



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:41 PM UTC

PDB ID : 6YAN / pdb_00006yan
EMDB ID : EMD-10762
Title : Mammalian 48S late-stage translation initiation complex with histone 4 mRNA
Authors : Bochler, A.; Simonetti, A.; Guca, E.; Hashem, Y.
Deposited on : 2020-03-12
Resolution : 3.48 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
Mogul : 2022.3.0, CSD as543be (2022)
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

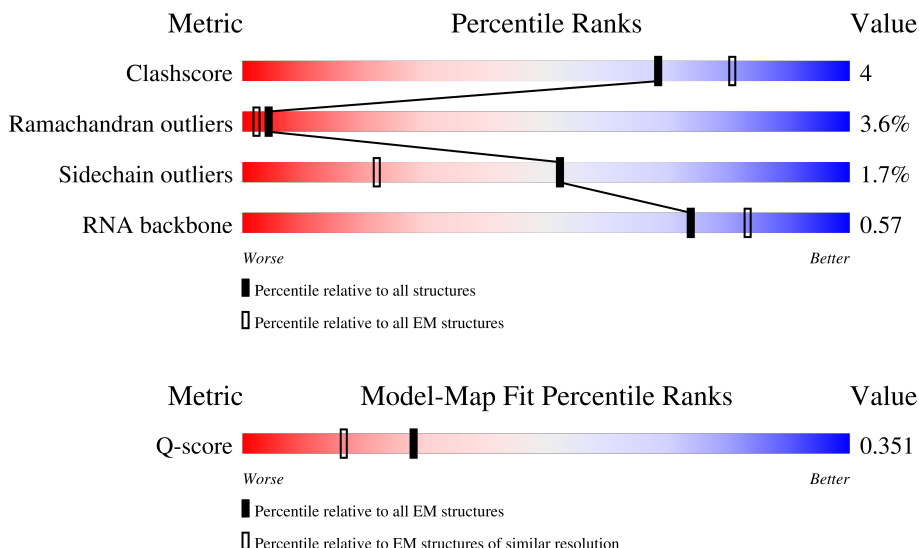
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 Å.

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



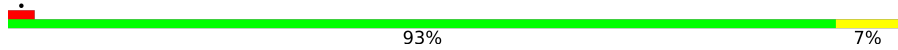
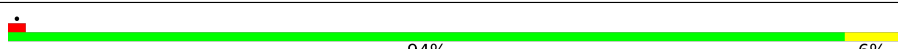
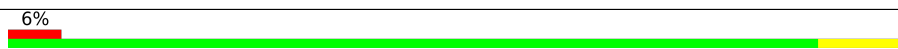
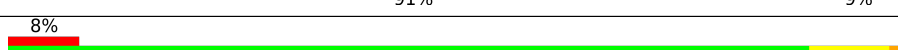
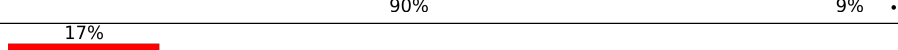
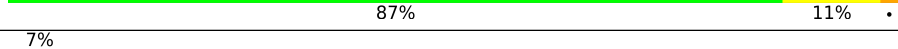
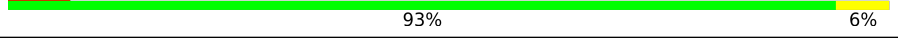
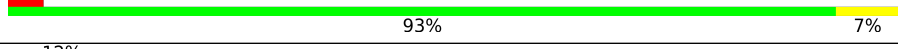
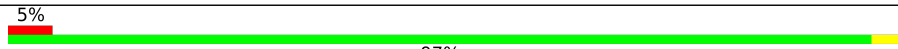
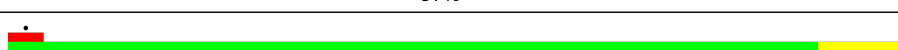
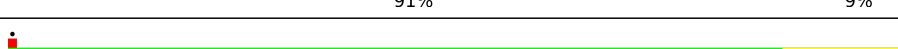
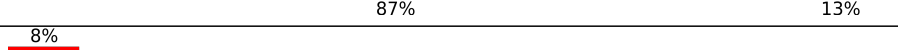
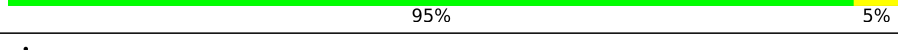
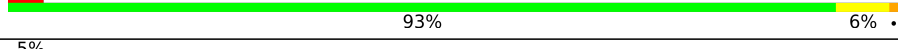
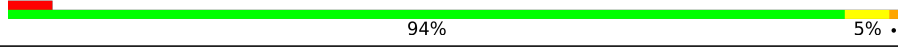
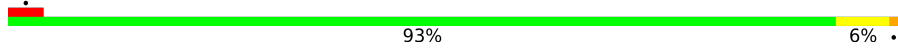
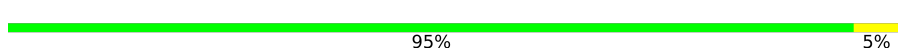
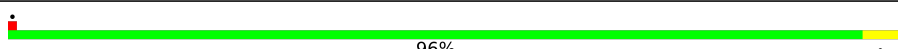
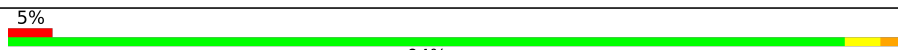
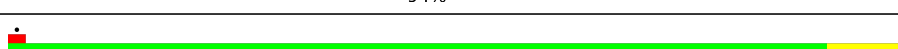
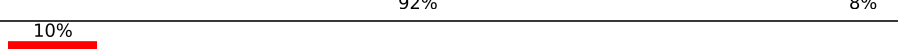
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13672 (2.98 - 3.98)

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	25	16% 88% 12%
2	C	208	92% 8%
3	D	215	90% 8%

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Mol	Chain	Length	Quality of chain
4	E	226	
5	F	227	
6	G	263	
7	H	191	
8	I	237	
9	J	190	
10	K	206	
11	L	182	
12	M	98	
13	N	158	
14	O	124	
15	P	150	
16	Q	136	
17	S	141	
18	T	126	
19	V	141	
20	W	104	
21	X	82	
22	Y	129	
23	Z	142	
24	a	126	
25	b	99	
26	c	84	
27	d	64	
28	e	53	

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Mol	Chain	Length	Quality of chain
29	f	71	
30	g	313	
31	h	75	
32	i	59	
33	2	1863	
34	3	36	
35	A	266	
36	B	422	
37	U	142	
38	R	135	
39	1	75	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	C4J	2	1244	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 84251 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 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1643	1045	289	301	8		

- Molecule 3 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	215	Total	C	N	O	S	0	0
			1742	1107	309	311	15		

- Molecule 4 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	226	Total	C	N	O	S	0	0
			1743	1127	300	307	9		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	227	Total	C	N	O	S	0	0
			1765	1124	317	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	237	Total	C	N	O	S	0	0
			1924	1200	387	330	7		

- Molecule 9 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	190	Total	C	N	O	S	0	0
			1530	975	281	273	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 12 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 15 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 16 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 18 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	126	Total	C	N	O	S	0	0
			1020	639	188	188	5		

- Molecule 19 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 20 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	82	Total	C	N	O	S	0	0
			620	378	117	120	5		

- Molecule 22 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 23 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 24 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	126	Total	C	N	O	S	0	0
			1022	645	198	174	5		

- Molecule 25 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	99	Total	C	N	O	S	0	0
			790	491	162	131	6		

- Molecule 26 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

- Molecule 27 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	64	Total	C	N	O	S	0	0
			507	308	102	95	2		

- Molecule 28 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 29 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

- Molecule 30 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	313	Total	C	N	O	S	0	0
			2437	1535	424	466	12		

- Molecule 31 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

- Molecule 32 is a protein called 40S ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

- Molecule 33 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	1744	Total	C	N	O	P	0	0
			37202	16613	6663	12186	1740		

- Molecule 34 is a RNA chain called histone 4 (H4) mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	36	Total	C	N	O	P	0	0
			774	346	144	249	35		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 36 is a protein called eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 37 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	142	Total	C	N	O	S	0	0
			1172	733	239	199	1		

- Molecule 38 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	135	Total	C	N	O	S	0	0
			1111	704	211	189	7		

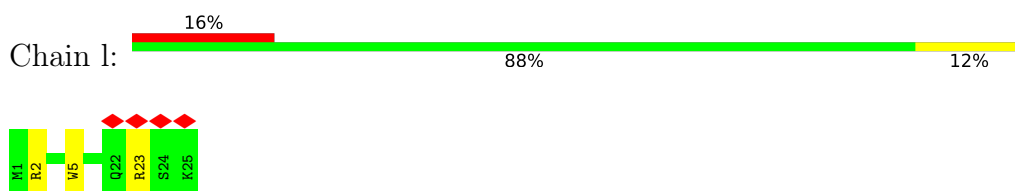
- Molecule 39 is a RNA chain called initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	75	Total	C	N	O	P	0	0
			1614	722	299	519	74		

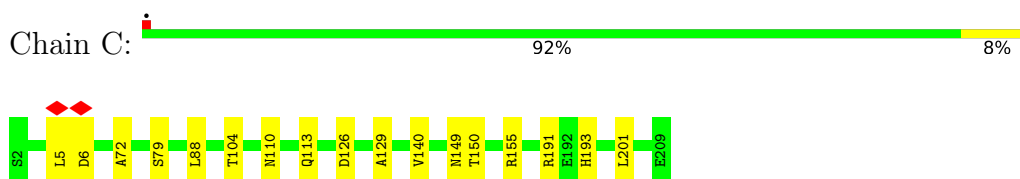
3 Residue-property plots

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.

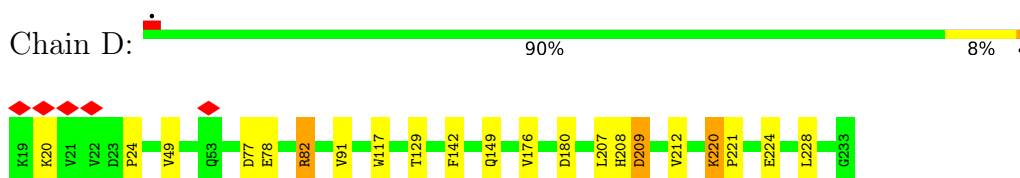
- Molecule 1: 60s ribosomal protein l41



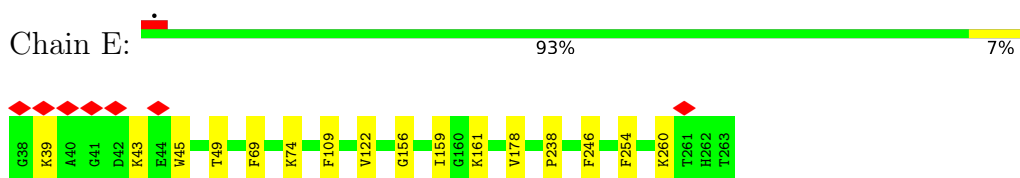
- Molecule 2: 40S ribosomal protein SA



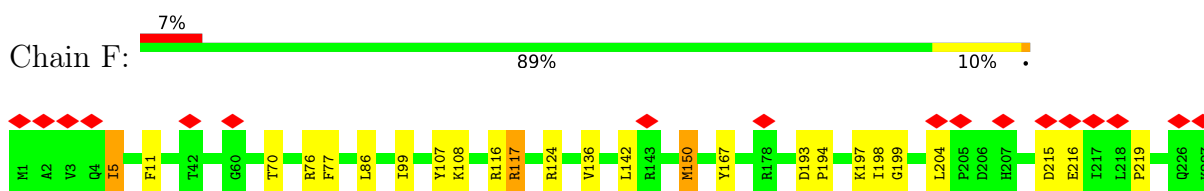
- Molecule 3: ribosomal protein eS1



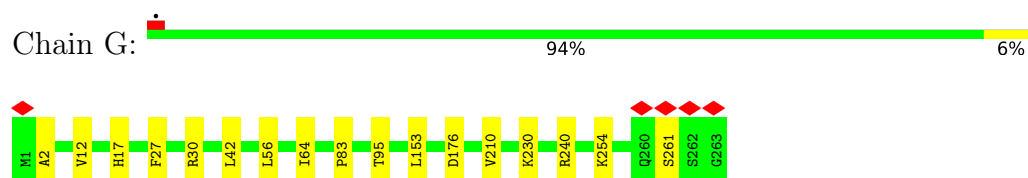
- Molecule 4: 40S ribosomal protein uS5



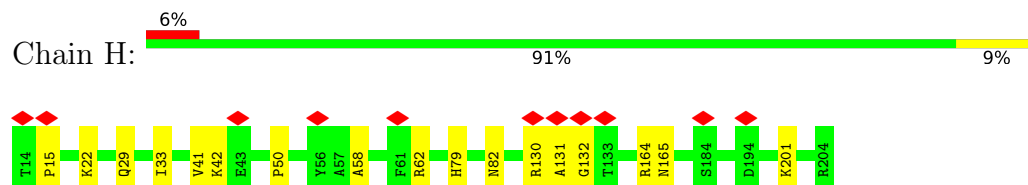
- Molecule 5: Ribosomal protein S3



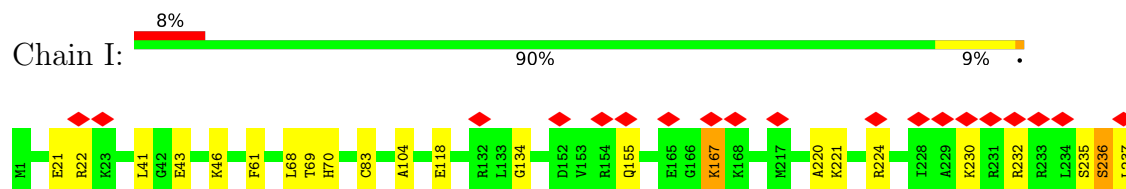
- Molecule 6: 40S ribosomal protein S4



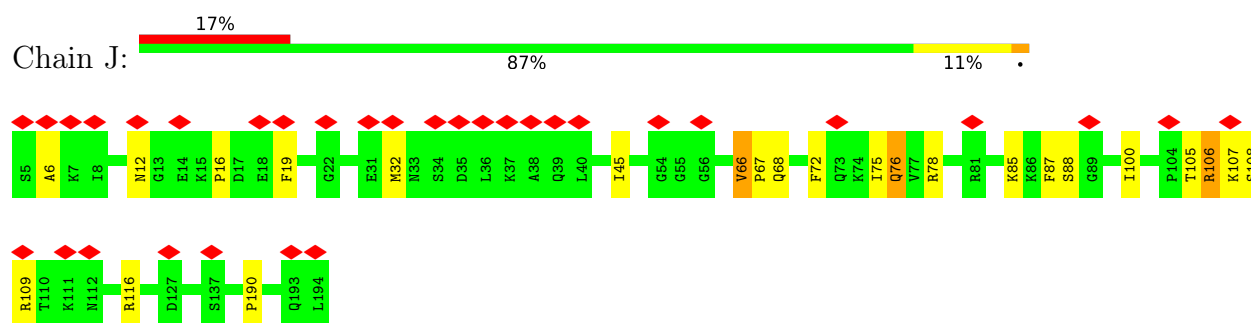
- Molecule 7: Ribosomal protein S5



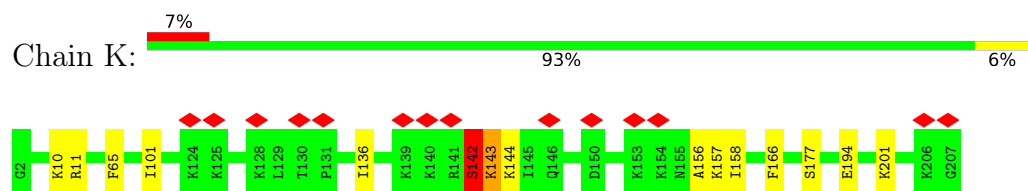
- Molecule 8: 40S ribosomal protein S6



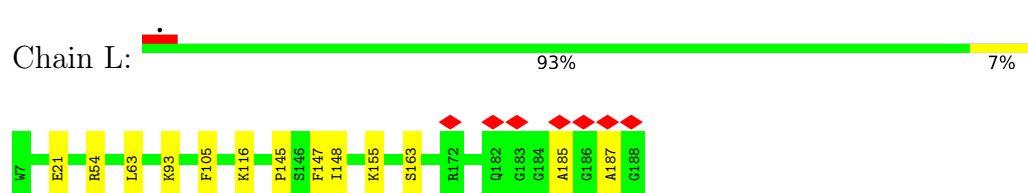
- Molecule 9: ribosomal protein eS7



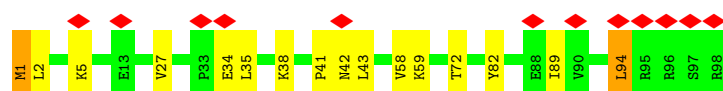
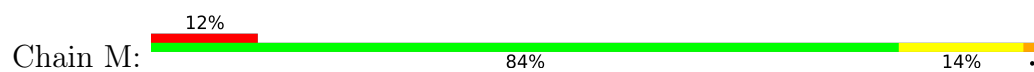
- Molecule 10: 40S ribosomal protein S8



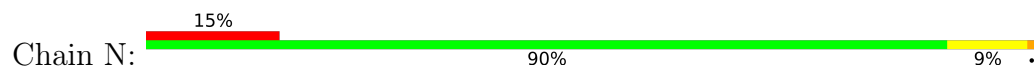
- Molecule 11: Ribosomal protein S9 (Predicted)



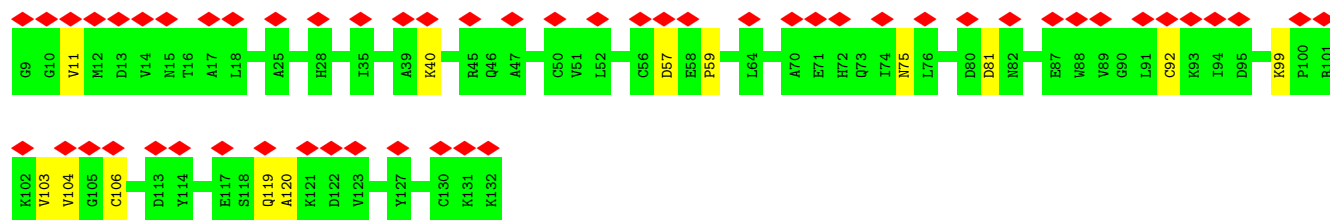
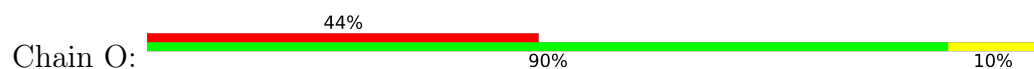
- Molecule 12: 40S ribosomal protein eS10



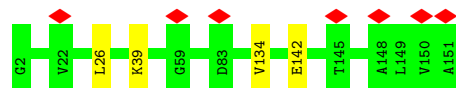
• Molecule 13: Ribosomal protein S11



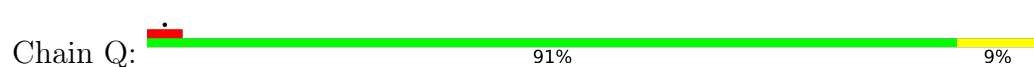
• Molecule 14: 40S ribosomal protein S12



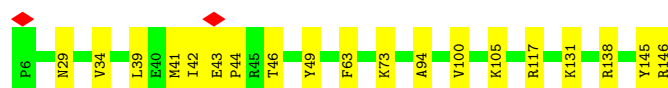
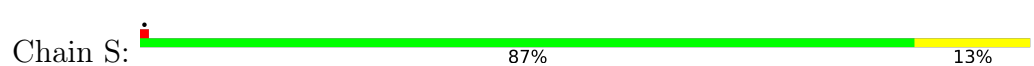
• Molecule 15: ribosomal protein uS15



• Molecule 16: 40S ribosomal protein uS11

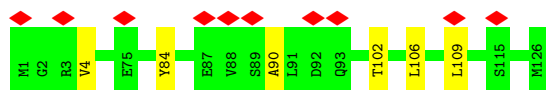


• Molecule 17: ribosomal protein uS9



• Molecule 18: ribosomal protein eS17





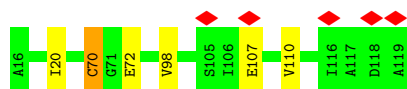
- Molecule 19: 40S ribosomal protein eS19

Chain V: 93% 6% .



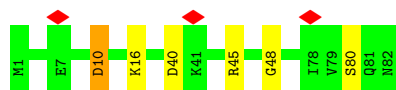
- Molecule 20: Ribosomal_S10 domain-containing protein

Chain W: 5% 94% 5% .



- Molecule 21: 40S ribosomal protein S21

Chain X: 93% 6% .



- Molecule 22: Ribosomal protein S15a

Chain Y: 95% 5% .



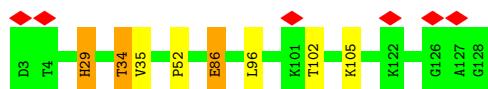
- Molecule 23: 40S ribosomal protein uS12

Chain Z: 96% .



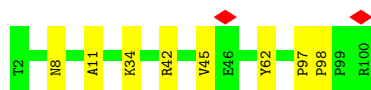
- Molecule 24: 40S ribosomal protein S24

Chain a: 5% 94% . .

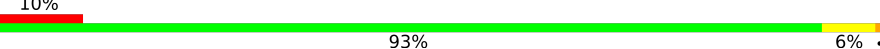


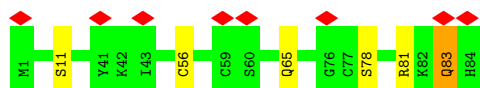
- Molecule 25: 40S ribosomal protein eS26

Chain b:  92% 8%

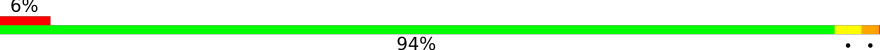


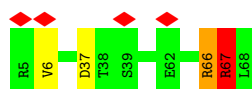
- Molecule 26: 40S ribosomal protein S27

Chain c:  10% 93% 6%



- Molecule 27: ribosomal protein eS28

Chain d:  6% 94% . . .



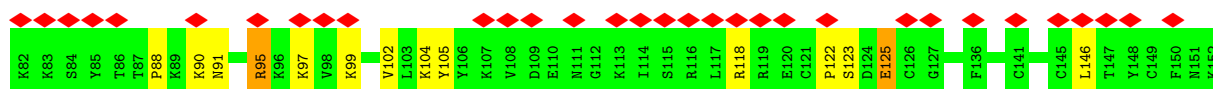
- Molecule 28: ribosomal protein uS14

Chain e:  85% 15%

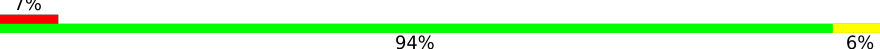


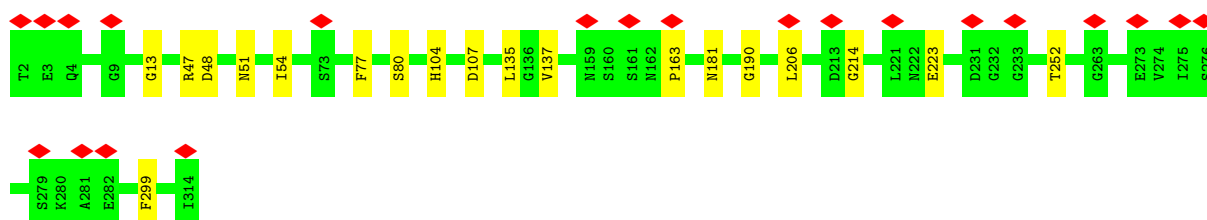
- Molecule 29: ribosomal protein eS31

Chain f:  45% 80% 17% .



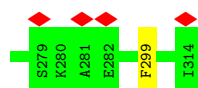
- Molecule 30: ribosomal protein RACK1

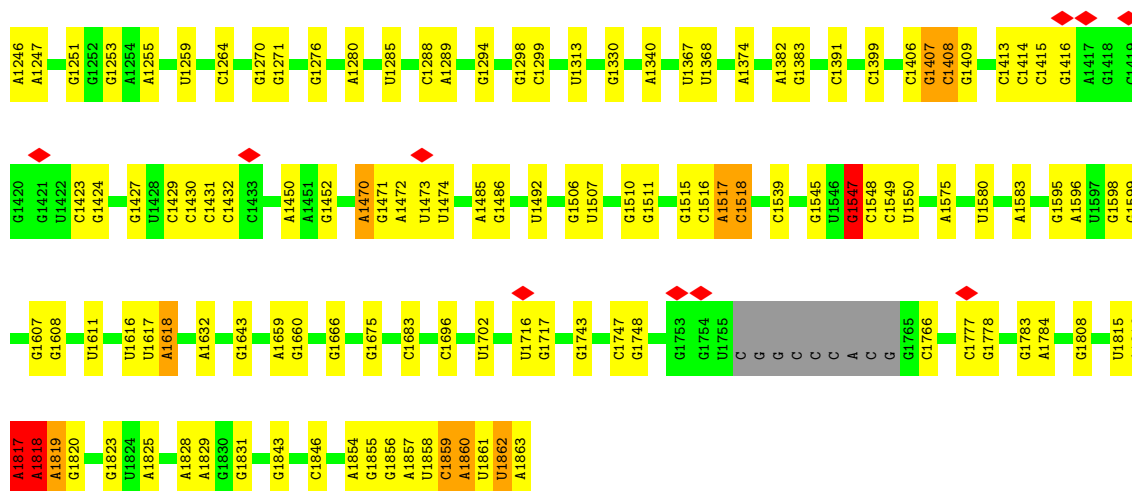
Chain g:  7% 94% 6%



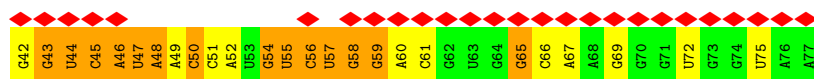
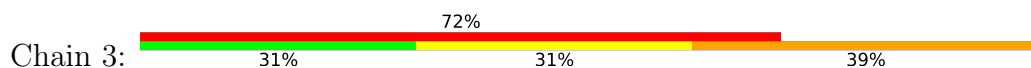
- Molecule 31: ribosomal protein eS25

Chain h:  12% 85% 13%

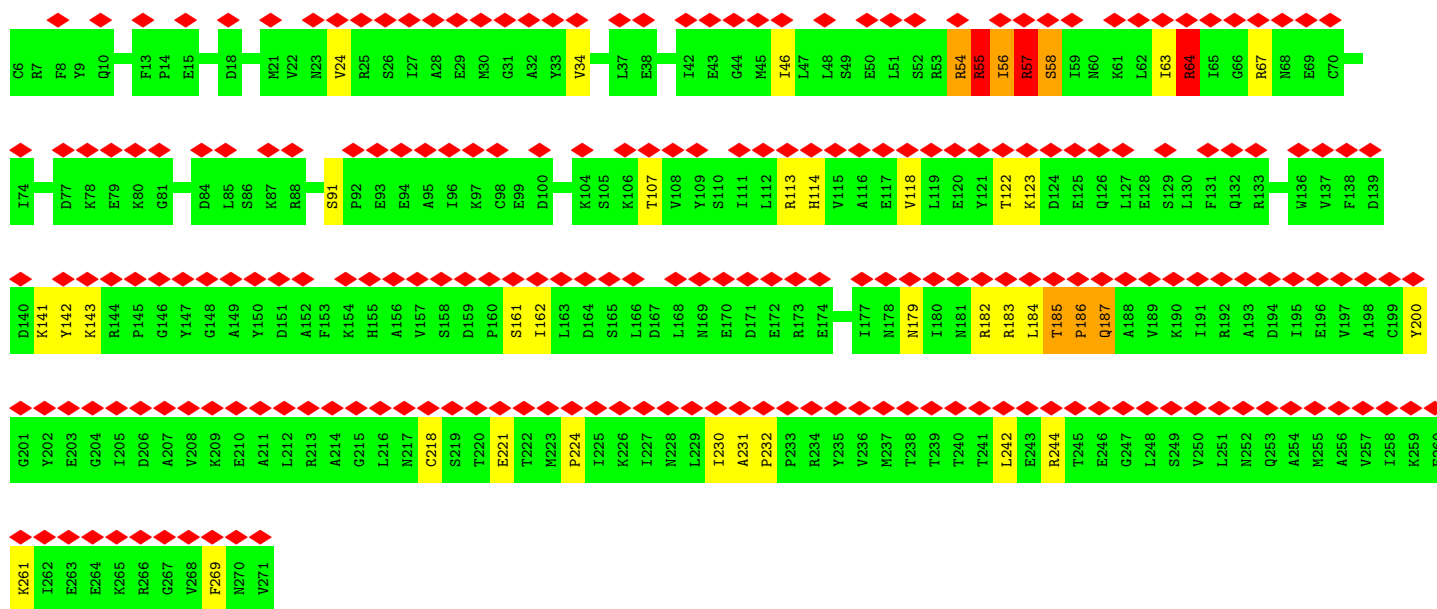
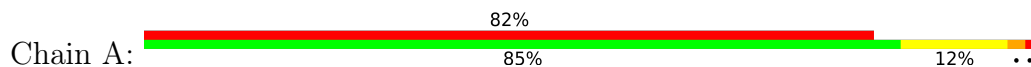




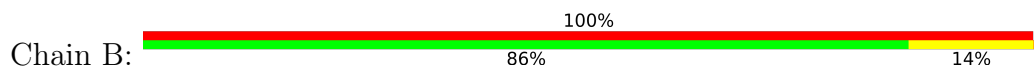
• Molecule 34: histone 4 (H4) mRNA

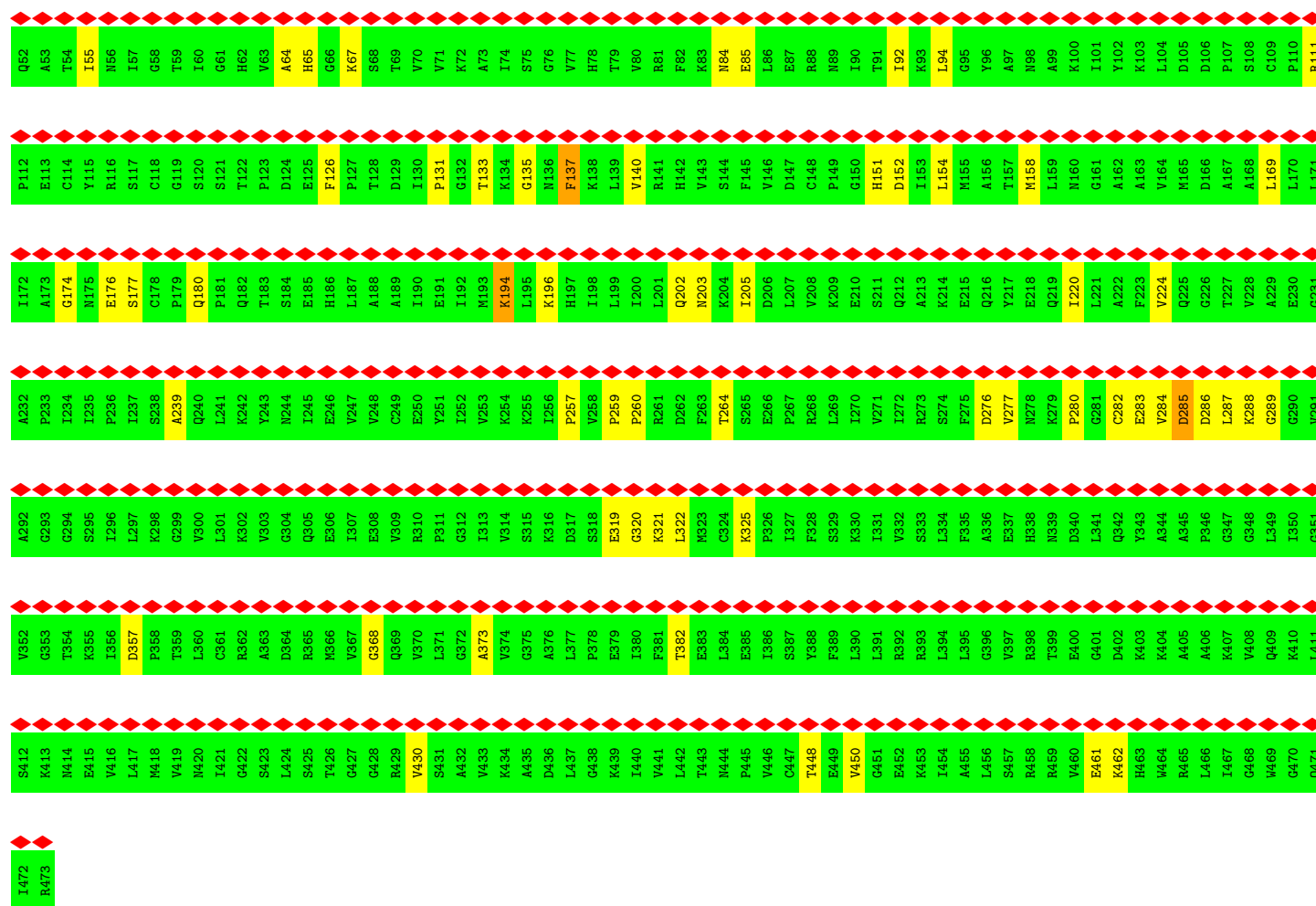


• Molecule 35: Eukaryotic translation initiation factor 2 subunit 1

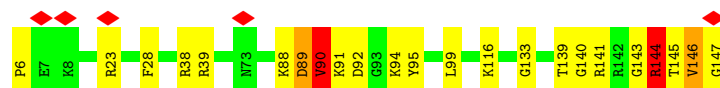
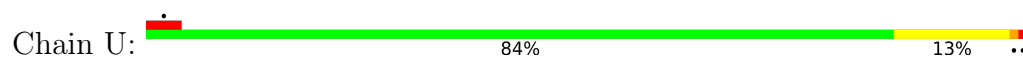


• Molecule 36: eukaryotic translation initiation factor 2 subunit gamma

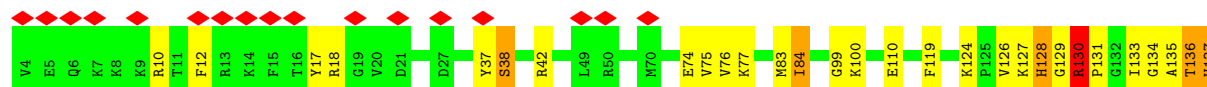
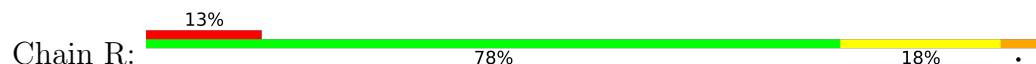




- Molecule 37: 40S ribosomal protein uS13

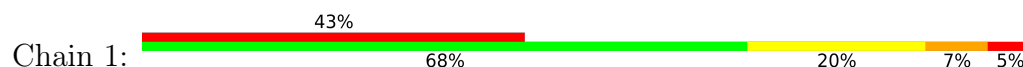


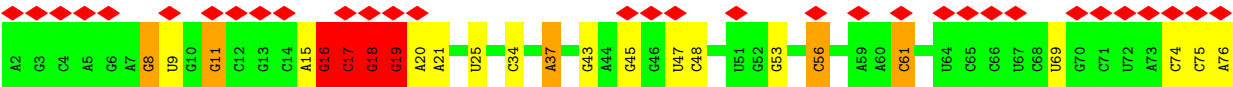
- Molecule 38: Ribosomal protein S15



S138

- Molecule 39: initiator methionylated tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0109	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, C4J

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	I	1.58	0/241	1.45	0/305
2	C	1.26	0/1680	1.42	3/2283 (0.1%)
3	D	1.23	0/1770	1.47	13/2367 (0.5%)
4	E	1.22	0/1779	1.37	10/2399 (0.4%)
5	F	1.27	0/1793	1.45	7/2412 (0.3%)
6	G	1.29	0/2125	1.42	9/2856 (0.3%)
7	H	1.28	0/1531	1.44	5/2059 (0.2%)
8	I	1.37	0/1946	1.44	18/2587 (0.7%)
9	J	1.26	0/1553	1.46	9/2079 (0.4%)
10	K	1.32	0/1709	1.44	7/2278 (0.3%)
11	L	1.36	0/1523	1.45	3/2031 (0.1%)
12	M	1.27	0/852	1.52	6/1147 (0.5%)
13	N	1.30	0/1319	1.36	6/1761 (0.3%)
14	O	1.20	0/968	1.68	12/1296 (0.9%)
15	P	1.25	0/1232	1.50	3/1656 (0.2%)
16	Q	1.32	0/1029	1.47	7/1380 (0.5%)
17	S	1.30	0/1141	1.47	6/1528 (0.4%)
18	T	1.27	0/1032	1.43	3/1383 (0.2%)
19	V	1.26	0/1133	1.53	7/1517 (0.5%)
20	W	1.28	0/832	1.46	3/1117 (0.3%)
21	X	1.33	0/627	1.39	6/839 (0.7%)
22	Y	1.31	0/1051	1.40	6/1406 (0.4%)
23	Z	1.32	0/1125	1.40	0/1500
24	a	1.30	0/1038	1.47	5/1377 (0.4%)
25	b	1.38	0/803	1.44	2/1076 (0.2%)
26	c	1.25	0/673	1.43	5/902 (0.6%)
27	d	1.44	0/509	1.30	1/680 (0.1%)
28	e	1.38	0/455	1.37	2/603 (0.3%)
29	f	1.27	0/594	1.43	4/786 (0.5%)
30	g	1.26	0/2494	1.41	11/3394 (0.3%)
31	h	1.25	0/605	1.48	7/810 (0.9%)
32	i	1.37	0/478	1.47	4/628 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2	0.92	11/41562 (0.0%)	1.06	39/64770 (0.1%)
34	3	0.71	0/867	0.86	0/1352
35	A	1.27	1/2178 (0.0%)	1.62	28/2935 (1.0%)
36	B	1.22	0/3267	1.55	42/4415 (1.0%)
37	U	1.28	0/1190	1.45	3/1592 (0.2%)
38	R	1.24	0/1132	1.38	6/1510 (0.4%)
39	1	1.77	9/1770 (0.5%)	1.64	17/2759 (0.6%)
All	All	1.14	21/89606 (0.0%)	1.27	325/129775 (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
2	C	0	1
3	D	0	1
5	F	0	2
8	I	0	2
9	J	0	2
11	L	0	2
12	M	0	5
17	S	0	2
26	c	0	1
28	e	0	2
29	f	0	1
31	h	0	1
32	i	0	2
33	2	1	64
34	3	1	0
35	A	0	8
36	B	0	11
37	U	0	3
39	1	3	3
All	All	5	113

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	19	G	O3'-P	34.80	2.13	1.61
39	1	16	G	O3'-P	-31.34	1.14	1.61
39	1	17	C	O3'-P	25.68	1.99	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	1815	U	O3'-P	-23.38	1.26	1.61
39	1	17	C	C2'-O2'	-22.58	1.07	1.41
39	1	18	G	O3'-P	17.34	1.87	1.61
33	2	350	A	O3'-P	16.96	1.86	1.61
33	2	1172	G	O3'-P	-15.96	1.37	1.61
39	1	18	G	C3'-O3'	-15.66	1.18	1.42
33	2	675	A	O3'-P	15.56	1.84	1.61
33	2	676	U	O3'-P	-15.28	1.38	1.61
33	2	797	U	O3'-P	-11.58	1.43	1.61
33	2	351	U	O3'-P	-10.89	1.44	1.61
39	1	37	T6A	O3'-P	8.82	1.65	1.56
33	2	1170	U	O3'-P	-8.22	1.48	1.61
39	1	18	G	C1'-N9	-8.13	1.35	1.48
33	2	1171	G	O3'-P	-7.43	1.50	1.61
33	2	1170	U	C1'-N1	6.22	1.57	1.48
33	2	1816	A	O3'-P	-6.17	1.51	1.61
35	A	57	ARG	C-N	-6.15	1.25	1.33
39	1	17	C	C3'-O3'	-5.93	1.34	1.43

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	1	19	G	O3'-P-O5'	40.40	164.60	104.00
39	1	17	C	C4'-C3'-O3'	24.13	145.59	109.40
33	2	797	U	O3'-P-O5'	-22.57	70.15	104.00
33	2	676	U	O3'-P-O5'	-22.25	70.62	104.00
35	A	54	ARG	CA-C-N	21.29	151.05	122.30
35	A	54	ARG	C-N-CA	21.29	151.05	122.30
39	1	16	G	P-O3'-C3'	18.27	147.60	120.20
39	1	17	C	O3'-P-O5'	17.52	130.28	104.00
39	1	18	G	O3'-P-O5'	16.96	129.44	104.00
33	2	351	U	P-O3'-C3'	14.54	142.01	120.20
33	2	1817	A	P-O3'-C3'	-14.24	98.83	120.20
39	1	19	G	OP1-P-O3'	-13.50	67.51	108.00
33	2	1171	G	O3'-P-O5'	13.15	123.73	104.00
39	1	8	G	P-O3'-C3'	10.72	136.28	120.20
33	2	1854	A	P-O3'-C3'	10.47	135.91	120.20
33	2	351	U	O3'-P-O5'	10.32	119.48	104.00
33	2	677	C	O3'-P-O5'	9.62	118.44	104.00
33	2	1172	G	P-O3'-C3'	9.49	134.43	120.20
35	A	54	ARG	O-C-N	-9.22	112.27	122.88
17	S	46	THR	N-CA-C	-9.22	104.11	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	g	54	ILE	N-CA-C	-9.01	101.80	109.19
35	A	56	ILE	CA-C-N	-8.75	106.47	122.31
35	A	56	ILE	C-N-CA	-8.75	106.47	122.31
33	2	1816	A	P-O3'-C3'	-8.74	107.08	120.20
6	G	12	VAL	N-CA-C	-8.52	104.72	112.90
33	2	1816	A	O3'-P-O5'	-8.43	91.36	104.00
33	2	1818	A	C4'-C3'-O3'	8.31	121.87	109.40
39	1	16	G	OP1-P-O3'	8.18	132.53	108.00
22	Y	84	LYS	N-CA-C	-8.17	104.46	114.75
25	b	34	LYS	N-CA-C	-8.16	105.31	114.62
33	2	675	A	O3'-P-O5'	-8.15	91.78	104.00
39	1	19	G	P-O3'-C3'	8.13	132.40	120.20
35	A	230	ILE	N-CA-C	-8.10	104.86	112.96
6	G	64	ILE	N-CA-C	-8.07	103.95	111.45
33	2	1818	A	C2'-C3'-O3'	8.04	121.56	109.50
33	2	1170	U	P-O3'-C3'	7.99	132.19	120.20
14	O	59	PRO	N-CA-C	-7.93	104.53	114.68
14	O	92	CYS	N-CA-C	-7.91	105.60	114.62
10	K	142	SER	CA-C-N	7.86	135.85	121.70
10	K	142	SER	C-N-CA	7.86	135.85	121.70
33	2	351	U	OP1-P-O3'	-7.75	84.74	108.00
18	T	102	THR	N-CA-C	-7.70	103.50	113.12
36	B	319	GLU	N-CA-C	-7.67	105.08	114.75
35	A	113	ARG	N-CA-C	-7.62	103.84	113.43
9	J	87	PHE	CA-CB-CG	-7.61	106.19	113.80
36	B	239	ALA	N-CA-C	-7.61	105.16	114.75
39	1	19	G	OP2-P-O3'	-7.60	85.19	108.00
33	2	1470	A	P-O3'-C3'	7.57	131.55	120.20
17	S	117	ARG	N-CA-C	-7.56	101.49	110.41
36	B	276	ASP	CA-C-N	7.41	135.04	121.70
36	B	276	ASP	C-N-CA	7.41	135.04	121.70
30	g	181	ASN	N-CA-C	-7.40	106.18	114.62
39	1	18	G	C4'-C3'-O3'	7.33	124.00	113.00
10	K	157	LYS	N-CA-C	-7.26	104.28	113.43
10	K	65	PHE	CA-CB-CG	-7.15	106.65	113.80
33	2	1407	G	P-O3'-C3'	7.14	130.91	120.20
35	A	57	ARG	CA-C-N	7.11	135.12	121.54
35	A	57	ARG	C-N-CA	7.11	135.12	121.54
7	H	33	ILE	N-CA-C	-7.07	106.11	112.90
12	M	27	VAL	N-CA-C	-7.04	105.95	112.43
4	E	69	PHE	CA-CB-CG	-6.95	106.85	113.80
15	P	134	VAL	N-CA-C	-6.86	106.32	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	43	GLU	N-CA-C	-6.84	105.87	114.56
22	Y	6	VAL	N-CA-C	-6.83	105.10	111.45
35	A	232	PRO	N-CA-C	6.81	119.00	110.70
24	a	105	LYS	N-CA-C	-6.80	104.14	113.18
33	2	798	A	O5'-C5'-C4'	6.79	121.69	111.50
36	B	220	ILE	N-CA-CB	6.77	118.47	110.55
39	1	16	G	O3'-P-O5'	-6.70	93.95	104.00
33	2	1218	G	O3'-P-O5'	-6.69	93.97	104.00
37	U	28	PHE	CA-CB-CG	-6.68	107.12	113.80
18	T	109	LEU	N-CA-C	-6.68	105.03	113.72
29	f	105	TYR	N-CA-C	-6.62	105.24	113.38
24	a	102	THR	N-CA-C	6.58	118.24	111.14
39	1	17	C	P-O3'-C3'	6.56	130.04	120.20
33	2	581	U	P-O3'-C3'	6.55	130.03	120.20
5	F	197	LYS	CA-C-N	6.55	133.49	121.70
5	F	197	LYS	C-N-CA	6.55	133.49	121.70
14	O	104	VAL	CA-C-N	6.51	126.29	120.10
14	O	104	VAL	C-N-CA	6.51	126.29	120.10
33	2	676	U	OP2-P-O3'	6.50	127.50	108.00
14	O	119	GLN	CA-C-N	6.49	131.08	120.63
14	O	119	GLN	C-N-CA	6.49	131.08	120.63
36	B	94	LEU	CA-C-N	6.39	126.41	120.34
36	B	94	LEU	C-N-CA	6.39	126.41	120.34
32	i	118	ASN	CA-C-N	6.38	133.19	121.70
32	i	118	ASN	C-N-CA	6.38	133.19	121.70
14	O	120	ALA	CA-C-N	6.38	129.12	120.38
14	O	120	ALA	C-N-CA	6.38	129.12	120.38
36	B	84	ASN	CA-C-N	6.32	133.08	121.70
36	B	84	ASN	C-N-CA	6.32	133.08	121.70
14	O	57	ASP	N-CA-C	-6.31	107.42	114.62
36	B	357	ASP	CA-C-N	6.30	127.71	119.84
36	B	357	ASP	C-N-CA	6.30	127.71	119.84
5	F	11	PHE	CA-CB-CG	-6.23	107.57	113.80
11	L	105	PHE	CA-CB-CG	-6.23	107.57	113.80
21	X	48	GLY	CA-C-N	6.21	130.21	121.02
21	X	48	GLY	C-N-CA	6.21	130.21	121.02
36	B	382	THR	N-CA-C	-6.18	106.33	114.31
36	B	137	PHE	CA-CB-CG	6.16	119.96	113.80
33	2	320	G	C5'-C4'-C3'	-6.13	106.80	116.00
3	D	209	ASP	N-CA-CB	6.10	120.80	110.49
36	B	55	ILE	N-CA-C	-6.08	99.72	108.42
33	2	537	G	P-O5'-C5'	6.06	129.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	545	A	P-O3'-C3'	6.05	129.28	120.20
7	H	15	PRO	N-CA-C	-6.05	107.72	114.92
12	M	1	MET	CA-C-N	6.05	132.59	121.70
12	M	1	MET	C-N-CA	6.05	132.59	121.70
16	Q	91	THR	N-CA-C	-6.03	107.15	114.75
3	D	24	PRO	N-CA-C	-6.02	107.75	114.92
3	D	78	GLU	CA-C-N	5.99	128.68	120.35
3	D	78	GLU	C-N-CA	5.99	128.68	120.35
37	U	92	ASP	N-CA-C	-5.99	107.79	114.62
6	G	56	LEU	N-CA-C	-5.98	107.21	114.75
39	1	18	G	OP1-P-O3'	-5.96	90.11	108.00
10	K	101	ILE	N-CA-C	-5.92	99.60	108.12
36	B	152	ASP	CA-C-N	5.91	128.56	120.46
36	B	152	ASP	C-N-CA	5.91	128.56	120.46
19	V	46	ALA	CA-C-N	5.90	125.91	119.89
19	V	46	ALA	C-N-CA	5.90	125.91	119.89
35	A	46	ILE	N-CA-C	-5.87	99.87	108.97
20	W	70	CYS	CA-C-N	5.86	125.54	119.92
20	W	70	CYS	C-N-CA	5.86	125.54	119.92
9	J	72	PHE	CA-CB-CG	-5.86	107.94	113.80
31	h	51	ASP	CA-C-N	5.85	128.92	120.79
31	h	51	ASP	C-N-CA	5.85	128.92	120.79
36	B	92	ILE	N-CA-C	-5.84	107.05	112.83
36	B	140	VAL	N-CA-C	-5.81	106.82	111.81
4	E	109	PHE	CA-CB-CG	-5.80	108.00	113.80
3	D	82	ARG	N-CA-CB	5.76	120.23	110.49
31	h	52	LYS	CA-C-N	5.76	128.00	120.28
31	h	52	LYS	C-N-CA	5.76	128.00	120.28
33	2	79	A	C4'-C3'-C2'	-5.76	96.84	102.60
33	2	675	A	P-O3'-C3'	-5.74	111.59	120.20
9	J	68	GLN	CA-C-N	5.72	128.22	120.38
9	J	68	GLN	C-N-CA	5.72	128.22	120.38
35	A	231	ALA	N-CA-C	-5.72	103.07	108.22
33	2	1424	G	C5'-C4'-C3'	5.67	124.50	116.00
38	R	119	PHE	CA-CB-CG	-5.65	108.15	113.80
22	Y	3	ARG	N-CA-C	-5.64	98.78	110.80
4	E	74	LYS	N-CA-C	-5.64	107.64	114.75
9	J	19	PHE	CA-CB-CG	-5.63	108.17	113.80
14	O	120	ALA	N-CA-C	5.62	119.64	112.34
22	Y	62	VAL	N-CA-C	-5.60	100.17	108.45
36	B	259	PRO	CA-C-N	5.59	126.83	119.84
36	B	259	PRO	C-N-CA	5.59	126.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	210	VAL	N-CA-C	-5.58	100.44	108.42
11	L	145	PRO	N-CA-C	-5.58	108.28	114.92
30	g	214	GLY	N-CA-C	-5.57	107.01	114.25
39	1	17	C	OP2-P-O3'	-5.56	91.31	108.00
35	A	122	THR	N-CA-C	-5.55	104.06	112.99
36	B	158	MET	CA-C-N	5.55	127.65	120.44
36	B	158	MET	C-N-CA	5.55	127.65	120.44
13	N	62	PHE	CA-CB-CG	-5.54	108.25	113.80
13	N	134	LEU	N-CA-C	-5.54	107.06	113.88
30	g	77	PHE	CA-CB-CG	-5.53	108.27	113.80
22	Y	119	LYS	N-CA-C	-5.53	106.58	113.38
33	2	1172	G	OP2-P-O3'	-5.53	91.41	108.00
12	M	5	LYS	N-CA-C	-5.53	106.38	113.23
4	E	254	PHE	CA-CB-CG	-5.53	108.28	113.80
21	X	80	SER	N-CA-C	-5.52	107.79	114.75
14	O	106	CYS	N-CA-C	-5.52	106.71	113.50
16	Q	139	SER	CA-C-N	5.52	132.08	121.54
16	Q	139	SER	C-N-CA	5.52	132.08	121.54
16	Q	107	THR	CA-C-N	5.49	125.49	119.89
16	Q	107	THR	C-N-CA	5.49	125.49	119.89
3	D	220	LYS	N-CA-C	-5.48	103.29	108.22
35	A	118	VAL	N-CA-C	-5.47	105.34	113.39
3	D	224	GLU	CA-C-N	5.47	127.88	120.38
3	D	224	GLU	C-N-CA	5.47	127.88	120.38
30	g	47	ARG	N-CA-C	-5.47	105.97	113.30
33	2	869	G	P-O3'-C3'	5.46	128.38	120.20
37	U	90	VAL	N-CA-C	-5.46	97.99	109.34
8	I	232	ARG	CA-C-N	5.44	127.51	120.44
8	I	232	ARG	C-N-CA	5.44	127.51	120.44
26	c	65	GLN	CA-C-N	5.43	125.44	119.90
26	c	65	GLN	C-N-CA	5.43	125.44	119.90
33	2	536	G	O3'-P-O5'	5.42	112.13	104.00
18	T	4	VAL	N-CA-C	-5.41	100.69	108.48
24	a	35	VAL	CA-C-N	5.41	125.41	119.89
24	a	35	VAL	C-N-CA	5.41	125.41	119.89
35	A	123	LYS	CA-C-N	5.41	128.07	120.28
35	A	123	LYS	C-N-CA	5.41	128.07	120.28
36	B	180	GLN	CA-C-N	5.41	126.60	119.84
36	B	180	GLN	C-N-CA	5.41	126.60	119.84
8	I	21	GLU	CA-C-N	5.40	127.78	120.44
8	I	21	GLU	C-N-CA	5.40	127.78	120.44
39	1	16	G	OP2-P-O3'	-5.39	91.84	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	40	ALA	CA-C-N	5.38	127.49	120.28
19	V	40	ALA	C-N-CA	5.38	127.49	120.28
21	X	10	ASP	N-CA-CB	5.38	119.58	110.49
24	a	86	GLU	N-CA-CB	5.37	119.94	110.37
3	D	176	VAL	N-CA-C	-5.37	108.27	113.53
5	F	204	LEU	CA-C-N	5.37	126.55	119.84
5	F	204	LEU	C-N-CA	5.37	126.55	119.84
10	K	143	LYS	N-CA-CB	5.37	119.62	110.50
36	B	194	LYS	N-CA-CB	5.36	119.55	110.49
12	M	72	THR	CA-C-N	5.36	127.47	120.28
12	M	72	THR	C-N-CA	5.36	127.47	120.28
6	G	27	PHE	CA-CB-CG	-5.36	108.44	113.80
6	G	42	LEU	CA-C-N	5.34	125.34	119.89
6	G	42	LEU	C-N-CA	5.34	125.34	119.89
26	c	56	CYS	N-CA-C	-5.34	101.24	109.52
30	g	80	SER	CA-C-N	5.34	125.28	121.65
30	g	80	SER	C-N-CA	5.34	125.28	121.65
32	i	87	ARG	N-CA-C	-5.33	108.54	114.62
8	I	224	ARG	CA-C-N	5.33	127.36	120.44
8	I	224	ARG	C-N-CA	5.33	127.36	120.44
33	2	224	U	P-O3'-C3'	5.32	128.19	120.20
6	G	95	THR	N-CA-C	-5.32	107.80	114.56
35	A	162	ILE	N-CA-C	-5.31	107.20	113.42
33	2	229	A	O3'-P-O5'	-5.31	96.04	104.00
35	A	114	HIS	CA-C-N	5.30	127.72	120.46
35	A	114	HIS	C-N-CA	5.30	127.72	120.46
35	A	269	PHE	CA-CB-CG	-5.30	108.50	113.80
31	h	55	TYR	CB-CA-C	-5.29	101.86	110.85
38	R	38	SER	CA-C-N	5.28	128.75	120.82
38	R	38	SER	C-N-CA	5.28	128.75	120.82
10	K	136	ILE	N-CA-C	-5.28	107.98	113.10
33	2	536	G	P-O3'-C3'	5.28	128.12	120.20
36	B	67	LYS	N-CA-C	-5.28	106.52	113.12
8	I	118	GLU	N-CA-C	-5.27	107.02	113.50
14	O	11	VAL	N-CA-C	-5.27	107.84	112.90
6	G	261	SER	N-CA-C	-5.27	106.36	114.16
29	f	95	ARG	N-CA-CB	5.27	119.39	110.49
36	B	202	GLN	CA-C-N	5.26	127.28	120.44
36	B	202	GLN	C-N-CA	5.26	127.28	120.44
38	R	124	LYS	CA-C-N	5.26	125.32	119.32
38	R	124	LYS	C-N-CA	5.26	125.32	119.32
36	B	126	PHE	CA-CB-CG	-5.26	108.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	70	SER	CA-C-N	5.25	124.43	118.97
16	Q	70	SER	C-N-CA	5.25	124.43	118.97
20	W	110	VAL	N-CA-C	-5.24	101.43	108.35
22	Y	97	ARG	N-CA-C	-5.24	106.93	113.38
30	g	299	PHE	N-CA-C	-5.23	101.45	109.41
30	g	252	THR	N-CA-C	-5.23	102.45	110.14
36	B	320	GLY	N-CA-C	-5.23	105.12	112.13
33	2	181	A	P-O5'-C5'	5.22	128.73	120.90
33	2	1203	G	C4'-C3'-O3'	-5.22	105.17	113.00
8	I	134	GLY	CA-C-N	5.21	126.35	119.84
8	I	134	GLY	C-N-CA	5.21	126.35	119.84
9	J	116	ARG	CA-C-N	5.21	125.20	119.89
9	J	116	ARG	C-N-CA	5.21	125.20	119.89
27	d	6	VAL	N-CA-C	-5.21	107.68	112.83
39	1	18	G	P-O3'-C3'	5.19	127.99	120.20
13	N	129	GLY	CA-C-N	5.19	128.08	120.71
13	N	129	GLY	C-N-CA	5.19	128.08	120.71
2	C	79	SER	N-CA-C	-5.19	108.70	114.62
33	2	1766	C	O3'-P-O5'	5.19	111.78	104.00
8	I	221	LYS	CA-C-N	5.18	127.18	120.44
8	I	221	LYS	C-N-CA	5.18	127.18	120.44
3	D	180	ASP	CA-C-N	5.18	128.59	120.82
3	D	180	ASP	C-N-CA	5.18	128.59	120.82
36	B	169	LEU	N-CA-C	-5.18	98.84	107.80
7	H	82	ASN	CA-CB-CG	-5.17	107.43	112.60
33	2	543	U	P-O5'-C5'	5.17	128.66	120.90
4	E	238	PRO	CA-C-N	5.17	127.46	120.38
4	E	238	PRO	C-N-CA	5.17	127.46	120.38
4	E	49	THR	CA-C-N	5.15	127.13	120.44
4	E	49	THR	C-N-CA	5.15	127.13	120.44
5	F	77	PHE	CA-CB-CG	-5.15	108.65	113.80
17	S	34	VAL	N-CA-C	-5.14	101.22	108.27
36	B	325	LYS	CA-C-N	5.13	125.13	119.89
36	B	325	LYS	C-N-CA	5.13	125.13	119.89
11	L	93	LYS	N-CA-C	-5.13	101.49	109.24
2	C	129	ALA	N-CA-C	-5.13	108.05	114.56
29	f	97	LYS	CA-C-N	5.12	127.47	120.35
29	f	97	LYS	C-N-CA	5.12	127.47	120.35
3	D	142	PHE	CA-CB-CG	-5.12	108.68	113.80
9	J	87	PHE	CA-C-N	5.12	131.31	121.54
9	J	87	PHE	C-N-CA	5.12	131.31	121.54
7	H	165	ASN	CA-C-N	5.11	127.47	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	165	ASN	C-N-CA	5.11	127.47	120.46
17	S	94	ALA	CA-C-N	5.11	127.13	120.28
17	S	94	ALA	C-N-CA	5.11	127.13	120.28
3	D	91	VAL	N-CA-C	-5.11	101.13	108.48
38	R	76	VAL	N-CA-C	-5.11	101.13	108.53
8	I	61	PHE	CA-CB-CG	-5.10	108.70	113.80
26	c	11	SER	CA-C-N	5.10	125.13	119.32
26	c	11	SER	C-N-CA	5.10	125.13	119.32
35	A	185	THR	CA-C-N	5.09	126.21	119.84
35	A	185	THR	C-N-CA	5.09	126.21	119.84
4	E	178	VAL	N-CA-C	-5.08	100.58	108.86
36	B	264	THR	N-CA-C	-5.07	106.34	112.88
36	B	176	GLU	CA-C-N	5.07	131.22	121.54
36	B	176	GLU	C-N-CA	5.07	131.22	121.54
31	h	103	HIS	CA-C-N	5.07	127.07	120.28
31	h	103	HIS	C-N-CA	5.07	127.07	120.28
30	g	135	LEU	N-CA-C	-5.06	106.79	113.17
13	N	16	ILE	N-CA-C	-5.06	101.18	108.42
36	B	151	HIS	CA-C-N	5.06	127.06	120.28
36	B	151	HIS	C-N-CA	5.06	127.06	120.28
8	I	22	ARG	CA-C-N	5.06	127.56	120.28
8	I	22	ARG	C-N-CA	5.06	127.56	120.28
35	A	64	ARG	CA-C-N	5.06	127.28	120.50
35	A	64	ARG	C-N-CA	5.06	127.28	120.50
36	B	448	THR	CA-C-N	5.06	127.32	120.44
36	B	448	THR	C-N-CA	5.06	127.32	120.44
32	i	130	ASN	N-CA-C	-5.05	101.61	109.14
35	A	142	TYR	CB-CA-C	-5.05	104.47	110.94
33	2	1547	G	C5'-C4'-C3'	5.05	123.58	116.00
8	I	167	LYS	N-CA-C	-5.05	108.39	114.75
28	e	42	CYS	CA-C-N	5.05	127.36	120.54
28	e	42	CYS	C-N-CA	5.05	127.36	120.54
36	B	111	ARG	CA-C-N	5.05	126.15	119.84
36	B	111	ARG	C-N-CA	5.05	126.15	119.84
17	S	63	PHE	CA-CB-CG	-5.05	108.75	113.80
25	b	45	VAL	N-CA-C	-5.04	107.84	112.83
30	g	137	VAL	N-CA-C	-5.03	101.45	108.80
19	V	113	VAL	N-CA-C	-5.03	101.36	108.65
4	E	246	PHE	N-CA-CB	5.03	118.99	110.49
15	P	142	GLU	CA-C-N	5.02	126.97	120.44
15	P	142	GLU	C-N-CA	5.02	126.97	120.44
5	F	136	VAL	N-CA-C	-5.02	101.24	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	63	ILE	N-CA-C	-5.02	100.34	107.77
13	N	4	ILE	N-CA-C	-5.02	108.38	113.20
19	V	72	VAL	CA-C-N	5.01	125.41	119.94
19	V	72	VAL	C-N-CA	5.01	125.41	119.94
8	I	220	ALA	CA-C-N	5.01	126.96	120.44
8	I	220	ALA	C-N-CA	5.01	126.96	120.44
2	C	150	THR	N-CA-C	-5.01	105.24	113.50
21	X	45	ARG	CA-C-N	5.01	127.96	120.90
21	X	45	ARG	C-N-CA	5.01	127.96	120.90
35	A	91	SER	CA-C-N	5.00	124.78	119.28
35	A	91	SER	C-N-CA	5.00	124.78	119.28

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'
34	3	65	G	C3'
39	1	17	C	C2',C3'
39	1	18	G	C3'

All (113) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	1	18	G	Sidechain
39	1	48	C	Sidechain
39	1	69	U	Sidechain
33	2	112	U	Sidechain
33	2	1125	G	Sidechain
33	2	1139	A	Sidechain
33	2	1170	U	Sidechain
33	2	1171	G	Sidechain
33	2	1192	A	Sidechain
33	2	1251	G	Sidechain
33	2	1259	U	Sidechain
33	2	1285	U	Sidechain
33	2	1288	C	Sidechain
33	2	1289	A	Sidechain
33	2	1383	G	Sidechain
33	2	1416	G	Sidechain
33	2	1423	C	Sidechain
33	2	145	G	Sidechain
33	2	1452	G	Sidechain

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Mol	Chain	Res	Type	Group
33	2	146	G	Sidechain
33	2	1511	G	Sidechain
33	2	1515	G	Sidechain
33	2	1545	G	Sidechain
33	2	1547	G	Sidechain
33	2	1595	G	Sidechain
33	2	1598	G	Sidechain
33	2	1599	G	Sidechain
33	2	1607	G	Sidechain
33	2	1611	U	Sidechain
33	2	167	G	Sidechain
33	2	170	A	Sidechain
33	2	1702	U	Sidechain
33	2	1783	G	Sidechain
33	2	1784	A	Sidechain
33	2	1808	G	Sidechain
33	2	188	U	Sidechain
33	2	190	A	Sidechain
33	2	196	U	Sidechain
33	2	228	A	Sidechain
33	2	318	U	Sidechain
33	2	319	G	Sidechain
33	2	321	C	Sidechain
33	2	361	A	Sidechain
33	2	39	A	Sidechain
33	2	41	G	Sidechain
33	2	421	G	Sidechain
33	2	435	A	Sidechain
33	2	44	U	Sidechain
33	2	452	C	Sidechain
33	2	519	A	Sidechain
33	2	525	G	Sidechain
33	2	528	U	Sidechain
33	2	574	A	Sidechain
33	2	576	G	Sidechain
33	2	581	U	Sidechain
33	2	649	G	Sidechain
33	2	652	G	Sidechain
33	2	657	U	Sidechain
33	2	66	G	Sidechain
33	2	82	G	Sidechain
33	2	869	G	Sidechain

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Mol	Chain	Res	Type	Group
33	2	874	G	Sidechain
33	2	877	G	Sidechain
33	2	88	G	Sidechain
33	2	903	G	Sidechain
33	2	92	A	Sidechain
33	2	955	G	Sidechain
35	A	184	LEU	Peptide
35	A	185	THR	Peptide
35	A	186	PRO	Peptide
35	A	187	GLN	Peptide
35	A	200	TYR	Sidechain
35	A	54	ARG	Mainchain
35	A	55	ARG	Sidechain
35	A	57	ARG	Peptide
36	B	133	THR	Peptide
36	B	280	PRO	Peptide
36	B	282	CYS	Peptide
36	B	284	VAL	Peptide
36	B	285	ASP	Peptide
36	B	286	ASP	Peptide
36	B	287	LEU	Peptide
36	B	288	LYS	Peptide
36	B	289	GLY	Peptide
36	B	322	LEU	Peptide
36	B	373	ALA	Peptide
2	C	193	HIS	Peptide
3	D	208	HIS	Peptide
5	F	107	TYR	Sidechain
5	F	167	TYR	Sidechain
8	I	68	LEU	Peptide
8	I	69	THR	Peptide
9	J	105	THR	Peptide
9	J	66	VAL	Peptide
11	L	147	PHE	Peptide
11	L	54	ARG	Sidechain
12	M	1	MET	Peptide
12	M	34	GLU	Peptide
12	M	35	LEU	Peptide
12	M	43	LEU	Peptide
12	M	82	TYR	Sidechain
17	S	42	ILE	Peptide
17	S	43	GLU	Peptide

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Mol	Chain	Res	Type	Group
37	U	89	ASP	Peptide
37	U	94	LYS	Peptide
37	U	99	LEU	Peptide
26	c	81	ARG	Peptide
28	e	28	HIS	Peptide
28	e	49	ASP	Peptide
29	f	90	LYS	Peptide
31	h	109	TYR	Sidechain
32	i	120	VAL	Peptide
32	i	126	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	240	0	289	0	0
2	C	1643	0	1646	1	0
3	D	1742	0	1815	0	0
4	E	1743	0	1836	0	0
5	F	1765	0	1863	23	0
6	G	2083	0	2189	0	0
7	H	1509	0	1563	8	0
8	I	1924	0	2086	12	0
9	J	1530	0	1623	27	0
10	K	1680	0	1762	1	0
11	L	1499	0	1608	0	0
12	M	828	0	854	0	0
13	N	1296	0	1374	0	0
14	O	958	0	993	0	0
15	P	1208	0	1294	1	0
16	Q	1016	0	1039	0	0
17	S	1123	0	1193	2	0
18	T	1020	0	1075	0	0
19	V	1113	0	1149	5	0
20	W	822	0	887	1	0
21	X	620	0	622	0	0
22	Y	1034	0	1080	0	0
23	Z	1107	0	1179	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	1022	0	1084	1	0
25	b	790	0	839	5	0
26	c	659	0	683	0	0
27	d	507	0	536	2	0
28	e	445	0	442	0	0
29	f	582	0	599	1	0
30	g	2437	0	2393	0	0
31	h	599	0	655	17	0
32	i	473	0	524	2	0
33	2	37202	0	18777	315	0
34	3	774	0	390	80	0
35	A	2147	0	2189	26	0
36	B	3214	0	3354	0	0
37	U	1172	0	1226	66	0
38	R	1111	0	1166	58	0
39	1	1614	0	824	59	0
All	All	84251	0	66700	545	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 4.

All (545) 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)
37:U:147:GLY:CA	38:R:131:PRO:HG3	1.22	1.68
37:U:147:GLY:HA3	38:R:131:PRO:CG	1.34	1.55
39:1:16:G:O3'	39:1:17:C:P	1.14	1.52
33:2:1817:A:C2'	33:2:1818:A:H5'	1.47	1.42
5:F:117:ARG:HH12	34:3:67:A:N6	1.14	1.41
35:A:183:ARG:NE	39:1:18:G:O6	1.59	1.33
8:I:230:LYS:NZ	33:2:747:G:OP2	1.57	1.33
5:F:117:ARG:NH1	34:3:67:A:N6	1.79	1.29
8:I:236:SER:O	8:I:237:LEU:HG	1.21	1.29
33:2:1817:A:O2'	33:2:1818:A:H5'	1.19	1.29
33:2:1518:C:OP1	37:U:143:GLY:HA2	1.17	1.25
33:2:1517:A:C2	38:R:128:HIS:CE1	2.26	1.24
33:2:1518:C:OP1	37:U:143:GLY:CA	1.86	1.23
31:h:48:VAL:HG22	37:U:23:ARG:NH1	1.52	1.23
33:2:1696:C:H5'	34:3:54:G:O6	1.38	1.23
5:F:117:ARG:NH2	34:3:65:G:H2'	1.50	1.23
33:2:740:G:H21	33:2:794:G:C1'	1.50	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:16:G:C8	39:1:17:C:C6	2.27	1.23
39:1:16:G:HO3'	39:1:17:C:P	1.07	1.22
39:1:16:G:C2'	39:1:17:C:H5''	1.71	1.21
39:1:17:C:O3'	39:1:18:G:P	1.99	1.21
8:I:230:LYS:NZ	33:2:747:G:P	2.17	1.18
39:1:16:G:C8	39:1:17:C:H6	1.61	1.18
31:h:50:PHE:HB2	37:U:6:PRO:N	1.58	1.17
5:F:116:ARG:HE	5:F:150:MET:HE2	1.09	1.16
33:2:1817:A:H2'	33:2:1818:A:H5'	1.30	1.13
9:J:108:SER:HA	33:2:740:G:O3'	1.47	1.12
9:J:108:SER:HA	33:2:740:G:C3'	1.65	1.12
33:2:740:G:N2	33:2:794:G:H1'	1.62	1.12
35:A:183:ARG:NE	39:1:18:G:C6	2.19	1.11
9:J:107:LYS:HE3	33:2:738:U:C4'	1.81	1.09
34:3:57:U:H5'	34:3:58:G:OP2	1.51	1.09
5:F:116:ARG:HE	5:F:150:MET:CE	1.65	1.09
39:1:16:G:H2'	39:1:17:C:H5''	1.28	1.08
7:H:130:ARG:CD	34:3:47:U:H4'	1.83	1.08
38:R:128:HIS:HB3	38:R:129:GLY:HA3	1.28	1.08
7:H:130:ARG:HD3	34:3:47:U:C4'	1.84	1.07
39:1:19:G:O3'	39:1:20:A:P	2.13	1.06
33:2:1817:A:C2'	33:2:1818:A:C5'	2.31	1.06
39:1:16:G:C3'	39:1:17:C:H5''	1.84	1.06
5:F:117:ARG:NH1	34:3:67:A:H61	1.42	1.03
39:1:16:G:C3'	39:1:17:C:P	2.46	1.03
9:J:106:ARG:HG3	33:2:794:G:N7	1.68	1.02
33:2:1817:A:H2'	33:2:1818:A:C5'	1.87	1.02
7:H:132:GLY:O	35:A:55:ARG:NH2	1.91	1.02
37:U:147:GLY:HA2	38:R:131:PRO:HG3	1.37	1.01
33:2:742:C:C2'	33:2:743:U:H5'	1.91	1.01
9:J:107:LYS:HE3	33:2:738:U:H4'	1.38	1.01
34:3:57:U:C5'	34:3:58:G:OP2	2.08	1.01
8:I:236:SER:O	8:I:237:LEU:CG	2.09	1.00
33:2:1817:A:O2'	33:2:1818:A:C5'	2.09	1.00
37:U:143:GLY:O	37:U:144:ARG:NH1	1.93	1.00
33:2:737:C:H3'	33:2:738:U:H5''	1.42	1.00
33:2:683:G:N2	33:2:731:C:N3	2.10	1.00
33:2:1518:C:O2'	37:U:146:VAL:CG1	2.08	0.99
33:2:749:C:H3'	33:2:750:G:H5''	1.43	0.99
33:2:740:G:H21	33:2:794:G:H1'	0.81	0.97
33:2:684:A:C2	33:2:731:C:N3	2.32	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:237:LEU:HB2	33:2:784:G:H4'	1.42	0.97
9:J:107:LYS:HE2	33:2:737:C:H2'	1.46	0.97
5:F:117:ARG:HH22	34:3:65:G:H2'	1.16	0.97
34:3:51:C:H4'	39:1:37:T6A:ODB	1.64	0.97
23:Z:61:GLN:HG3	33:2:1818:A:OP1	1.64	0.96
33:2:1518:C:O2'	37:U:146:VAL:HG13	1.64	0.96
35:A:183:ARG:CZ	39:1:18:G:H1	1.80	0.95
33:2:740:G:N2	33:2:794:G:C1'	2.21	0.95
39:1:16:G:H8	39:1:17:C:H6	1.04	0.94
5:F:116:ARG:NE	5:F:150:MET:HE2	1.83	0.94
37:U:147:GLY:HA3	38:R:131:PRO:CB	1.96	0.94
33:2:745:U:H2'	33:2:746:C:C6	2.01	0.94
34:3:42:G:H2'	34:3:43:G:N7	1.83	0.94
35:A:183:ARG:CZ	39:1:18:G:O6	2.16	0.94
33:2:1818:A:O2'	33:2:1819:A:H5''	1.67	0.93
33:2:680:G:H1	33:2:734:C:H42	1.00	0.93
33:2:742:C:O2'	33:2:743:U:H5'	1.68	0.93
33:2:738:U:O2'	33:2:740:G:OP2	1.86	0.93
39:1:16:G:C8	39:1:17:C:C5	2.56	0.92
33:2:742:C:H2'	33:2:743:U:H5'	1.49	0.92
39:1:16:G:H2'	39:1:17:C:C5'	1.98	0.92
33:2:683:G:H1	33:2:731:C:H42	1.18	0.92
31:h:48:VAL:HG22	37:U:23:ARG:HH11	1.26	0.91
9:J:107:LYS:CE	33:2:738:U:C4'	2.38	0.91
9:J:106:ARG:CG	33:2:794:G:N7	2.23	0.91
5:F:117:ARG:HH22	34:3:65:G:C2'	1.82	0.91
33:2:733:G:N7	33:2:738:U:O4	2.04	0.90
33:2:1696:C:C5'	34:3:54:G:O6	2.19	0.90
33:2:680:G:H1	33:2:734:C:N4	1.68	0.90
39:1:16:G:H8	39:1:17:C:C6	1.75	0.90
38:R:136:THR:O	38:R:138:SER:N	2.05	0.90
39:1:16:G:O3'	39:1:17:C:OP2	1.90	0.90
33:2:734:C:H2'	33:2:735:C:H5''	1.53	0.90
33:2:787:C:H2'	33:2:788:C:C6	2.06	0.89
33:2:739:U:O2'	33:2:740:G:OP1	1.88	0.89
35:A:183:ARG:CZ	39:1:18:G:N1	2.36	0.89
8:I:235:SER:O	8:I:237:LEU:N	2.07	0.88
33:2:949:C:C3'	33:2:950:U:P	2.62	0.88
9:J:107:LYS:HD2	33:2:740:G:P	2.13	0.88
33:2:751:C:O2'	33:2:752:C:H5'	1.74	0.87
35:A:183:ARG:CZ	39:1:18:G:C6	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:117:ARG:NH1	34:3:67:A:H62	1.69	0.87
33:2:746:C:H2'	33:2:747:G:C8	2.10	0.87
7:H:130:ARG:HD3	34:3:47:U:H4'	0.92	0.87
8:I:230:LYS:HZ2	33:2:747:G:P	1.91	0.87
33:2:742:C:O2'	33:2:743:U:C5'	2.23	0.87
33:2:685:G:N2	33:2:730:C:N3	2.22	0.87
37:U:147:GLY:CA	38:R:131:PRO:CG	2.13	0.85
33:2:740:G:N1	33:2:793:C:C2	2.44	0.85
33:2:684:A:H2'	33:2:685:G:C8	2.12	0.85
33:2:732:C:H2'	33:2:733:G:O4'	1.76	0.85
33:2:1244:C4J:C3	33:2:1244:C4J:O36	2.23	0.84
33:2:740:G:N1	33:2:793:C:O2	2.09	0.84
33:2:731:C:H2'	33:2:732:C:H5''	1.57	0.84
9:J:107:LYS:HG2	33:2:737:C:O2'	1.77	0.83
31:h:48:VAL:HG21	37:U:23:ARG:HD3	1.60	0.83
37:U:91:LYS:HA	38:R:18:ARG:H	1.42	0.82
39:1:16:G:H2'	39:1:17:C:O4'	1.80	0.81
39:1:11:G:H1	39:1:25:U:H3	1.27	0.81
39:1:16:G:C2'	39:1:17:C:C5'	2.56	0.81
9:J:108:SER:CA	33:2:740:G:C3'	2.54	0.81
37:U:147:GLY:HA3	38:R:131:PRO:CD	2.11	0.81
33:2:1518:C:OP1	37:U:143:GLY:N	2.12	0.80
33:2:1518:C:O2'	37:U:146:VAL:HG11	1.81	0.80
33:2:1518:C:C5'	33:2:1518:C:H6	1.95	0.80
31:h:50:PHE:HB2	37:U:6:PRO:CD	2.11	0.80
33:2:1518:C:H6	33:2:1518:C:H5''	1.47	0.79
33:2:743:U:H1'	33:2:744:C:C1'	2.12	0.79
33:2:1264:C:C4'	38:R:100:LYS:HE3	2.13	0.79
33:2:743:U:O2'	33:2:744:C:O4'	2.00	0.79
39:1:17:C:H2'	39:1:18:G:H5'	1.63	0.79
33:2:748:G:O2'	33:2:749:C:O5'	2.01	0.79
34:3:51:C:C4'	39:1:37:T6A:ODB	2.30	0.79
33:2:1510:G:C3'	33:2:1510:G:C5'	2.61	0.78
38:R:128:HIS:HB3	38:R:129:GLY:CA	2.13	0.78
33:2:734:C:C2'	33:2:735:C:H5''	2.13	0.78
33:2:1517:A:H2	38:R:128:HIS:CE1	2.01	0.78
39:1:18:G:O4'	39:1:61:C:H5'	1.84	0.78
5:F:117:ARG:HH21	34:3:65:G:H2'	1.45	0.77
39:1:16:G:O3'	39:1:17:C:O5'	2.01	0.77
8:I:236:SER:C	8:I:237:LEU:HG	2.09	0.77
34:3:47:U:P	34:3:47:U:H6	2.07	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:743:U:O4	33:2:791:A:N1	2.18	0.77
23:Z:61:GLN:CG	33:2:1818:A:OP1	2.33	0.76
33:2:749:C:H2'	33:2:750:G:O4'	1.86	0.76
33:2:1696:C:C4'	34:3:54:G:C6	2.68	0.76
9:J:106:ARG:N	33:2:794:G:N7	2.34	0.75
35:A:183:ARG:CD	39:1:18:G:C6	2.69	0.75
37:U:147:GLY:C	38:R:131:PRO:HG3	2.09	0.75
34:3:59:G:H5''	34:3:59:G:N3	2.02	0.74
35:A:183:ARG:NH2	39:1:18:G:H1	1.84	0.74
33:2:1817:A:C8	33:2:1817:A:OP2	2.41	0.74
35:A:107:THR:HG22	39:1:18:G:C6	2.23	0.74
37:U:147:GLY:HA3	38:R:131:PRO:HG3	0.76	0.74
33:2:1232:G:H5'	38:R:134:GLY:O	1.88	0.74
33:2:797:U:H2'	33:2:798:A:O4'	1.88	0.73
33:2:748:G:C2	33:2:749:C:C2	2.77	0.73
34:3:42:G:H2'	34:3:43:G:C8	2.23	0.73
31:h:48:VAL:CG2	37:U:23:ARG:HD3	2.19	0.72
34:3:58:G:O2'	34:3:59:G:O5'	2.06	0.72
33:2:684:A:C2	33:2:731:C:C4	2.78	0.72
37:U:143:GLY:C	37:U:144:ARG:HG3	2.13	0.72
25:b:98:PRO:O	33:2:1862:U:H5	1.71	0.72
33:2:749:C:C3'	33:2:750:G:H5''	2.18	0.72
33:2:683:G:H1	33:2:731:C:N4	1.87	0.72
9:J:107:LYS:HA	33:2:740:G:O5'	1.89	0.71
9:J:107:LYS:CE	33:2:737:C:H2'	2.18	0.71
33:2:68:A:H61	33:2:81:U:H3	1.38	0.71
33:2:733:G:C5	33:2:738:U:O4	2.44	0.71
33:2:748:G:N2	33:2:749:C:O2	2.23	0.71
34:3:56:C:H1'	34:3:57:U:OP1	1.89	0.71
33:2:683:G:H2'	33:2:684:A:C8	2.24	0.71
9:J:107:LYS:CG	33:2:737:C:O2'	2.37	0.71
33:2:745:U:H2'	33:2:746:C:C5	2.25	0.70
39:1:19:G:O3'	39:1:20:A:OP1	2.08	0.70
39:1:18:G:O4'	39:1:61:C:C5'	2.39	0.70
33:2:740:G:N2	33:2:794:G:O4'	2.23	0.70
34:3:51:C:H1'	39:1:37:T6A:O14	1.92	0.70
33:2:1236:A:N1	38:R:99:GLY:HA3	2.06	0.69
33:2:737:C:C3'	33:2:738:U:H5''	2.22	0.69
8:I:235:SER:C	8:I:237:LEU:H	2.02	0.68
33:2:793:C:O2'	33:2:794:G:H4'	1.93	0.68
34:3:49:A:H2'	34:3:50:C:H5'	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:117:ARG:HH12	34:3:67:A:H61	0.68	0.68
39:1:16:G:C3'	39:1:17:C:C5'	2.70	0.68
33:2:685:G:N2	33:2:730:C:C2	2.62	0.68
33:2:795:U:OP2	33:2:795:U:H4'	1.93	0.68
34:3:59:G:N3	34:3:59:G:H3'	2.08	0.67
5:F:117:ARG:NH2	34:3:65:G:C2'	2.39	0.67
33:2:740:G:O6	33:2:793:C:N3	2.27	0.67
35:A:179:ASN:OD1	35:A:183:ARG:NH2	2.28	0.67
33:2:526:A:H62	33:2:537:G:H21	1.42	0.66
34:3:55:U:H5	34:3:56:C:C5	2.13	0.66
39:1:16:G:O3'	39:1:17:C:C5'	2.43	0.66
8:I:237:LEU:HB2	33:2:784:G:C4'	2.20	0.66
5:F:116:ARG:NE	5:F:150:MET:CE	2.48	0.66
33:2:1608:G:H5''	38:R:42:ARG:HH22	1.60	0.66
33:2:1859:C:H4'	33:2:1860:A:OP2	1.95	0.66
33:2:1510:G:C5'	33:2:1510:G:O4'	2.44	0.66
9:J:109:ARG:HB2	33:2:740:G:H2'	1.77	0.65
33:2:1232:G:H4'	38:R:135:ALA:HB2	1.79	0.65
33:2:739:U:H4'	33:2:740:G:OP2	1.96	0.65
24:a:29:HIS:CE1	24:a:34:THR:H	2.15	0.65
33:2:785:G:N2	33:2:786:C:O2	2.30	0.65
33:2:1232:G:C4'	38:R:135:ALA:HB2	2.27	0.64
33:2:743:U:H1'	33:2:744:C:H1'	1.78	0.64
33:2:1518:C:P	37:U:143:GLY:HA2	2.35	0.64
25:b:97:PRO:HB3	33:2:1862:U:C6	2.33	0.64
33:2:1696:C:O4'	34:3:54:G:C6	2.50	0.64
33:2:683:G:C6	33:2:684:A:C6	2.86	0.64
33:2:1518:C:H5''	33:2:1518:C:C6	2.31	0.64
34:3:46:A:O5'	34:3:46:A:H8	1.81	0.64
34:3:58:G:HO2'	34:3:59:G:P	2.21	0.64
37:U:91:LYS:H	38:R:18:ARG:HG2	1.62	0.64
39:1:16:G:C2'	39:1:17:C:O4'	2.44	0.63
19:V:38:LYS:CG	37:U:39:ARG:NH1	2.61	0.63
38:R:129:GLY:O	38:R:130:ARG:HB2	1.99	0.63
33:2:743:U:H1'	33:2:744:C:O4'	1.99	0.63
33:2:784:G:H2'	33:2:785:G:H5'	1.79	0.63
33:2:790:A:O5'	33:2:790:A:H8	1.81	0.63
39:1:16:G:H2'	39:1:17:C:C4'	2.28	0.63
33:2:740:G:C6	33:2:793:C:N3	2.67	0.62
9:J:106:ARG:CA	33:2:794:G:N7	2.46	0.62
33:2:685:G:H1	33:2:730:C:H42	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:688:U:H6	33:2:688:U:O5'	1.83	0.62
33:2:740:G:C2	33:2:793:C:O2	2.52	0.62
37:U:91:LYS:HG2	38:R:17:TYR:HA	1.82	0.62
33:2:746:C:H2'	33:2:747:G:N7	2.14	0.62
7:H:130:ARG:HH11	34:3:47:U:H5'	1.64	0.62
19:V:38:LYS:HG2	37:U:39:ARG:NH1	2.15	0.62
38:R:133:ILE:O	38:R:133:ILE:HG22	2.01	0.61
33:2:745:U:O2'	33:2:746:C:O4'	2.18	0.61
33:2:1696:C:H4'	34:3:54:G:C5	2.35	0.61
33:2:682:G:C2	33:2:683:G:N7	2.69	0.61
33:2:733:G:N7	33:2:738:U:C4	2.69	0.61
33:2:751:C:H2'	33:2:752:C:C6	2.35	0.61
33:2:1618:A:C5'	37:U:133:GLY:HA3	2.30	0.61
39:1:19:G:N1	39:1:56:C:N3	2.49	0.61
33:2:734:C:C3'	33:2:735:C:H5''	2.31	0.61
33:2:790:A:C6	33:2:791:A:N6	2.69	0.61
33:2:1618:A:H5''	37:U:133:GLY:CA	2.31	0.60
33:2:793:C:C2'	33:2:794:G:H4'	2.31	0.60
34:3:56:C:H1'	34:3:57:U:P	2.41	0.60
33:2:744:C:C4	33:2:745:U:O4	2.55	0.60
33:2:1817:A:HO2'	33:2:1818:A:H5'	1.57	0.60
5:F:116:ARG:HE	5:F:150:MET:HE1	1.64	0.60
5:F:117:ARG:NH2	34:3:65:G:C8	2.70	0.60
19:V:45:LEU:HD11	37:U:38:ARG:NH2	2.17	0.59
35:A:107:THR:HG22	39:1:18:G:O6	2.01	0.59
33:2:686:G:O5'	33:2:686:G:H8	1.84	0.59
32:i:118:ASN:H	32:i:119:VAL:HA	1.68	0.59
33:2:790:A:H2'	33:2:791:A:C8	2.37	0.59
33:2:682:G:C2	33:2:683:G:C5	2.91	0.59
33:2:743:U:C6	33:2:744:C:C2	2.91	0.59
33:2:1264:C:H4'	38:R:100:LYS:HE3	1.85	0.59
31:h:48:VAL:CG2	37:U:23:ARG:HH11	2.09	0.59
38:R:128:HIS:CB	38:R:129:GLY:HA3	2.15	0.58
31:h:48:VAL:HG22	37:U:23:ARG:CZ	2.30	0.58
33:2:683:G:N1	33:2:684:A:C6	2.71	0.58
33:2:682:G:H2'	33:2:683:G:H8	1.68	0.58
33:2:784:G:C5	33:2:785:G:N7	2.71	0.58
33:2:1517:A:C2	38:R:128:HIS:NE2	2.71	0.58
33:2:793:C:H4'	33:2:793:C:OP1	2.03	0.58
33:2:743:U:H3	33:2:791:A:H2	1.51	0.58
31:h:50:PHE:CB	37:U:6:PRO:CD	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:107:LYS:HD2	33:2:740:G:O5'	2.03	0.57
33:2:683:G:O2'	33:2:684:A:H5'	2.04	0.57
33:2:784:G:C2'	33:2:785:G:H5'	2.33	0.57
38:R:135:ALA:O	38:R:136:THR:HB	2.04	0.57
33:2:1170:U:H2'	33:2:1171:G:C8	2.38	0.57
33:2:746:C:C2'	33:2:747:G:C8	2.86	0.57
33:2:787:C:H2'	33:2:788:C:C5	2.38	0.57
25:b:98:PRO:O	33:2:1862:U:C5	2.57	0.57
33:2:750:G:C6	33:2:751:C:N4	2.73	0.57
33:2:683:G:C6	33:2:684:A:N6	2.73	0.57
34:3:49:A:H2	34:3:49:A:OP1	1.88	0.57
19:V:38:LYS:HG3	37:U:39:ARG:NH1	2.20	0.57
33:2:740:G:H2'	33:2:741:C:H5''	1.87	0.57
35:A:64:ARG:HE	35:A:67:ARG:HG3	1.70	0.56
37:U:147:GLY:HA3	38:R:131:PRO:HB3	1.85	0.56
33:2:1244:C4J:O2	33:2:1244:C4J:C31	2.53	0.56
35:A:183:ARG:NH2	39:1:18:G:N1	2.51	0.56
33:2:1618:A:H5''	37:U:133:GLY:N	2.20	0.56
9:J:107:LYS:CA	33:2:740:G:O5'	2.54	0.56
33:2:745:U:C2	33:2:746:C:C4	2.94	0.56
31:h:103:HIS:CD2	31:h:104:ARG:H	2.24	0.56
33:2:1618:A:H5''	37:U:133:GLY:HA3	1.87	0.56
33:2:734:C:C5	33:2:737:C:N4	2.73	0.56
34:3:56:C:C1'	34:3:57:U:P	2.94	0.56
34:3:54:G:O2'	34:3:55:U:OP1	2.18	0.55
33:2:848:G:H3'	33:2:849:C:H5''	1.88	0.55
34:3:54:G:O5'	34:3:54:G:H8	1.89	0.55
31:h:48:VAL:HG11	37:U:23:ARG:HD3	1.88	0.55
7:H:131:ALA:O	34:3:49:A:OP2	2.23	0.55
33:2:1862:U:O2	33:2:1862:U:H2'	2.06	0.55
33:2:681:U:H2'	33:2:681:U:O2	2.07	0.55
34:3:49:A:H2'	34:3:50:C:C5'	2.36	0.55
34:3:49:A:C5'	34:3:49:A:N3	2.70	0.55
39:1:18:G:C1'	39:1:61:C:H5'	2.36	0.55
7:H:131:ALA:C	34:3:49:A:OP2	2.50	0.55
9:J:75:ILE:HG23	9:J:76:GLN:H	1.72	0.55
33:2:687:G:H2'	33:2:688:U:H5'	1.89	0.55
33:2:739:U:O2	33:2:739:U:H2'	2.06	0.55
33:2:1232:G:C2	33:2:1518:C:N4	2.75	0.55
33:2:1696:C:H4'	34:3:54:G:C6	2.40	0.55
33:2:787:C:N3	33:2:788:C:N4	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:64:ARG:HD3	35:A:64:ARG:N	2.23	0.54
33:2:684:A:O5'	33:2:684:A:H8	1.91	0.54
33:2:1330:G:H22	33:2:1492:U:H3	1.55	0.54
33:2:1518:C:C5'	33:2:1518:C:C6	2.85	0.54
9:J:108:SER:CA	33:2:740:G:O3'	2.38	0.54
35:A:64:ARG:HD3	35:A:64:ARG:H	1.73	0.54
34:3:42:G:H2'	34:3:43:G:C5	2.41	0.54
37:U:88:LYS:CG	38:R:37:TYR:CD2	2.91	0.54
33:2:786:C:H6	33:2:786:C:O5'	1.91	0.54
33:2:683:G:N2	33:2:731:C:C2	2.66	0.53
10:K:142:SER:H	10:K:143:LYS:HB2	1.73	0.53
5:F:117:ARG:CZ	34:3:67:A:H62	2.22	0.53
33:2:1407:G:H3'	33:2:1408:C:H5''	1.90	0.53
5:F:5:ILE:HD13	5:F:5:ILE:H	1.73	0.53
33:2:1518:C:C1'	37:U:146:VAL:HG13	2.38	0.53
37:U:91:LYS:HZ3	38:R:17:TYR:HD1	1.52	0.53
33:2:1294:G:P	38:R:77:LYS:HE2	2.49	0.53
33:2:682:G:N3	33:2:683:G:C8	2.76	0.53
33:2:744:C:C5	33:2:745:U:O4	2.62	0.53
34:3:54:G:H4'	34:3:55:U:OP1	2.07	0.53
33:2:687:G:C5	33:2:729:C:N4	2.77	0.53
27:d:67:ARG:HG2	27:d:67:ARG:HH11	1.73	0.53
33:2:743:U:HO2'	33:2:744:C:C1'	2.21	0.53
33:2:685:G:H1	33:2:730:C:N4	2.06	0.52
34:3:50:C:H2'	34:3:51:C:H5'	1.92	0.52
5:F:117:ARG:CZ	34:3:67:A:N6	2.67	0.52
5:F:99:ILE:HD12	5:F:99:ILE:H	1.74	0.52
33:2:683:G:C2	33:2:684:A:C4	2.97	0.52
33:2:682:G:O5'	33:2:682:G:H8	1.92	0.52
34:3:54:G:O2'	34:3:55:U:H5''	2.09	0.52
33:2:745:U:H3'	33:2:745:U:H6	1.75	0.52
33:2:794:G:O2'	33:2:795:U:OP1	2.20	0.52
9:J:100:ILE:CD1	33:2:736:C:O2	2.58	0.51
33:2:734:C:C3'	33:2:735:C:C5'	2.88	0.51
33:2:747:G:O5'	33:2:747:G:H8	1.91	0.51
33:2:1294:G:OP1	38:R:77:LYS:HE2	2.10	0.51
7:H:130:ARG:HD3	34:3:47:U:C5'	2.40	0.51
34:3:51:C:O2'	39:1:37:T6A:ODB	2.14	0.51
39:1:16:G:C8	39:1:17:C:H5	2.26	0.51
20:W:20:ILE:HG21	20:W:98:VAL:HG21	1.93	0.51
33:2:687:G:C6	33:2:729:C:N4	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:790:A:C5	33:2:791:A:N6	2.78	0.51
33:2:1817:A:H2'	33:2:1818:A:O5'	2.10	0.51
35:A:64:ARG:N	35:A:64:ARG:CD	2.74	0.51
33:2:682:G:C4	33:2:683:G:N7	2.79	0.51
34:3:57:U:C4'	34:3:58:G:OP2	2.59	0.51
34:3:59:G:N3	34:3:59:G:C3'	2.73	0.51
33:2:687:G:C2'	33:2:688:U:H5'	2.41	0.51
33:2:749:C:H3'	33:2:750:G:C5'	2.29	0.51
34:3:50:C:C2'	34:3:51:C:H5'	2.41	0.50
33:2:787:C:O5'	33:2:787:C:H6	1.94	0.50
34:3:55:U:C5	34:3:56:C:C5	2.98	0.50
19:V:38:LYS:HG2	37:U:39:ARG:CZ	2.42	0.50
34:3:46:A:O3'	34:3:47:U:H6	1.95	0.50
33:2:1264:C:O2'	38:R:100:LYS:HG3	2.12	0.50
34:3:55:U:H3'	34:3:56:C:H5''	1.94	0.50
39:1:19:G:C3'	39:1:20:A:OP1	2.59	0.50
39:1:16:G:C3'	39:1:17:C:OP2	2.53	0.50
33:2:679:U:H2'	33:2:680:G:C8	2.47	0.49
33:2:683:G:C2	33:2:684:A:C5	3.00	0.49
33:2:745:U:N3	33:2:746:C:N4	2.60	0.49
25:b:97:PRO:CB	33:2:1862:U:C6	2.95	0.49
33:2:741:C:N3	33:2:792:G:O6	2.46	0.49
33:2:743:U:O4	33:2:791:A:C2	2.65	0.49
34:3:47:U:P	34:3:47:U:C6	2.97	0.49
39:1:16:G:O2'	39:1:17:C:O4'	2.28	0.49
8:I:236:SER:O	8:I:237:LEU:CB	2.60	0.49
33:2:225:C:H3'	33:2:226:A:C5'	2.42	0.49
33:2:740:G:C3'	33:2:741:C:H5''	2.43	0.49
31:h:48:VAL:HG11	37:U:23:ARG:CD	2.42	0.49
34:3:49:A:OP1	34:3:49:A:C2	2.66	0.49
31:h:48:VAL:CG1	37:U:23:ARG:HD3	2.42	0.48
33:2:740:G:H3'	33:2:741:C:H5''	1.95	0.48
34:3:49:A:N3	34:3:49:A:O5'	2.46	0.48
34:3:58:G:N3	34:3:58:G:H2'	2.28	0.48
33:2:784:G:C6	33:2:785:G:C5	3.01	0.48
37:U:147:GLY:C	38:R:131:PRO:CG	2.77	0.48
33:2:1264:C:O4'	38:R:100:LYS:HE3	2.13	0.48
33:2:745:U:C2	33:2:746:C:N4	2.81	0.48
39:1:19:G:N2	39:1:56:C:C2	2.81	0.48
37:U:143:GLY:C	37:U:144:ARG:CG	2.85	0.47
33:2:1264:C:H4'	38:R:100:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:1517:A:C2	38:R:128:HIS:HE1	2.16	0.47
33:2:743:U:O2'	33:2:744:C:O5'	2.32	0.47
33:2:1264:C:O4'	38:R:100:LYS:NZ	2.46	0.47
33:2:1105:C:H3'	33:2:1106:G:H5''	1.97	0.47
33:2:742:C:O2'	33:2:743:U:H5''	2.09	0.47
33:2:1244:C4J:C4	39:1:34:C:H5'	2.44	0.47
35:A:179:ASN:HB3	35:A:183:ARG:NH1	2.30	0.47
37:U:146:VAL:HG12	37:U:147:GLY:H	1.79	0.47
33:2:784:G:H8	33:2:784:G:P	2.38	0.47
33:2:784:G:C4	33:2:785:G:C8	3.02	0.47
33:2:1860:A:O2'	33:2:1861:U:H5'	2.15	0.47
35:A:182:ARG:HB3	39:1:53:G:H21	1.80	0.47
37:U:147:GLY:CA	38:R:131:PRO:CB	2.76	0.47
33:2:741:C:H3'	33:2:741:C:H6	1.80	0.47
34:3:43:G:H2'	34:3:44:U:C5	2.50	0.47
33:2:684:A:H2'	33:2:685:G:H8	1.73	0.47
33:2:731:C:C2'	33:2:732:C:H5''	2.37	0.47
33:2:749:C:C3'	33:2:750:G:C5'	2.89	0.47
33:2:682:G:C2	33:2:683:G:C8	3.03	0.46
33:2:742:C:H3'	33:2:742:C:H6	1.80	0.46
33:2:793:C:H2'	33:2:794:G:H4'	1.97	0.46
33:2:685:G:H8	33:2:685:G:O5'	1.98	0.46
34:3:55:U:C5	34:3:56:C:C6	3.03	0.46
39:1:16:G:H3'	39:1:17:C:OP2	2.15	0.46
33:2:676:U:O2	33:2:913:U:C2	2.68	0.46
33:2:745:U:C2'	33:2:746:C:C6	2.89	0.46
39:1:19:G:H3'	39:1:20:A:OP1	2.15	0.46
33:2:1547:G:OP2	33:2:1547:G:C8	2.68	0.46
34:3:55:U:H3'	34:3:56:C:C5'	2.45	0.46
35:A:55:ARG:HD3	35:A:55:ARG:HA	1.64	0.46
33:2:748:G:N2	33:2:749:C:C2	2.84	0.46
33:2:1517:A:N3	38:R:128:HIS:NE2	2.64	0.46
39:1:17:C:H2'	39:1:18:G:C5'	2.41	0.46
17:S:145:TYR:O	17:S:146:ARG:HB3	2.16	0.46
33:2:741:C:H2'	33:2:742:C:O4'	2.15	0.46
33:2:751:C:C2'	33:2:752:C:H5'	2.44	0.46
33:2:1518:C:C2'	37:U:146:VAL:HG13	2.44	0.46
33:2:679:U:H3'	33:2:679:U:H6	1.81	0.46
33:2:1517:A:N3	38:R:128:HIS:CE1	2.78	0.46
33:2:1236:A:C4	38:R:100:LYS:HE2	2.16	0.45
33:2:1294:G:C5'	38:R:77:LYS:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:183:ARG:NH1	39:1:18:G:O6	2.49	0.45
32:i:118:ASN:H	32:i:119:VAL:CA	2.28	0.45
37:U:91:LYS:HA	38:R:18:ARG:N	2.22	0.45
33:2:785:G:C2	33:2:786:C:C2	3.04	0.45
33:2:684:A:H2	33:2:731:C:N3	2.09	0.45
33:2:740:G:C2'	33:2:741:C:H5''	2.46	0.45
33:2:1518:C:H1'	37:U:146:VAL:HG13	1.99	0.45
37:U:139:THR:HG22	37:U:140:GLY:N	2.30	0.45
38:R:84:ILE:HD12	38:R:84:ILE:H	1.81	0.45
5:F:116:ARG:CZ	5:F:150:MET:HE2	2.46	0.45
38:R:136:THR:O	38:R:136:THR:HG23	2.16	0.45
34:3:45:C:H3'	34:3:45:C:O2	2.17	0.45
5:F:198:ILE:HD12	5:F:198:ILE:H	1.82	0.44
17:S:39:LEU:H	17:S:39:LEU:HD23	1.81	0.44
33:2:743:U:OP2	33:2:743:U:H2'	2.17	0.44
33:2:743:U:C5	33:2:744:C:N3	2.85	0.44
35:A:24:VAL:HA	35:A:34:VAL:HG12	1.98	0.44
8:I:237:LEU:OXT	33:2:784:G:O3'	2.35	0.44
33:2:684:A:C6	33:2:685:G:O6	2.70	0.44
33:2:1407:G:H3'	33:2:1408:C:C5'	2.46	0.44
33:2:1429:C:C5	33:2:1430:C:C5	3.06	0.44
33:2:792:G:H8	33:2:792:G:P	2.40	0.44
33:2:1236:A:H1'	38:R:100:LYS:HE2	1.99	0.44
35:A:57:ARG:O	35:A:57:ARG:HG2	2.17	0.44
35:A:64:ARG:NE	35:A:67:ARG:HG3	2.30	0.44
39:1:17:C:H2'	39:1:18:G:P	2.58	0.44
33:2:784:G:C5	33:2:785:G:C5	3.04	0.44
33:2:682:G:H2'	33:2:683:G:C8	2.52	0.44
33:2:735:C:H3'	33:2:736:C:H5''	2.00	0.44
33:2:737:C:H3'	33:2:738:U:C5'	2.30	0.44
33:2:787:C:O5'	33:2:787:C:C6	2.70	0.44
34:3:47:U:C6	34:3:47:U:OP2	2.70	0.44
37:U:88:LYS:HG3	38:R:37:TYR:CD2	2.52	0.44
31:h:50:PHE:CB	37:U:6:PRO:HD3	2.46	0.43
33:2:1518:C:C6	33:2:1518:C:C4'	3.01	0.43
33:2:682:G:N3	33:2:683:G:N7	2.66	0.43
33:2:745:U:C2	33:2:746:C:N3	2.86	0.43
33:2:785:G:C2	33:2:786:C:O2	2.70	0.43
33:2:1232:G:O4'	38:R:135:ALA:HB2	2.18	0.43
9:J:107:LYS:HG3	33:2:737:C:O2'	2.17	0.43
33:2:201:G:H3'	33:2:202:U:H5''	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2:683:G:H2'	33:2:684:A:H8	1.78	0.43
33:2:1818:A:HO2'	33:2:1819:A:H5''	1.77	0.43
9:J:100:ILE:HG13	33:2:736:C:O2	2.18	0.43
33:2:746:C:H5''	33:2:747:G:OP2	2.19	0.43
35:A:183:ARG:HD2	39:1:18:G:C6	2.49	0.43
38:R:128:HIS:CB	38:R:129:GLY:CA	2.85	0.43
9:J:100:ILE:HD12	33:2:736:C:O2	2.19	0.43
15:P:26:LEU:H	15:P:26:LEU:HD12	1.83	0.43
33:2:790:A:H8	33:2:790:A:P	2.42	0.43
37:U:147:GLY:C	38:R:131:PRO:CB	2.92	0.43
33:2:734:C:H5	33:2:737:C:N4	2.17	0.43
33:2:748:G:O2'	33:2:749:C:C6	2.71	0.43
34:3:46:A:O3'	34:3:47:U:C6	2.70	0.43
33:2:682:G:N1	33:2:683:G:C5	2.87	0.43
33:2:684:A:H2'	33:2:685:G:N7	2.32	0.43
33:2:734:C:H3'	33:2:735:C:C5'	2.49	0.43
33:2:790:A:N6	33:2:791:A:N6	2.67	0.43
34:3:59:G:N3	34:3:59:G:C5'	2.78	0.43
33:2:1172:G:C6	33:2:1173:U:C4	3.07	0.42
9:J:109:ARG:N	33:2:741:C:OP1	2.52	0.42
29:f:146:LEU:HD23	29:f:146:LEU:H	1.84	0.42
33:2:737:C:H5'	33:2:738:U:OP2	2.19	0.42
25:b:42:ARG:HH22	34:3:44:U:H1'	1.84	0.42
33:2:791:A:C8	33:2:791:A:O5'	2.72	0.42
34:3:47:U:O2'	34:3:48:A:P	2.77	0.42
39:1:16:G:C2'	39:1:17:C:C4'	2.93	0.42
31:h:50:PHE:CG	37:U:6:PRO:CD	3.02	0.42
33:2:786:C:O5'	33:2:786:C:C6	2.71	0.42
37:U:141:ARG:HD2	37:U:141:ARG:HA	1.78	0.42
33:2:791:A:O5'	33:2:791:A:H8	2.03	0.42
33:2:1618:A:C5'	37:U:133:GLY:H	2.33	0.42
33:2:1828:A:H2	33:2:1831:G:H1	1.66	0.42
34:3:57:U:H3'	34:3:57:U:O2	2.20	0.42
33:2:1276:G:H1	33:2:1313:U:H3	1.66	0.42
33:2:1408:C:H2'	33:2:1409:G:C8	2.54	0.42
37:U:90:VAL:HG13	38:R:18:ARG:HH11	1.85	0.42
33:2:519:A:N6	33:2:545:A:H61	2.17	0.41
33:2:737:C:C3'	33:2:738:U:C5'	2.97	0.41
33:2:1264:C:C5'	38:R:100:LYS:HE3	2.49	0.41
34:3:46:A:C3'	34:3:47:U:C6	3.03	0.41
33:2:1696:C:C5'	34:3:54:G:C6	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:3:44:U:O2'	34:3:45:C:OP2	2.34	0.41
37:U:146:VAL:HG12	37:U:147:GLY:N	2.35	0.41
27:d:66:ARG:HD2	27:d:66:ARG:O	2.21	0.41
33:2:745:U:C4	33:2:746:C:N4	2.88	0.41
35:A:56:ILE:O	35:A:58:SER:N	2.52	0.41
2:C:5:LEU:HD22	2:C:5:LEU:H	1.85	0.41
37:U:90:VAL:HG22	38:R:18:ARG:HD3	2.01	0.41
37:U:91:LYS:NZ	38:R:17:TYR:HD1	2.19	0.41
33:2:741:C:C6	33:2:741:C:C3'	3.03	0.41
33:2:790:A:H2'	33:2:791:A:H8	1.83	0.41
9:J:107:LYS:HD2	33:2:740:G:OP2	2.20	0.41
37:U:116:LYS:HG2	38:R:110:GLU:OE2	2.20	0.41
39:1:18:G:H1'	39:1:61:C:H5'	2.01	0.41
33:2:686:G:O5'	33:2:686:G:C8	2.70	0.41
33:2:746:C:C3'	33:2:747:G:C8	3.03	0.41
33:2:924:G:H1	33:2:1009:U:H3	1.67	0.41
33:2:546:U:H3'	33:2:547:U:H5''	2.03	0.41
33:2:552:U:H2'	33:2:553:G:C8	2.56	0.41
33:2:742:C:C3'	33:2:742:C:C6	3.04	0.41
33:2:874:G:H22	33:2:904:A:H2	1.68	0.41
34:3:51:C:C2'	34:3:52:A:OP2	2.68	0.41
33:2:124:U:H3	33:2:330:C:H42	1.68	0.41
33:2:734:C:H41	33:2:737:C:N4	2.19	0.41
33:2:745:U:C3'	33:2:745:U:C6	3.03	0.41
33:2:1264:C:O4'	38:R:100:LYS:CE	2.68	0.41
33:2:1618:A:H5''	37:U:133:GLY:H	1.84	0.41
34:3:43:G:O2'	34:3:44:U:C6	2.70	0.41
33:2:987:G:C6	33:2:1130:G:H4'	2.56	0.40
31:h:86:ALA:HA	31:h:89:GLN:HE21	1.86	0.40
33:2:516:A:N6	33:2:578:G:H22	2.20	0.40
31:h:48:VAL:CG1	37:U:23:ARG:CD	2.99	0.40
33:2:739:U:HO2'	33:2:740:G:P	2.42	0.40
33:2:744:C:OP1	33:2:744:C:H4'	2.21	0.40
34:3:42:G:C2'	34:3:43:G:C5	3.04	0.40
5:F:70:THR:HG22	5:F:86:LEU:HD13	2.03	0.40
33:2:745:U:H3'	33:2:745:U:C6	2.56	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	
1	I	23/25 (92%)	23 (100%)	0	0	100	100
2	C	206/208 (99%)	176 (85%)	21 (10%)	9 (4%)	2	17
3	D	213/215 (99%)	185 (87%)	19 (9%)	9 (4%)	2	18
4	E	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	5	30
5	F	225/227 (99%)	205 (91%)	13 (6%)	7 (3%)	3	25
6	G	261/263 (99%)	229 (88%)	26 (10%)	6 (2%)	5	30
7	H	189/191 (99%)	165 (87%)	16 (8%)	8 (4%)	2	18
8	I	233/237 (98%)	206 (88%)	20 (9%)	7 (3%)	3	25
9	J	188/190 (99%)	162 (86%)	18 (10%)	8 (4%)	2	18
10	K	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	3	26
11	L	180/182 (99%)	167 (93%)	6 (3%)	7 (4%)	2	20
12	M	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	1	12
13	N	156/158 (99%)	130 (83%)	19 (12%)	7 (4%)	2	17
14	O	122/124 (98%)	103 (84%)	15 (12%)	4 (3%)	3	23
15	P	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
16	Q	134/136 (98%)	116 (87%)	11 (8%)	7 (5%)	1	14
17	S	139/141 (99%)	123 (88%)	12 (9%)	4 (3%)	3	26
18	T	124/126 (98%)	114 (92%)	8 (6%)	2 (2%)	7	36
19	V	139/141 (99%)	124 (89%)	10 (7%)	5 (4%)	2	21
20	W	102/104 (98%)	95 (93%)	4 (4%)	3 (3%)	3	26
21	X	80/82 (98%)	66 (82%)	13 (16%)	1 (1%)	9	39
22	Y	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	36
23	Z	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	38
24	a	122/126 (97%)	106 (87%)	12 (10%)	4 (3%)	3	23
25	b	97/99 (98%)	81 (84%)	13 (13%)	3 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	82/84 (98%)	72 (88%)	8 (10%)	2 (2%)	4	29
27	d	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	2	16
28	e	51/53 (96%)	39 (76%)	8 (16%)	4 (8%)	1	8
29	f	69/71 (97%)	56 (81%)	6 (9%)	7 (10%)	0	6
30	g	311/313 (99%)	273 (88%)	31 (10%)	7 (2%)	5	30
31	h	73/75 (97%)	70 (96%)	2 (3%)	1 (1%)	9	38
32	i	57/59 (97%)	45 (79%)	7 (12%)	5 (9%)	0	7
35	A	264/266 (99%)	225 (85%)	29 (11%)	10 (4%)	2	20
36	B	420/422 (100%)	350 (83%)	48 (11%)	22 (5%)	1	14
37	U	140/142 (99%)	121 (86%)	14 (10%)	5 (4%)	2	21
38	R	133/135 (98%)	105 (79%)	18 (14%)	10 (8%)	1	9
All	All	5534/5610 (99%)	4836 (87%)	500 (9%)	198 (4%)	4	21

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	209	ASP
3	D	221	PRO
5	F	193	ASP
5	F	219	PRO
6	G	2	ALA
6	G	17	HIS
8	I	46	LYS
8	I	104	ALA
8	I	155	GLN
8	I	236	SER
9	J	67	PRO
9	J	88	SER
10	K	158	ILE
10	K	177	SER
11	L	63	LEU
11	L	148	ILE
11	L	155	LYS
12	M	89	ILE
13	N	66	VAL
14	O	99	LYS
19	V	143	LYS
22	Y	3	ARG

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Mol	Chain	Res	Type
24	a	86	GLU
29	f	91	ASN
29	f	95	ARG
35	A	58	SER
35	A	186	PRO
35	A	187	GLN
36	B	194	LYS
37	U	90	VAL
38	R	126	VAL
38	R	137	HIS
2	C	6	ASP
3	D	149	GLN
5	F	142	LEU
5	F	215	ASP
5	F	216	GLU
6	G	153	LEU
7	H	79	HIS
7	H	164	ARG
8	I	41	LEU
9	J	106	ARG
9	J	190	PRO
11	L	21	GLU
12	M	2	LEU
12	M	42	ASN
13	N	81	LYS
14	O	103	VAL
16	Q	99	ALA
16	Q	140	THR
17	S	29	ASN
17	S	44	PRO
19	V	34	VAL
19	V	40	ALA
21	X	10	ASP
27	d	67	ARG
28	e	8	TRP
29	f	122	PRO
30	g	107	ASP
32	i	131	ALA
35	A	218	CYS
35	A	221	GLU
36	B	65	HIS
36	B	283	GLU

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Mol	Chain	Res	Type
36	B	285	ASP
36	B	462	LYS
37	U	145	THR
38	R	12	PHE
38	R	136	THR
2	C	155	ARG
3	D	82	ARG
4	E	156	GLY
4	E	159	ILE
4	E	260	LYS
5	F	199	GLY
6	G	240	ARG
7	H	22	LYS
7	H	41	VAL
7	H	50	PRO
7	H	58	ALA
7	H	62	ARG
8	I	83	CYS
10	K	11	ARG
10	K	142	SER
10	K	144	LYS
11	L	187	ALA
13	N	42	LEU
13	N	119	ASP
13	N	148	ALA
14	O	75	ASN
14	O	81	ASP
16	Q	66	ARG
16	Q	138	ASP
18	T	84	TYR
18	T	90	ALA
20	W	72	GLU
23	Z	126	ALA
25	b	11	ALA
26	c	83	GLN
28	e	24	CYS
29	f	123	SER
30	g	13	GLY
30	g	48	ASP
31	h	111	ARG
32	i	84	GLY
35	A	242	LEU

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Mol	Chain	Res	Type
35	A	244	ARG
36	B	131	PRO
36	B	174	GLY
36	B	177	SER
36	B	224	VAL
36	B	277	VAL
37	U	144	ARG
38	R	10	ARG
38	R	83	MET
38	R	128	HIS
38	R	130	ARG
2	C	113	GLN
2	C	149	ASN
3	D	20	LYS
3	D	77	ASP
5	F	194	PRO
6	G	30	ARG
6	G	83	PRO
7	H	42	LYS
9	J	6	ALA
9	J	12	ASN
9	J	16	PRO
9	J	45	ILE
11	L	185	ALA
12	M	38	LYS
12	M	94	LEU
17	S	138	ARG
19	V	90	SER
24	a	52	PRO
25	b	8	ASN
27	d	37	ASP
30	g	163	PRO
30	g	190	GLY
30	g	223	GLU
32	i	85	LYS
35	A	143	LYS
35	A	161	SER
35	A	224	PRO
36	B	64	ALA
36	B	196	LYS
36	B	205	ILE
36	B	257	PRO

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Mol	Chain	Res	Type
36	B	321	LYS
36	B	461	GLU
37	U	89	ASP
37	U	95	TYR
2	C	72	ALA
2	C	104	THR
2	C	110	ASN
2	C	191	ARG
3	D	117	TRP
3	D	129	THR
3	D	207	LEU
4	E	45	TRP
4	E	161	LYS
8	I	70	HIS
12	M	41	PRO
13	N	31	GLU
19	V	28	LEU
20	W	70	CYS
20	W	107	GLU
22	Y	58	ALA
24	a	34	THR
24	a	96	LEU
25	b	62	TYR
27	d	66	ARG
29	f	125	GLU
30	g	104	HIS
32	i	83	VAL
32	i	86	VAL
36	B	85	GLU
36	B	260	PRO
38	R	38	SER
38	R	74	GLU
10	K	156	ALA
13	N	6	THR
16	Q	64	ALA
16	Q	129	ILE
16	Q	134	PRO
23	Z	127	ASN
26	c	78	SER
36	B	135	GLY
36	B	154	LEU
2	C	126	ASP

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Mol	Chain	Res	Type
28	e	50	ILE
29	f	102	VAL
29	f	88	PRO
36	B	368	GLY
11	L	163	SER
17	S	100	VAL
28	e	51	GLY
36	B	450	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	I	24/24 (100%)	21 (88%)	3 (12%)	4	22
2	C	174/174 (100%)	171 (98%)	3 (2%)	53	69
3	D	196/196 (100%)	192 (98%)	4 (2%)	48	66
4	E	187/187 (100%)	184 (98%)	3 (2%)	55	70
5	F	190/190 (100%)	184 (97%)	6 (3%)	34	59
6	G	225/225 (100%)	222 (99%)	3 (1%)	61	72
7	H	161/161 (100%)	159 (99%)	2 (1%)	63	73
8	I	207/207 (100%)	206 (100%)	1 (0%)	81	80
9	J	170/170 (100%)	165 (97%)	5 (3%)	37	61
10	K	177/177 (100%)	173 (98%)	4 (2%)	44	64
11	L	157/157 (100%)	156 (99%)	1 (1%)	78	79
12	M	89/89 (100%)	86 (97%)	3 (3%)	32	58
13	N	142/142 (100%)	136 (96%)	6 (4%)	26	52
14	O	104/104 (100%)	103 (99%)	1 (1%)	68	75
15	P	130/130 (100%)	129 (99%)	1 (1%)	73	76
16	Q	106/106 (100%)	105 (99%)	1 (1%)	70	75
17	S	117/117 (100%)	112 (96%)	5 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	T	114/114 (100%)	113 (99%)	1 (1%)	70	75
19	V	113/113 (100%)	113 (100%)	0	100	100
20	W	94/94 (100%)	94 (100%)	0	100	100
21	X	67/67 (100%)	65 (97%)	2 (3%)	36	60
22	Y	112/112 (100%)	112 (100%)	0	100	100
23	Z	114/114 (100%)	112 (98%)	2 (2%)	51	69
24	a	108/108 (100%)	107 (99%)	1 (1%)	70	75
25	b	87/87 (100%)	87 (100%)	0	100	100
26	c	76/76 (100%)	75 (99%)	1 (1%)	61	72
27	d	57/57 (100%)	56 (98%)	1 (2%)	51	69
28	e	47/47 (100%)	46 (98%)	1 (2%)	47	66
29	f	64/64 (100%)	60 (94%)	4 (6%)	16	43
30	g	272/272 (100%)	270 (99%)	2 (1%)	76	77
31	h	66/66 (100%)	66 (100%)	0	100	100
32	i	49/49 (100%)	49 (100%)	0	100	100
35	A	238/238 (100%)	234 (98%)	4 (2%)	53	69
36	B	354/354 (100%)	351 (99%)	3 (1%)	73	76
37	U	122/122 (100%)	120 (98%)	2 (2%)	55	70
38	R	121/121 (100%)	116 (96%)	5 (4%)	27	53
All	All	4831/4831 (100%)	4750 (98%)	81 (2%)	52	69

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	2	ARG
1	l	5	TRP
1	l	23	ARG
2	C	88	LEU
2	C	140	VAL
2	C	201	LEU
3	D	49	VAL
3	D	212	VAL
3	D	220	LYS
3	D	228	LEU
4	E	39	LYS

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Mol	Chain	Res	Type
4	E	43	LYS
4	E	122	VAL
5	F	5	ILE
5	F	76	ARG
5	F	108	LYS
5	F	117	ARG
5	F	124	ARG
5	F	150	MET
6	G	176	ASP
6	G	230	LYS
6	G	254	LYS
7	H	29	GLN
7	H	201	LYS
8	I	167	LYS
9	J	32	MET
9	J	66	VAL
9	J	76	GLN
9	J	78	ARG
9	J	85	LYS
10	K	10	LYS
10	K	166	PHE
10	K	194	GLU
10	K	201	LYS
11	L	116	LYS
12	M	58	VAL
12	M	59	LYS
12	M	94	LEU
13	N	1	MET
13	N	4	ILE
13	N	31	GLU
13	N	39	ASN
13	N	111	VAL
13	N	157	LYS
14	O	40	LYS
15	P	39	LYS
16	Q	39	ASP
17	S	41	MET
17	S	49	TYR
17	S	73	LYS
17	S	105	LYS
17	S	131	LYS
18	T	106	LEU

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Mol	Chain	Res	Type
21	X	16	LYS
21	X	40	ASP
23	Z	32	LEU
23	Z	105	PHE
24	a	29	HIS
26	c	83	GLN
27	d	67	ARG
28	e	39	CYS
29	f	99	LYS
29	f	104	LYS
29	f	118	ARG
29	f	125	GLU
30	g	51	ASN
30	g	206	LEU
35	A	55	ARG
35	A	64	ARG
35	A	141	LYS
35	A	261	LYS
36	B	137	PHE
36	B	203	ASN
36	B	430	VAL
37	U	144	ARG
37	U	146	VAL
38	R	75	VAL
38	R	84	ILE
38	R	127	LYS
38	R	130	ARG
38	R	137	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	22	GLN
2	C	113	GLN
2	C	149	ASN
2	C	164	ASN
3	D	158	HIS
4	E	220	ASN
4	E	257	HIS
5	F	74	GLN
5	F	101	GLN
5	F	145	GLN

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Mol	Chain	Res	Type
5	F	207	HIS
6	G	50	ASN
6	G	98	ASN
6	G	112	HIS
6	G	157	ASN
6	G	209	HIS
7	H	29	GLN
7	H	36	GLN
7	H	65	GLN
7	H	79	HIS
7	H	95	HIS
7	H	186	ASN
8	I	4	ASN
8	I	65	GLN
8	I	81	HIS
8	I	105	ASN
8	I	146	ASN
9	J	91	HIS
9	J	97	GLN
9	J	112	ASN
9	J	163	GLN
9	J	193	GLN
10	K	22	HIS
10	K	64	ASN
10	K	88	ASN
11	L	143	ASN
11	L	156	HIS
12	M	28	HIS
12	M	32	HIS
12	M	61	GLN
13	N	13	GLN
13	N	106	HIS
13	N	108	ASN
13	N	121	GLN
14	O	55	ASN
14	O	73	GLN
15	P	36	GLN
15	P	49	GLN
15	P	105	ASN
15	P	138	ASN
16	Q	32	HIS
16	Q	79	GLN

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Mol	Chain	Res	Type
19	V	42	HIS
19	V	51	ASN
19	V	105	GLN
20	W	47	ASN
22	Y	24	GLN
22	Y	113	HIS
23	Z	16	HIS
23	Z	46	HIS
24	a	19	GLN
24	a	29	HIS
25	b	8	ASN
25	b	17	HIS
25	b	43	ASN
25	b	72	HIS
25	b	80	HIS
26	c	19	HIS
27	d	29	GLN
28	e	4	GLN
28	e	5	GLN
28	e	10	HIS
28	e	16	GLN
28	e	45	GLN
29	f	93	HIS
30	g	14	HIS
30	g	62	HIS
30	g	104	HIS
30	g	133	ASN
30	g	143	GLN
30	g	159	ASN
30	g	187	ASN
30	g	188	HIS
30	g	222	ASN
30	g	311	GLN
31	h	46	ASN
31	h	89	GLN
31	h	103	HIS
35	A	41	ASN
35	A	68	ASN
35	A	132	GLN
35	A	169	ASN
35	A	181	ASN
35	A	187	GLN

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Mol	Chain	Res	Type
36	B	65	HIS
36	B	98	ASN
36	B	160	ASN
36	B	180	GLN
36	B	202	GLN
36	B	203	ASN
36	B	420	ASN
37	U	42	HIS
37	U	87	GLN
37	U	120	HIS
38	R	79	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1733/1863 (93%)	264 (15%)	11 (0%)
34	3	35/36 (97%)	20 (57%)	5 (14%)
39	1	74/75 (98%)	16 (21%)	5 (6%)
All	All	1842/1974 (93%)	300 (16%)	21 (1%)

All (300) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	4	C
33	2	33	G
33	2	41	G
33	2	42	A
33	2	44	U
33	2	46	A
33	2	55	U
33	2	56	G
33	2	59	U
33	2	60	A
33	2	67	C
33	2	68	A
33	2	73	C
33	2	74	G
33	2	75	G
33	2	76	U
33	2	79	A
33	2	80	G

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Mol	Chain	Res	Type
33	2	94	G
33	2	113	G
33	2	126	G
33	2	143	U
33	2	147	A
33	2	148	U
33	2	178	C
33	2	179	C
33	2	181	A
33	2	182	C
33	2	183	G
33	2	184	G
33	2	191	C
33	2	197	U
33	2	202	U
33	2	223	A
33	2	224	U
33	2	225	C
33	2	226	A
33	2	271	G
33	2	274	G
33	2	277	U
33	2	278	U
33	2	285	U
33	2	296	U
33	2	299	G
33	2	300	G
33	2	309	A
33	2	310	G
33	2	311	C
33	2	315	C
33	2	316	C
33	2	317	G
33	2	322	G
33	2	337	G
33	2	347	C
33	2	352	C
33	2	354	A
33	2	358	U
33	2	375	G
33	2	376	C
33	2	397	G

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Mol	Chain	Res	Type
33	2	398	A
33	2	399	C
33	2	418	U
33	2	438	A
33	2	439	A
33	2	440	C
33	2	442	G
33	2	457	G
33	2	462	C
33	2	463	A
33	2	464	G
33	2	472	G
33	2	477	U
33	2	483	A
33	2	492	C
33	2	513	A
33	2	515	A
33	2	522	C
33	2	542	G
33	2	543	U
33	2	546	U
33	2	547	U
33	2	554	A
33	2	558	C
33	2	579	G
33	2	580	A
33	2	581	U
33	2	582	C
33	2	583	C
33	2	584	A
33	2	596	G
33	2	597	U
33	2	598	C
33	2	604	G
33	2	618	A
33	2	633	A
33	2	658	A
33	2	659	A
33	2	661	A
33	2	662	A
33	2	678	U
33	2	679	U

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Mol	Chain	Res	Type
33	2	680	G
33	2	681	U
33	2	682	G
33	2	729	C
33	2	732	C
33	2	733	G
33	2	734	C
33	2	735	C
33	2	736	C
33	2	737	C
33	2	738	U
33	2	739	U
33	2	740	G
33	2	741	C
33	2	742	C
33	2	743	U
33	2	744	C
33	2	746	C
33	2	747	G
33	2	748	G
33	2	749	C
33	2	750	G
33	2	751	C
33	2	785	G
33	2	786	C
33	2	787	C
33	2	788	C
33	2	789	G
33	2	790	A
33	2	791	A
33	2	793	C
33	2	794	G
33	2	795	U
33	2	807	A
33	2	817	G
33	2	818	U
33	2	819	U
33	2	820	C
33	2	833	A
33	2	835	C
33	2	843	A
33	2	849	C

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Mol	Chain	Res	Type
33	2	865	A
33	2	867	U
33	2	868	A
33	2	869	G
33	2	870	G
33	2	874	G
33	2	883	U
33	2	884	U
33	2	906	G
33	2	907	C
33	2	909	A
33	2	915	A
33	2	916	A
33	2	918	A
33	2	929	G
33	2	951	A
33	2	966	G
33	2	967	G
33	2	986	A
33	2	988	A
33	2	1004	A
33	2	1012	U
33	2	1013	U
33	2	1019	A
33	2	1041	U
33	2	1045	A
33	2	1057	U
33	2	1058	A
33	2	1081	C
33	2	1082	G
33	2	1106	G
33	2	1112	C
33	2	1113	C
33	2	1144	A
33	2	1145	A
33	2	1153	G
33	2	1154	G
33	2	1203	G
33	2	1211	C
33	2	1217	G
33	2	1238	U
33	2	1246	A

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Mol	Chain	Res	Type
33	2	1247	A
33	2	1253	G
33	2	1255	A
33	2	1270	G
33	2	1271	G
33	2	1280	A
33	2	1298	G
33	2	1299	C
33	2	1340	A
33	2	1367	U
33	2	1368	U
33	2	1374	A
33	2	1382	A
33	2	1391	C
33	2	1399	C
33	2	1406	C
33	2	1408	C
33	2	1413	C
33	2	1414	C
33	2	1415	C
33	2	1427	G
33	2	1431	C
33	2	1432	C
33	2	1450	A
33	2	1470	A
33	2	1471	G
33	2	1472	A
33	2	1473	U
33	2	1474	U
33	2	1485	A
33	2	1486	G
33	2	1506	G
33	2	1507	U
33	2	1516	C
33	2	1517	A
33	2	1518	C
33	2	1539	C
33	2	1547	G
33	2	1548	C
33	2	1549	C
33	2	1550	U
33	2	1575	A

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Mol	Chain	Res	Type
33	2	1580	U
33	2	1583	A
33	2	1596	A
33	2	1616	U
33	2	1617	U
33	2	1618	A
33	2	1632	A
33	2	1643	G
33	2	1659	A
33	2	1660	G
33	2	1666	G
33	2	1675	G
33	2	1683	C
33	2	1716	U
33	2	1717	G
33	2	1743	G
33	2	1747	C
33	2	1748	G
33	2	1777	C
33	2	1778	G
33	2	1817	A
33	2	1819	A
33	2	1820	G
33	2	1823	G
33	2	1825	A
33	2	1829	A
33	2	1843	G
33	2	1846	C
33	2	1855	G
33	2	1856	G
33	2	1857	A
33	2	1858	U
33	2	1859	C
33	2	1860	A
33	2	1862	U
33	2	1863	A
34	3	43	G
34	3	44	U
34	3	45	C
34	3	46	A
34	3	47	U
34	3	48	A

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Mol	Chain	Res	Type
34	3	50	C
34	3	54	G
34	3	55	U
34	3	56	C
34	3	57	U
34	3	58	G
34	3	59	G
34	3	60	A
34	3	61	C
34	3	65	G
34	3	66	C
34	3	69	G
34	3	72	U
34	3	75	U
39	1	9	U
39	1	11	G
39	1	15	A
39	1	16	G
39	1	17	C
39	1	18	G
39	1	19	G
39	1	21	A
39	1	43	G
39	1	45	G
39	1	47	U
39	1	56	C
39	1	61	C
39	1	74	C
39	1	75	C
39	1	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	2	224	U
33	2	397	G
33	2	739	U
33	2	817	G
33	2	866	A
33	2	1012	U
33	2	1057	U
33	2	1153	G

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Mol	Chain	Res	Type
33	2	1549	C
33	2	1616	U
33	2	1818	A
34	3	54	G
34	3	56	C
34	3	57	U
34	3	58	G
34	3	65	G
39	1	8	G
39	1	16	G
39	1	17	C
39	1	18	G
39	1	74	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	T6A	1	37	39	31,34,35	1.41	4 (12%)	43,49,52	2.50	18 (41%)
33	C4J	2	1244	33	25,29,30	1.04	2 (8%)	28,42,45	2.91	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	T6A	1	37	39	-	6/23/41/42	0/3/3/3
33	C4J	2	1244	33	1/1/7/7	9/16/34/35	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	37	T6A	C5-C4	4.75	1.47	1.39
33	2	1244	C4J	C4-C5	-3.51	1.39	1.47
39	1	37	T6A	C5-C6	2.76	1.48	1.41
39	1	37	T6A	C5-N7	-2.33	1.34	1.39
39	1	37	T6A	C8-N7	2.25	1.36	1.31
33	2	1244	C4J	C1'-C5	-2.12	1.45	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2	1244	C4J	C1'-C5-C4	14.41	139.48	117.61
39	1	37	T6A	C12-N11-C10	8.54	136.20	121.99
39	1	37	T6A	C5-C4-N3	-5.55	119.07	126.72
39	1	37	T6A	N3-C4-N9	4.45	134.74	127.17
39	1	37	T6A	C14-C12-C13	3.69	116.47	110.03
39	1	37	T6A	C2-N3-C4	3.69	120.84	111.83
33	2	1244	C4J	C4-N3-C2	-3.63	121.15	125.62
39	1	37	T6A	N3-C2-N1	-3.62	123.09	128.58
39	1	37	T6A	C2'-C1'-N9	-3.59	104.39	113.30
39	1	37	T6A	C4-C5-N7	-3.56	106.51	110.58
39	1	37	T6A	C6-C5-N7	3.49	136.23	132.43
39	1	37	T6A	O10-C10-N6	-2.84	118.60	123.64
39	1	37	T6A	C4-N9-C8	2.77	108.64	105.74
39	1	37	T6A	C5-N7-C8	2.68	107.67	103.45
39	1	37	T6A	C14-C12-N11	2.61	118.63	111.70
39	1	37	T6A	C2-N1-C6	2.22	122.61	115.24
39	1	37	T6A	N6-C10-N11	2.13	116.70	113.77
39	1	37	T6A	O4'-C1'-N9	2.08	112.08	108.09
39	1	37	T6A	N9-C8-N7	-2.07	110.99	113.94
39	1	37	T6A	N6-C6-N1	2.03	122.79	117.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	2	1244	C4J	C4'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	2	1244	C4J	C31-C3-N3-C2
33	2	1244	C4J	C31-C3-N3-C4
33	2	1244	C4J	C3-C31-C32-C34
33	2	1244	C4J	C3-C31-C32-N33

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Mol	Chain	Res	Type	Atoms
39	1	37	T6A	C14-C12-N11-C10
33	2	1244	C4J	N33-C32-C34-O35
39	1	37	T6A	N11-C12-C13-ODB
39	1	37	T6A	N11-C12-C13-ODA
39	1	37	T6A	O4'-C4'-C5'-O5'
39	1	37	T6A	C13-C12-N11-C10
33	2	1244	C4J	C31-C32-C34-O35
39	1	37	T6A	C13-C12-C14-C15
33	2	1244	C4J	C31-C32-C34-O36
33	2	1244	C4J	N3-C3-C31-C32
33	2	1244	C4J	N33-C32-C34-O36

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	37	T6A	4	0
33	2	1244	C4J	3	0

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
33	2	6
39	1	5
8	I	1

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Mol	Chain	Number of breaks
24	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	P	8.58
1	I	217:MET	C	218:LYS	N	3.94
1	a	9:THR	C	10:ARG	N	3.27
1	1	19:G	O3'	20:A	P	2.13
1	1	17:C	O3'	18:G	P	1.99
1	1	18:G	O3'	19:G	P	1.87
1	2	350:A	O3'	351:U	P	1.86
1	2	675:A	O3'	676:U	P	1.84
1	2	676:U	O3'	677:C	P	1.38
1	2	1172:G	O3'	1173:U	P	1.37
1	1	36:U	O3'	37:T6A	P	1.28
1	2	1815:U	O3'	1816:A	P	1.26
1	1	16:G	O3'	17:C	P	1.14

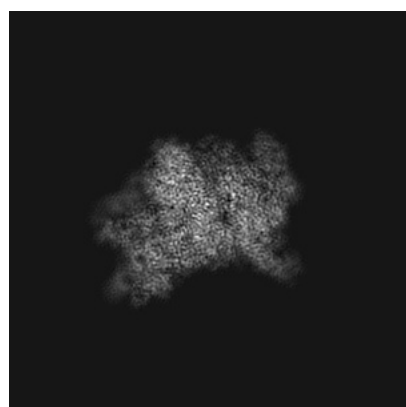
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10762. These allow visual inspection of the internal detail of the map and identification of artifacts.

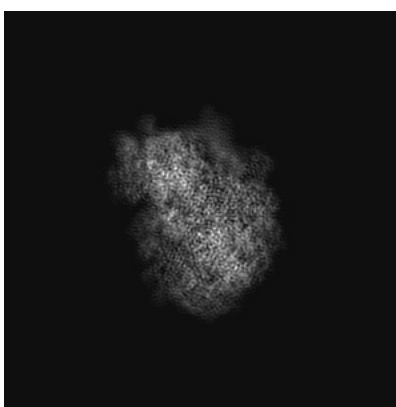
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

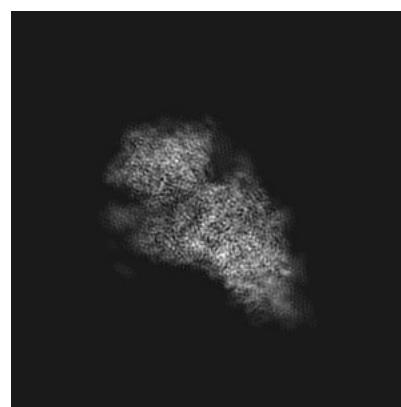
6.1.1 Primary map



X



Y

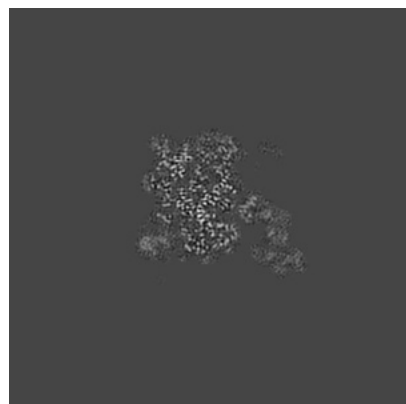


Z

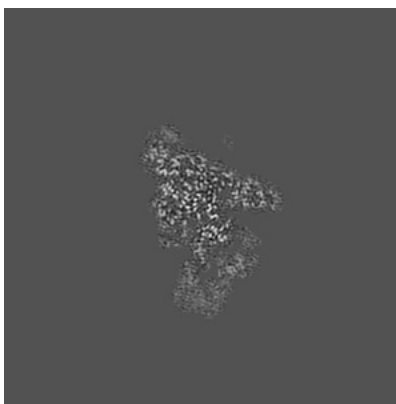
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

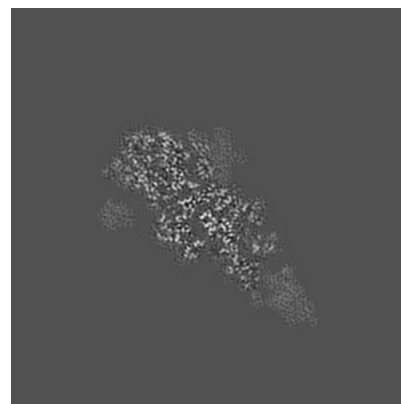
6.2.1 Primary map



X Index: 192



Y Index: 192

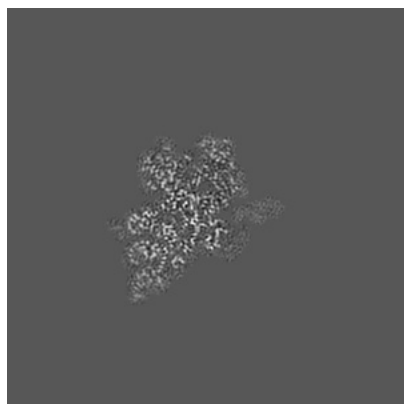


Z Index: 192

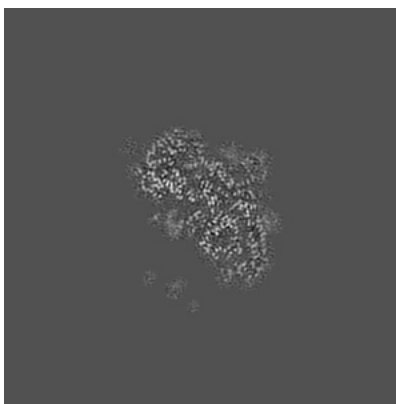
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

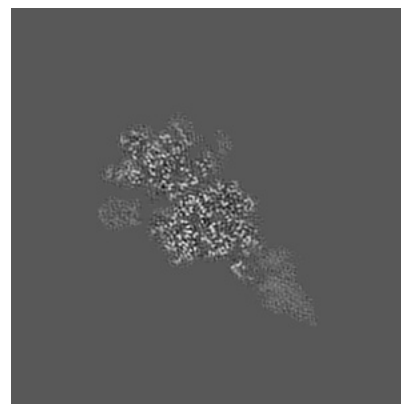
6.3.1 Primary map



X Index: 208



Y Index: 160

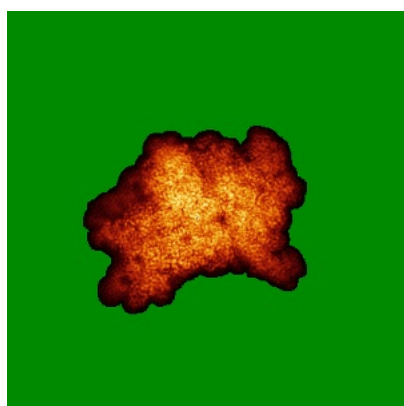


Z Index: 199

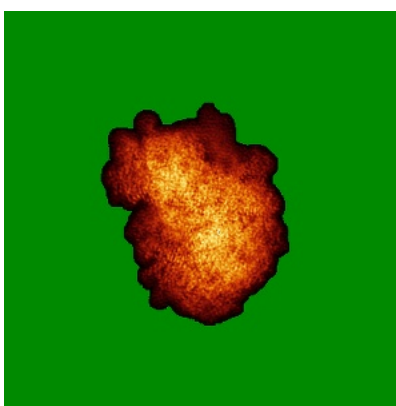
The images above show the largest variance slices of the map in three orthogonal directions.

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

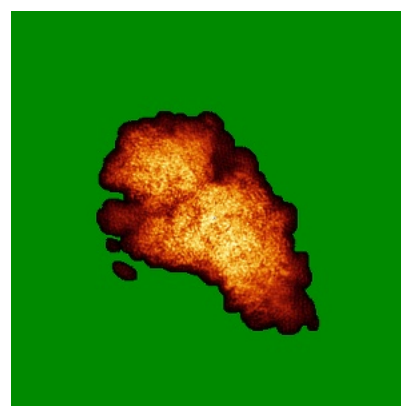
6.4.1 Primary map



X



Y

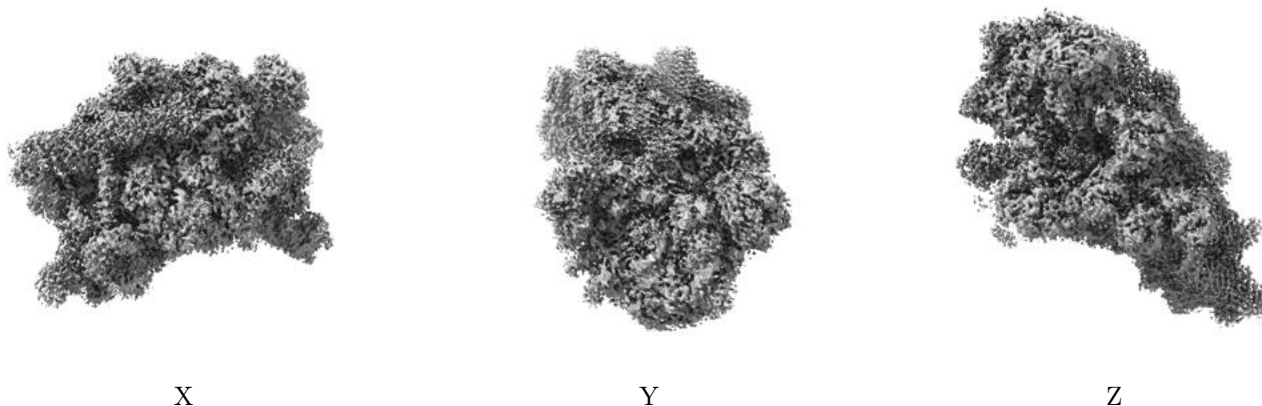


Z

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 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

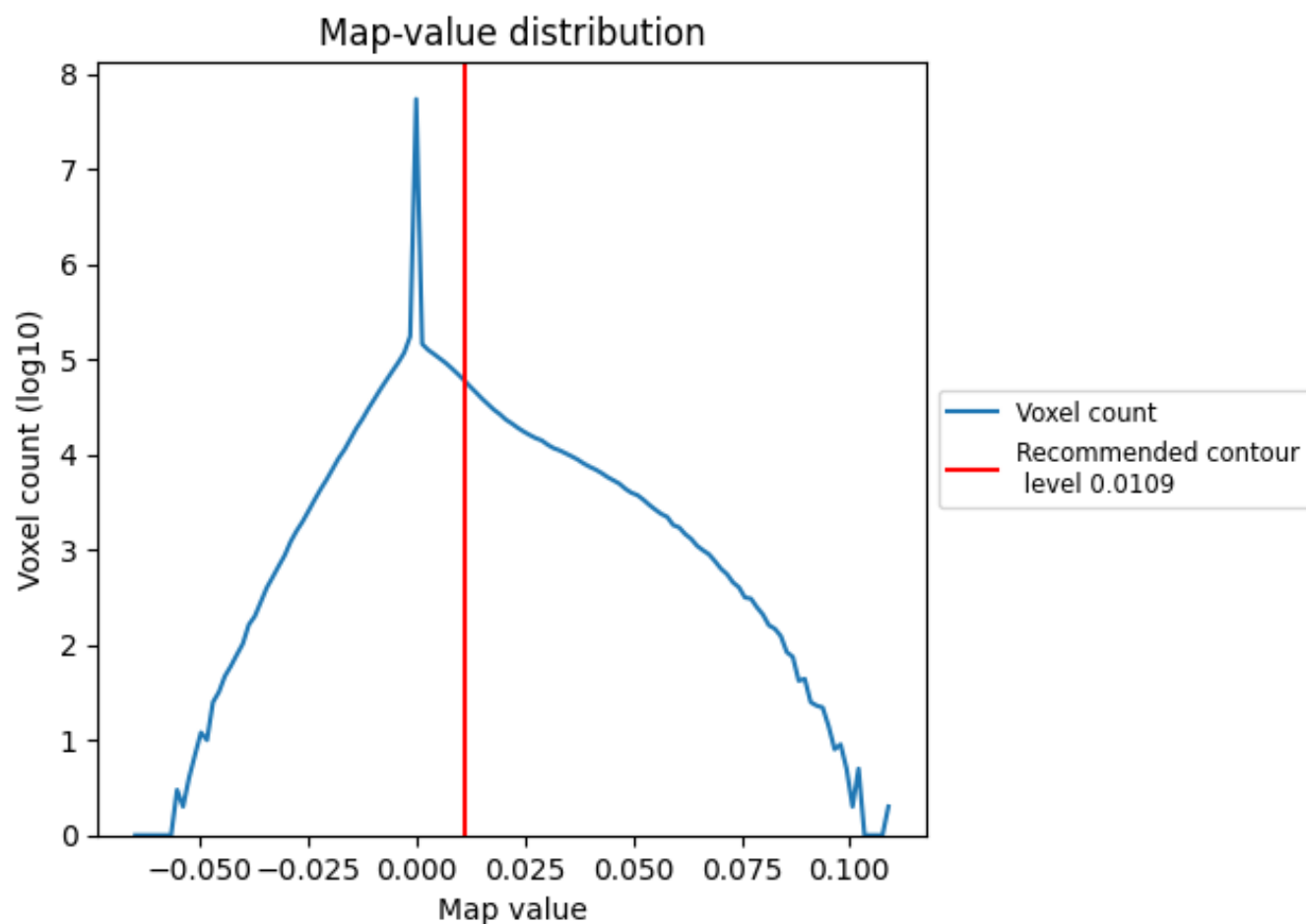
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

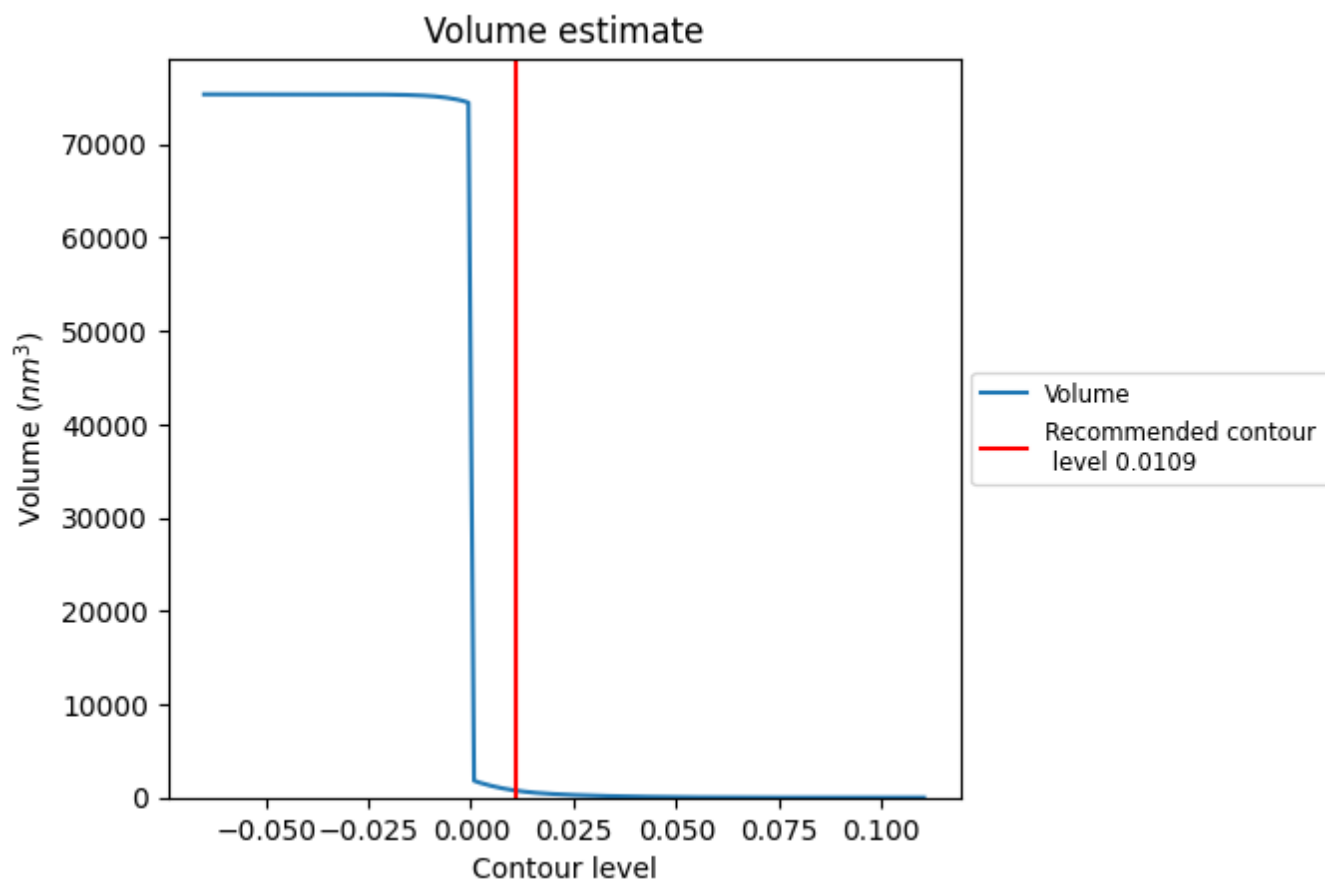
This section contains the results of statistical analysis of the map.

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.

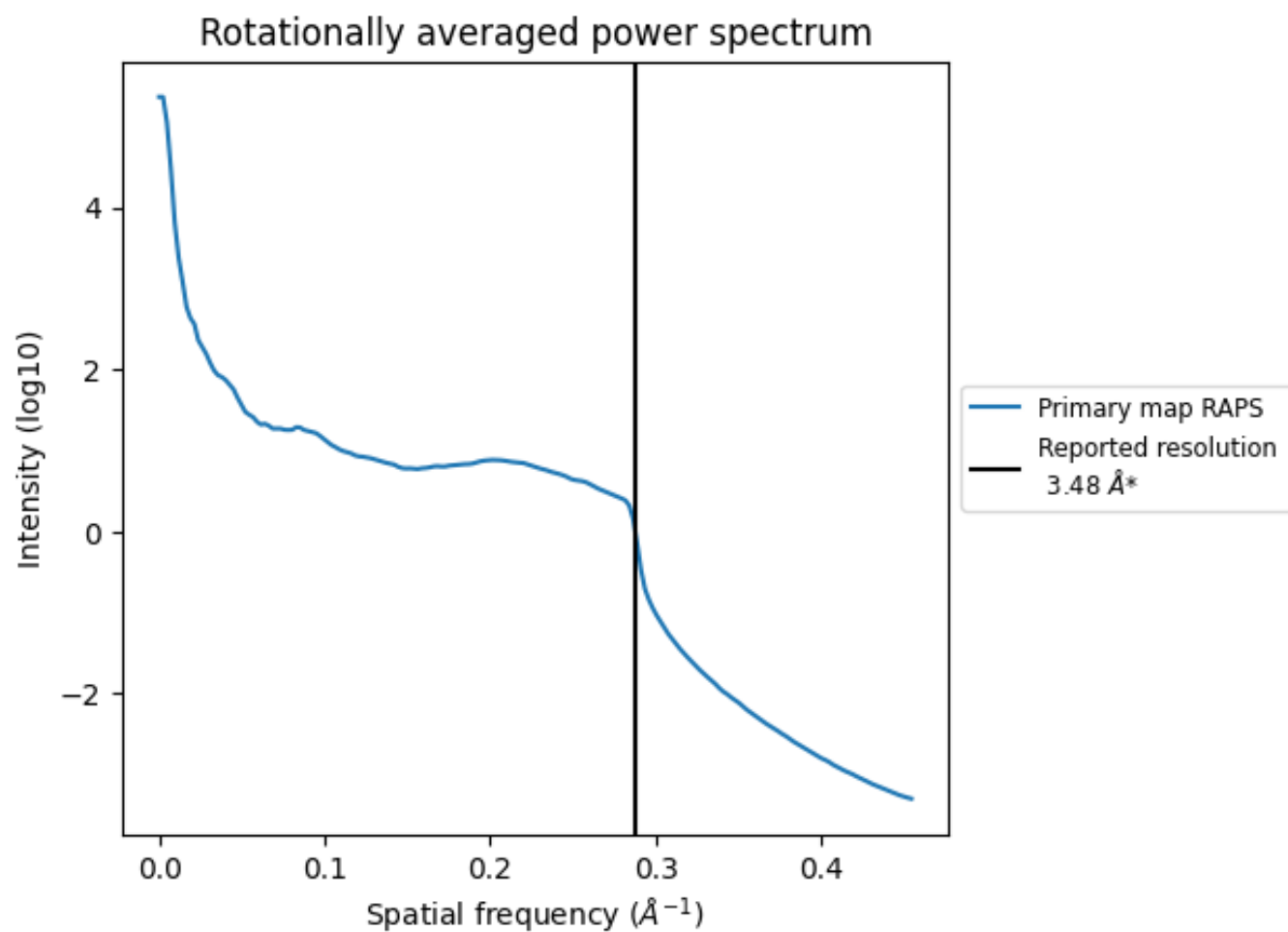
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 0.287 Å⁻¹

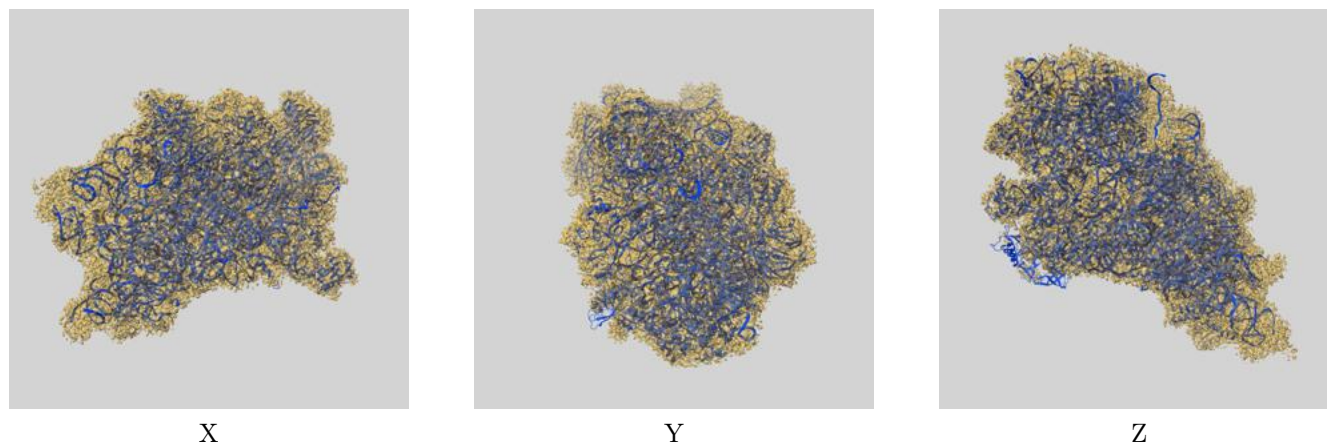
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

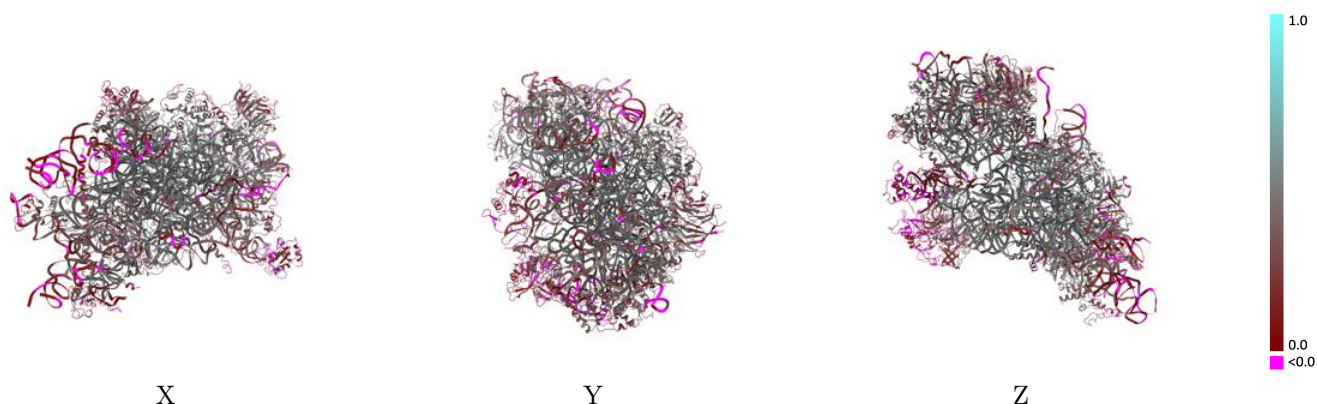
This section contains information regarding the fit between EMDB map EMD-10762 and PDB model 6YAN. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



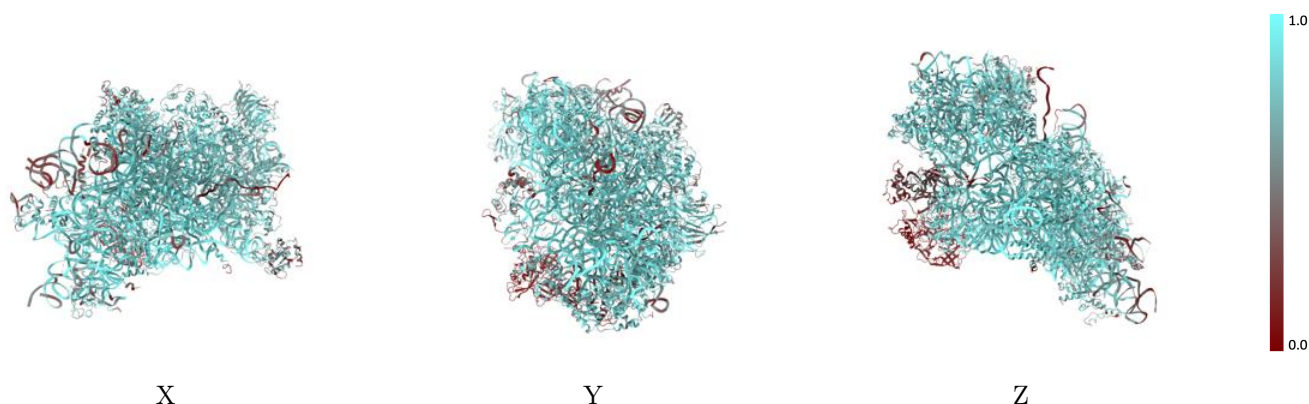
The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



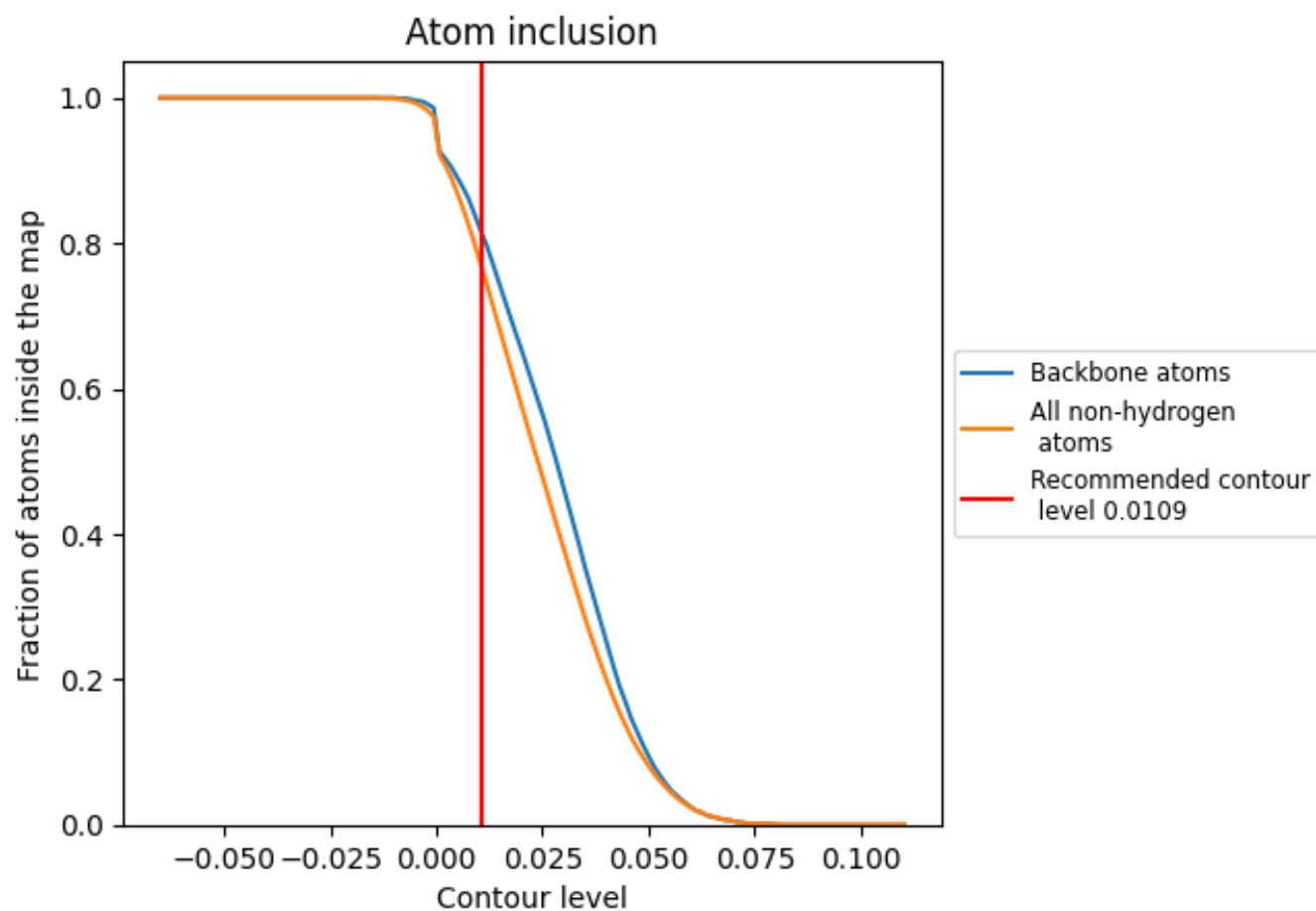
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0109).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.3510
1	 0.5060	 0.1520
2	 0.8840	 0.4010
3	 0.3270	 0.1390
A	 0.1820	 0.0510
B	 0.0080	 -0.0120
C	 0.8300	 0.4210
D	 0.7890	 0.4010
E	 0.8250	 0.4440
F	 0.7360	 0.3530
G	 0.8140	 0.4160
H	 0.7840	 0.3830
I	 0.7260	 0.2980
J	 0.6340	 0.2810
K	 0.7710	 0.3630
L	 0.8230	 0.4160
M	 0.7420	 0.3150
N	 0.7490	 0.3830
O	 0.4360	 0.1240
P	 0.8050	 0.3960
Q	 0.8060	 0.4090
R	 0.7000	 0.3020
S	 0.8140	 0.4180
T	 0.7290	 0.3300
U	 0.7690	 0.3430
V	 0.7770	 0.3790
W	 0.7500	 0.3450
X	 0.7920	 0.3780
Y	 0.8680	 0.4780
Z	 0.8510	 0.4510
a	 0.7970	 0.3730
b	 0.8330	 0.4320
c	 0.7400	 0.3230
d	 0.7540	 0.3660
e	 0.8100	 0.3800



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Chain	Atom inclusion	Q-score
f	 0.4430	 0.0750
g	 0.7390	 0.3250
h	 0.7060	 0.3110
i	 0.6230	 0.2840
l	 0.7670	 0.3910