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	r	140	Total	C	N	O	S	0	0
			1113	706	212	192	3		

- Molecule 4 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	t	119	Total	C	N	O	S	0	0
			969	615	185	165	4		

- Molecule 5 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	u	120	Total	C	N	O	S	0	0
			981	614	194	169	4		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	258	Total	C	N	O	S	0	0
			2038	1290	383	354	11		

- Molecule 7 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	142	Total	C	N	O	S	0	0
			1116	706	220	188	2		

- Molecule 8 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	190	Total	C	N	O	S	0	0
			1493	932	286	269	6		

- Molecule 9 is a protein called Ribosomal protein S7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	200	Total	C	N	O	S	0	0
			1670	1063	324	277	6		

- Molecule 10 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	141	Total	C	N	O	S	0	0
			1143	724	221	190	8		

- Molecule 11 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	82	Total	C	N	O	S	0	0
			630	384	121	116	9		

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	104	Total	C	N	O	S	0	0
			829	510	177	132	10		

- Molecule 13 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	68	Total	C	N	O	S	0	0
			526	315	107	100	4		

- Molecule 14 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	135	Total	C	N	O	S	0	0
			1011	620	195	187	9		

- Molecule 15 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	217	Total	C	N	O	S	0	0
			1781	1124	337	313	7		

- Molecule 16 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	148	Total	C	N	O	S	0	0
			1212	760	239	207	6		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	123	Total	C	N	O	S	0	0
			989	628	194	165	2		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	175	Total	C	N	O	S	0	0
			1404	885	283	233	3		

- Molecule 19 is a protein called 40S ribosomal protein S9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	164	Total	C	N	O	S	0	0
			1365	864	266	227	8		

- Molecule 20 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	207	Total	C	N	O	S	0	0
			1658	1060	299	288	11		

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	223	Total	C	N	O	S	0	0
			1726	1098	304	314	10		

- Molecule 22 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	129	Total	C	N	O	S	0	0
			1019	647	188	176	8		

- Molecule 23 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	83	Total	C	N	O	S	0	0
			635	395	116	122	2		

- Molecule 24 is a protein called Ribosomal protein S25, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	70	Total	C	N	O	S	0	0
			553	356	97	97	3		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	121	Total	C	N	O	S	0	0
			958	594	174	185	5		

- Molecule 26 is a protein called Ubiquitin/ribosomal protein S27a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	64	Total	C	N	O	S	0	0
			518	324	98	90	6		

- Molecule 27 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	249	Total	C	N	O	S	0	0
			1983	1244	402	333	4		

- Molecule 28 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	118	Total	C	N	O	S	0	0
			972	610	187	170	5		

- Molecule 29 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	99	Total	C	N	O	S	0	0
			784	497	144	140	3		

- Molecule 30 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	200	Total	C	N	O	S	0	0
			1587	995	302	279	11		

- Molecule 31 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	93	Total	C	N	O	S	0	0
			780	508	136	132	4		

- Molecule 32 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	o	140	Total	C	N	O	S	0	0
			1116	702	221	185	8		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	60	Total	C	N	O	S	0	0
			480	303	98	78	1		

- Molecule 34 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	173	Total	C	N	O	S	0	0
			1358	862	259	234	3		

- Molecule 35 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	2022	Total	C	N	O	P	0	0
			43106	19268	7710	14111	2017		

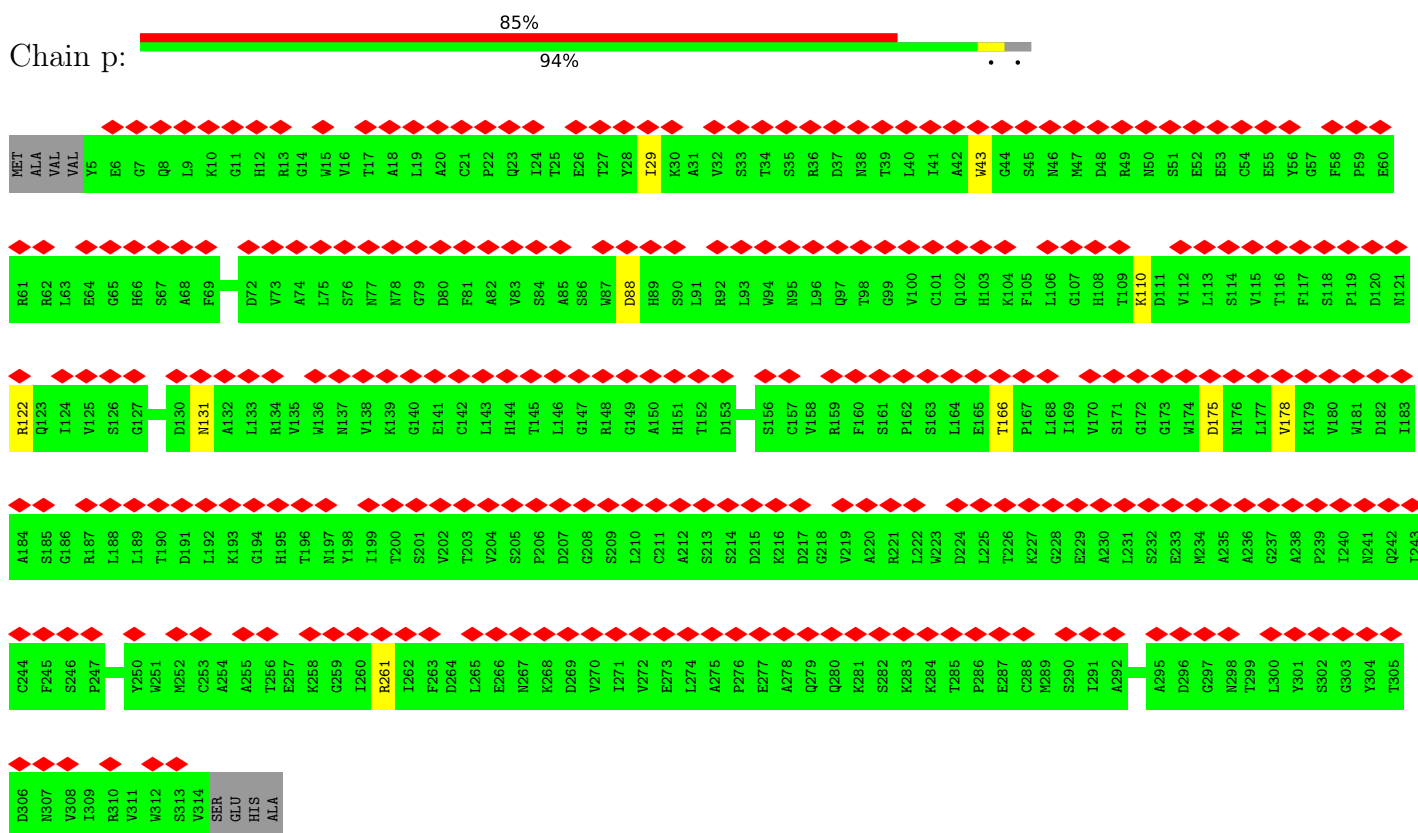
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	143	C	A	conflict	GB 320364483
E	805	C	U	conflict	GB 320364483
E	2316	U	-	insertion	GB 320364483
E	2317	U	-	insertion	GB 320364483
E	2318	U	-	insertion	GB 320364483

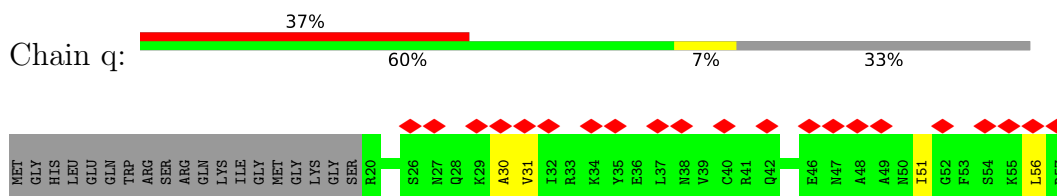
3 Residue-property plots

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: Activated protein kinase C receptor, putative

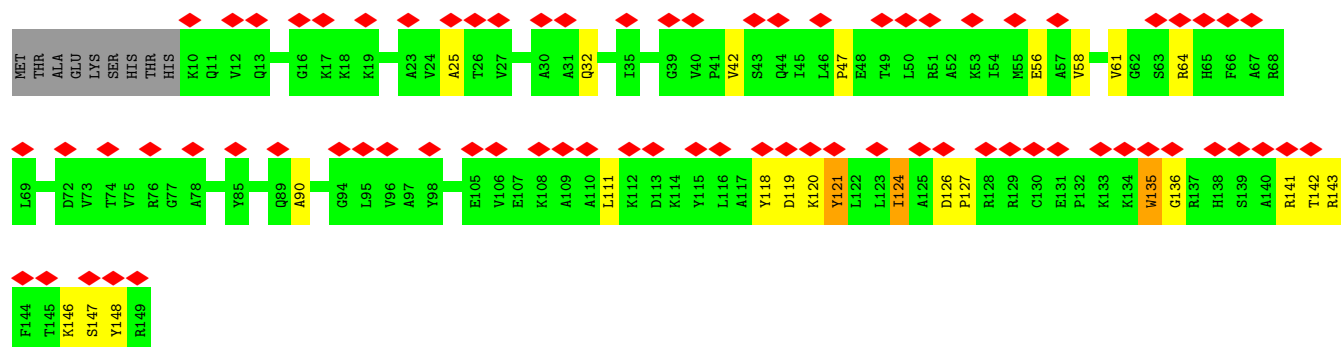


- Molecule 2: Ribosomal protein S29, putative

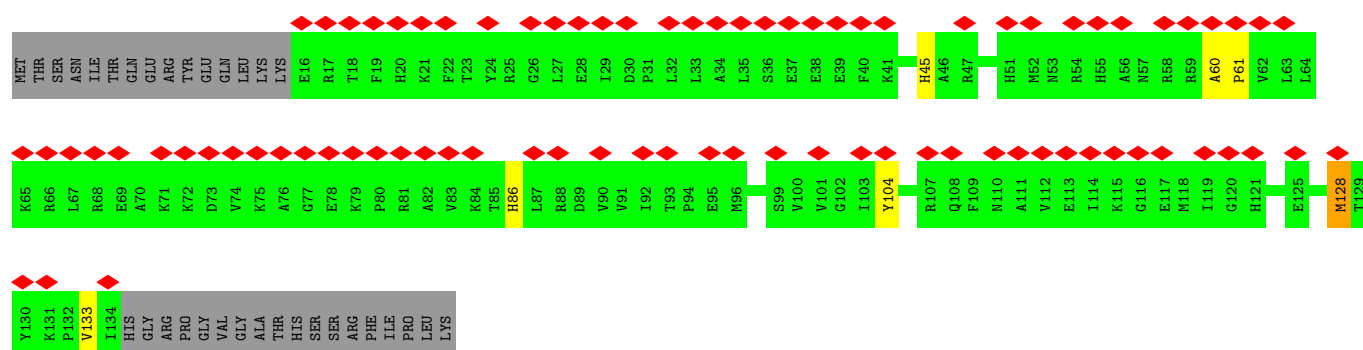


- Molecule 3: 40S ribosomal protein S16, putative

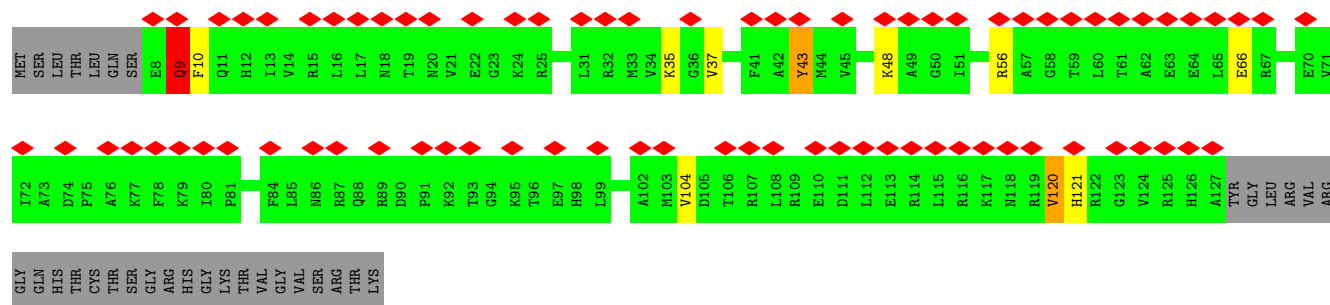




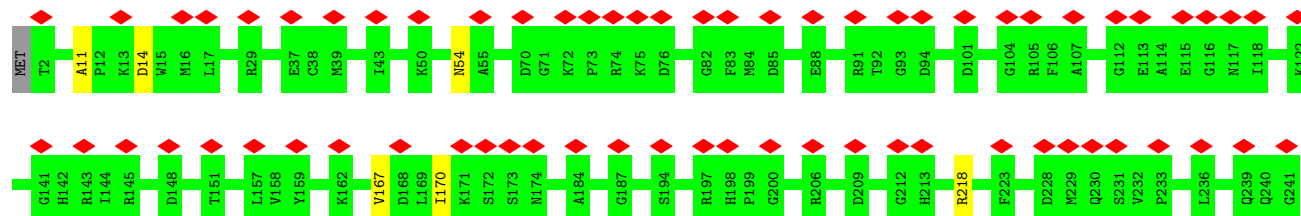
• Molecule 4: 40S ribosomal protein S15, putative

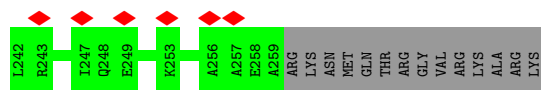


• Molecule 5: 40S ribosomal protein S18, putative

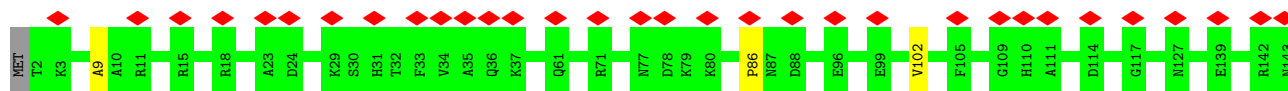


• Molecule 6: 40S ribosomal protein S4

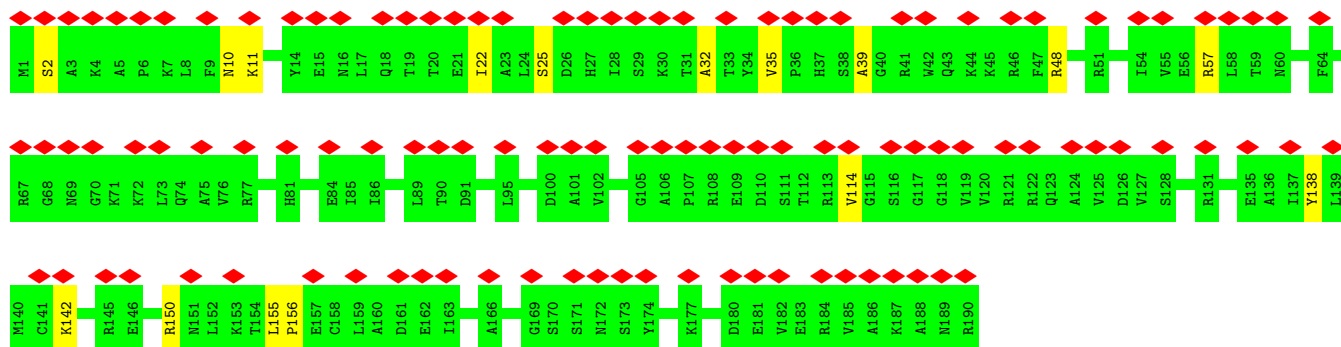
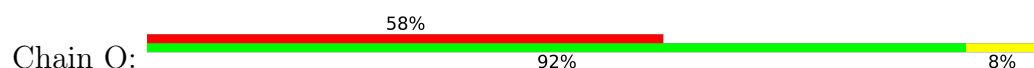




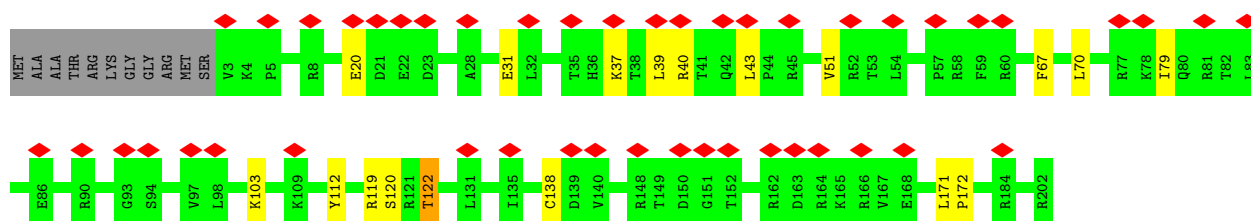
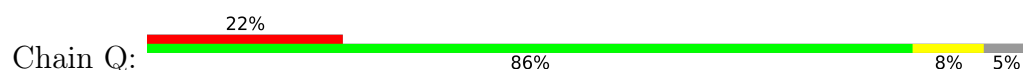
- Molecule 7: 40S ribosomal protein S23, putative



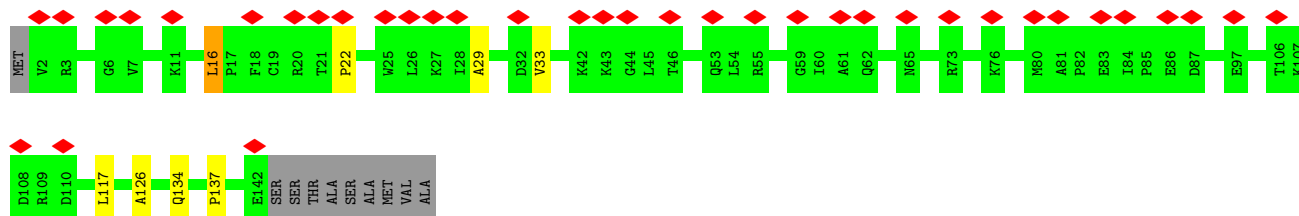
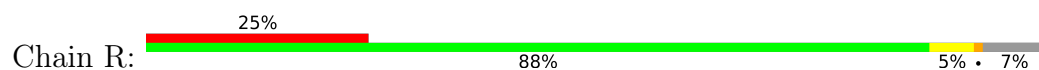
- Molecule 8: 40S ribosomal protein S5, putative



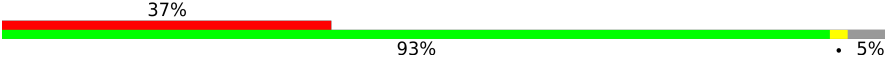
- Molecule 9: Ribosomal protein S7, putative

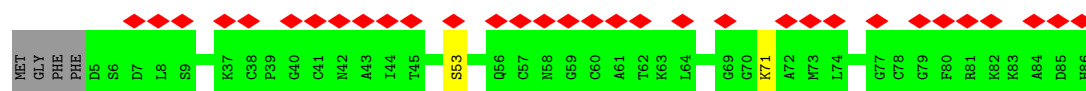


- Molecule 10: 40S ribosomal protein S13, putative



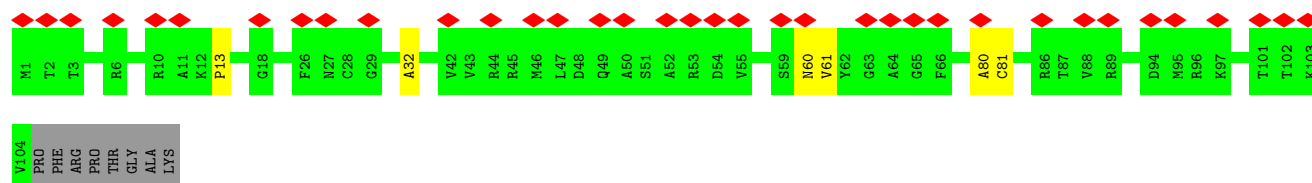
- Molecule 11: 40S ribosomal protein S27, putative

Chain S: 



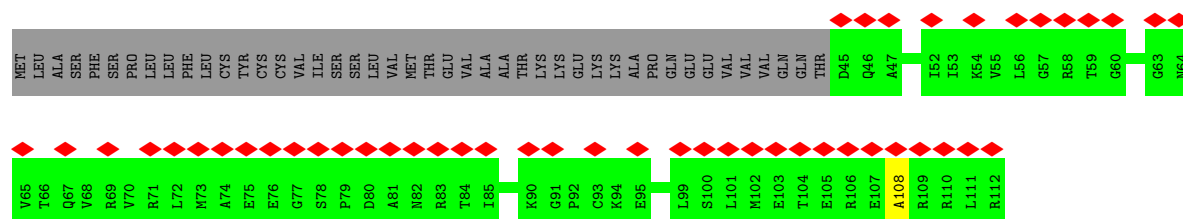
- Molecule 12: 40S ribosomal protein S26

Chain T: 

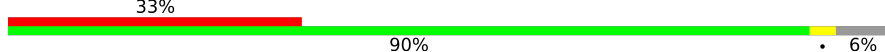


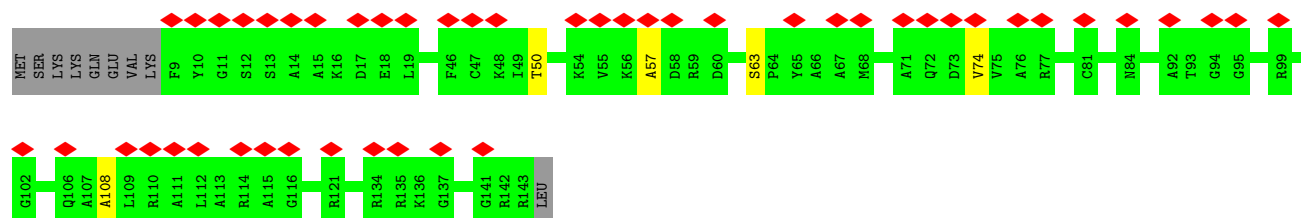
- Molecule 13: 40S ribosomal protein S33, putative

Chain U: 



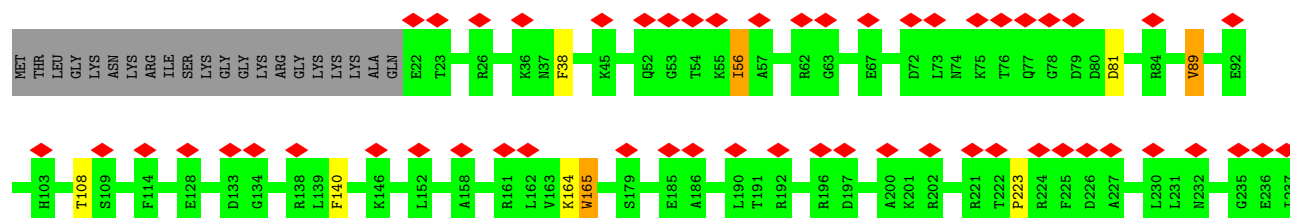
- Molecule 14: 40S ribosomal protein S14, putative

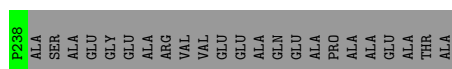
Chain V: 



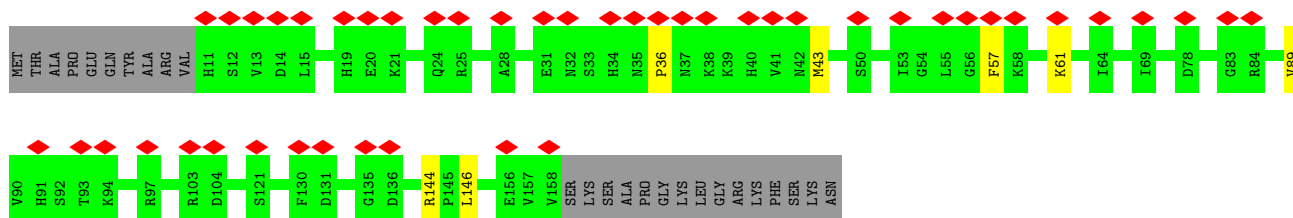
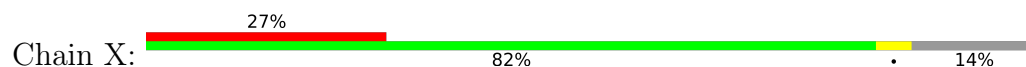
- Molecule 15: 40S ribosomal protein S3a-2

Chain W: 

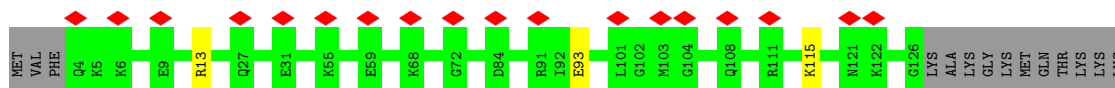
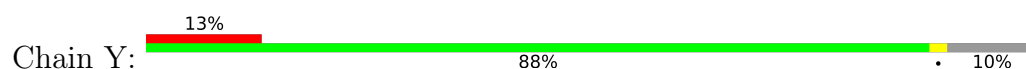




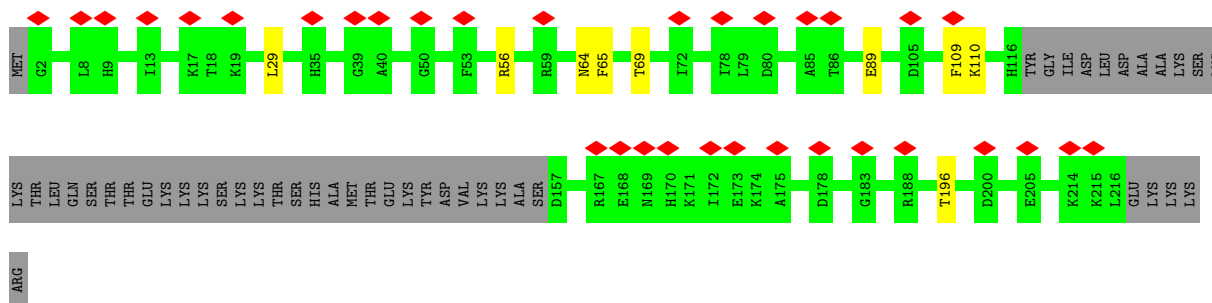
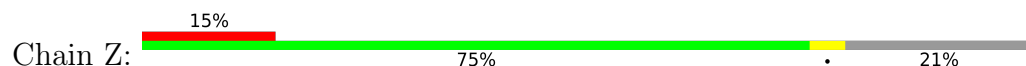
- Molecule 16: 40S ribosomal protein S11, putative



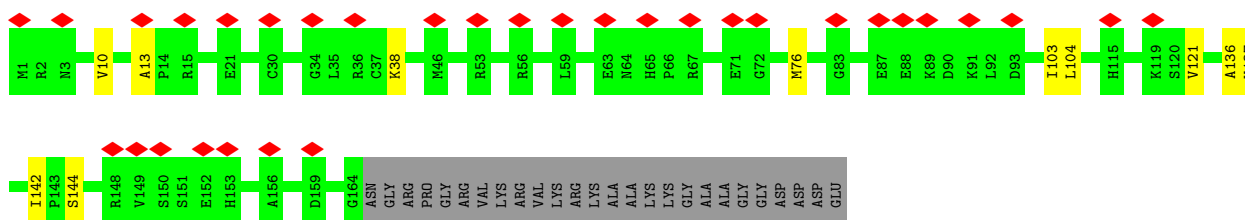
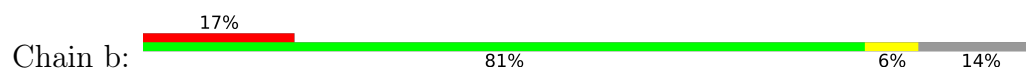
- Molecule 17: 40S ribosomal protein S24



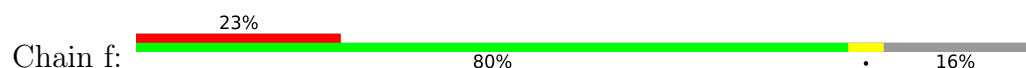
- Molecule 18: 40S ribosomal protein S8

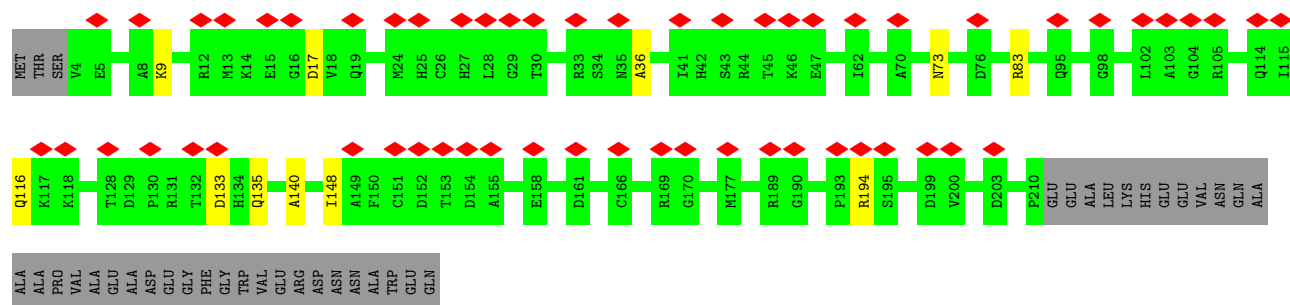


- Molecule 19: 40S ribosomal protein S9, putative

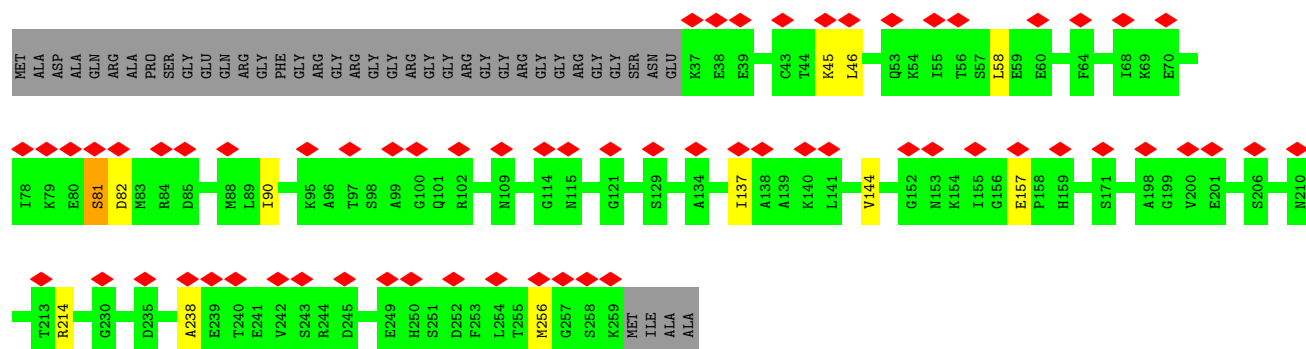
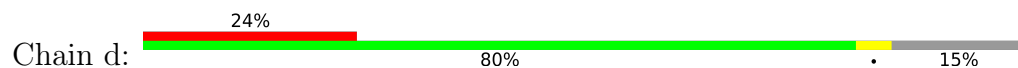


- Molecule 20: 40S ribosomal protein SA

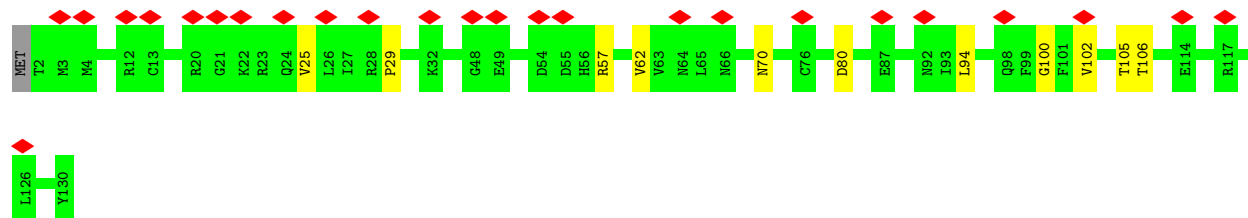
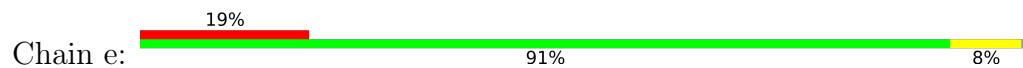




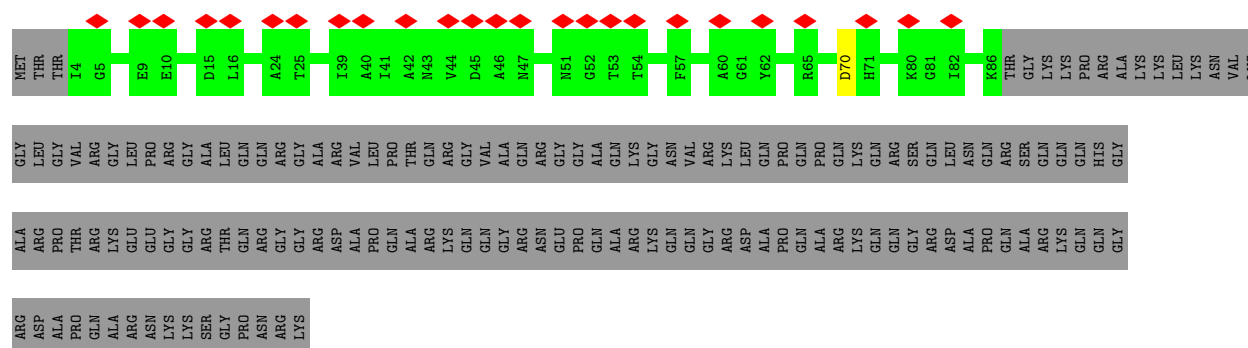
- Molecule 21: 40S ribosomal protein S2, putative



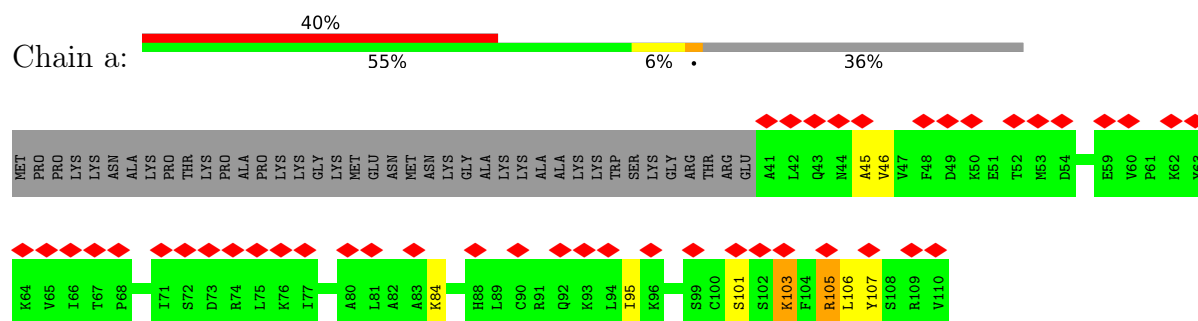
- Molecule 22: 40S ribosomal protein S15a, putative



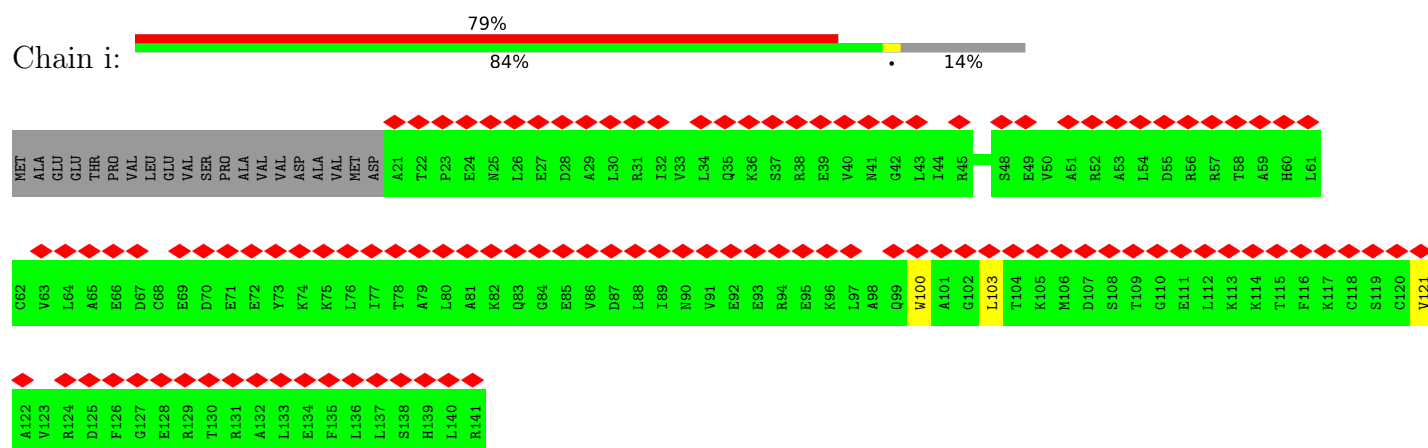
- Molecule 23: 40S ribosomal protein S21, putative



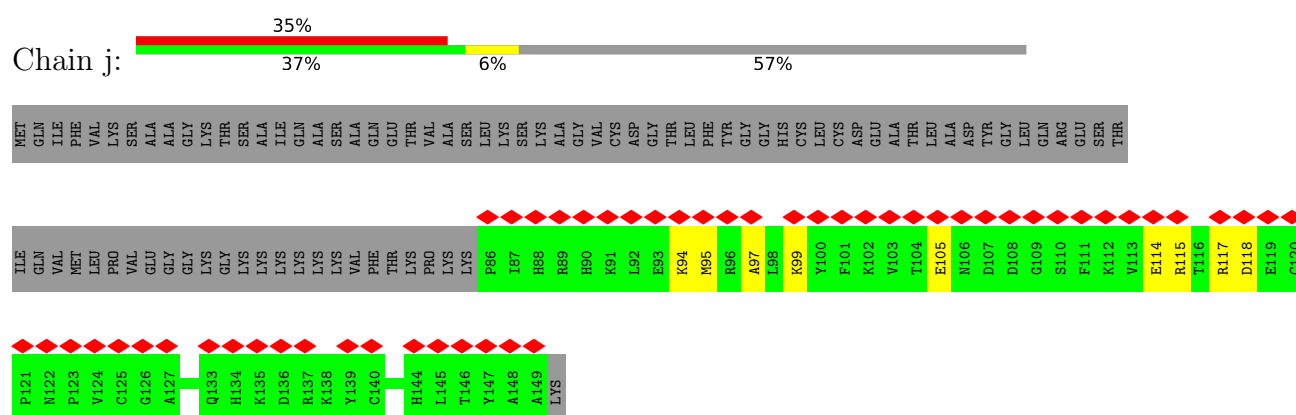
- Molecule 24: Ribosomal protein S25, putative



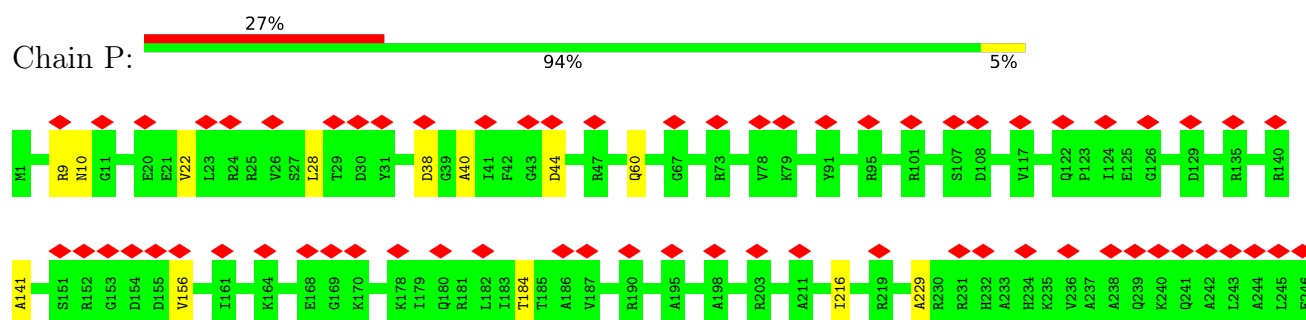
- Molecule 25: 40S ribosomal protein S12

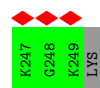


- Molecule 26: Ubiquitin/ribosomal protein S27a, putative

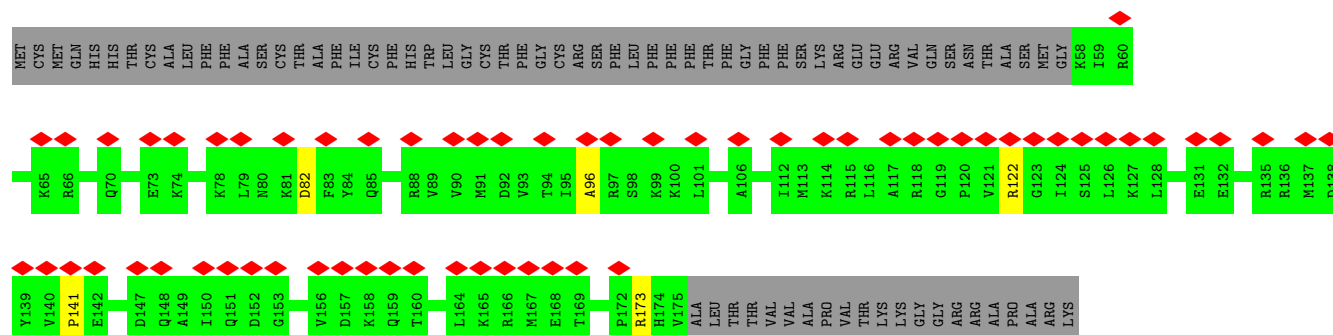


- Molecule 27: 40S ribosomal protein S6

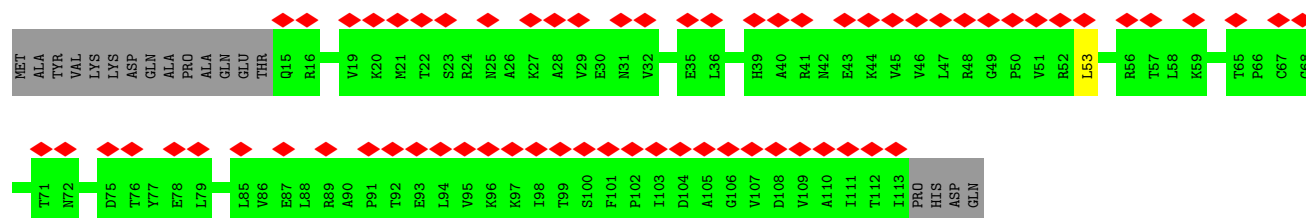
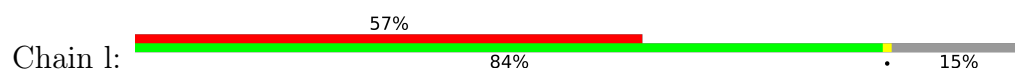




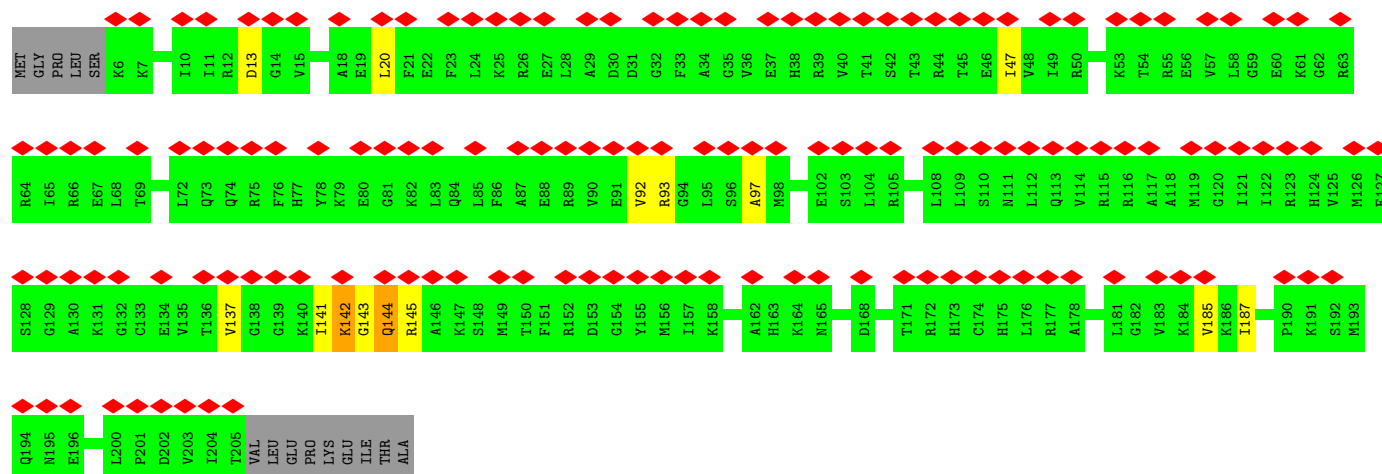
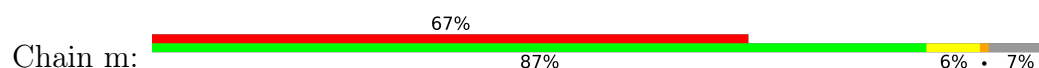
- Molecule 28: 40S ribosomal protein S17, putative



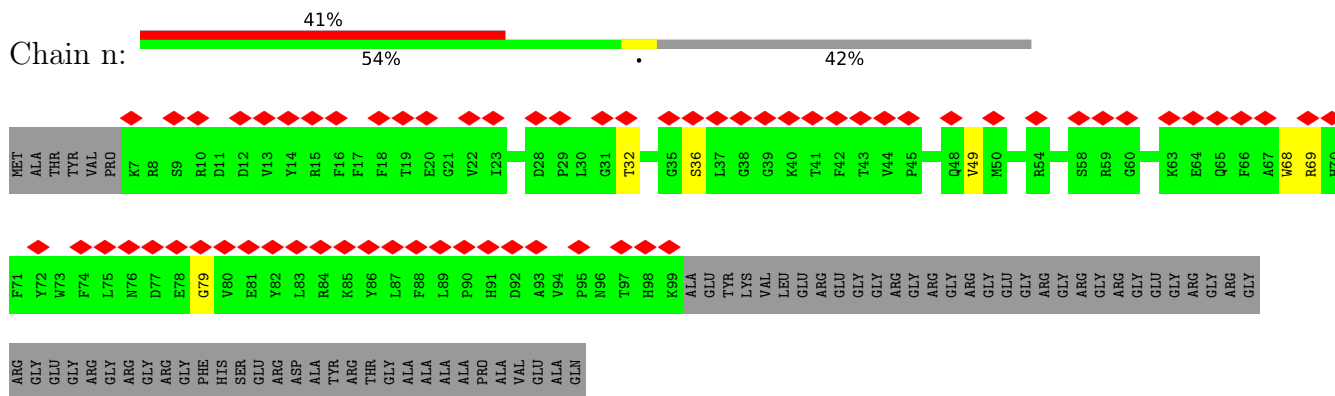
- Molecule 29: Ribosomal protein S20, putative



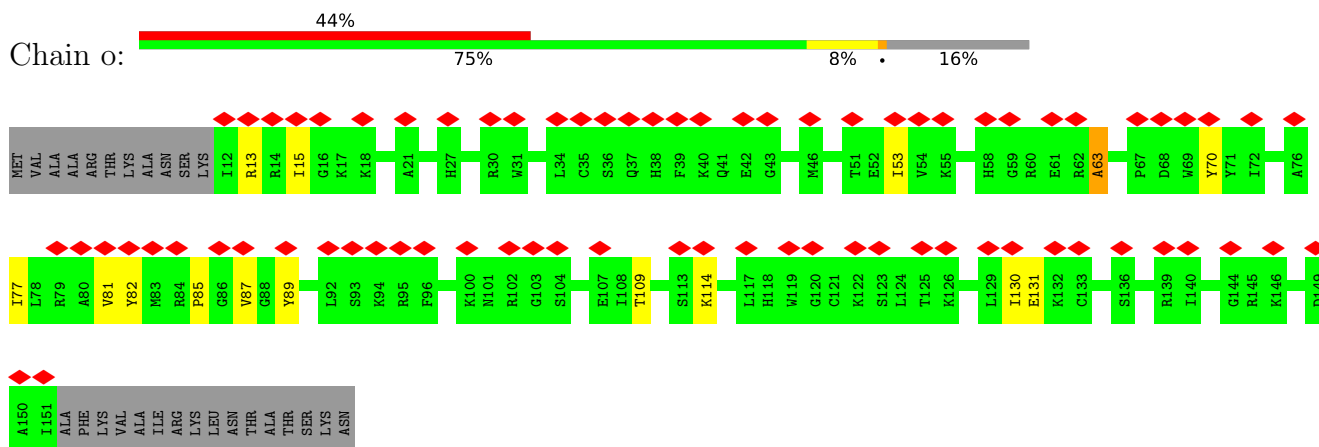
- Molecule 30: 40S ribosomal protein S3, putative



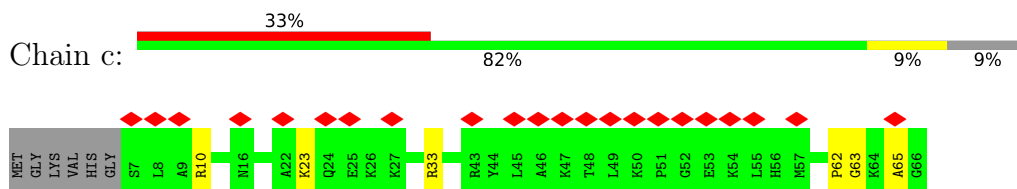
- Molecule 31: 40S ribosomal protein S10, putative



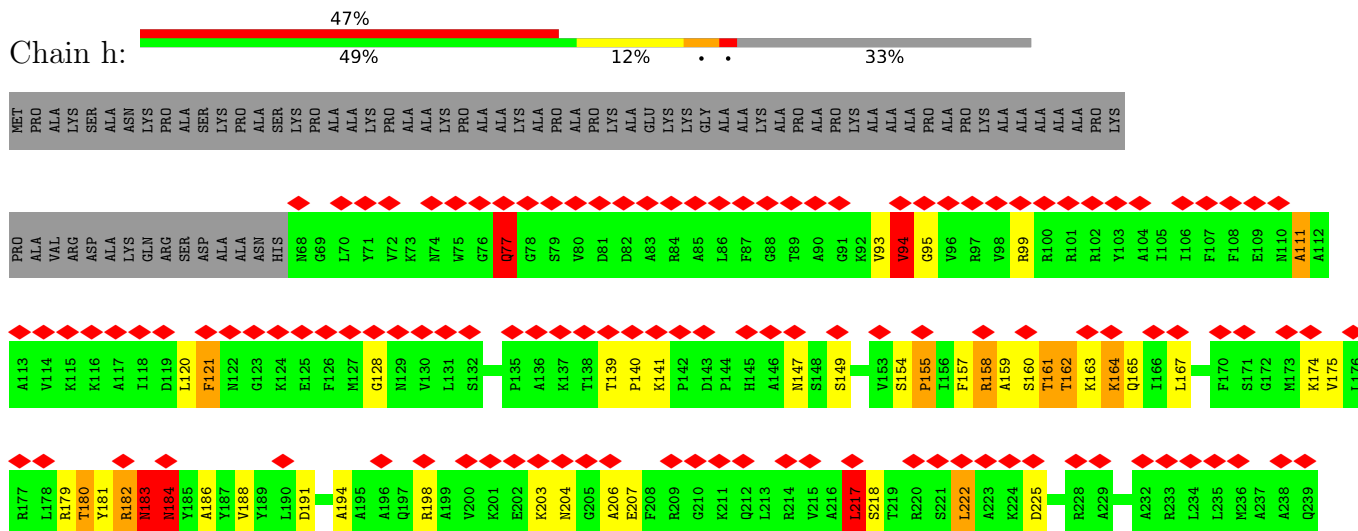
- Molecule 32: Ribosomal protein S19, putative



- Molecule 33: 40S ribosomal protein S30

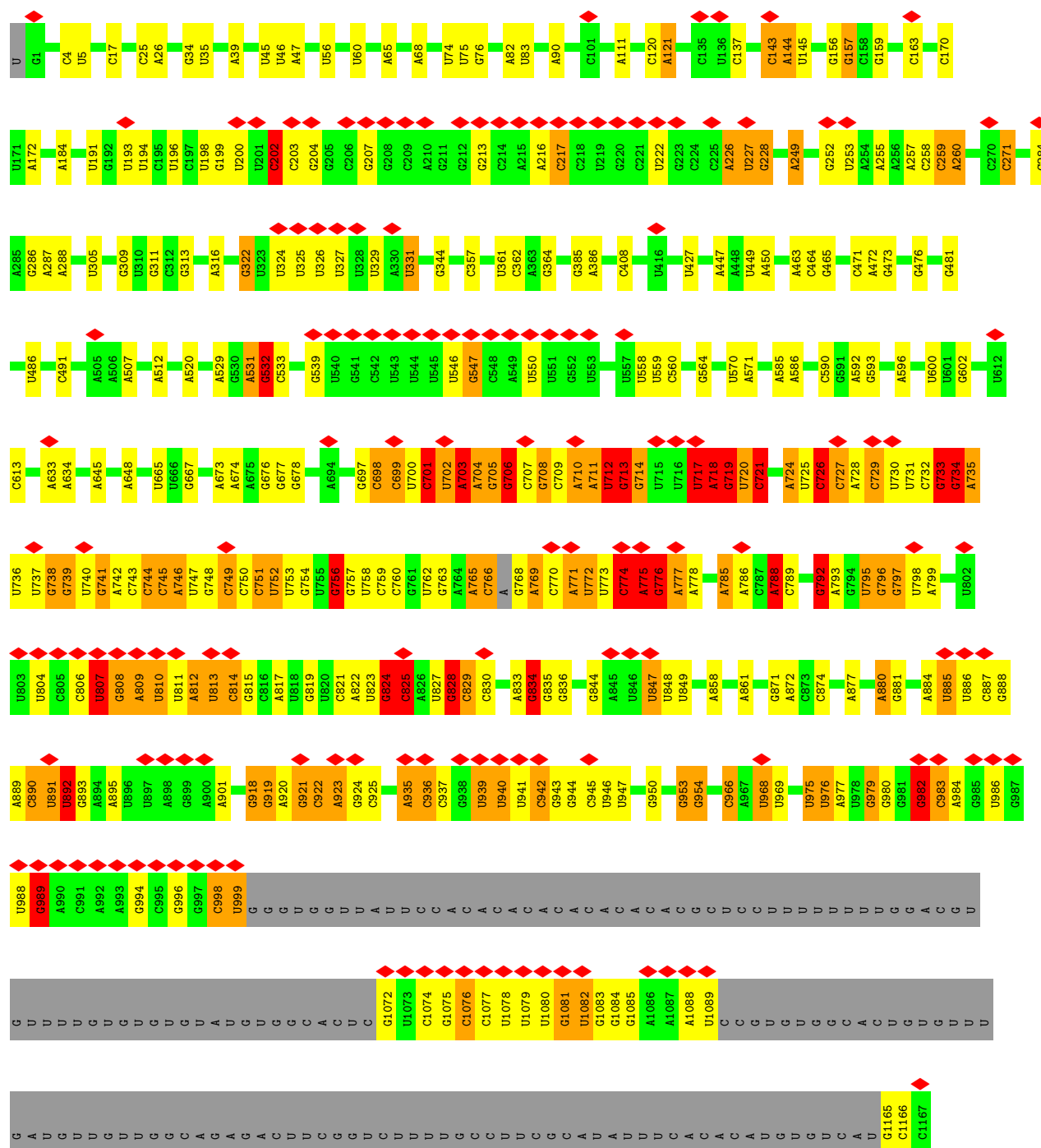


- Molecule 34: RNA-binding protein, putative





• Molecule 35: 18S rRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0549	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	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	p	1.23	0/2461	1.35	3/3347 (0.1%)
2	q	1.36	0/314	1.45	2/416 (0.5%)
3	r	1.29	0/1131	1.63	14/1520 (0.9%)
4	t	1.29	0/988	1.57	2/1325 (0.2%)
5	u	1.32	0/996	1.65	10/1334 (0.7%)
6	L	1.29	0/2073	1.41	8/2787 (0.3%)
7	M	1.27	0/1137	1.45	3/1520 (0.2%)
8	O	1.26	0/1515	1.59	8/2034 (0.4%)
9	Q	1.33	0/1703	1.57	17/2290 (0.7%)
10	R	1.28	0/1164	1.64	11/1559 (0.7%)
11	S	1.28	0/641	1.43	0/858
12	T	1.40	0/845	1.54	10/1129 (0.9%)
13	U	1.43	0/527	1.32	0/702
14	V	1.31	0/1026	1.51	8/1376 (0.6%)
15	W	1.30	0/1809	1.47	10/2437 (0.4%)
16	X	1.31	0/1238	1.39	7/1662 (0.4%)
17	Y	1.28	0/1004	1.48	5/1335 (0.4%)
18	Z	1.36	0/1424	1.45	7/1904 (0.4%)
19	b	1.31	0/1394	1.60	13/1874 (0.7%)
20	f	1.24	0/1693	1.56	15/2290 (0.7%)
21	d	1.22	0/1760	1.57	18/2376 (0.8%)
22	e	1.27	0/1037	1.54	5/1391 (0.4%)
23	g	1.23	0/644	1.42	2/875 (0.2%)
24	a	1.18	0/559	1.58	2/748 (0.3%)
25	i	1.24	0/966	1.43	2/1295 (0.2%)
26	j	1.28	0/530	1.47	3/707 (0.4%)
27	P	1.35	0/2008	1.51	18/2678 (0.7%)
28	k	1.27	0/985	1.55	3/1313 (0.2%)
29	l	1.28	0/794	1.42	2/1076 (0.2%)
30	m	1.32	0/1606	1.57	13/2141 (0.6%)
31	n	1.20	0/804	1.60	5/1082 (0.5%)
32	o	1.27	0/1140	1.65	13/1524 (0.9%)
33	c	1.23	0/488	1.55	5/644 (0.8%)
34	h	1.30	0/1381	1.67	23/1857 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	E	0.91	1/48215 (0.0%)	1.13	169/75140 (0.2%)
All	All	1.10	1/88000 (0.0%)	1.31	436/128546 (0.3%)

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
1	p	0	3
3	r	0	7
4	t	0	2
5	u	0	4
8	O	0	3
9	Q	0	3
15	W	0	1
18	Z	0	1
22	e	0	1
24	a	0	2
26	j	0	1
27	P	0	2
28	k	0	1
30	m	0	2
32	o	0	2
33	c	0	2
34	h	0	22
35	E	4	121
All	All	4	180

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	734	G	N9-C4	-5.42	1.27	1.38

All (436) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	774	C	P-O3'-C3'	29.99	165.19	120.20
35	E	1187	C	P-O3'-C3'	26.78	160.37	120.20
35	E	703	A	P-O3'-C3'	18.68	148.22	120.20
35	E	975	U	O3'-P-O5'	18.32	131.48	104.00
35	E	531	A	P-O3'-C3'	17.55	146.52	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	1904	U	P-O3'-C3'	16.96	145.65	120.20
35	E	807	U	P-O3'-C3'	16.31	144.67	120.20
35	E	769	A	P-O3'-C3'	15.69	143.74	120.20
35	E	998	C	P-O3'-C3'	14.65	142.18	120.20
35	E	1546	C	P-O3'-C3'	14.53	141.99	120.20
35	E	1191	G	P-O3'-C3'	14.52	141.98	120.20
35	E	2048	A	P-O3'-C3'	14.39	141.78	120.20
35	E	2049	C	P-O3'-C3'	13.38	140.26	120.20
35	E	1188	C	P-O5'-C5'	13.36	140.94	120.90
35	E	939	U	P-O3'-C3'	13.12	139.87	120.20
35	E	756	G	P-O3'-C3'	12.78	139.37	120.20
35	E	808	G	P-O3'-C3'	12.67	139.21	120.20
35	E	227	U	P-O3'-C3'	12.52	138.97	120.20
35	E	701	C	P-O3'-C3'	12.21	138.51	120.20
35	E	706	G	P-O5'-C5'	12.07	139.00	120.90
35	E	918	G	P-O3'-C3'	11.92	138.08	120.20
35	E	810	U	P-O3'-C3'	11.76	137.83	120.20
35	E	697	G	P-O3'-C3'	11.34	137.21	120.20
35	E	795	U	P-O3'-C3'	11.31	137.17	120.20
35	E	890	C	P-O3'-C3'	11.24	137.05	120.20
35	E	765	A	P-O3'-C3'	11.14	136.91	120.20
35	E	727	C	P-O3'-C3'	11.08	136.82	120.20
35	E	705	G	P-O3'-C3'	10.89	136.54	120.20
35	E	942	C	P-O3'-C3'	10.69	136.24	120.20
35	E	777	A	P-O3'-C3'	10.58	136.07	120.20
35	E	813	U	P-O3'-C3'	10.57	136.05	120.20
35	E	1903	A	P-O3'-C3'	10.44	135.86	120.20
35	E	775	A	P-O5'-C5'	10.25	136.28	120.90
35	E	2217	G	P-O3'-C3'	10.18	135.47	120.20
35	E	892	U	P-O3'-C3'	10.05	135.27	120.20
35	E	1191	G	C2'-C3'-O3'	9.99	124.49	109.50
35	E	702	U	P-O3'-C3'	9.85	134.97	120.20
35	E	1082	U	P-O3'-C3'	9.83	134.94	120.20
35	E	202	C	P-O3'-C3'	9.76	134.84	120.20
35	E	2234	A	P-O3'-C3'	9.67	134.70	120.20
35	E	814	C	P-O3'-C3'	9.67	134.70	120.20
35	E	935	A	P-O3'-C3'	9.62	134.62	120.20
35	E	2012	C	P-O5'-C5'	9.55	135.23	120.90
35	E	1192	A	P-O3'-C3'	9.55	134.52	120.20
35	E	1913	U	P-O3'-C3'	9.40	134.30	120.20
35	E	891	U	P-O3'-C3'	9.28	134.12	120.20
35	E	698	C	P-O3'-C3'	9.26	134.08	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	1902	G	P-O3'-C3'	9.24	134.06	120.20
35	E	829	C	P-O3'-C3'	9.05	133.78	120.20
35	E	729	C	P-O3'-C3'	9.01	133.71	120.20
35	E	976	U	O5'-P-OP2	-8.92	81.23	108.00
35	E	885	U	P-O3'-C3'	8.91	133.57	120.20
35	E	942	C	C2'-C3'-O3'	8.90	122.85	109.50
35	E	975	U	OP2-P-O3'	-8.90	81.31	108.00
35	E	1076	C	P-O3'-C3'	8.90	133.54	120.20
35	E	2227	U	P-O3'-C3'	8.89	133.53	120.20
35	E	532	G	P-O3'-C3'	8.88	133.52	120.20
35	E	976	U	O5'-P-OP1	-8.85	81.44	108.00
35	E	1081	G	P-O3'-C3'	8.85	133.48	120.20
35	E	719	G	P-O3'-C3'	8.81	133.42	120.20
35	E	968	U	P-O3'-C3'	8.80	133.40	120.20
35	E	2213	G	P-O3'-C3'	8.71	133.27	120.20
35	E	709	C	P-O3'-C3'	8.67	133.20	120.20
35	E	940	U	P-O3'-C3'	8.62	133.14	120.20
5	u	37	VAL	CA-C-N	8.53	129.63	119.99
5	u	37	VAL	C-N-CA	8.53	129.63	119.99
35	E	975	U	OP1-P-O3'	-8.43	82.72	108.00
35	E	795	U	C2'-C3'-O3'	8.39	122.08	109.50
35	E	1082	U	P-O5'-C5'	8.38	133.47	120.90
35	E	217	C	C5'-C4'-C3'	8.37	128.56	116.00
30	m	143	GLY	CA-C-N	8.35	136.72	121.70
30	m	143	GLY	C-N-CA	8.35	136.72	121.70
35	E	788	A	P-O3'-C3'	8.33	132.70	120.20
35	E	2051	C	P-O3'-C3'	8.25	132.58	120.20
3	r	135	TRP	CA-C-N	8.24	136.53	121.70
3	r	135	TRP	C-N-CA	8.24	136.53	121.70
35	E	1886	G	P-O3'-C3'	8.21	132.51	120.20
35	E	1186	U	P-O3'-C3'	8.11	132.36	120.20
27	P	10	ASN	N-CA-C	-8.09	105.40	114.62
35	E	711	A	O3'-P-O5'	-8.09	91.87	104.00
35	E	712	U	P-O3'-C3'	8.02	132.24	120.20
35	E	2017	G	P-O3'-C3'	8.02	132.22	120.20
35	E	1187	C	O3'-P-O5'	8.00	116.00	104.00
16	X	36	PRO	N-CA-C	-7.90	105.52	114.92
35	E	1880	U	C4'-C3'-C2'	-7.80	94.80	102.60
35	E	1545	U	P-O3'-C3'	7.80	131.90	120.20
35	E	1903	A	P-O5'-C5'	7.78	132.58	120.90
35	E	2152	C	P-O3'-C3'	7.70	131.76	120.20
35	E	713	G	P-O3'-C3'	7.70	131.75	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	717	U	P-O3'-C3'	7.63	131.64	120.20
35	E	774	C	O3'-P-O5'	7.60	115.41	104.00
35	E	785	A	P-O3'-C3'	7.60	131.60	120.20
22	e	62	VAL	N-CA-C	-7.59	98.33	108.35
35	E	772	U	P-O3'-C3'	7.54	131.51	120.20
21	d	82	ASP	N-CA-C	-7.40	106.18	114.62
35	E	633	A	P-O3'-C3'	7.29	131.13	120.20
35	E	919	G	P-O3'-C3'	7.23	131.05	120.20
35	E	812	A	P-O3'-C3'	7.22	131.03	120.20
2	q	56	LEU	N-CA-C	-7.21	105.67	114.75
35	E	792	G	P-O3'-C3'	7.18	130.97	120.20
5	u	9	GLN	CA-C-N	7.05	134.39	121.70
5	u	9	GLN	C-N-CA	7.05	134.39	121.70
35	E	847	U	P-O3'-C3'	7.04	130.77	120.20
35	E	772	U	O4'-C1'-C2'	-7.01	98.79	105.80
35	E	785	A	C2'-C3'-O3'	6.98	119.98	109.50
8	O	35	VAL	N-CA-C	-6.97	103.48	109.19
35	E	2050	C	P-O3'-C3'	6.88	130.52	120.20
28	k	96	ALA	N-CA-C	-6.83	106.84	114.62
35	E	776	G	P-O5'-C5'	6.81	131.11	120.90
35	E	833	A	P-O3'-C3'	6.81	130.41	120.20
35	E	227	U	C2'-C3'-O3'	6.79	119.68	109.50
27	P	38	ASP	CA-C-N	6.78	127.62	120.03
27	P	38	ASP	C-N-CA	6.78	127.62	120.03
35	E	772	U	C4'-C3'-C2'	-6.77	95.83	102.60
8	O	22	ILE	N-CA-C	-6.76	106.64	113.47
35	E	935	A	C2'-C3'-O3'	6.76	119.64	109.50
35	E	1903	A	C5'-C4'-C3'	6.74	126.11	116.00
2	q	51	ILE	N-CA-C	-6.72	106.45	112.90
32	o	53	ILE	N-CA-C	-6.72	106.59	113.10
35	E	2011	A	P-O3'-C3'	6.70	130.25	120.20
4	t	133	VAL	N-CA-C	-6.70	99.51	108.35
32	o	85	PRO	CA-C-N	6.62	127.44	120.03
32	o	85	PRO	C-N-CA	6.62	127.44	120.03
34	h	149	SER	CA-C-N	6.56	133.51	121.70
34	h	149	SER	C-N-CA	6.56	133.51	121.70
32	o	114	LYS	CA-C-N	6.53	127.37	119.99
32	o	114	LYS	C-N-CA	6.53	127.37	119.99
8	O	142	LYS	CA-C-N	6.53	127.37	119.99
8	O	142	LYS	C-N-CA	6.53	127.37	119.99
35	E	923	A	P-O3'-C3'	6.47	129.90	120.20
35	E	989	G	C5'-C4'-C3'	-6.44	106.34	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	80	ALA	CA-C-N	6.42	129.72	120.79
12	T	80	ALA	C-N-CA	6.42	129.72	120.79
12	T	60	ASN	N-CA-C	-6.42	107.31	114.62
35	E	749	C	P-O3'-C3'	6.38	129.76	120.20
35	E	976	U	OP1-P-OP2	6.37	138.71	119.60
35	E	922	C	P-O3'-C3'	6.35	129.72	120.20
30	m	93	ARG	CA-C-N	6.34	127.13	120.03
30	m	93	ARG	C-N-CA	6.34	127.13	120.03
7	M	102	VAL	N-CA-C	-6.32	100.00	108.35
31	n	69	ARG	N-CA-C	-6.28	106.83	114.75
35	E	771	A	P-O3'-C3'	6.28	129.62	120.20
35	E	1904	U	C2'-C3'-O3'	6.21	118.82	109.50
35	E	547	G	C5'-C4'-C3'	6.21	125.31	116.00
34	h	99	ARG	CA-C-N	6.20	128.88	120.44
34	h	99	ARG	C-N-CA	6.20	128.88	120.44
35	E	751	C	O3'-P-O5'	6.19	113.28	104.00
35	E	1875	G	P-O3'-C3'	6.19	129.49	120.20
35	E	769	A	C2'-C3'-O3'	6.17	118.76	109.50
27	P	40	ALA	CA-C-N	6.17	129.23	120.53
27	P	40	ALA	C-N-CA	6.17	129.23	120.53
35	E	834	G	P-O3'-C3'	6.15	129.42	120.20
35	E	559	U	P-O3'-C3'	6.14	129.41	120.20
35	E	753	U	C4'-C3'-C2'	-6.14	96.46	102.60
35	E	982	G	P-O3'-C3'	6.14	129.41	120.20
35	E	772	U	C2'-C3'-O3'	6.09	118.63	109.50
35	E	2048	A	C2'-C3'-O3'	6.08	118.61	109.50
35	E	776	G	C2'-C3'-O3'	6.05	118.58	109.50
35	E	1872	G	C1'-C2'-O2'	-6.04	102.74	111.80
30	m	144	GLN	N-CA-CB	6.01	120.71	110.50
32	o	109	THR	CA-C-N	6.00	128.64	120.77
32	o	109	THR	C-N-CA	6.00	128.64	120.77
35	E	921	G	P-O3'-C3'	5.99	129.19	120.20
35	E	998	C	C2'-C3'-O3'	5.99	118.48	109.50
35	E	810	U	C2'-C3'-O3'	5.97	122.66	113.70
35	E	324	U	C2'-C3'-O3'	5.95	118.43	109.50
22	e	106	THR	N-CA-C	-5.95	100.09	108.96
21	d	144	VAL	N-CA-C	-5.94	104.32	109.19
6	L	14	ASP	N-CA-C	-5.94	106.04	113.28
20	f	73	ASN	CA-C-N	5.92	126.34	119.47
20	f	73	ASN	C-N-CA	5.92	126.34	119.47
35	E	752	U	O5'-C5'-C4'	5.92	120.38	111.50
35	E	706	G	O4'-C1'-C2'	-5.91	101.69	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	e	80	ASP	CA-CB-CG	-5.88	106.72	112.60
22	e	70	ASN	N-CA-C	-5.88	107.92	114.62
10	R	126	ALA	CA-C-N	5.87	128.46	120.54
10	R	126	ALA	C-N-CA	5.87	128.46	120.54
34	h	222	LEU	CA-C-N	5.87	132.26	121.70
34	h	222	LEU	C-N-CA	5.87	132.26	121.70
35	E	705	G	O3'-P-O5'	5.87	112.80	104.00
35	E	828	G	P-O3'-C3'	5.87	129.00	120.20
35	E	1832	A	P-O3'-C3'	5.86	128.99	120.20
35	E	1887	U	C5'-C4'-C3'	-5.86	107.22	116.00
35	E	1187	C	C4'-C3'-C2'	-5.85	96.75	102.60
18	Z	65	PHE	CA-CB-CG	-5.84	107.96	113.80
19	b	10	VAL	N-CA-C	-5.83	107.45	113.10
16	X	57	PHE	CA-CB-CG	-5.81	107.99	113.80
22	e	105	THR	N-CA-C	-5.79	100.75	109.95
18	Z	110	LYS	CA-C-N	5.78	128.34	120.54
18	Z	110	LYS	C-N-CA	5.78	128.34	120.54
3	r	58	VAL	CA-C-N	5.78	129.49	120.82
3	r	58	VAL	C-N-CA	5.78	129.49	120.82
3	r	47	PRO	CA-C-N	5.78	128.29	120.38
3	r	47	PRO	C-N-CA	5.78	128.29	120.38
35	E	1686	G	P-O5'-C5'	-5.78	112.24	120.90
35	E	788	A	C2'-C3'-O3'	5.77	118.16	109.50
34	h	225	ASP	N-CA-C	5.77	118.31	111.33
15	W	140	PHE	CA-CB-CG	-5.72	108.08	113.80
16	X	146	LEU	N-CA-C	-5.72	107.54	114.75
20	f	133	ASP	CA-C-N	5.71	128.21	120.38
20	f	133	ASP	C-N-CA	5.71	128.21	120.38
3	r	64	ARG	N-CA-C	-5.70	104.56	112.03
35	E	1880	U	P-O3'-C3'	5.70	128.74	120.20
27	P	28	LEU	N-CA-C	-5.68	107.35	114.56
14	V	63	SER	CA-C-N	5.68	125.14	119.24
14	V	63	SER	C-N-CA	5.68	125.14	119.24
34	h	167	LEU	CA-C-N	5.67	128.19	120.54
34	h	167	LEU	C-N-CA	5.67	128.19	120.54
21	d	256	MET	CA-C-N	5.67	126.23	119.94
21	d	256	MET	C-N-CA	5.67	126.23	119.94
27	P	156	VAL	N-CA-C	-5.66	107.22	112.43
15	W	56	ILE	CA-C-N	5.66	128.13	120.38
15	W	56	ILE	C-N-CA	5.66	128.13	120.38
19	b	104	LEU	CA-C-N	5.65	128.63	120.38
19	b	104	LEU	C-N-CA	5.65	128.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	f	194	ARG	CA-C-N	5.64	128.30	120.29
20	f	194	ARG	C-N-CA	5.64	128.30	120.29
35	E	1188	C	P-O3'-C3'	5.63	128.65	120.20
21	d	90	ILE	N-CA-C	-5.62	99.97	108.17
34	h	184	ASN	N-CA-C	-5.62	98.84	110.80
30	m	97	ALA	CA-C-N	5.61	128.57	120.38
30	m	97	ALA	C-N-CA	5.61	128.57	120.38
35	E	726	C	P-O3'-C3'	5.61	128.61	120.20
9	Q	79	ILE	CA-C-N	5.58	128.07	120.54
9	Q	79	ILE	C-N-CA	5.58	128.07	120.54
35	E	797	G	P-O3'-C3'	5.58	128.57	120.20
14	V	50	THR	CA-C-N	5.58	126.29	119.99
14	V	50	THR	C-N-CA	5.58	126.29	119.99
35	E	1201	G	C5'-C4'-C3'	5.56	124.34	116.00
8	O	32	ALA	N-CA-C	-5.55	107.75	114.75
35	E	324	U	C4'-C3'-O3'	5.53	117.70	109.40
30	m	142	LYS	N-CA-C	-5.53	99.02	110.80
10	R	137	PRO	N-CA-C	-5.52	108.36	114.92
35	E	766	C	O4'-C1'-N1	5.51	116.47	108.20
35	E	834	G	P-O5'-C5'	5.51	129.17	120.90
35	E	1177	C	O5'-C5'-C4'	5.51	119.97	111.70
25	i	100	TRP	CA-C-N	5.51	127.93	120.38
25	i	100	TRP	C-N-CA	5.51	127.93	120.38
35	E	891	U	C2'-C3'-O3'	5.50	117.76	109.50
21	d	46	LEU	CA-C-N	5.49	126.20	119.99
21	d	46	LEU	C-N-CA	5.49	126.20	119.99
19	b	38	LYS	CA-C-N	5.49	127.90	120.38
19	b	38	LYS	C-N-CA	5.49	127.90	120.38
31	n	49	VAL	CA-C-N	5.48	127.94	120.54
31	n	49	VAL	C-N-CA	5.48	127.94	120.54
35	E	699	C	O3'-P-O5'	5.47	112.21	104.00
24	a	84	LYS	CA-C-N	5.47	126.15	120.03
24	a	84	LYS	C-N-CA	5.47	126.15	120.03
35	E	702	U	O4'-C1'-N1	5.47	116.40	108.20
6	L	218	ARG	CA-C-N	5.47	127.92	120.54
6	L	218	ARG	C-N-CA	5.47	127.92	120.54
19	b	76	MET	CA-C-N	5.46	127.87	120.38
19	b	76	MET	C-N-CA	5.46	127.87	120.38
33	c	10	ARG	N-CA-C	-5.46	105.56	113.21
9	Q	120	SER	N-CA-C	-5.46	106.98	113.97
19	b	13	ALA	CA-C-N	5.46	125.46	119.89
19	b	13	ALA	C-N-CA	5.46	125.46	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	43	LEU	CA-C-N	5.45	125.12	119.56
9	Q	43	LEU	C-N-CA	5.45	125.12	119.56
21	d	214	ARG	CA-C-N	5.44	126.14	119.99
21	d	214	ARG	C-N-CA	5.44	126.14	119.99
35	E	1546	C	P-O5'-C5'	5.44	129.06	120.90
35	E	2213	G	C2'-C3'-O3'	5.44	121.86	113.70
12	T	13	PRO	CA-C-N	5.43	125.42	119.89
12	T	13	PRO	C-N-CA	5.43	125.42	119.89
1	p	178	VAL	N-CA-C	-5.42	99.75	107.77
35	E	774	C	C2'-C3'-O3'	5.42	117.62	109.50
8	O	156	PRO	CA-C-N	5.41	127.79	120.38
8	O	156	PRO	C-N-CA	5.41	127.79	120.38
27	P	229	ALA	CA-C-N	5.40	127.83	120.54
27	P	229	ALA	C-N-CA	5.40	127.83	120.54
20	f	148	ILE	N-CA-C	-5.40	100.46	108.45
27	P	141	ALA	CA-C-N	5.40	128.06	120.28
27	P	141	ALA	C-N-CA	5.40	128.06	120.28
12	T	61	VAL	N-CA-C	-5.39	107.47	112.43
34	h	121	PHE	N-CA-CB	5.39	119.59	110.49
30	m	20	LEU	CA-C-N	5.39	127.50	120.28
30	m	20	LEU	C-N-CA	5.39	127.50	120.28
10	R	33	VAL	CA-C-N	5.38	127.82	120.77
10	R	33	VAL	C-N-CA	5.38	127.82	120.77
35	E	983	C	O4'-C1'-N1	5.38	116.57	108.50
35	E	996	G	P-O3'-C3'	-5.38	112.13	120.20
18	Z	109	PHE	CA-CB-CG	-5.36	108.44	113.80
1	p	166	THR	N-CA-C	-5.36	100.82	109.40
33	c	63	GLY	CA-C-N	5.36	128.46	120.90
33	c	63	GLY	C-N-CA	5.36	128.46	120.90
34	h	184	ASN	N-CA-CB	5.34	119.52	110.49
35	E	271	C	P-O5'-C5'	5.33	128.90	120.90
35	E	1075	G	C5'-C4'-C3'	5.33	124.00	116.00
8	O	48	ARG	N-CA-C	-5.32	104.73	113.50
34	h	140	PRO	N-CA-C	5.31	123.41	112.47
35	E	713	G	P-O5'-C5'	5.31	128.87	120.90
30	m	185	VAL	N-CA-C	-5.31	100.83	108.42
21	d	81	SER	N-CA-CB	5.29	119.43	110.49
35	E	1887	U	C3'-C2'-C1'	5.29	106.59	101.30
21	d	137	ILE	CA-C-N	5.29	127.62	120.38
21	d	137	ILE	C-N-CA	5.29	127.62	120.38
21	d	58	LEU	CA-C-N	5.28	127.66	120.54
21	d	58	LEU	C-N-CA	5.28	127.66	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	43	TYR	CA-C-N	5.28	127.61	120.38
5	u	43	TYR	C-N-CA	5.28	127.61	120.38
34	h	165	GLN	CA-C-N	5.27	127.67	120.77
34	h	165	GLN	C-N-CA	5.27	127.67	120.77
9	Q	40	ARG	N-CA-C	-5.26	105.84	113.21
34	h	77	GLN	N-CA-CB	5.26	119.38	110.49
9	Q	70	LEU	CA-C-N	5.25	127.32	120.28
9	Q	70	LEU	C-N-CA	5.25	127.32	120.28
35	E	771	A	C2'-C3'-O3'	5.25	117.38	109.50
7	M	9	ALA	CA-C-N	5.23	127.61	120.54
7	M	9	ALA	C-N-CA	5.23	127.61	120.54
20	f	17	ASP	CA-C-N	5.23	127.35	120.60
20	f	17	ASP	C-N-CA	5.23	127.35	120.60
32	o	82	TYR	N-CA-C	-5.23	108.66	114.62
34	h	164	LYS	N-CA-C	5.23	121.94	110.80
35	E	1877	U	C4'-C3'-C2'	5.23	107.83	102.60
35	E	1198	G	P-O3'-C3'	5.23	128.04	120.20
35	E	792	G	C5'-C4'-C3'	5.22	123.84	116.00
35	E	717	U	C2'-C3'-O3'	5.21	117.32	109.50
35	E	825	C	O5'-C5'-C4'	5.21	119.32	111.50
35	E	2052	C	C2'-C3'-O3'	5.21	117.31	109.50
3	r	111	LEU	CA-C-N	5.21	127.21	120.44
3	r	111	LEU	C-N-CA	5.21	127.21	120.44
3	r	118	TYR	CA-C-N	5.20	131.47	121.54
3	r	118	TYR	C-N-CA	5.20	131.47	121.54
34	h	141	LYS	N-CA-C	5.19	120.67	113.45
16	X	61	LYS	CA-C-N	5.19	127.55	120.54
16	X	61	LYS	C-N-CA	5.19	127.55	120.54
34	h	183	ASN	CA-CB-CG	5.19	117.79	112.60
14	V	74	VAL	CA-C-N	5.19	127.85	120.53
14	V	74	VAL	C-N-CA	5.19	127.85	120.53
20	f	135	GLN	CA-C-N	5.19	127.18	120.44
20	f	135	GLN	C-N-CA	5.19	127.18	120.44
29	l	53	LEU	CA-C-N	5.19	126.32	119.84
29	l	53	LEU	C-N-CA	5.19	126.32	119.84
15	W	165	TRP	CA-CB-CG	5.19	123.45	113.60
33	c	33	ARG	CA-C-N	5.18	127.48	120.38
33	c	33	ARG	C-N-CA	5.18	127.48	120.38
26	j	94	LYS	N-CA-C	-5.18	107.02	113.55
21	d	157	GLU	CA-C-N	5.18	125.47	119.93
21	d	157	GLU	C-N-CA	5.18	125.47	119.93
26	j	114	GLU	CA-C-N	5.18	131.43	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	j	114	GLU	C-N-CA	5.18	131.43	121.54
32	o	70	TYR	CA-C-N	5.18	127.53	120.54
32	o	70	TYR	C-N-CA	5.18	127.53	120.54
35	E	144	A	C2'-C3'-O3'	5.17	117.25	109.50
12	T	81	CYS	CA-C-N	5.17	127.97	120.79
12	T	81	CYS	C-N-CA	5.17	127.97	120.79
27	P	216	ILE	CA-C-N	5.16	125.67	119.94
27	P	216	ILE	C-N-CA	5.16	125.67	119.94
9	Q	172	PRO	CA-C-N	5.16	127.53	120.77
9	Q	172	PRO	C-N-CA	5.16	127.53	120.77
18	Z	89	GLU	CA-C-N	5.16	127.50	120.54
18	Z	89	GLU	C-N-CA	5.16	127.50	120.54
34	h	194	ALA	CA-C-N	5.16	127.91	120.38
34	h	194	ALA	C-N-CA	5.16	127.91	120.38
5	u	104	VAL	CA-C-N	5.16	127.44	120.38
5	u	104	VAL	C-N-CA	5.16	127.44	120.38
35	E	2234	A	C4'-C3'-C2'	-5.15	97.45	102.60
19	b	121	VAL	CA-C-N	5.15	127.43	120.38
19	b	121	VAL	C-N-CA	5.15	127.43	120.38
20	f	140	ALA	CA-C-N	5.14	127.43	120.38
20	f	140	ALA	C-N-CA	5.14	127.43	120.38
31	n	79	GLY	CA-C-N	5.14	127.04	120.56
31	n	79	GLY	C-N-CA	5.14	127.04	120.56
9	Q	31	GLU	CA-C-N	5.14	127.47	120.54
9	Q	31	GLU	C-N-CA	5.14	127.47	120.54
15	W	164	LYS	CA-C-N	5.13	127.88	120.38
15	W	164	LYS	C-N-CA	5.13	127.88	120.38
30	m	13	ASP	CA-C-N	5.13	125.79	119.99
30	m	13	ASP	C-N-CA	5.13	125.79	119.99
17	Y	115	LYS	CA-C-N	5.13	127.41	120.38
17	Y	115	LYS	C-N-CA	5.13	127.41	120.38
18	Z	196	THR	N-CA-C	-5.13	108.29	114.75
27	P	184	THR	CA-C-N	5.13	129.34	121.19
27	P	184	THR	C-N-CA	5.13	129.34	121.19
35	E	775	A	P-O3'-C3'	5.13	127.89	120.20
9	Q	20	GLU	CA-C-N	5.12	127.90	120.79
9	Q	20	GLU	C-N-CA	5.12	127.90	120.79
12	T	32	ALA	CA-C-N	5.11	125.11	119.90
12	T	32	ALA	C-N-CA	5.11	125.11	119.90
3	r	148	TYR	N-CA-C	5.10	116.84	111.28
5	u	66	GLU	CA-C-N	5.09	127.42	120.54
5	u	66	GLU	C-N-CA	5.09	127.42	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	54	ASN	CA-C-N	5.09	127.41	120.54
6	L	54	ASN	C-N-CA	5.09	127.41	120.54
10	R	117	LEU	CA-C-N	5.09	127.71	120.53
10	R	117	LEU	C-N-CA	5.09	127.71	120.53
15	W	89	VAL	N-CA-C	-5.09	102.32	108.53
19	b	103	ILE	CA-C-N	5.09	127.35	120.38
19	b	103	ILE	C-N-CA	5.09	127.35	120.38
35	E	834	G	O5'-C5'-C4'	5.09	119.13	111.50
32	o	131	GLU	CA-C-N	5.09	127.35	120.38
32	o	131	GLU	C-N-CA	5.09	127.35	120.38
16	X	144	ARG	CA-C-N	5.08	125.08	119.90
16	X	144	ARG	C-N-CA	5.08	125.08	119.90
34	h	218	SER	N-CA-C	-5.08	101.19	108.60
10	R	22	PRO	CA-C-N	5.07	126.18	119.84
10	R	22	PRO	C-N-CA	5.07	126.18	119.84
9	Q	171	LEU	CA-C-N	5.07	124.52	119.24
9	Q	171	LEU	C-N-CA	5.07	124.52	119.24
3	r	56	GLU	CA-C-N	5.07	127.38	120.54
3	r	56	GLU	C-N-CA	5.07	127.38	120.54
35	E	819	G	P-O3'-C3'	5.07	127.80	120.20
35	E	1880	U	O4'-C1'-N1	5.07	116.10	108.50
15	W	38	PHE	CA-CB-CG	-5.07	108.73	113.80
4	t	86	HIS	N-CA-C	-5.06	106.52	113.30
15	W	108	THR	CA-C-N	5.05	127.30	120.38
15	W	108	THR	C-N-CA	5.05	127.30	120.38
32	o	130	ILE	N-CA-C	-5.05	108.05	112.90
1	p	88	ASP	CA-CB-CG	5.05	117.65	112.60
35	E	2050	C	O5'-C5'-C4'	5.05	119.28	111.70
21	d	45	LYS	CA-C-N	5.04	127.35	120.54
21	d	45	LYS	C-N-CA	5.04	127.35	120.54
23	g	70	ASP	CA-C-N	5.04	127.35	120.54
23	g	70	ASP	C-N-CA	5.04	127.35	120.54
6	L	170	ILE	N-CA-C	-5.04	101.69	108.35
14	V	108	ALA	CA-C-N	5.03	127.33	120.54
14	V	108	ALA	C-N-CA	5.03	127.33	120.54
20	f	83	ARG	CA-C-N	5.03	127.27	120.38
20	f	83	ARG	C-N-CA	5.03	127.27	120.38
35	E	809	A	C2'-C3'-O3'	5.03	117.04	109.50
6	L	11	ALA	CA-C-N	5.02	125.01	119.89
6	L	11	ALA	C-N-CA	5.02	125.01	119.89
17	Y	13	ARG	N-CA-C	-5.02	101.81	108.74
17	Y	93	GLU	CA-C-N	5.02	126.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	93	GLU	C-N-CA	5.02	126.11	119.84
10	R	29	ALA	CA-C-N	5.02	127.25	120.38
10	R	29	ALA	C-N-CA	5.02	127.25	120.38
34	h	186	ALA	N-CA-C	-5.02	101.78	109.41
27	P	22	VAL	CA-C-N	5.02	127.31	120.54
27	P	22	VAL	C-N-CA	5.02	127.31	120.54
28	k	82	ASP	CA-C-N	5.01	127.25	120.38
28	k	82	ASP	C-N-CA	5.01	127.25	120.38
27	P	60	GLN	N-CA-C	-5.01	105.23	113.50
35	E	721	C	P-O5'-C5'	5.01	128.41	120.90
9	Q	67	PHE	CA-CB-CG	-5.01	108.79	113.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	E	325	U	C3'
35	E	702	U	C1'
35	E	810	U	C3'
35	E	1903	A	C3'

All (180) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	E	1080	U	Sidechain
35	E	1084	G	Sidechain
35	E	1169	U	Sidechain
35	E	1170	C	Sidechain
35	E	1171	C	Sidechain
35	E	1182	G	Sidechain
35	E	1186	U	Sidechain
35	E	1187	C	Sidechain
35	E	1188	C	Sidechain
35	E	1190	G	Sidechain
35	E	1253	G	Sidechain
35	E	1271	G	Sidechain
35	E	1300	C	Sidechain
35	E	1358	G	Sidechain
35	E	1376	G	Sidechain
35	E	143	C	Sidechain
35	E	1542	U	Sidechain
35	E	1543	C	Sidechain
35	E	1559	U	Sidechain

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Mol	Chain	Res	Type	Group
35	E	1560	G	Sidechain
35	E	159	G	Sidechain
35	E	1625	A	Sidechain
35	E	1638	G	Sidechain
35	E	1651	A	Sidechain
35	E	1652	A	Sidechain
35	E	1667	G	Sidechain
35	E	1670	A	Sidechain
35	E	1686	G	Sidechain
35	E	1714	U	Sidechain
35	E	172	A	Sidechain
35	E	1735	G	Sidechain
35	E	1737	U	Sidechain
35	E	1825	A	Sidechain
35	E	1867	G	Sidechain
35	E	1870	G	Sidechain
35	E	1872	G	Sidechain
35	E	1873	G	Sidechain
35	E	1874	C	Sidechain
35	E	1876	G	Sidechain
35	E	1880	U	Sidechain
35	E	1886	G	Sidechain
35	E	1903	A	Sidechain
35	E	1924	G	Sidechain
35	E	1925	A	Sidechain
35	E	1928	U	Sidechain
35	E	1941	C	Sidechain
35	E	1989	G	Sidechain
35	E	2003	G	Sidechain
35	E	2012	C	Sidechain
35	E	2019	C	Sidechain
35	E	202	C	Sidechain
35	E	2044	G	Sidechain
35	E	2075	G	Sidechain
35	E	2113	G	Sidechain
35	E	2129	U	Sidechain
35	E	213	G	Sidechain
35	E	2153	C	Sidechain
35	E	2215	C	Sidechain
35	E	2239	A	Sidechain
35	E	2240	A	Sidechain
35	E	226	A	Sidechain

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Mol	Chain	Res	Type	Group
35	E	228	G	Sidechain
35	E	2283	A	Sidechain
35	E	249	A	Sidechain
35	E	259	C	Sidechain
35	E	260	A	Sidechain
35	E	344	G	Sidechain
35	E	361	U	Sidechain
35	E	39	A	Sidechain
35	E	476	G	Sidechain
35	E	481	G	Sidechain
35	E	512	A	Sidechain
35	E	60	U	Sidechain
35	E	600	U	Sidechain
35	E	667	G	Sidechain
35	E	700	U	Sidechain
35	E	701	C	Sidechain
35	E	706	G	Sidechain
35	E	708	G	Sidechain
35	E	710	A	Sidechain
35	E	712	U	Sidechain
35	E	713	G	Sidechain
35	E	717	U	Sidechain
35	E	718	A	Sidechain
35	E	719	G	Sidechain
35	E	720	U	Sidechain
35	E	721	C	Sidechain
35	E	724	A	Sidechain
35	E	726	C	Sidechain
35	E	733	G	Sidechain
35	E	734	G	Sidechain
35	E	735	A	Sidechain
35	E	738	G	Sidechain
35	E	739	G	Sidechain
35	E	741	G	Sidechain
35	E	744	C	Sidechain
35	E	746	A	Sidechain
35	E	754	G	Sidechain
35	E	756	G	Sidechain
35	E	758	U	Sidechain
35	E	759	C	Sidechain
35	E	774	C	Sidechain
35	E	776	G	Sidechain

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Mol	Chain	Res	Type	Group
35	E	788	A	Sidechain
35	E	792	G	Sidechain
35	E	796	G	Sidechain
35	E	807	U	Sidechain
35	E	824	G	Sidechain
35	E	828	G	Sidechain
35	E	834	G	Sidechain
35	E	849	U	Sidechain
35	E	874	C	Sidechain
35	E	936	C	Sidechain
35	E	937	C	Sidechain
35	E	953	G	Sidechain
35	E	954	G	Sidechain
35	E	966	C	Sidechain
35	E	979	G	Sidechain
35	E	982	G	Sidechain
35	E	984	A	Sidechain
35	E	989	G	Sidechain
8	O	138	TYR	Sidechain
8	O	150	ARG	Peptide
8	O	57	ARG	Sidechain
27	P	44	ASP	Peptide
27	P	9	ARG	Peptide
9	Q	112	TYR	Sidechain
9	Q	119	ARG	Sidechain
9	Q	37	LYS	Peptide
15	W	81	ASP	Peptide
18	Z	56	ARG	Sidechain
24	a	107	TYR	Sidechain
24	a	46	VAL	Peptide
33	c	62	PRO	Peptide
33	c	65	ALA	Peptide
22	e	57	ARG	Sidechain
34	h	111	ALA	Peptide
34	h	120	LEU	Peptide
34	h	139	THR	Peptide
34	h	147	ASN	Peptide
34	h	154	SER	Peptide
34	h	155	PRO	Peptide
34	h	157	PHE	Peptide
34	h	158	ARG	Peptide
34	h	159	ALA	Peptide

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Mol	Chain	Res	Type	Group
34	h	160	SER	Peptide
34	h	174	LYS	Peptide
34	h	179	ARG	Peptide
34	h	180	THR	Peptide
34	h	182	ARG	Peptide
34	h	183	ASN	Peptide
34	h	184	ASN	Peptide
34	h	203	LYS	Peptide
34	h	207	GLU	Peptide
34	h	217	LEU	Peptide
34	h	77	GLN	Peptide
34	h	93	VAL	Peptide
34	h	94	VAL	Peptide
26	j	99	LYS	Peptide
28	k	173	ARG	Sidechain
30	m	142	LYS	Peptide
30	m	145	ARG	Peptide
32	o	63	ALA	Peptide
32	o	89	TYR	Sidechain
1	p	110	LYS	Peptide
1	p	261	ARG	Sidechain
1	p	43	TRP	Peptide
3	r	120	LYS	Peptide
3	r	121	TYR	Peptide
3	r	141	ARG	Peptide
3	r	142	THR	Peptide
3	r	147	SER	Peptide
3	r	32	GLN	Peptide
3	r	42	VAL	Peptide
4	t	104	TYR	Sidechain
4	t	128	MET	Peptide
5	u	43	TYR	Sidechain
5	u	48	LYS	Peptide
5	u	56	ARG	Peptide
5	u	9	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	p	2405	0	2323	0	0
2	q	311	0	319	0	0
3	r	1113	0	1175	3	0
4	t	969	0	1003	0	0
5	u	981	0	1021	2	0
6	L	2038	0	2142	0	0
7	M	1116	0	1169	0	0
8	O	1493	0	1562	0	0
9	Q	1670	0	1778	1	0
10	R	1143	0	1226	1	0
11	S	630	0	630	0	0
12	T	829	0	866	0	0
13	U	526	0	550	0	0
14	V	1011	0	1019	0	0
15	W	1781	0	1853	0	0
16	X	1212	0	1250	0	0
17	Y	989	0	1065	0	0
18	Z	1404	0	1503	1	0
19	b	1365	0	1410	1	0
20	f	1658	0	1704	0	0
21	d	1726	0	1774	0	0
22	e	1019	0	1050	2	0
23	g	635	0	631	0	0
24	a	553	0	608	1	0
25	i	958	0	981	0	0
26	j	518	0	513	1	0
27	P	1983	0	2131	0	0
28	k	972	0	1031	1	0
29	l	784	0	848	0	0
30	m	1587	0	1662	0	0
31	n	780	0	771	0	0
32	o	1116	0	1166	0	0
33	c	480	0	532	0	0
34	h	1358	0	1419	4	0
35	E	43106	0	21756	88	0
All	All	82219	0	62441	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (102) 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)
35:E:725:U:H3	35:E:733:G:H1	1.12	0.96
35:E:1849:U:H3	35:E:1869:G:H1	1.26	0.83
35:E:207:G:H1	35:E:222:U:H3	1.30	0.78
35:E:2220:G:H1	35:E:2232:U:H3	1.32	0.77
35:E:711:A:N1	35:E:746:A:N1	2.33	0.77
35:E:1085:G:H1	35:E:1169:U:H3	1.33	0.76
35:E:322:G:H1	35:E:331:U:H3	1.31	0.76
35:E:546:U:H2'	35:E:547:G:H5'	1.68	0.75
35:E:539:G:H1	35:E:550:U:H3	1.35	0.74
35:E:259:C:N3	35:E:954:G:N1	2.35	0.73
35:E:724:A:C4	35:E:735:A:C2	2.80	0.70
35:E:216:A:H2'	35:E:217:C:H5'	1.74	0.69
35:E:1088:A:N1	35:E:1166:C:N3	2.41	0.69
35:E:532:G:H1	35:E:558:U:H3	1.38	0.69
35:E:1089:U:H3	35:E:1165:G:H1	1.39	0.68
35:E:1381:G:H1	35:E:1537:U:H3	1.40	0.67
35:E:880:A:H62	35:E:892:U:H3	1.43	0.64
35:E:546:U:C2'	35:E:547:G:H5'	2.28	0.63
35:E:724:A:C2	35:E:734:G:N1	2.65	0.63
35:E:259:C:C2	35:E:954:G:C2	2.88	0.62
35:E:2124:G:H22	35:E:2140:U:H3	1.48	0.61
35:E:1852:G:C2	35:E:1866:A:C2	2.93	0.57
35:E:216:A:C2'	35:E:217:C:H5'	2.35	0.56
35:E:1872:G:C6	35:E:1873:G:C6	2.94	0.55
35:E:724:A:C2	35:E:725:U:C2	2.96	0.54
35:E:2004:A:H61	35:E:2052:C:H41	1.57	0.53
35:E:259:C:N3	35:E:954:G:C6	2.77	0.53
35:E:817:A:C2	35:E:828:G:C2	2.97	0.52
35:E:1856:G:H3'	35:E:1857:U:H5''	1.92	0.52
5:u:120:VAL:HG22	5:u:121:HIS:H	1.74	0.51
35:E:989:G:H1	35:E:1177:C:H42	1.57	0.51
35:E:1689:A:H1'	35:E:1691:G:H1	1.74	0.51
35:E:718:A:C2	35:E:719:G:C2	2.99	0.51
3:r:135:TRP:HB3	3:r:136:GLY:HA3	1.92	0.51
35:E:1911:U:H3	35:E:1917:G:H1	1.59	0.50
35:E:1852:G:N1	35:E:1866:A:C2	2.80	0.50
35:E:1184:C:H2'	35:E:1185:A:C8	2.46	0.50
3:r:124:ILE:HG13	3:r:126:ASP:H	1.77	0.50
35:E:724:A:N1	35:E:734:G:C6	2.80	0.50
35:E:1866:A:C2	35:E:1867:G:C4	3.00	0.49
35:E:260:A:N1	35:E:953:G:C6	2.81	0.49
35:E:744:C:H2'	35:E:745:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:259:C:C4	35:E:954:G:N1	2.81	0.48
35:E:202:C:N3	35:E:226:A:N1	2.61	0.48
35:E:1200:A:N1	35:E:1300:C:C4	2.81	0.48
35:E:1848:U:H3	35:E:1870:G:H1	1.60	0.48
35:E:1384:G:N1	35:E:1534:A:C2	2.82	0.48
35:E:2091:U:H3'	35:E:2092:A:H5''	1.96	0.48
24:a:103:LYS:H	24:a:105:ARG:HH11	1.62	0.47
34:h:198:ARG:HE	34:h:217:LEU:HD22	1.80	0.47
35:E:1987:A:H3'	35:E:1988:U:H5'	1.96	0.47
35:E:260:A:C6	35:E:953:G:N1	2.82	0.47
35:E:711:A:C2	35:E:746:A:C2	3.03	0.47
35:E:120:C:H3'	35:E:121:A:H5''	1.97	0.47
22:e:94:LEU:HD11	22:e:102:VAL:HG23	1.96	0.46
35:E:1908:U:H3'	35:E:1909:U:H5'	1.98	0.46
35:E:734:G:C6	35:E:735:A:C6	3.04	0.46
35:E:1375:U:H3	35:E:1543:C:N4	2.13	0.45
3:r:25:ALA:HB2	3:r:90:ALA:HB1	1.97	0.45
35:E:774:C:H1'	35:E:775:A:H5''	1.98	0.45
35:E:259:C:C2	35:E:954:G:C4	3.05	0.45
22:e:94:LEU:HD13	22:e:100:GLY:HA3	1.99	0.45
35:E:2051:C:H3'	35:E:2052:C:H4'	1.99	0.45
26:j:117:ARG:HG2	26:j:118:ASP:H	1.81	0.44
35:E:1846:C:C2	35:E:1873:G:N2	2.85	0.44
34:h:94:VAL:HG12	34:h:95:GLY:H	1.82	0.44
35:E:1923:U:H3	35:E:1927:A:H62	1.66	0.44
35:E:156:G:H3'	35:E:157:G:H5''	1.99	0.44
35:E:1169:U:C4	35:E:1170:C:C4	3.05	0.44
35:E:743:C:H2'	35:E:744:C:C6	2.52	0.43
35:E:999:U:H3	35:E:1072:G:H1	1.66	0.43
35:E:1872:G:N1	35:E:1873:G:N1	2.66	0.43
35:E:824:G:H5''	35:E:825:C:H5''	1.99	0.43
5:u:9:GLN:CB	5:u:10:PHE:HA	2.49	0.43
35:E:711:A:C5	35:E:712:U:C4	3.07	0.43
18:Z:64:ASN:HD21	35:E:305:U:H2'	1.83	0.43
35:E:1380:U:H3	35:E:1538:G:H1	1.65	0.43
35:E:1542:U:H2'	35:E:1543:C:H5''	2.01	0.43
10:R:16:LEU:HD11	35:E:1196:A:H5''	2.01	0.43
28:k:122:ARG:HE	35:E:1786:G:H5'	1.83	0.42
35:E:711:A:N1	35:E:746:A:C2	2.86	0.42
35:E:1905:U:H3	35:E:1922:G:H22	1.68	0.42
35:E:714:G:H2'	35:E:718:A:H62	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:1629:C:H1'	35:E:2153:C:H41	1.84	0.42
35:E:1852:G:C6	35:E:1866:A:N1	2.88	0.42
35:E:260:A:C2	35:E:953:G:C2	3.08	0.42
34:h:180:THR:HB	34:h:182:ARG:H	1.83	0.41
35:E:1993:G:H21	35:E:1994:U:H2'	1.84	0.41
35:E:703:A:C2	35:E:704:A:C5	3.09	0.41
35:E:260:A:C2	35:E:953:G:C4	3.08	0.41
35:E:724:A:C6	35:E:735:A:N1	2.88	0.41
35:E:1825:A:C2	35:E:1879:U:O4	2.73	0.41
35:E:1852:G:N2	35:E:1866:A:C2	2.89	0.41
35:E:817:A:N1	35:E:828:G:N1	2.69	0.41
19:b:142:ILE:HG22	19:b:144:SER:H	1.86	0.41
35:E:718:A:C2	35:E:744:C:O2	2.73	0.41
35:E:602:G:N1	35:E:645:A:N1	2.69	0.41
35:E:1856:G:C3'	35:E:1857:U:H5''	2.51	0.41
9:Q:103:LYS:HA	35:E:763:G:H1	1.85	0.41
35:E:1384:G:C2	35:E:1534:A:C2	3.09	0.40
35:E:216:A:C2	35:E:217:C:C6	3.10	0.40
34:h:161:THR:HG23	34:h:162:THR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	p	308/318 (97%)	288 (94%)	18 (6%)	2 (1%)	21	57
2	q	36/57 (63%)	28 (78%)	6 (17%)	2 (6%)	1	17
3	r	138/149 (93%)	113 (82%)	18 (13%)	7 (5%)	1	18
4	t	117/152 (77%)	105 (90%)	8 (7%)	4 (3%)	3	24
5	u	118/153 (77%)	102 (86%)	13 (11%)	3 (2%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	L	256/273 (94%)	239 (93%)	16 (6%)	1 (0%)	30	65
7	M	140/143 (98%)	131 (94%)	8 (6%)	1 (1%)	18	54
8	O	188/190 (99%)	165 (88%)	16 (8%)	7 (4%)	2	22
9	Q	198/211 (94%)	178 (90%)	16 (8%)	4 (2%)	6	33
10	R	139/151 (92%)	127 (91%)	11 (8%)	1 (1%)	18	54
11	S	80/86 (93%)	73 (91%)	5 (6%)	2 (2%)	4	29
12	T	102/112 (91%)	90 (88%)	12 (12%)	0	100	100
13	U	66/112 (59%)	62 (94%)	3 (4%)	1 (2%)	8	38
14	V	133/144 (92%)	116 (87%)	16 (12%)	1 (1%)	16	52
15	W	215/261 (82%)	200 (93%)	13 (6%)	2 (1%)	14	48
16	X	146/173 (84%)	133 (91%)	11 (8%)	2 (1%)	9	39
17	Y	121/137 (88%)	113 (93%)	8 (7%)	0	100	100
18	Z	171/221 (77%)	157 (92%)	12 (7%)	2 (1%)	10	42
19	b	162/190 (85%)	143 (88%)	17 (10%)	2 (1%)	10	42
20	f	205/245 (84%)	190 (93%)	12 (6%)	3 (2%)	8	38
21	d	221/263 (84%)	205 (93%)	14 (6%)	2 (1%)	14	48
22	e	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	52
23	g	81/236 (34%)	78 (96%)	3 (4%)	0	100	100
24	a	68/110 (62%)	58 (85%)	6 (9%)	4 (6%)	1	16
25	i	119/141 (84%)	111 (93%)	7 (6%)	1 (1%)	16	52
26	j	62/150 (41%)	47 (76%)	11 (18%)	4 (6%)	1	15
27	P	247/250 (99%)	226 (92%)	21 (8%)	0	100	100
28	k	116/196 (59%)	102 (88%)	13 (11%)	1 (1%)	14	48
29	l	97/117 (83%)	82 (84%)	15 (16%)	0	100	100
30	m	198/214 (92%)	179 (90%)	14 (7%)	5 (2%)	4	29
31	n	91/161 (56%)	83 (91%)	5 (6%)	3 (3%)	3	24
32	o	138/167 (83%)	112 (81%)	21 (15%)	5 (4%)	2	23
33	c	58/66 (88%)	53 (91%)	4 (7%)	1 (2%)	7	36
34	h	171/257 (66%)	123 (72%)	31 (18%)	17 (10%)	0	8
All	All	4833/5936 (81%)	4330 (90%)	412 (8%)	91 (2%)	8	34

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	r	121	TYR
3	r	124	ILE
5	u	120	VAL
9	Q	138	CYS
21	d	81	SER
26	j	95	MET
26	j	97	ALA
30	m	144	GLN
34	h	77	GLN
34	h	121	PHE
34	h	155	PRO
34	h	158	ARG
34	h	162	THR
34	h	183	ASN
34	h	184	ASN
34	h	204	ASN
2	q	31	VAL
3	r	119	ASP
3	r	146	LYS
4	t	45	HIS
5	u	35	LYS
8	O	10	ASN
8	O	114	VAL
9	Q	122	THR
11	S	53	SER
11	S	71	LYS
19	b	136	ALA
24	a	101	SER
24	a	103	LYS
24	a	105	ARG
30	m	141	ILE
30	m	187	ILE
32	o	81	VAL
34	h	94	VAL
34	h	164	LYS
34	h	191	ASP
1	p	131	ASN
2	q	30	ALA
3	r	127	PRO
8	O	155	LEU
9	Q	51	VAL
16	X	43	MET
18	Z	69	THR

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Mol	Chain	Res	Type
20	f	36	ALA
20	f	116	GLN
26	j	105	GLU
26	j	115	ARG
32	o	13	ARG
32	o	15	ILE
34	h	128	GLY
34	h	163	LYS
4	t	60	ALA
4	t	128	MET
7	M	86	PRO
8	O	25	SER
8	O	39	ALA
10	R	134	GLN
13	U	108	ALA
14	V	57	ALA
18	Z	29	LEU
24	a	45	ALA
25	i	103	LEU
28	k	141	PRO
31	n	32	THR
31	n	36	SER
31	n	68	TRP
34	h	161	THR
1	p	122	ARG
3	r	143	ARG
5	u	9	GLN
8	O	2	SER
8	O	11	LYS
9	Q	39	LEU
15	W	56	ILE
19	b	137	LYS
20	f	9	LYS
21	d	238	ALA
32	o	77	ILE
34	h	175	VAL
34	h	206	ALA
30	m	92	VAL
32	o	63	ALA
33	c	23	LYS
34	h	111	ALA
22	e	29	PRO

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Mol	Chain	Res	Type
4	t	61	PRO
3	r	61	VAL
30	m	47	ILE
6	L	167	VAL
15	W	223	PRO
16	X	89	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	262/268 (98%)	260 (99%)	2 (1%)	73	77
2	q	34/49 (69%)	34 (100%)	0	100	100
3	r	113/121 (93%)	113 (100%)	0	100	100
4	t	102/131 (78%)	102 (100%)	0	100	100
5	u	104/132 (79%)	104 (100%)	0	100	100
6	L	217/230 (94%)	217 (100%)	0	100	100
7	M	116/117 (99%)	116 (100%)	0	100	100
8	O	160/160 (100%)	160 (100%)	0	100	100
9	Q	188/195 (96%)	187 (100%)	1 (0%)	81	82
10	R	125/132 (95%)	124 (99%)	1 (1%)	73	77
11	S	70/73 (96%)	70 (100%)	0	100	100
12	T	87/93 (94%)	87 (100%)	0	100	100
13	U	57/97 (59%)	57 (100%)	0	100	100
14	V	103/112 (92%)	103 (100%)	0	100	100
15	W	194/223 (87%)	192 (99%)	2 (1%)	68	76
16	X	137/157 (87%)	137 (100%)	0	100	100
17	Y	104/116 (90%)	104 (100%)	0	100	100
18	Z	143/184 (78%)	143 (100%)	0	100	100
19	b	148/165 (90%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	f	182/211 (86%)	182 (100%)	0	100	100
21	d	187/208 (90%)	187 (100%)	0	100	100
22	e	110/111 (99%)	109 (99%)	1 (1%)	70	76
23	g	68/186 (37%)	68 (100%)	0	100	100
24	a	64/96 (67%)	62 (97%)	2 (3%)	35	56
25	i	103/120 (86%)	102 (99%)	1 (1%)	68	76
26	j	55/123 (45%)	55 (100%)	0	100	100
27	P	204/205 (100%)	204 (100%)	0	100	100
28	k	108/172 (63%)	108 (100%)	0	100	100
29	l	89/104 (86%)	89 (100%)	0	100	100
30	m	167/179 (93%)	166 (99%)	1 (1%)	78	81
31	n	84/125 (67%)	84 (100%)	0	100	100
32	o	118/139 (85%)	117 (99%)	1 (1%)	73	77
33	c	49/53 (92%)	49 (100%)	0	100	100
34	h	138/191 (72%)	133 (96%)	5 (4%)	31	53
All	All	4190/4978 (84%)	4173 (100%)	17 (0%)	81	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	29	ILE
1	p	175	ASP
9	Q	122	THR
10	R	16	LEU
15	W	89	VAL
15	W	165	TRP
22	e	25	VAL
24	a	95	ILE
24	a	106	LEU
25	i	121	VAL
30	m	137	VAL
32	o	87	VAL
34	h	94	VAL
34	h	181	TYR
34	h	188	VAL
34	h	217	LEU
34	h	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	12	HIS
1	p	46	ASN
1	p	78	ASN
1	p	102	GLN
1	p	108	HIS
1	p	131	ASN
1	p	144	HIS
1	p	151	HIS
1	p	195	HIS
1	p	298	ASN
2	q	47	ASN
3	r	44	GLN
3	r	65	HIS
3	r	80	GLN
3	r	104	ASN
4	t	51	HIS
4	t	110	ASN
5	u	126	HIS
6	L	33	HIS
6	L	47	ASN
6	L	54	ASN
6	L	64	GLN
6	L	142	HIS
6	L	152	HIS
6	L	239	GLN
7	M	8	HIS
7	M	77	ASN
8	O	27	HIS
8	O	37	HIS
8	O	43	GLN
8	O	69	ASN
8	O	93	ASN
9	Q	36	HIS
9	Q	42	GLN
9	Q	47	HIS
9	Q	132	ASN
10	R	77	HIS
10	R	101	HIS
10	R	105	ASN
10	R	123	HIS
10	R	134	GLN

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Mol	Chain	Res	Type
12	T	24	HIS
12	T	75	GLN
13	U	64	ASN
13	U	82	ASN
14	V	25	HIS
14	V	31	ASN
15	W	49	ASN
15	W	69	ASN
15	W	91	GLN
15	W	101	GLN
15	W	103	HIS
15	W	182	ASN
15	W	184	ASN
15	W	193	ASN
16	X	11	HIS
16	X	18	GLN
16	X	30	ASN
16	X	142	GLN
17	Y	4	GLN
17	Y	121	ASN
18	Z	21	HIS
18	Z	64	ASN
19	b	3	ASN
19	b	80	HIS
19	b	132	HIS
19	b	154	HIS
20	f	25	HIS
20	f	27	HIS
20	f	50	ASN
20	f	55	HIS
20	f	73	ASN
20	f	121	GLN
20	f	144	ASN
20	f	167	ASN
21	d	159	HIS
21	d	210	ASN
21	d	250	HIS
22	e	56	HIS
23	g	38	GLN
23	g	43	ASN
24	a	43	GLN
25	i	60	HIS

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Mol	Chain	Res	Type
25	i	139	HIS
26	j	88	HIS
26	j	90	HIS
27	P	54	GLN
27	P	142	ASN
27	P	232	HIS
27	P	239	GLN
28	k	145	HIS
28	k	159	GLN
29	l	25	ASN
29	l	69	ASN
30	m	77	HIS
30	m	163	HIS
30	m	165	ASN
31	n	98	HIS
32	o	41	GLN
32	o	49	ASN
32	o	58	HIS
32	o	65	GLN
32	o	101	ASN
32	o	118	HIS
33	c	16	ASN
33	c	17	GLN
34	h	129	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	E	2017/2319 (86%)	439 (21%)	86 (4%)

All (439) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	E	4	C
35	E	5	U
35	E	17	C
35	E	25	C
35	E	26	A
35	E	34	G
35	E	35	U
35	E	45	U

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Mol	Chain	Res	Type
35	E	46	U
35	E	47	A
35	E	56	U
35	E	65	A
35	E	74	U
35	E	75	U
35	E	76	G
35	E	82	A
35	E	83	U
35	E	90	A
35	E	111	A
35	E	121	A
35	E	137	C
35	E	143	C
35	E	144	A
35	E	145	U
35	E	157	G
35	E	163	C
35	E	170	C
35	E	184	A
35	E	191	U
35	E	193	U
35	E	194	U
35	E	196	U
35	E	198	U
35	E	199	G
35	E	200	U
35	E	202	C
35	E	203	C
35	E	204	G
35	E	227	U
35	E	228	G
35	E	249	A
35	E	252	G
35	E	253	U
35	E	255	A
35	E	257	A
35	E	258	C
35	E	271	C
35	E	284	C
35	E	286	G
35	E	287	A

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Mol	Chain	Res	Type
35	E	288	A
35	E	309	G
35	E	311	G
35	E	313	G
35	E	316	A
35	E	322	G
35	E	325	U
35	E	326	U
35	E	327	U
35	E	329	U
35	E	331	U
35	E	357	C
35	E	362	C
35	E	364	G
35	E	385	G
35	E	386	A
35	E	408	C
35	E	427	U
35	E	447	A
35	E	449	U
35	E	450	A
35	E	463	A
35	E	464	C
35	E	465	G
35	E	471	C
35	E	472	A
35	E	473	G
35	E	486	U
35	E	491	C
35	E	507	A
35	E	520	A
35	E	529	A
35	E	531	A
35	E	532	G
35	E	533	C
35	E	560	C
35	E	564	G
35	E	570	U
35	E	571	A
35	E	585	A
35	E	586	A
35	E	590	C

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Mol	Chain	Res	Type
35	E	592	A
35	E	593	G
35	E	596	A
35	E	613	C
35	E	634	A
35	E	648	A
35	E	665	U
35	E	673	A
35	E	674	A
35	E	676	G
35	E	677	G
35	E	678	G
35	E	698	C
35	E	699	C
35	E	702	U
35	E	703	A
35	E	704	A
35	E	705	G
35	E	706	G
35	E	707	C
35	E	708	G
35	E	710	A
35	E	713	G
35	E	714	G
35	E	717	U
35	E	718	A
35	E	720	U
35	E	721	C
35	E	726	C
35	E	727	C
35	E	728	A
35	E	729	C
35	E	730	U
35	E	731	U
35	E	732	C
35	E	733	G
35	E	736	U
35	E	737	U
35	E	738	G
35	E	739	G
35	E	740	U
35	E	741	G

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Mol	Chain	Res	Type
35	E	742	A
35	E	745	C
35	E	747	U
35	E	748	G
35	E	749	C
35	E	750	C
35	E	751	C
35	E	752	U
35	E	757	G
35	E	760	C
35	E	762	U
35	E	766	C
35	E	768	G
35	E	769	A
35	E	770	C
35	E	771	A
35	E	772	U
35	E	773	U
35	E	774	C
35	E	775	A
35	E	776	G
35	E	777	A
35	E	778	A
35	E	785	A
35	E	786	A
35	E	789	C
35	E	793	A
35	E	795	U
35	E	796	G
35	E	798	U
35	E	799	A
35	E	804	U
35	E	806	C
35	E	808	G
35	E	809	A
35	E	810	U
35	E	811	U
35	E	812	A
35	E	813	U
35	E	814	C
35	E	815	G
35	E	821	C

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Mol	Chain	Res	Type
35	E	822	A
35	E	823	U
35	E	824	G
35	E	825	C
35	E	827	U
35	E	829	C
35	E	830	C
35	E	834	G
35	E	835	G
35	E	836	G
35	E	844	G
35	E	847	U
35	E	848	U
35	E	858	A
35	E	861	A
35	E	871	G
35	E	872	A
35	E	877	A
35	E	880	A
35	E	881	G
35	E	884	A
35	E	885	U
35	E	886	U
35	E	887	C
35	E	888	G
35	E	889	A
35	E	891	U
35	E	892	U
35	E	893	G
35	E	895	A
35	E	901	A
35	E	919	G
35	E	920	A
35	E	921	G
35	E	922	C
35	E	923	A
35	E	924	G
35	E	925	C
35	E	935	A
35	E	936	C
35	E	940	U
35	E	941	U

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Mol	Chain	Res	Type
35	E	942	C
35	E	943	G
35	E	944	G
35	E	945	C
35	E	946	U
35	E	947	U
35	E	950	G
35	E	966	C
35	E	969	U
35	E	975	U
35	E	976	U
35	E	977	A
35	E	979	G
35	E	980	G
35	E	983	C
35	E	986	U
35	E	988	U
35	E	989	G
35	E	994	G
35	E	999	U
35	E	1074	C
35	E	1077	C
35	E	1078	U
35	E	1079	U
35	E	1081	G
35	E	1082	U
35	E	1083	G
35	E	1171	C
35	E	1172	C
35	E	1175	A
35	E	1177	C
35	E	1178	U
35	E	1187	C
35	E	1188	C
35	E	1189	A
35	E	1191	G
35	E	1192	A
35	E	1193	A
35	E	1194	U
35	E	1195	G
35	E	1197	A
35	E	1207	U

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Mol	Chain	Res	Type
35	E	1208	U
35	E	1211	G
35	E	1221	U
35	E	1247	U
35	E	1268	A
35	E	1270	A
35	E	1295	U
35	E	1301	A
35	E	1339	G
35	E	1340	A
35	E	1356	C
35	E	1359	C
35	E	1360	A
35	E	1361	A
35	E	1363	C
35	E	1375	U
35	E	1524	U
35	E	1541	U
35	E	1542	U
35	E	1543	C
35	E	1544	U
35	E	1545	U
35	E	1546	C
35	E	1547	A
35	E	1559	U
35	E	1560	G
35	E	1561	A
35	E	1606	A
35	E	1618	G
35	E	1626	C
35	E	1627	C
35	E	1628	A
35	E	1631	A
35	E	1638	G
35	E	1653	U
35	E	1659	U
35	E	1661	A
35	E	1664	A
35	E	1668	G
35	E	1669	G
35	E	1671	A
35	E	1672	C

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Mol	Chain	Res	Type
35	E	1685	G
35	E	1689	A
35	E	1690	G
35	E	1691	G
35	E	1695	A
35	E	1696	G
35	E	1701	G
35	E	1711	G
35	E	1712	U
35	E	1724	A
35	E	1725	U
35	E	1727	C
35	E	1738	G
35	E	1782	U
35	E	1783	U
35	E	1789	A
35	E	1813	G
35	E	1815	A
35	E	1829	C
35	E	1830	C
35	E	1831	C
35	E	1832	A
35	E	1833	U
35	E	1857	U
35	E	1872	G
35	E	1873	G
35	E	1874	C
35	E	1875	G
35	E	1876	G
35	E	1877	U
35	E	1878	A
35	E	1880	U
35	E	1881	C
35	E	1882	G
35	E	1883	C
35	E	1884	U
35	E	1885	U
35	E	1886	G
35	E	1887	U
35	E	1903	A
35	E	1904	U
35	E	1905	U

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Mol	Chain	Res	Type
35	E	1909	U
35	E	1910	G
35	E	1914	U
35	E	1927	A
35	E	1930	U
35	E	1943	G
35	E	1947	U
35	E	1950	G
35	E	1951	A
35	E	1955	U
35	E	1956	C
35	E	1959	C
35	E	1961	A
35	E	1965	U
35	E	1966	C
35	E	1974	C
35	E	1976	C
35	E	1977	G
35	E	1988	U
35	E	1990	U
35	E	1991	C
35	E	1992	A
35	E	1993	G
35	E	1994	U
35	E	2000	C
35	E	2002	A
35	E	2006	A
35	E	2007	A
35	E	2008	A
35	E	2009	C
35	E	2010	G
35	E	2012	C
35	E	2013	U
35	E	2016	U
35	E	2018	U
35	E	2019	C
35	E	2020	G
35	E	2021	G
35	E	2022	A
35	E	2030	G
35	E	2032	U
35	E	2033	C

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Mol	Chain	Res	Type
35	E	2034	A
35	E	2048	A
35	E	2049	C
35	E	2050	C
35	E	2051	C
35	E	2052	C
35	E	2053	G
35	E	2054	G
35	E	2060	C
35	E	2061	G
35	E	2063	A
35	E	2064	G
35	E	2068	C
35	E	2070	C
35	E	2071	U
35	E	2072	U
35	E	2075	G
35	E	2077	C
35	E	2087	C
35	E	2090	U
35	E	2091	U
35	E	2092	A
35	E	2097	U
35	E	2099	G
35	E	2102	C
35	E	2103	A
35	E	2107	A
35	E	2108	G
35	E	2118	G
35	E	2135	A
35	E	2153	C
35	E	2165	A
35	E	2214	A
35	E	2216	A
35	E	2217	G
35	E	2218	U
35	E	2225	C
35	E	2226	U
35	E	2227	U
35	E	2228	C
35	E	2235	C
35	E	2275	G

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Mol	Chain	Res	Type
35	E	2278	G
35	E	2280	A
35	E	2283	A
35	E	2284	A
35	E	2287	U
35	E	2288	A
35	E	2310	G
35	E	2311	G
35	E	2312	A
35	E	2314	C
35	E	2317	U

All (86) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	E	56	U
35	E	68	A
35	E	193	U
35	E	227	U
35	E	325	U
35	E	531	A
35	E	701	C
35	E	702	U
35	E	703	A
35	E	712	U
35	E	713	G
35	E	717	U
35	E	719	G
35	E	727	C
35	E	729	C
35	E	756	G
35	E	765	A
35	E	769	A
35	E	771	A
35	E	774	C
35	E	775	A
35	E	777	A
35	E	785	A
35	E	788	A
35	E	792	G
35	E	795	U
35	E	797	G

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Mol	Chain	Res	Type
35	E	807	U
35	E	808	G
35	E	810	U
35	E	812	A
35	E	813	U
35	E	814	C
35	E	822	A
35	E	828	G
35	E	829	C
35	E	847	U
35	E	885	U
35	E	890	C
35	E	891	U
35	E	892	U
35	E	918	G
35	E	919	G
35	E	921	G
35	E	922	C
35	E	923	A
35	E	935	A
35	E	939	U
35	E	940	U
35	E	942	C
35	E	968	U
35	E	975	U
35	E	982	G
35	E	988	U
35	E	998	C
35	E	1076	C
35	E	1186	U
35	E	1187	C
35	E	1188	C
35	E	1191	G
35	E	1192	A
35	E	1526	A
35	E	1545	U
35	E	1546	C
35	E	1695	A
35	E	1712	U
35	E	1872	G
35	E	1875	G
35	E	1876	G

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Mol	Chain	Res	Type
35	E	1882	G
35	E	1886	G
35	E	1903	A
35	E	1904	U
35	E	1913	U
35	E	2006	A
35	E	2017	G
35	E	2020	G
35	E	2048	A
35	E	2049	C
35	E	2050	C
35	E	2051	C
35	E	2052	C
35	E	2152	C
35	E	2213	G
35	E	2227	U
35	E	2234	A

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

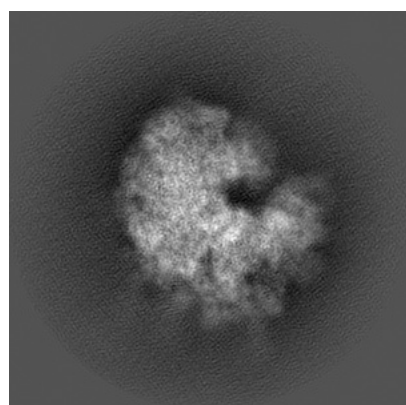
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3844. These allow visual inspection of the internal detail of the map and identification of artifacts.

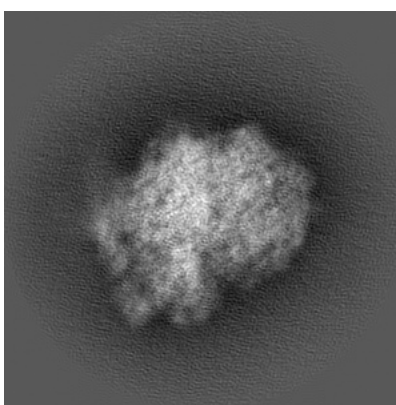
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

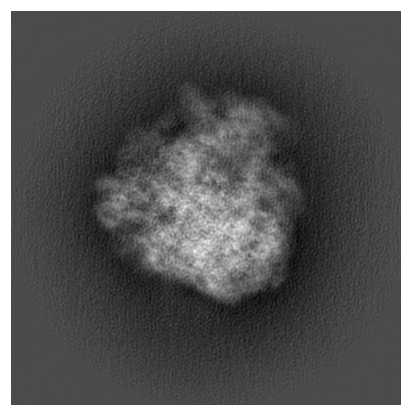
6.1.1 Primary map



X



Y

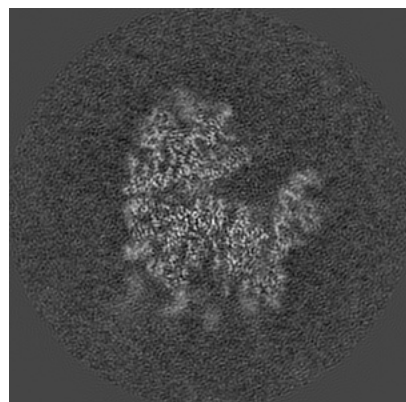


Z

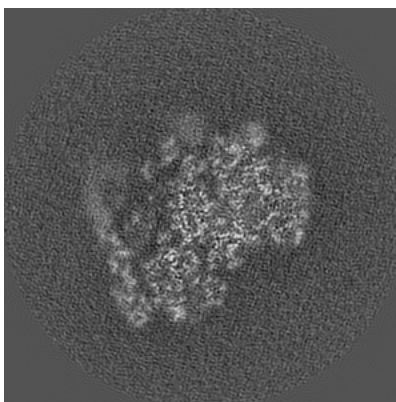
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

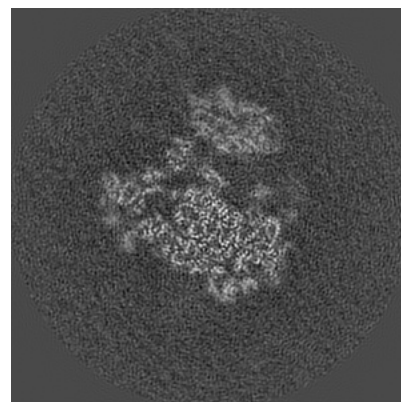
6.2.1 Primary map



X Index: 160



Y Index: 160

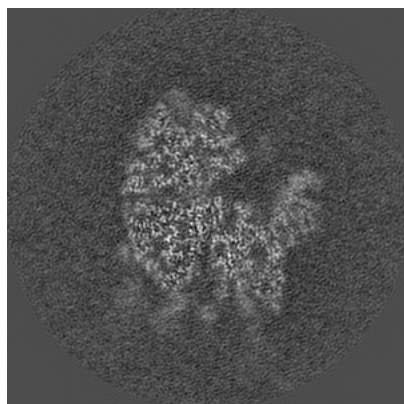


Z Index: 160

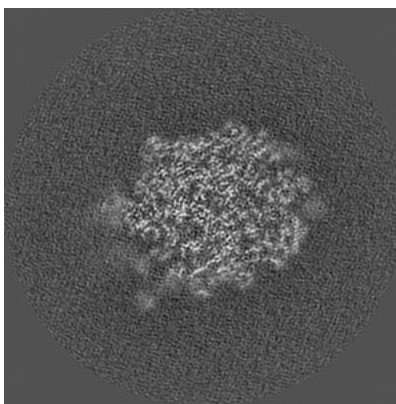
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

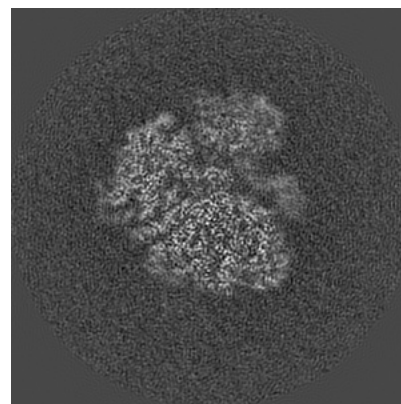
6.3.1 Primary map



X Index: 157



Y Index: 134

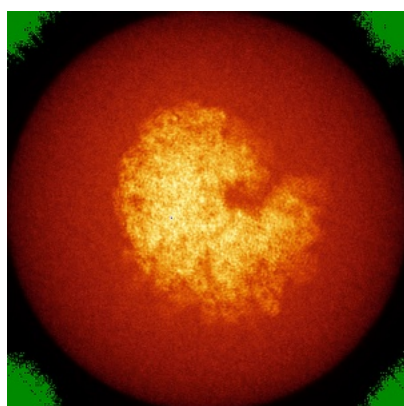


Z Index: 147

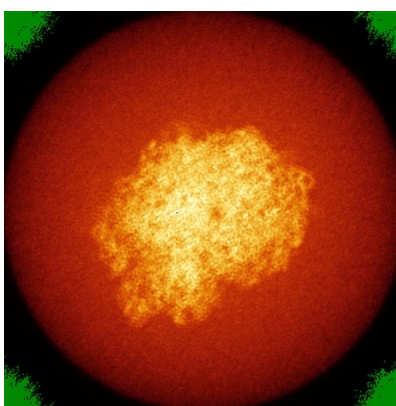
The images above show the largest variance slices of the map in three orthogonal directions.

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

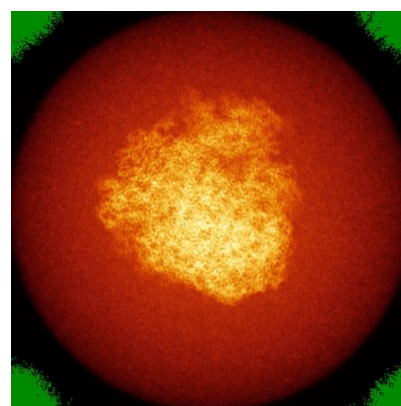
6.4.1 Primary map



X



Y

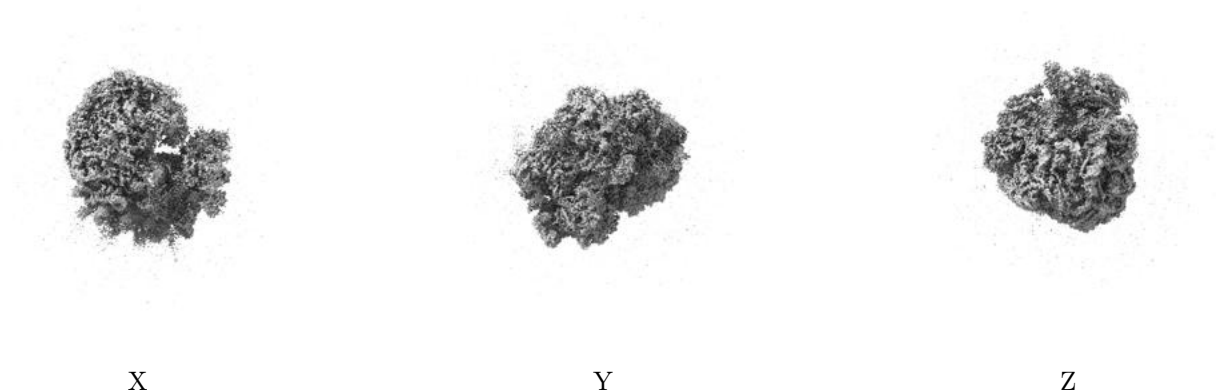


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0549. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

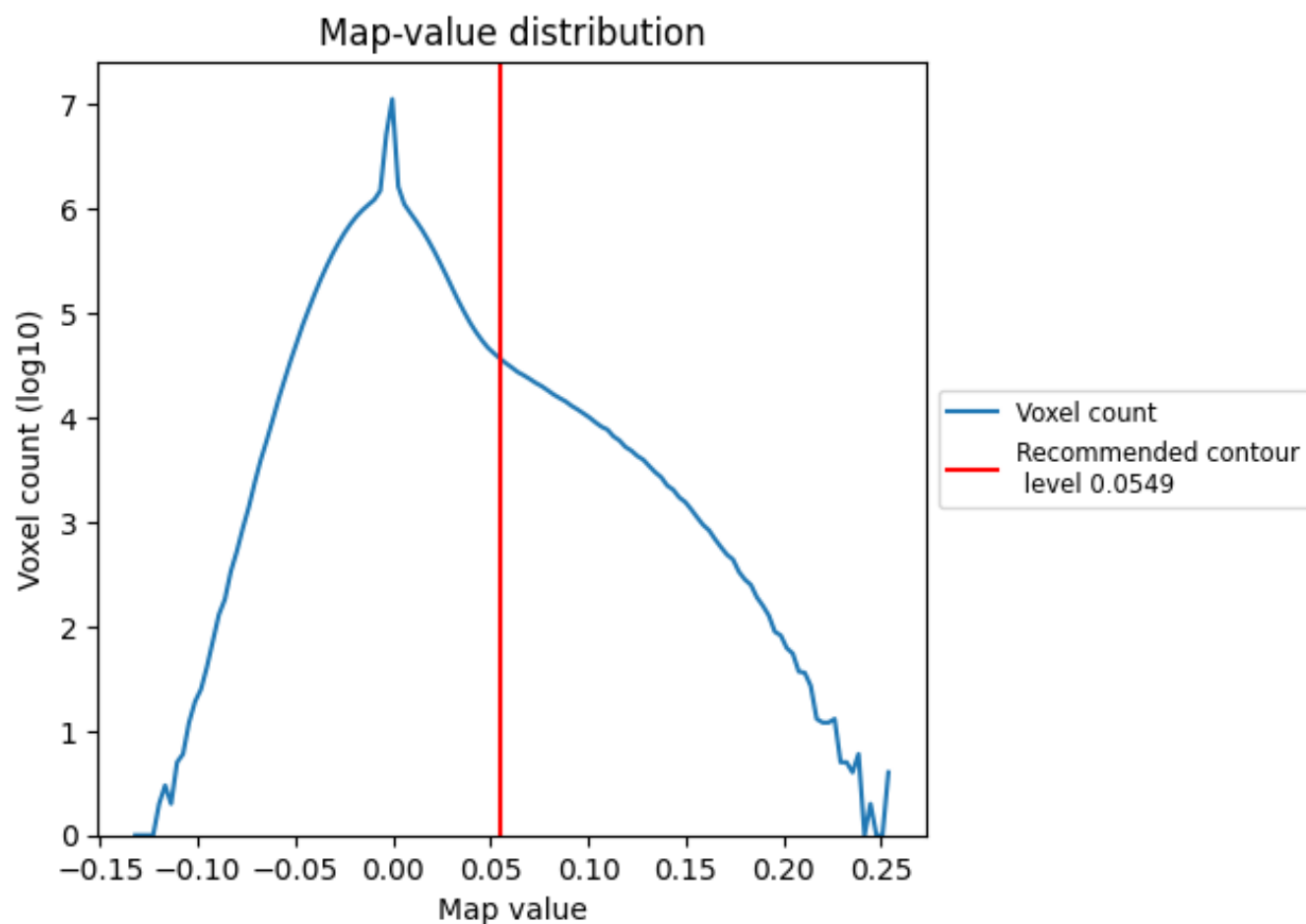
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

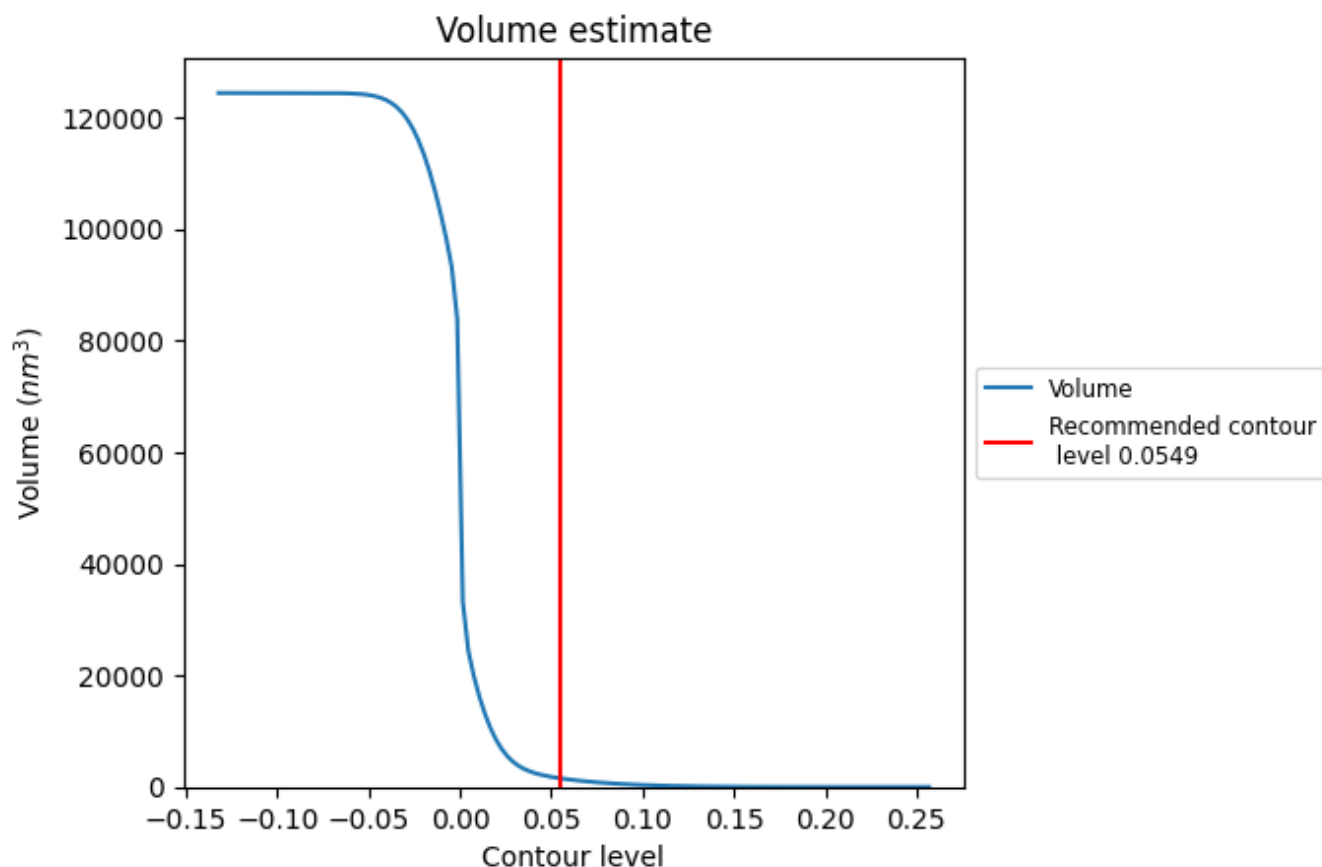
This section contains the results of statistical analysis of the map.

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.

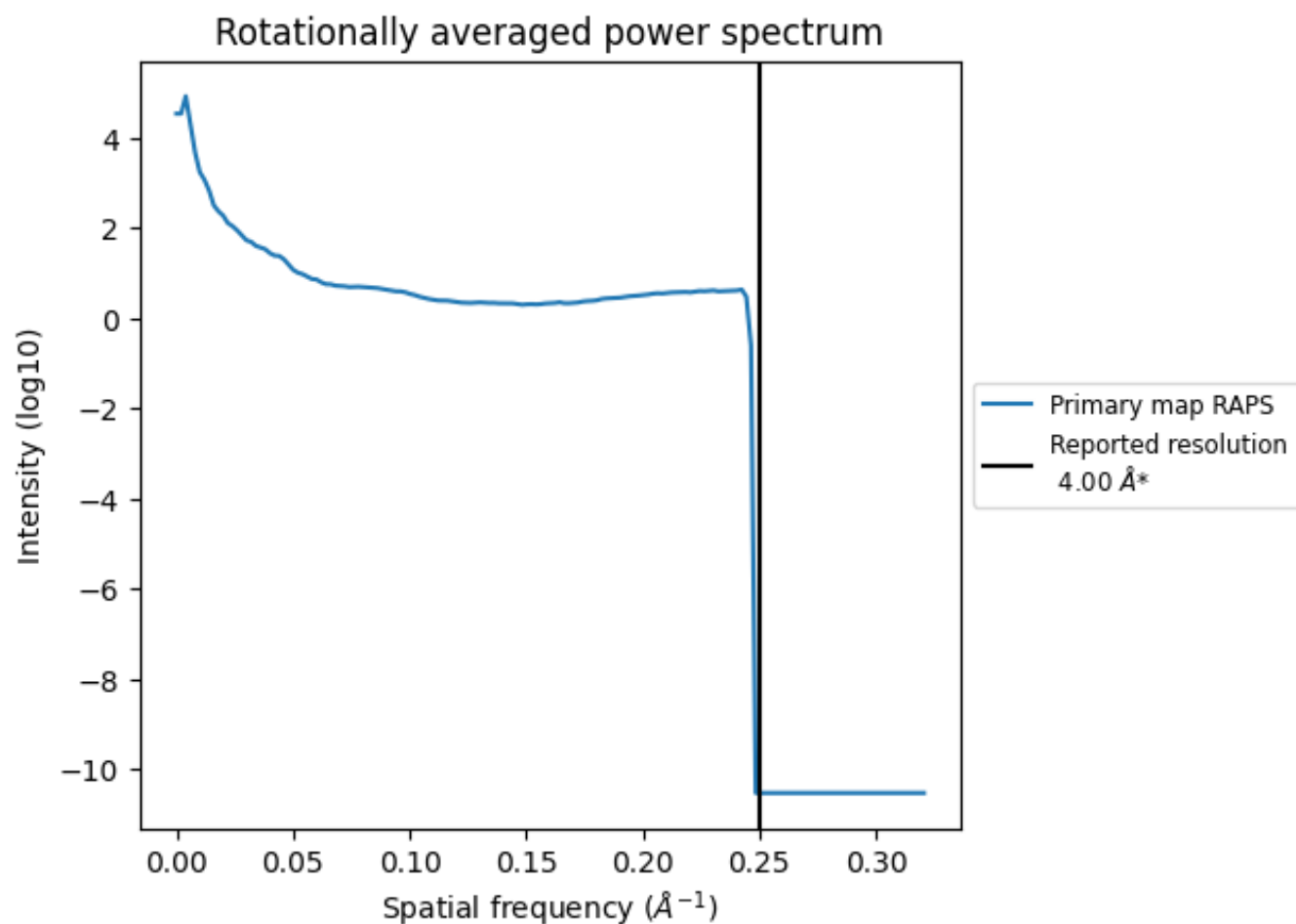
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1549 nm³; this corresponds to an approximate mass of 1400 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 0.250 Å⁻¹

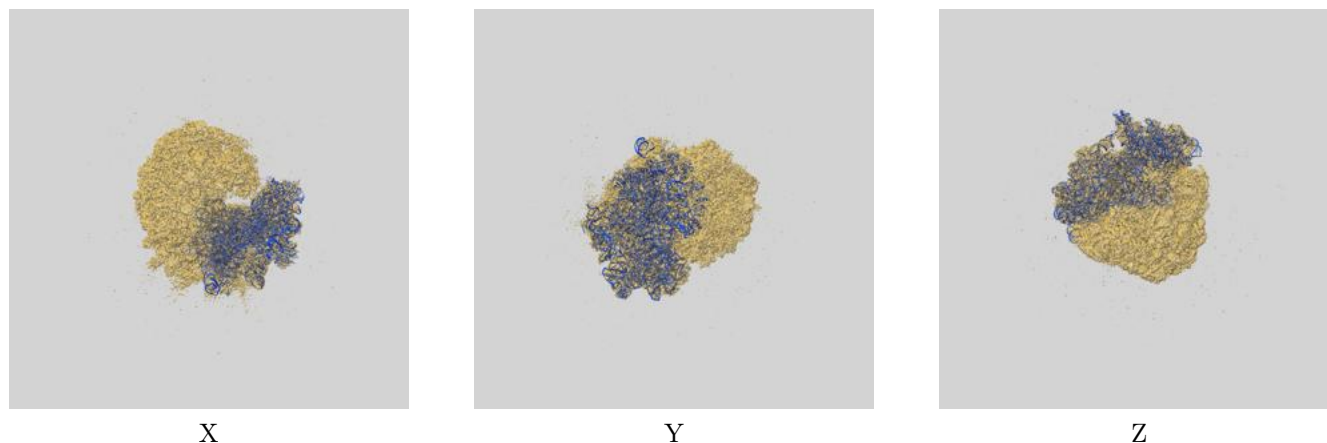
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

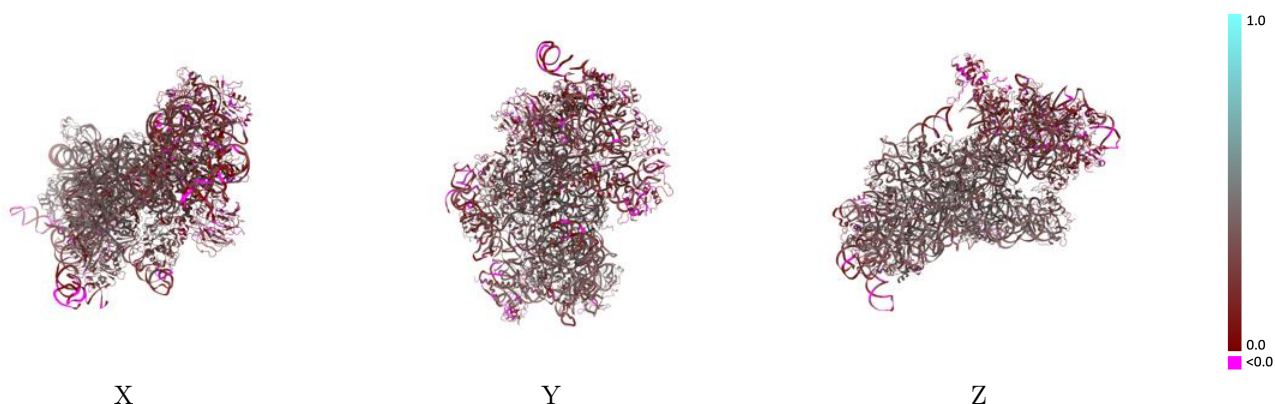
This section contains information regarding the fit between EMDB map EMD-3844 and PDB model 5OPT. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



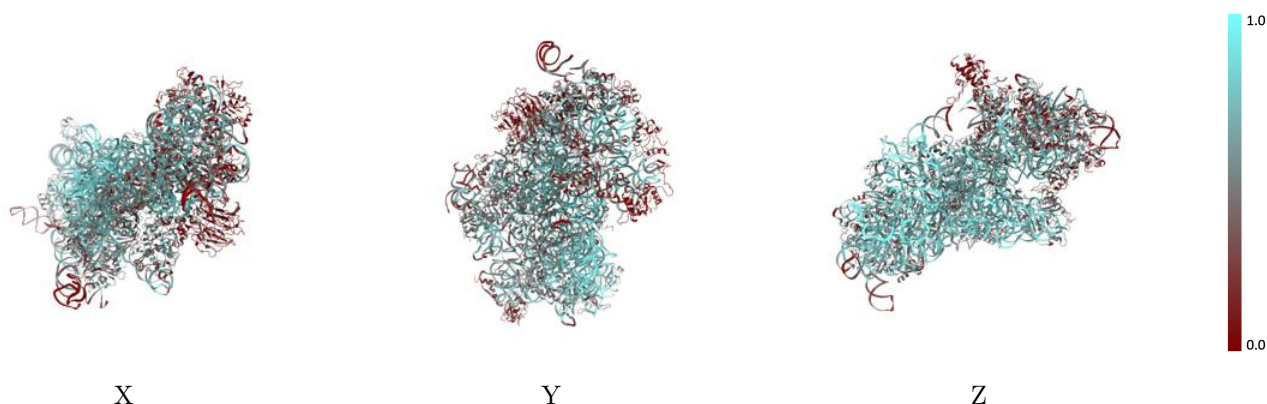
The images above show the 3D surface view of the map at the recommended contour level 0.0549 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



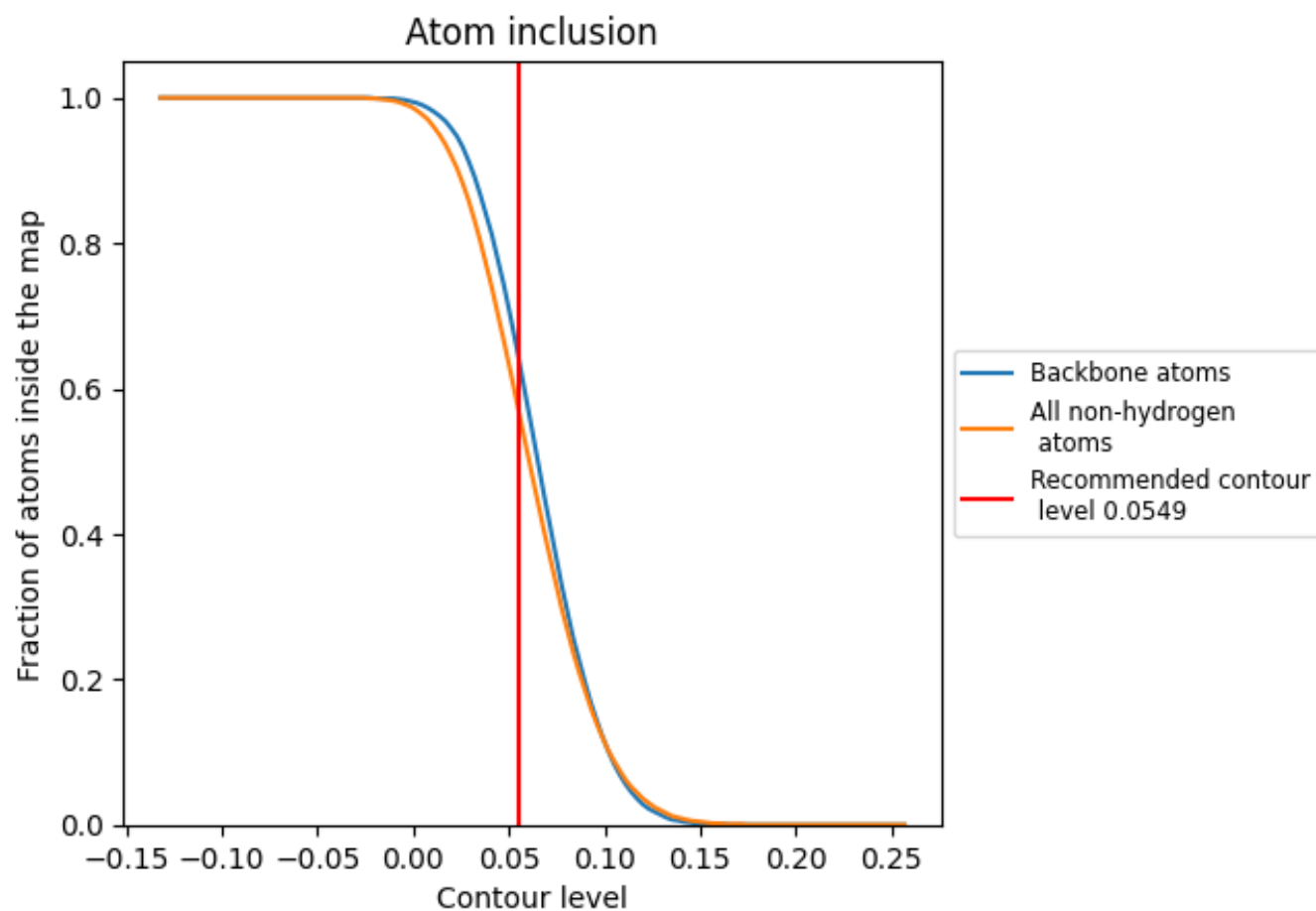
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0549).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (0.0549) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5720	 0.2840
E	 0.6990	 0.2970
L	 0.5230	 0.3590
M	 0.5610	 0.3500
O	 0.3580	 0.2240
P	 0.5280	 0.2910
Q	 0.5310	 0.3060
R	 0.5200	 0.3280
S	 0.4420	 0.3200
T	 0.5040	 0.3360
U	 0.2610	 0.2090
V	 0.4920	 0.3140
W	 0.5510	 0.3340
X	 0.5150	 0.3370
Y	 0.5850	 0.3250
Z	 0.5970	 0.3600
a	 0.2980	 0.1260
b	 0.5500	 0.3240
c	 0.4760	 0.2910
d	 0.5230	 0.3260
e	 0.5470	 0.3480
f	 0.5210	 0.3120
g	 0.5170	 0.3330
h	 0.2970	 0.1270
i	 0.1110	 0.0940
j	 0.1860	 0.1000
k	 0.3770	 0.2550
l	 0.2940	 0.2240
m	 0.2930	 0.2600
n	 0.2960	 0.2120
o	 0.3840	 0.1690
p	 0.1710	 0.1680
q	 0.3770	 0.2290
r	 0.3920	 0.2380
t	 0.2790	 0.1820
u	 0.3230	 0.1910

