



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 3J7A / pdb_00003j7a
EMDB ID : EMD-2660
Title : Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine, small subunit
Authors : Wong, W.; Bai, X.C.; Brown, A.; Fernandez, I.S.; Hanssen, E.; Condrón, M.; Tan, Y.H.; Baum, J.; Scheres, S.H.W.
Deposited on : 2014-06-03
Resolution : 3.20 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:

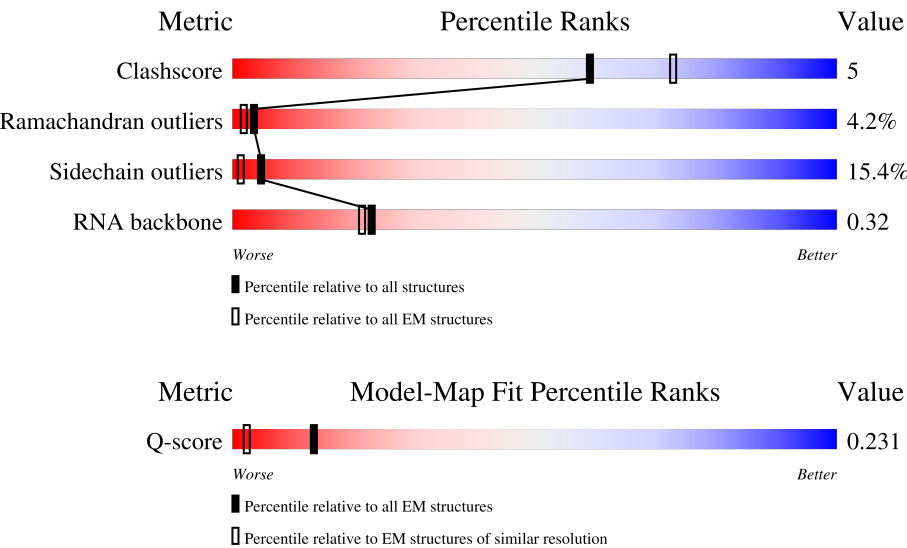
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	A	2092	44% 44%26%6%23%
2	B	262	76% 52%21%6%20%
3	C	263	70% 54%17%26%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	189	
6	F	261	
7	G	272	
8	H	306	
9	I	195	
10	J	194	
11	K	130	
12	L	218	
13	M	144	
14	N	118	
15	O	137	
16	P	151	
17	Q	145	
18	R	141	
19	S	156	
20	T	54	
21	U	151	
22	V	161	
23	W	137	
24	X	145	
25	Y	170	
26	Z	82	
27	1	133	
28	2	105	

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Mol	Chain	Length	Quality of chain
29	3	107	79% 67% 18% • 11%
30	4	82	87% 65% 24% • 7%
31	5	67	87% 78% 9% 13%
32	6	58	59% 57% 10% 7% 26%
33	7	74	100% 53% 46% •

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1608	Total	C	N	O	P	0	0
			34277	15347	6109	11213	1608		

- Molecule 2 is a protein called 40S ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	210	Total	C	N	O	S	0	0
			1713	1097	301	303	12		

- Molecule 3 is a protein called 40S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	195	Total	C	N	O	S	0	0
			1538	990	266	273	9		

- Molecule 4 is a protein called 40S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1228	782	225	214	7		

- Molecule 5 is a protein called 40S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1508	959	287	260	2		

- Molecule 6 is a protein called 40S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	257	Total	C	N	O	S	0	0
			2061	1320	377	356	8		

- Molecule 7 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	224	Total	C	N	O	S	0	0
			1757	1132	307	309	9		

- Molecule 8 is a protein called 40S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	204	Total	C	N	O	S	0	0
			1644	1042	313	283	6		

- Molecule 9 is a protein called 40S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	180	Total	C	N	O	S	0	0
			1424	893	263	258	10		

- Molecule 10 is a protein called 40S ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	188	Total	C	N	O	S	0	0
			1528	982	264	278	4		

- Molecule 11 is a protein called 40S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	129	Total	C	N	O	S	0	0
			1037	665	189	178	5		

- Molecule 12 is a protein called 40S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	172	Total	C	N	O	S	0	0
			1392	878	266	244	4		

- Molecule 13 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	138	Total	C	N	O	S	0	0
			1098	704	200	193	1		

- Molecule 14 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	98	Total	C	N	O	S	0	0
			772	484	135	148	5		

- Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	79	Total	C	N	O	S	0	0
			686	450	116	118	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	127	Total	C	N	O	S	0	0
			953	591	184	175	3		

- Molecule 17 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	144	Total	C	N	O	S	0	0
			1129	712	222	193	2		

- Molecule 18 is a protein called 40S ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	98	Total	C	N	O	S	0	0
			746	474	123	145	4		

- Molecule 19 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	128	Total	C	N	O	S	0	0
			1042	655	204	179	4		

- Molecule 20 is a protein called 40S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	48	Total	C	N	O	S	0	0
			404	252	85	63	4		

- Molecule 21 is a protein called 40S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	149	Total	C	N	O	S	0	0
			1202	769	220	210	3		

- Molecule 22 is a protein called 40S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	146	Total	C	N	O	S	0	0
			1206	772	227	200	7		

- Molecule 23 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	95	Total	C	N	O	S	0	0
			785	498	149	135	3		

- Molecule 24 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	96	Total	C	N	O	S	0	0
			776	497	137	138	4		

- Molecule 25 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	154	Total	C	N	O	S	0	0
			1266	811	239	214	2		

- Molecule 26 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	72	Total	C	N	O	S	0	0
			556	346	102	104	4		

- Molecule 27 is a protein called 40S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	120	Total	C	N	O	S	0	0
			981	629	188	162	2		

- Molecule 28 is a protein called 40S ribosomal protein eS25.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	41	Total	C	N	O	0	0
			320	208	56	56		

- Molecule 29 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	95	Total	C	N	O	S	0	0
			781	478	169	128	6		

- Molecule 30 is a protein called 40S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	76	Total	C	N	O	S	0	0
			586	368	102	107	9		

- Molecule 31 is a protein called 40S ribosomal protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	5	58	Total	C	N	O	0	0
			451	282	90	79		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
32	6	43	Total	C	N	O	0	0
			345	213	75	57		

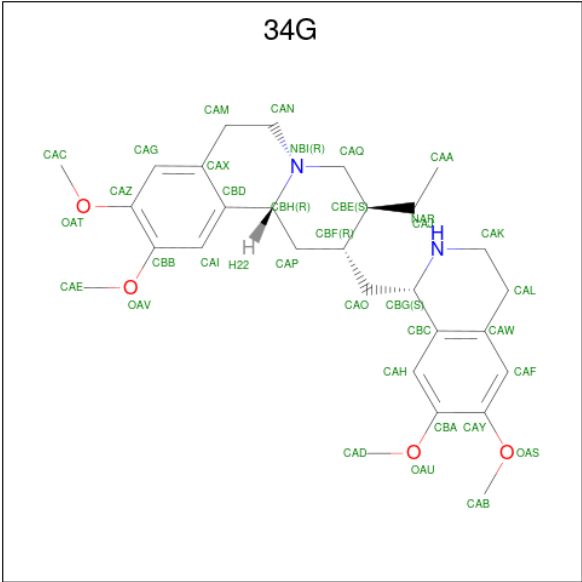
- Molecule 33 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	74	Total	C	N	O	P	0	0
			1571	702	275	521	73		

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	A	67	Total	Mg	0
			67	67	

- Molecule 35 is emetine (CCD ID: 34G) (formula: C₂₉H₄₀N₂O₄).

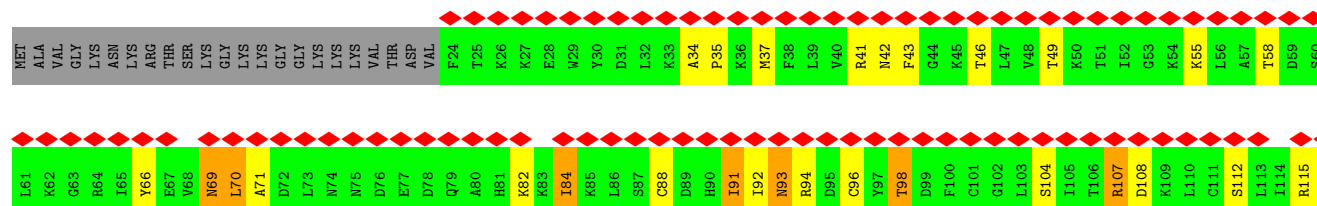
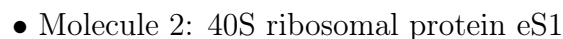


Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			35	29	2	4	

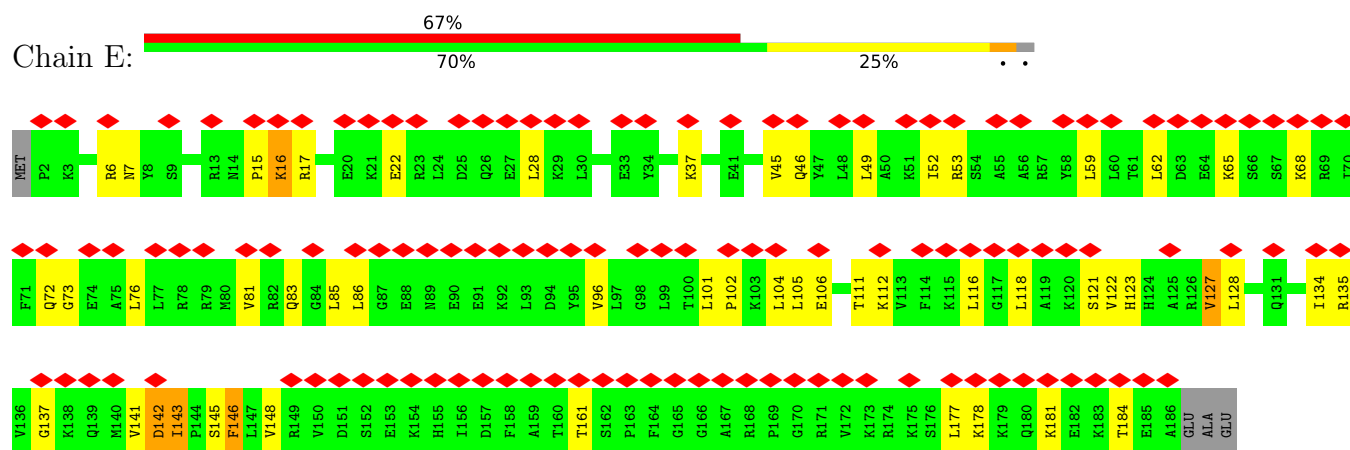
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	T	1	Total	Zn	0
			1	1	

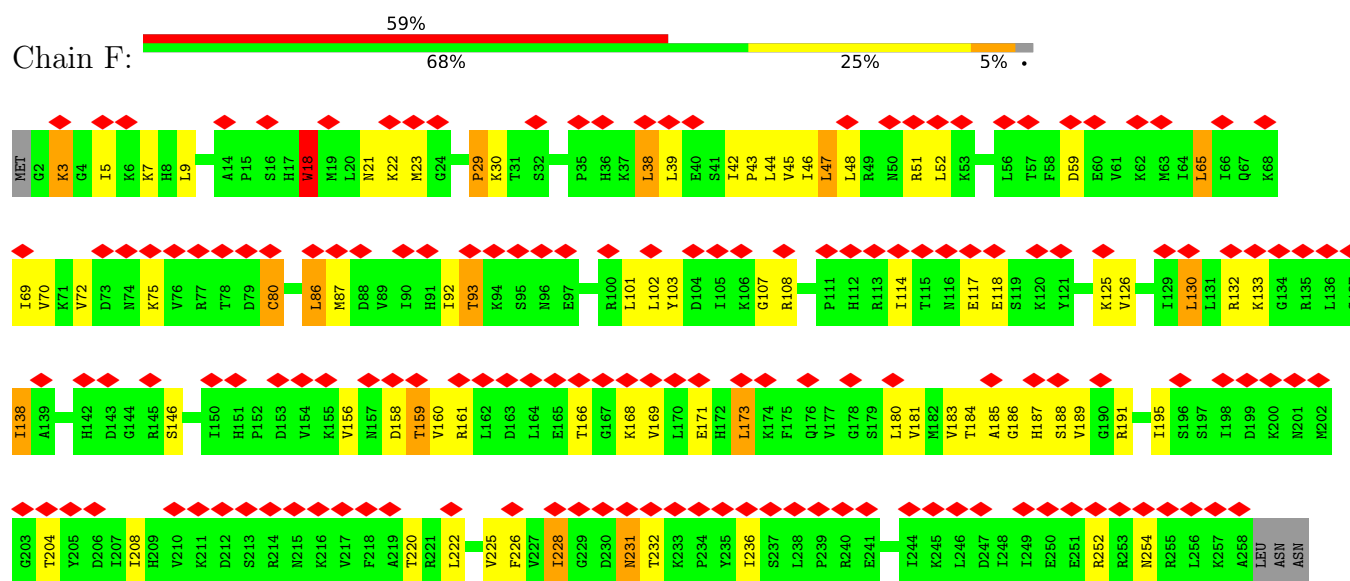




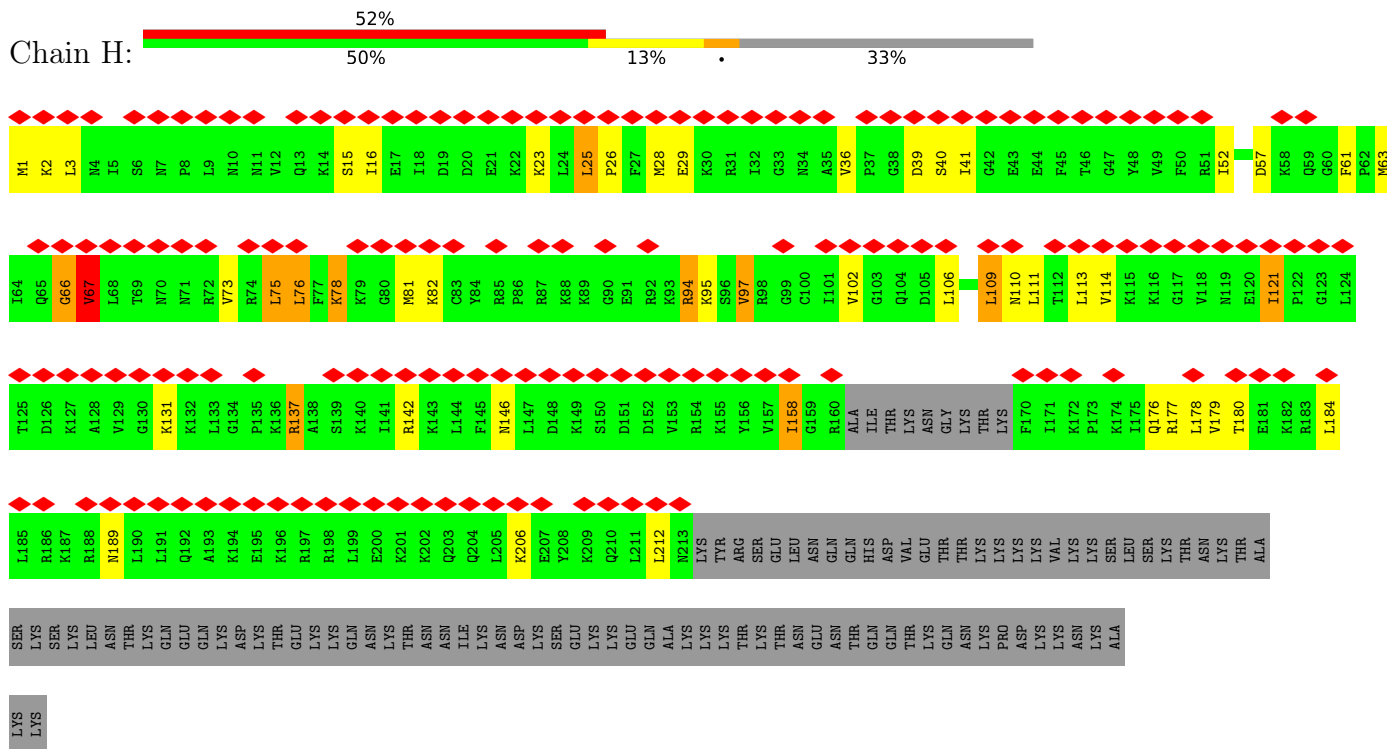




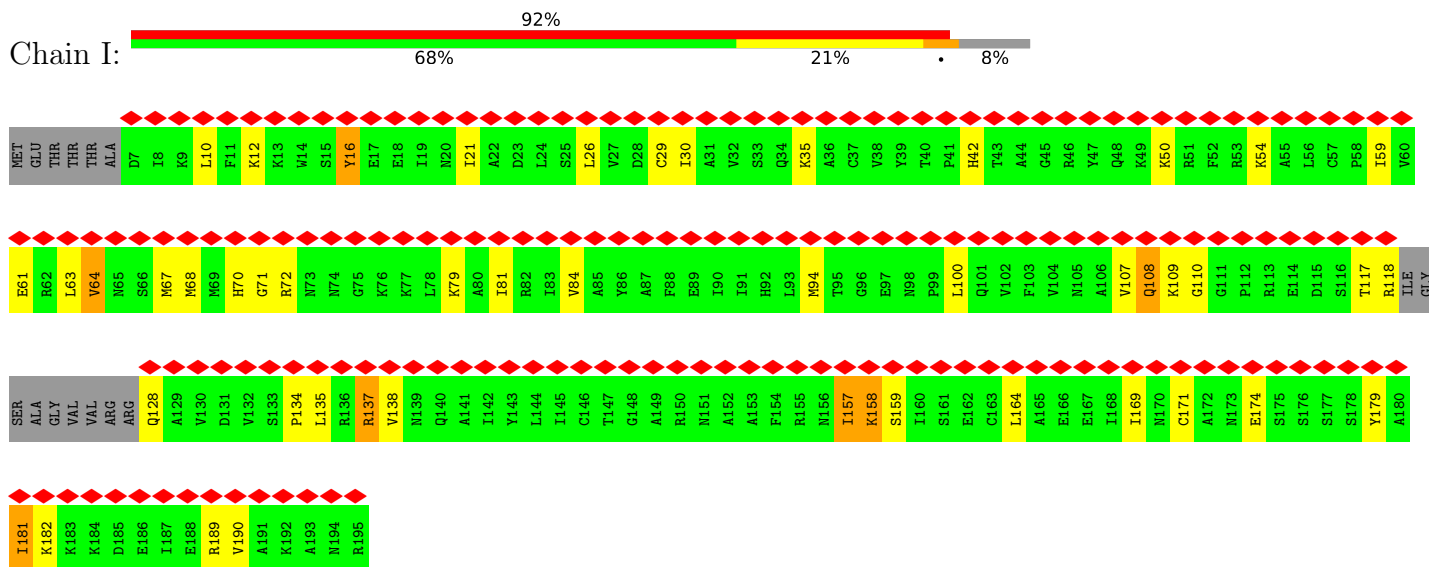
• Molecule 6: 40S ribosomal protein eS4



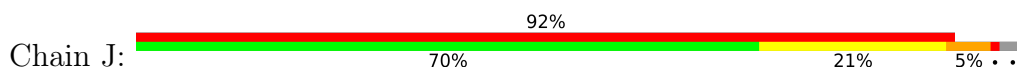
- Molecule 8: 40S ribosomal protein eS6



- Molecule 9: 40S ribosomal protein uS7

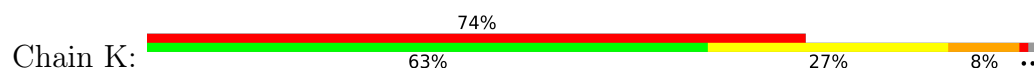


- Molecule 10: 40S ribosomal protein eS7

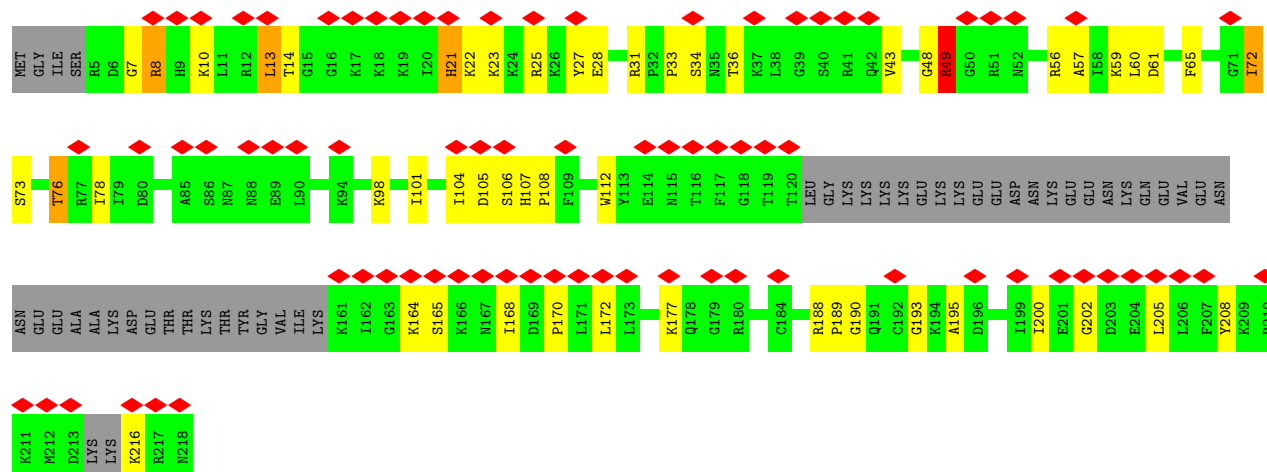




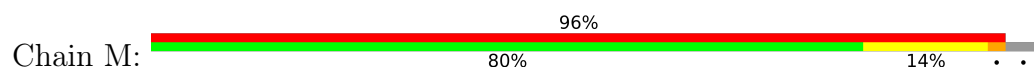
- Molecule 11: 40S ribosomal protein uS8

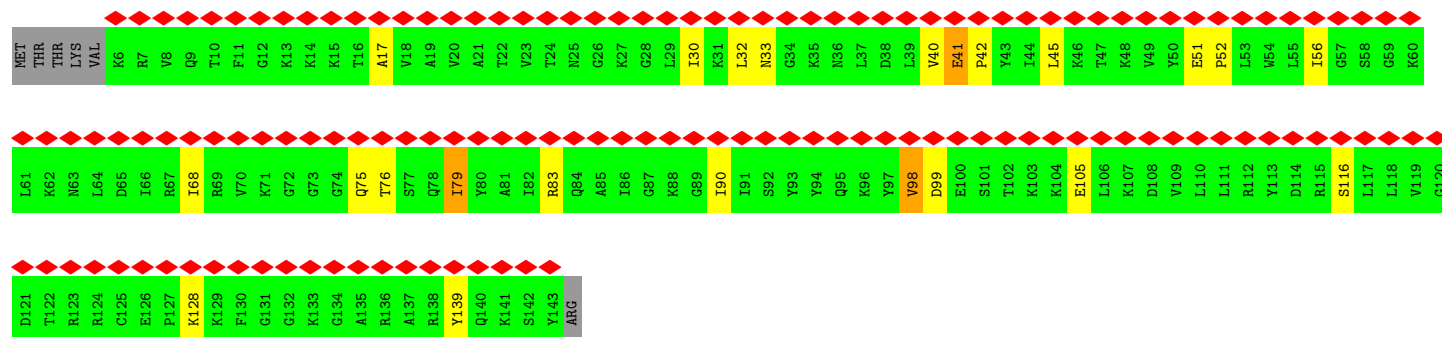


- Molecule 12: 40S ribosomal protein eS8

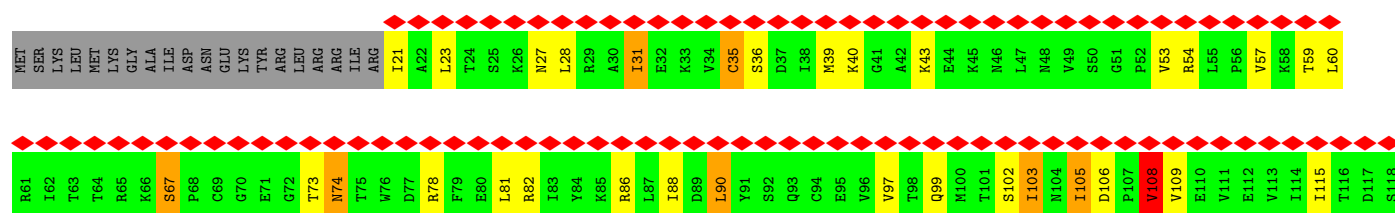
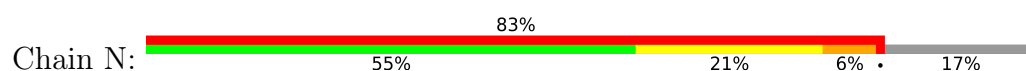


- Molecule 13: 40S ribosomal protein uS9

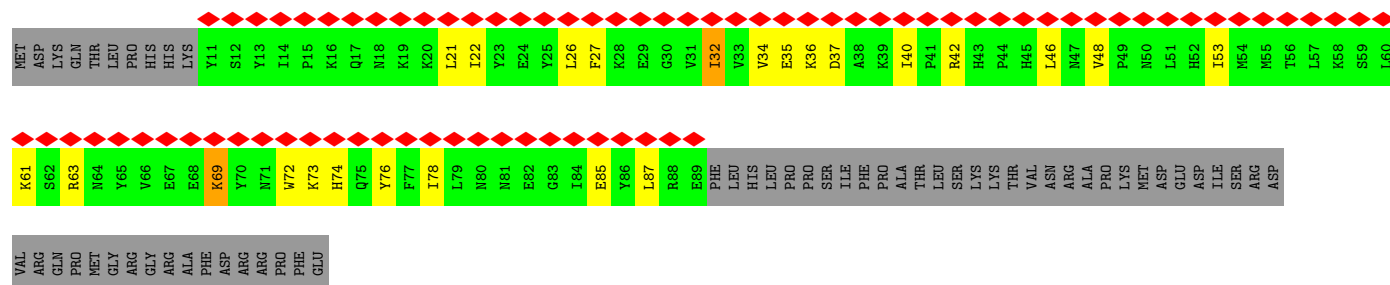




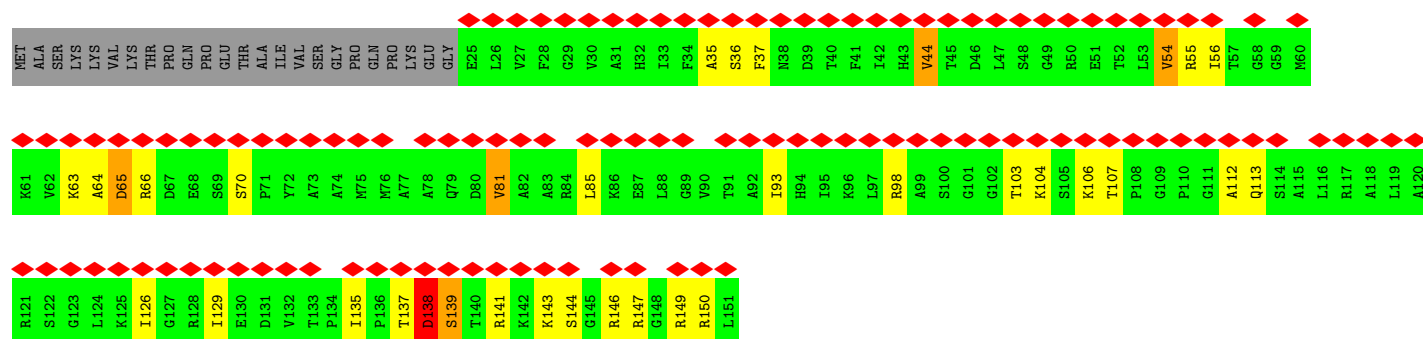
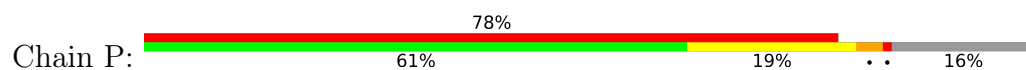
• Molecule 14: 40S ribosomal protein uS10



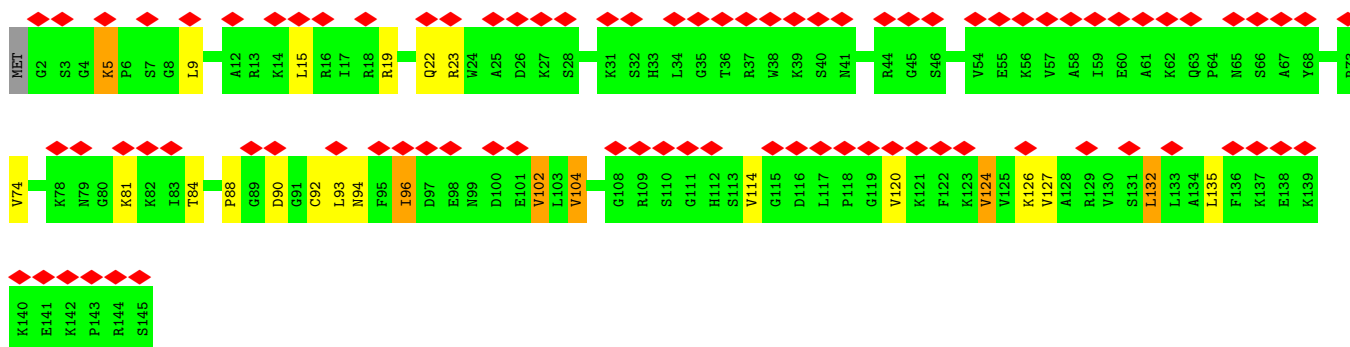
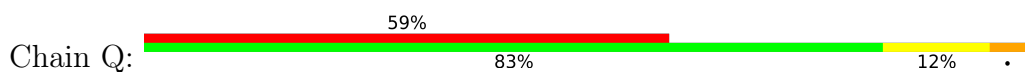
• Molecule 15: 40S ribosomal protein eS10



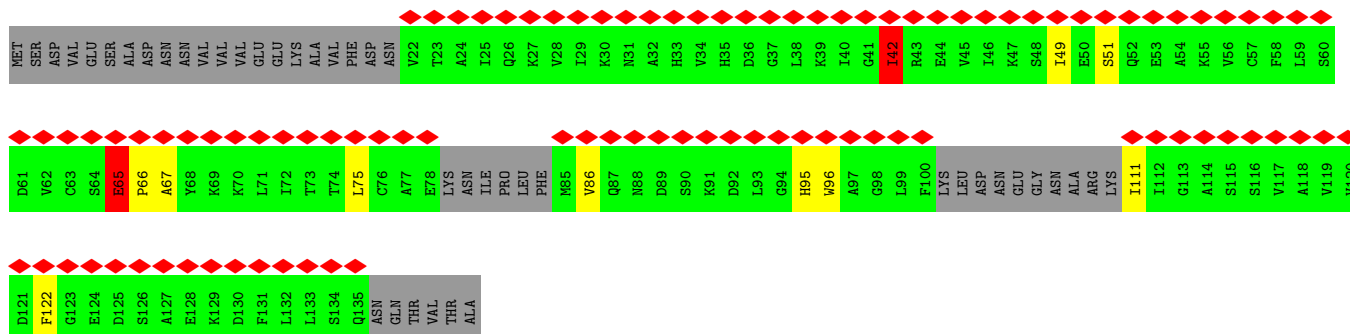
• Molecule 16: 40S ribosomal protein uS11



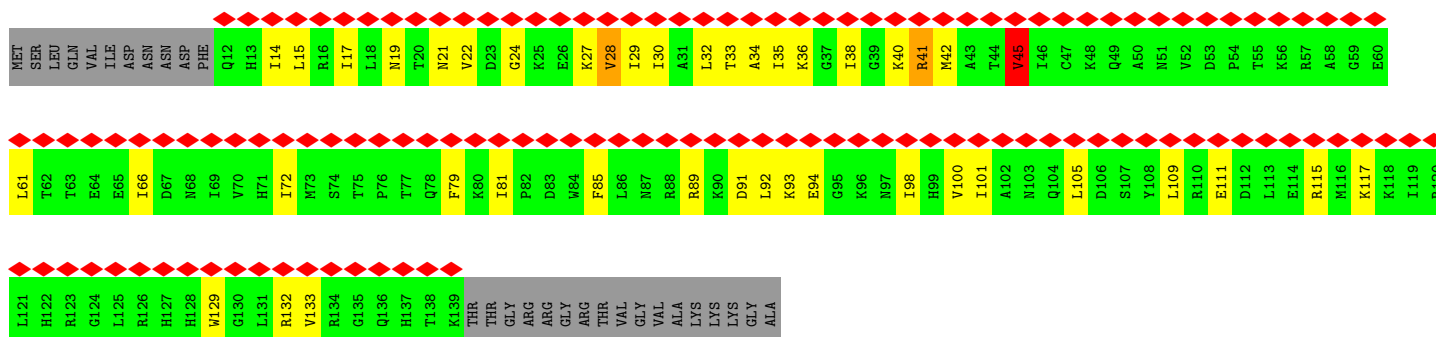
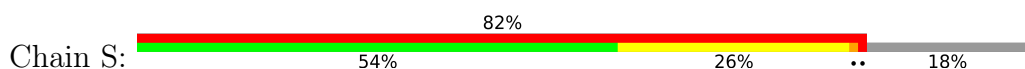
• Molecule 17: 40S ribosomal protein uS12



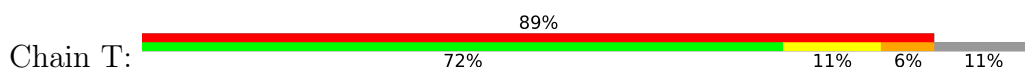
• Molecule 18: 40S ribosomal protein eS12



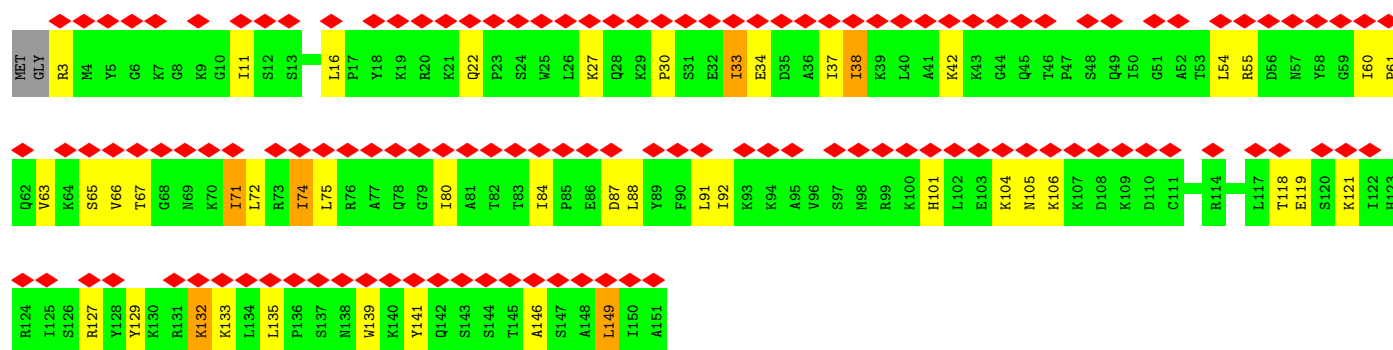
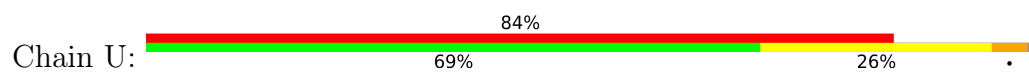
• Molecule 19: 40S ribosomal protein uS13



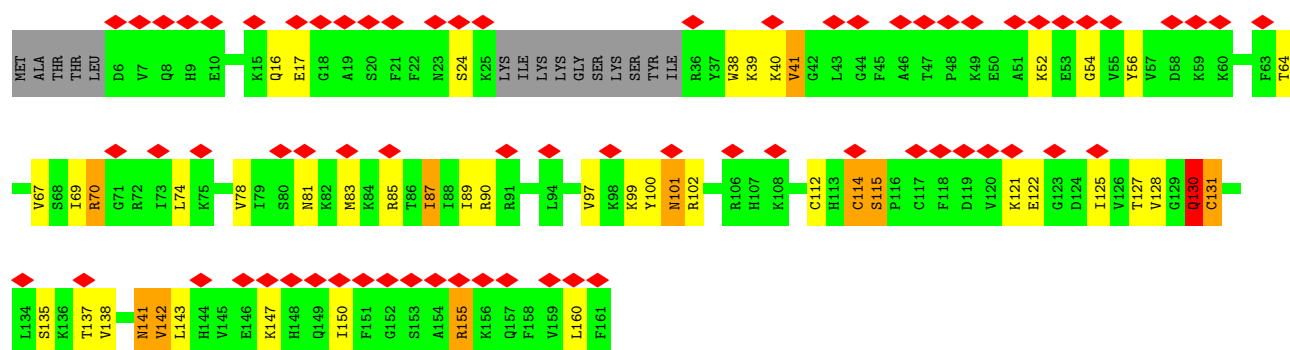
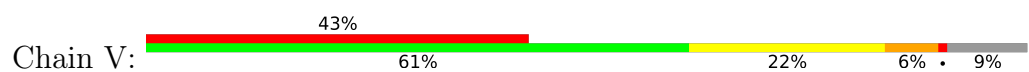
• Molecule 20: 40S ribosomal protein uS14



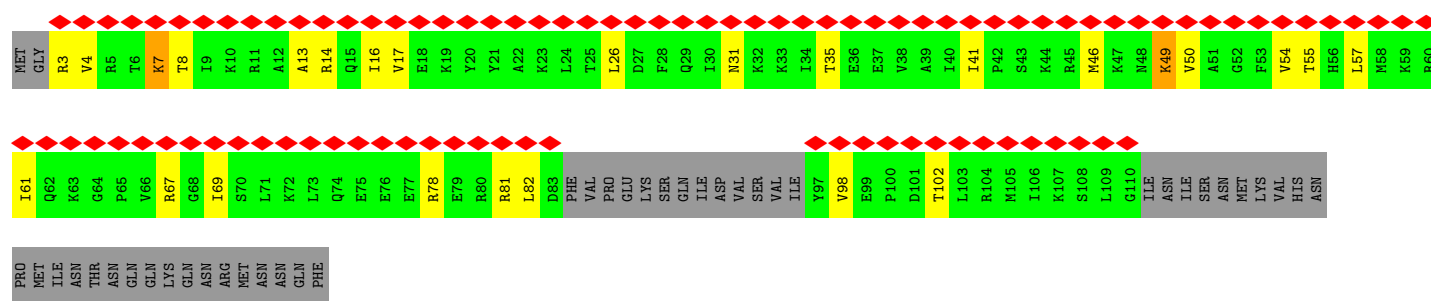
• Molecule 21: 40S ribosomal protein uS15



• Molecule 22: 40S ribosomal protein uS17

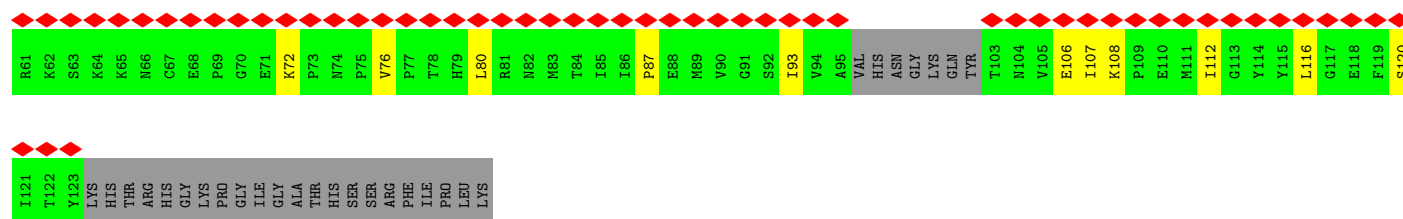


• Molecule 23: 40S ribosomal protein eS17



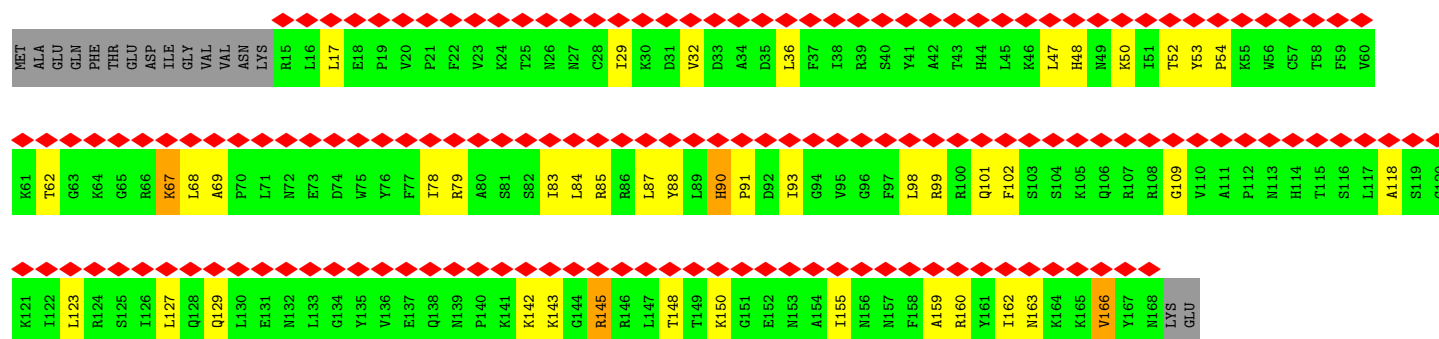
• Molecule 24: 40S ribosomal protein uS19





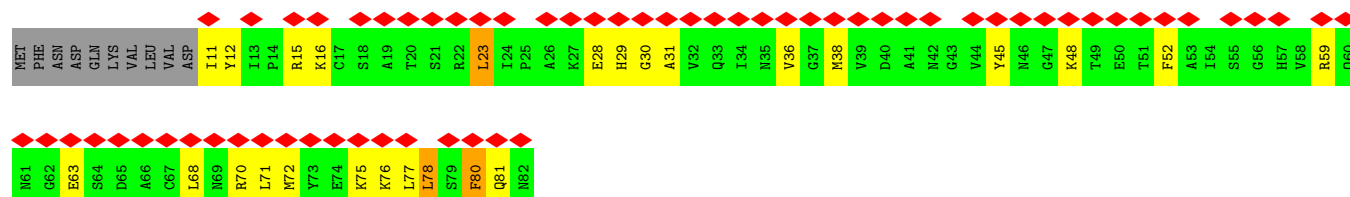
• Molecule 25: 40S ribosomal protein eS19

Chain Y:



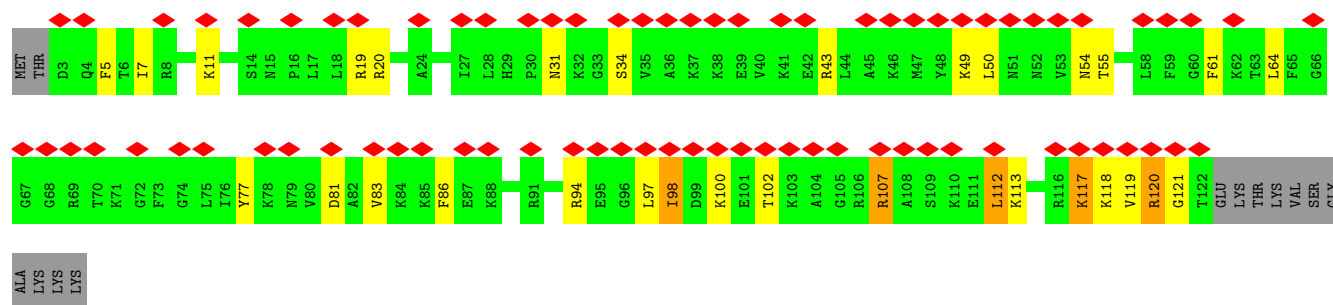
• Molecule 26: 40S ribosomal protein eS21

Chain Z:



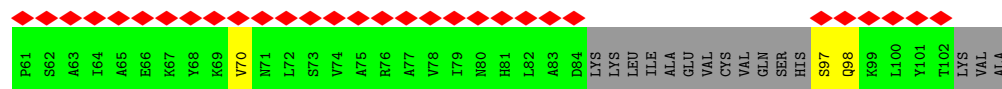
• Molecule 27: 40S ribosomal protein eS24

Chain 1:



• Molecule 28: 40S ribosomal protein eS25

Chain 2:



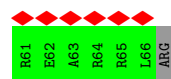
Chain 3:



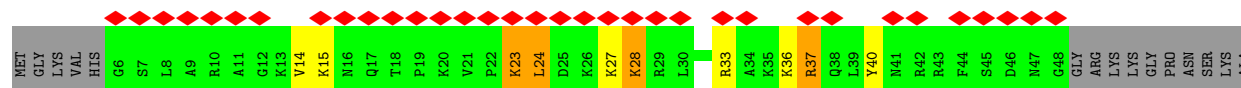
Chain 4: 87% 65% 24% 7%



Chain 5: 87% 78% 9% 13%



Chain 6:



Chain 7: 100% 53% 46%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	105247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	104748	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.545	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 34G, MG, ZN

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	A	0.42	3/38345 (0.0%)	0.83	63/59689 (0.1%)
2	B	0.63	0/1737	1.10	3/2321 (0.1%)
3	C	0.61	0/1569	1.12	3/2129 (0.1%)
4	D	0.62	0/1240	1.05	1/1652 (0.1%)
5	E	0.62	0/1532	1.18	1/2048 (0.0%)
6	F	0.63	0/2097	1.00	3/2819 (0.1%)
7	G	0.64	0/1799	1.07	2/2429 (0.1%)
8	H	0.59	0/1661	1.02	1/2205 (0.0%)
9	I	0.66	0/1443	1.22	3/1936 (0.2%)
10	J	0.63	0/1544	1.07	2/2064 (0.1%)
11	K	0.68	0/1054	1.23	4/1411 (0.3%)
12	L	0.65	0/1416	1.03	1/1890 (0.1%)
13	M	0.64	0/1113	0.95	0/1487
14	N	0.66	0/780	1.09	2/1053 (0.2%)
15	O	0.64	0/705	1.06	0/950
16	P	0.66	0/965	1.18	0/1295
17	Q	0.63	0/1149	0.96	1/1532 (0.1%)
18	R	0.67	0/754	1.03	3/1013 (0.3%)
19	S	0.70	0/1058	1.16	1/1420 (0.1%)
20	T	0.56	0/411	0.87	0/544
21	U	0.59	0/1223	1.23	1/1634 (0.1%)
22	V	0.66	0/1233	0.92	0/1645
23	W	0.67	0/792	1.17	0/1053
24	X	0.72	0/787	1.13	2/1050 (0.2%)
25	Y	0.61	0/1294	1.18	6/1742 (0.3%)
26	Z	0.58	0/564	1.02	0/758
27	1	0.63	0/994	1.15	3/1317 (0.2%)
28	2	0.71	0/323	1.04	1/435 (0.2%)
29	3	0.65	0/793	1.02	0/1055
30	4	0.66	0/597	0.93	1/801 (0.1%)
31	5	0.60	0/452	0.75	0/599
32	6	0.57	0/348	1.07	0/458

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	7	0.40	0/1754	0.70	0/2732
All	All	0.53	3/73526 (0.0%)	0.94	108/107166 (0.1%)

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	B	0	1
10	J	0	1
11	K	0	3
12	L	0	1
19	S	0	1
21	U	0	1
24	X	0	1
27	1	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	789	U	C1'-N1	7.13	1.59	1.48
1	A	788	A	O3'-P	6.41	1.70	1.61
1	A	788	A	C1'-N9	-5.60	1.39	1.48

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2053	U	C2'-C3'-O3'	11.38	126.57	109.50
1	A	1386	U	C2'-C3'-O3'	10.52	125.28	109.50
1	A	465	G	C2'-C3'-O3'	9.54	123.81	109.50
1	A	788	A	P-O3'-C3'	-9.01	106.69	120.20
1	A	1897	A	C4'-C3'-O3'	8.64	122.36	109.40
1	A	850	G	C2'-C3'-O3'	8.53	126.49	113.70
1	A	105	A	C2'-C3'-O3'	8.12	121.68	109.50
1	A	60	A	C2'-C3'-O3'	7.89	121.33	109.50
1	A	1381	C	C2'-C3'-O3'	7.80	125.40	113.70
1	A	635	G	C4'-C3'-O3'	-7.38	101.93	113.00
1	A	307	G	C4'-C3'-O3'	-7.38	101.93	113.00
19	S	45	VAL	N-CA-CB	7.33	119.12	110.55
3	C	181	VAL	N-CA-CB	7.32	120.49	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	7	GLY	N-CA-C	7.31	121.93	112.13
1	A	525	G	C2'-C3'-O3'	7.20	124.50	113.70
1	A	1865	G	C4'-C3'-O3'	7.14	120.10	109.40
27	1	107	ARG	N-CA-C	-7.09	104.78	113.50
1	A	788	A	O3'-P-O5'	-6.98	93.53	104.00
18	R	65	GLU	CA-C-N	6.93	128.50	119.84
18	R	65	GLU	C-N-CA	6.93	128.50	119.84
10	J	27	ILE	N-CA-CB	6.90	118.62	110.55
1	A	291	A	C2'-C3'-O3'	6.86	123.98	113.70
1	A	1818	A	C4'-C3'-O3'	6.82	119.63	109.40
3	C	63	ILE	N-CA-CB	6.65	118.33	110.55
2	B	149	GLN	N-CA-C	6.64	119.35	111.71
1	A	246	A	C2'-C3'-O3'	6.62	123.63	113.70
24	X	34	ILE	N-CA-CB	6.58	118.25	110.55
25	Y	53	TYR	CA-C-N	6.55	128.03	119.84
25	Y	53	TYR	C-N-CA	6.55	128.03	119.84
27	1	121	GLY	N-CA-C	-6.53	104.42	112.77
7	G	140	ALA	CA-C-O	-6.49	113.67	120.55
1	A	457	A	C4'-C3'-O3'	-6.45	103.33	113.00
2	B	69	ASN	N-CA-C	6.42	120.60	113.21
6	F	86	LEU	N-CA-C	6.37	118.76	111.11
1	A	250	A	C4'-C3'-O3'	6.34	118.91	109.40
9	I	64	VAL	N-CA-CB	6.33	117.95	110.55
1	A	628	A	C4'-C3'-O3'	-6.25	103.62	113.00
25	Y	69	ALA	CA-C-N	6.23	126.42	119.32
25	Y	69	ALA	C-N-CA	6.23	126.42	119.32
1	A	615	U	C4'-C3'-O3'	-6.23	103.66	113.00
1	A	25	C	C2'-C3'-O3'	6.20	118.80	109.50
1	A	465	G	C4'-C3'-O3'	-6.17	100.14	109.40
9	I	169	ILE	N-CA-CB	6.07	118.80	110.54
1	A	1094	A	C3'-C2'-O2'	6.03	119.74	110.70
1	A	409	A	C2'-C3'-O3'	-5.99	104.72	113.70
1	A	251	U	C2'-C3'-O3'	5.96	118.44	109.50
9	I	110	GLY	N-CA-C	5.95	121.35	113.37
7	G	78	PHE	N-CA-C	5.94	118.72	111.82
17	Q	114	VAL	N-CA-C	5.94	116.42	107.75
1	A	1870	A	C4'-C3'-O3'	5.87	118.20	109.40
6	F	29	PRO	N-CA-C	5.85	121.17	113.86
1	A	930	A	C2'-C3'-O3'	-5.81	100.78	109.50
1	A	246	A	C3'-C2'-O2'	5.78	119.37	110.70
27	1	20	ARG	N-CA-C	5.74	117.90	109.24
11	K	94	LEU	CA-C-N	5.72	125.34	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	94	LEU	C-N-CA	5.72	125.34	119.56
1	A	844	G	C2'-C3'-O3'	5.71	122.26	113.70
14	N	106	ASP	N-CA-C	5.67	113.11	108.07
25	Y	166	VAL	N-CA-CB	5.62	118.19	110.54
1	A	2082	A	C4'-C3'-O3'	-5.60	104.59	113.00
1	A	1786	U	C2'-C3'-O3'	5.60	122.10	113.70
1	A	463	G	C2'-C3'-O3'	5.59	122.08	113.70
1	A	50	C	C3'-C2'-O2'	5.57	119.06	110.70
1	A	98	G	C1'-C2'-O2'	5.51	116.67	108.40
1	A	1100	U	C4'-C3'-O3'	5.51	117.67	109.40
18	R	42	ILE	N-CA-C	5.51	120.80	109.34
8	H	189	ASN	CA-C-O	-5.50	114.72	120.55
1	A	306	A	C3'-C2'-O2'	5.50	118.95	110.70
5	E	127	VAL	N-CA-CB	5.50	118.82	110.58
1	A	331	G	C4'-C3'-O3'	-5.47	104.79	113.00
2	B	193	ILE	CB-CA-C	-5.47	104.97	111.97
1	A	359	A	C3'-C2'-O2'	5.41	118.81	110.70
21	U	118	THR	N-CA-CB	5.38	118.02	110.12
1	A	434	A	C2'-C3'-O3'	5.38	121.76	113.70
10	J	113	ILE	N-CA-CB	5.38	116.14	110.17
1	A	1416	U	C3'-C2'-O2'	5.35	118.72	110.70
1	A	1677	C	C4'-C3'-O3'	-5.34	104.99	113.00
1	A	983	G	C4'-C3'-O3'	5.34	117.40	109.40
6	F	18	TRP	CA-CB-CG	5.33	123.72	113.60
24	X	120	SER	N-CA-C	5.31	117.69	107.44
1	A	1819	U	C2'-C3'-O3'	5.31	117.47	109.50
28	2	59	ILE	N-CA-C	5.30	116.34	108.23
11	K	100	GLY	N-CA-C	-5.29	106.02	112.68
1	A	142	G	C4'-C3'-O3'	5.28	117.33	109.40
1	A	939	A	C4'-C3'-O3'	-5.26	105.12	113.00
1	A	455	C	C3'-C2'-O2'	5.25	118.57	110.70
1	A	307	G	C2'-C3'-O3'	5.21	121.51	113.70
1	A	476	A	C2'-C3'-O3'	5.19	121.48	113.70
1	A	930	A	C4'-C3'-O3'	5.17	117.16	109.40
4	D	73	VAL	N-CA-CB	5.16	117.55	110.54
1	A	1107	U	C4'-C3'-O3'	-5.13	105.31	113.00
1	A	1172	U	C2'-C3'-O3'	5.11	121.36	113.70
1	A	1059	U	C1'-C2'-O2'	5.10	116.06	108.40
1	A	1228	C	C3'-C2'-O2'	5.09	118.34	110.70
25	Y	145	ARG	N-CA-C	5.09	121.63	110.80
30	4	40	GLN	N-CA-C	5.08	116.24	108.52
1	A	2083	A	C3'-C2'-O2'	-5.07	106.99	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	34	VAL	N-CA-CB	5.07	117.44	110.54
1	A	423	A	C4'-C3'-O3'	5.06	116.99	109.40
1	A	1704	G	N9-C1'-C2'	5.06	119.59	112.00
1	A	14	U	C1'-C2'-O2'	5.06	115.99	108.40
14	N	103	ILE	N-CA-C	-5.04	107.42	111.91
3	C	142	PRO	N-CA-C	5.03	120.53	113.53
1	A	2063	U	C3'-C2'-O2'	5.03	118.25	110.70
1	A	2070	G	C3'-C2'-O2'	5.02	118.22	110.70
1	A	1870	A	C2'-C3'-O3'	5.01	117.02	109.50
1	A	1038	C	C4'-C3'-O3'	-5.01	105.48	113.00
1	A	1196	U	C4'-C3'-O3'	-5.00	105.50	113.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	1	118	LYS	Peptide
2	B	148	ASN	Peptide
10	J	132	SER	Peptide
11	K	27	ILE	Peptide
11	K	76	SER	Peptide
11	K	94	LEU	Peptide
12	L	164	LYS	Peptide
19	S	36	LYS	Peptide
21	U	104	LYS	Peptide
24	X	38	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	A	34277	0	17246	214	0
2	B	1713	0	1838	31	0
3	C	1538	0	1600	17	0
4	D	1228	0	1311	16	0
5	E	1508	0	1594	18	0
6	F	2061	0	2200	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1757	0	1811	14	0
8	H	1644	0	1795	18	0
9	I	1424	0	1471	11	0
10	J	1528	0	1680	21	0
11	K	1037	0	1099	17	0
12	L	1392	0	1447	22	0
13	M	1098	0	1183	7	0
14	N	772	0	813	8	0
15	O	686	0	695	7	0
16	P	953	0	997	19	0
17	Q	1129	0	1196	12	0
18	R	746	0	754	3	0
19	S	1042	0	1095	24	0
20	T	404	0	416	5	0
21	U	1202	0	1299	19	0
22	V	1206	0	1239	16	0
23	W	785	0	858	7	0
24	X	776	0	832	9	0
25	Y	1266	0	1316	12	0
26	Z	556	0	558	8	0
27	1	981	0	1065	10	0
28	2	320	0	338	1	0
29	3	781	0	818	13	0
30	4	586	0	604	5	0
31	5	451	0	485	2	0
32	6	345	0	381	5	0
33	7	1571	0	797	3	0
34	A	67	0	0	0	0
35	A	35	0	40	2	0
36	T	1	0	0	0	0
All	All	68866	0	52871	555	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 5.

All (555) 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)
19:S:33:THR:O	19:S:38:ILE:HG12	1.15	1.32
1:A:759:C:O2	1:A:788:A:C2	1.84	1.30
19:S:35:ILE:O	19:S:38:ILE:CG1	1.76	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:C:C2	1:A:788:A:C2	2.30	1.19
19:S:35:ILE:O	19:S:38:ILE:HG13	0.91	1.09
19:S:33:THR:O	19:S:38:ILE:CG1	2.05	1.04
1:A:759:C:C2	1:A:788:A:H2	1.77	0.96
1:A:1447:A:O2'	1:A:1448:U:OP2	1.85	0.94
1:A:1448:U:O2'	1:A:1449:U:O5'	1.85	0.93
1:A:759:C:O2	1:A:788:A:H2	1.40	0.89
1:A:759:C:C2	1:A:788:A:N1	2.39	0.89
1:A:788:A:H2'	1:A:789:U:H6	1.41	0.85
1:A:2044:G:C2'	1:A:2045:A:H5'	2.07	0.84
1:A:1447:A:O2'	1:A:1448:U:P	2.36	0.84
1:A:2044:G:O2'	1:A:2045:A:H5'	1.79	0.81
1:A:759:C:N3	1:A:788:A:N1	2.28	0.81
4:D:106:LEU:HD22	4:D:123:VAL:HG21	1.61	0.79
1:A:1447:A:HO2'	1:A:1448:U:P	2.04	0.79
1:A:338:U:P	12:L:56:ARG:HH22	2.07	0.78
1:A:788:A:H2'	1:A:789:U:C6	2.19	0.78
1:A:1448:U:HO2'	1:A:1449:U:P	2.09	0.76
19:S:38:ILE:HG22	19:S:38:ILE:O	1.86	0.75
11:K:111:MET:HE1	11:K:116:ALA:HB2	1.69	0.74
4:D:143:LEU:HD21	4:D:151:MET:HE2	1.70	0.73
16:P:35:ALA:CB	16:P:112:ALA:HB2	2.20	0.71
16:P:35:ALA:HB2	16:P:112:ALA:HB2	1.71	0.71
1:A:1387:U:O2'	1:A:1388:A:O4'	2.09	0.70
10:J:81:ILE:HD11	10:J:94:LEU:HD22	1.73	0.70
4:D:135:CYS:SG	4:D:136:GLU:N	2.64	0.70
5:E:86:LEU:HD11	5:E:96:VAL:HG12	1.72	0.70
17:Q:102:VAL:HG22	17:Q:127:VAL:HG12	1.75	0.68
1:A:1836:G:C5	19:S:30:ILE:HG13	2.29	0.68
2:B:37:MET:HE2	2:B:182:LYS:HA	1.75	0.68
5:E:28:LEU:HD11	32:6:40:TYR:HA	1.76	0.68
1:A:2044:G:H2'	1:A:2045:A:H5'	1.77	0.67
25:Y:29:ILE:HG22	25:Y:159:ALA:HB2	1.76	0.66
12:L:200:ILE:HD11	12:L:208:TYR:CD2	2.30	0.66
12:L:36:THR:HG21	12:L:189:PRO:HB2	1.78	0.66
1:A:1033:U:OP1	21:U:132:LYS:NZ	2.29	0.65
26:Z:38:MET:HE1	26:Z:77:LEU:HD22	1.78	0.65
26:Z:29:HIS:O	26:Z:31:ALA:N	2.31	0.64
1:A:981:U:OP1	1:A:982:A:O2'	2.13	0.64
18:R:49:ILE:HG21	18:R:75:LEU:HB3	1.80	0.63
10:J:61:LEU:HD11	10:J:175:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:U:O2'	1:A:166:A:N3	2.29	0.62
4:D:28:ILE:HD13	15:O:69:LYS:HD2	1.82	0.62
19:S:41:ARG:O	19:S:45:VAL:HG13	2.01	0.61
1:A:1049:G:H4'	1:A:2068:A:H4'	1.82	0.61
1:A:1061:A:O2'	1:A:2077:U:O2	2.17	0.61
10:J:23:CYS:O	10:J:27:ILE:HG23	2.01	0.61
16:P:113:GLN:HG2	29:3:45:VAL:HG12	1.82	0.60
13:M:45:LEU:HB3	13:M:79:ILE:HD13	1.81	0.60
1:A:1448:U:O2'	1:A:1449:U:H2'	2.02	0.60
1:A:1894:A:OP2	20:T:30:ARG:NH2	2.34	0.60
5:E:45:VAL:HG13	5:E:101:LEU:HD22	1.83	0.60
22:V:78:VAL:HG23	22:V:122:GLU:HA	1.84	0.59
1:A:1449:U:O2	1:A:1812:A:H5'	2.02	0.59
6:F:65:LEU:HD22	6:F:70:VAL:HG11	1.85	0.59
6:F:107:GLY:HA2	6:F:189:VAL:HG11	1.84	0.59
11:K:25:VAL:HG13	11:K:63:VAL:HG13	1.85	0.59
3:C:59:LEU:O	3:C:63:ILE:HG23	2.03	0.59
2:B:204:ILE:C	2:B:204:ILE:HD13	2.28	0.58
11:K:14:ILE:HG12	11:K:27:ILE:HD11	1.84	0.58
22:V:69:ILE:HD13	22:V:143:LEU:HD11	1.85	0.58
1:A:1907:G:O2'	1:A:1908:A:OP2	2.21	0.58
5:E:123:HIS:CE1	32:6:37:ARG:HD3	2.39	0.58
1:A:2027:C:C5	1:A:2028:U:C5	2.93	0.57
1:A:373:A:H2'	1:A:374:U:O4'	2.03	0.57
25:Y:32:VAL:HG21	25:Y:159:ALA:HB1	1.86	0.57
13:M:45:LEU:HD11	13:M:76:THR:HG22	1.86	0.57
21:U:55:ARG:NH1	30:4:49:GLN:OE1	2.38	0.57
1:A:145:A:H2'	1:A:146:A:C8	2.40	0.57
1:A:1075:C:N3	35:A:2168:34G:H1	2.19	0.57
1:A:1048:A:N3	1:A:2067:U:O2'	2.37	0.57
2:B:58:THR:HG23	2:B:91:ILE:HG12	1.87	0.57
1:A:1718:C:H2'	1:A:1832:U:O4	2.05	0.57
5:E:45:VAL:HG11	5:E:105:LEU:HD21	1.87	0.57
26:Z:52:PHE:CD1	26:Z:71:LEU:HD23	2.40	0.57
16:P:146:ARG:O	16:P:147:ARG:HG2	2.05	0.57
1:A:2029:A:H2'	1:A:2030:U:C6	2.40	0.57
1:A:334:A:H2'	1:A:335:G:O4'	2.05	0.56
1:A:1836:G:C4	19:S:30:ILE:HG13	2.40	0.56
1:A:106:A:OP2	1:A:314:A:N6	2.37	0.56
1:A:1967:G:O2'	1:A:2023:A:N6	2.38	0.56
11:K:8:ALA:CB	11:K:74:VAL:HG11	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:60:ILE:HB	10:J:92:VAL:HG12	1.86	0.56
1:A:142:G:O2'	1:A:143:A:H5'	2.05	0.56
1:A:1952:A:C2	1:A:2038:A:C2	2.94	0.56
24:X:30:GLN:O	24:X:34:ILE:HG23	2.06	0.56
25:Y:83:ILE:HD11	25:Y:123:LEU:CD1	2.36	0.56
1:A:1849:U:O4	24:X:40:ARG:NH2	2.39	0.56
6:F:18:TRP:O	6:F:51:ARG:NH2	2.39	0.56
12:L:65:PHE:CD2	12:L:104:ILE:HD11	2.41	0.56
2:B:34:ALA:HB3	2:B:41:ARG:HA	1.89	0.55
1:A:1267:C:H2'	1:A:1268:G:O4'	2.06	0.55
1:A:1841:U:H2'	1:A:1842:A:O4'	2.07	0.55
1:A:598:A:H2'	1:A:599:A:C8	2.41	0.55
5:E:59:LEU:HD13	5:E:73:GLY:HA2	1.88	0.55
9:I:30:ILE:HD13	9:I:59:ILE:HD12	1.88	0.55
1:A:2028:U:H2'	1:A:2028:U:O2	2.06	0.55
6:F:86:LEU:HD13	6:F:103:TYR:CE2	2.42	0.55
15:O:27:PHE:HB2	15:O:87:LEU:HD23	1.88	0.55
1:A:1881:G:H1	1:A:1907:G:HO2'	1.45	0.55
12:L:21:HIS:CG	12:L:21:HIS:O	2.60	0.55
23:W:98:VAL:HG12	23:W:102:THR:HG23	1.88	0.55
29:3:50:GLN:O	29:3:53:ILE:HG22	2.07	0.54
1:A:543:A:C5	1:A:544:G:C8	2.95	0.54
1:A:366:A:H2'	1:A:367:C:H4'	1.88	0.54
1:A:521:G:N7	1:A:544:G:N2	2.56	0.54
1:A:2029:A:H2'	1:A:2030:U:O4'	2.08	0.54
2:B:88:CYS:SG	2:B:96:CYS:SG	3.04	0.54
19:S:33:THR:HB	19:S:38:ILE:HG23	1.90	0.54
1:A:2045:A:O2'	1:A:2046:G:H5'	2.07	0.54
17:Q:102:VAL:HG13	17:Q:124:VAL:HG23	1.90	0.54
26:Z:78:LEU:HD11	26:Z:80:PHE:CZ	2.43	0.54
3:C:89:PHE:O	3:C:93:THR:HG22	2.08	0.54
1:A:56:A:N1	1:A:93:G:O2'	2.37	0.53
12:L:34:SER:HB2	12:L:56:ARG:HD2	1.90	0.53
3:C:164:ASN:HD22	3:C:170:ILE:HD11	1.73	0.53
6:F:87:MET:HE3	6:F:226:PHE:CE2	2.43	0.53
2:B:164:ILE:HG13	2:B:204:ILE:HD12	1.91	0.53
12:L:65:PHE:CZ	12:L:78:ILE:HG21	2.43	0.53
1:A:1423:A:N6	3:C:135:GLU:OE2	2.42	0.53
1:A:338:U:P	12:L:56:ARG:NH2	2.79	0.53
21:U:33:ILE:HD11	21:U:63:VAL:HG12	1.91	0.53
1:A:879:A:N1	1:A:925:C:O2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:2168:34G:H41	35:A:2168:34G:CAE	2.39	0.53
12:L:72:ILE:HD12	12:L:73:SER:N	2.23	0.53
16:P:138:ASP:CG	16:P:139:SER:N	2.67	0.53
12:L:76:THR:OG1	12:L:104:ILE:HG23	2.09	0.52
1:A:401:U:H2'	1:A:402:G:O4'	2.10	0.52
1:A:1387:U:O2'	1:A:1388:A:O5'	2.27	0.52
3:C:177:LEU:O	3:C:181:VAL:HG13	2.08	0.52
3:C:146:LEU:O	3:C:164:ASN:ND2	2.41	0.52
12:L:60:LEU:HD13	12:L:195:ALA:HB2	1.92	0.52
2:B:120:LEU:HD12	2:B:120:LEU:C	2.35	0.52
1:A:45:U:O2	1:A:440:G:H1'	2.10	0.52
1:A:647:C:O2	1:A:647:C:O4'	2.27	0.52
10:J:128:GLU:O	10:J:131:VAL:O	2.27	0.52
2:B:171:ILE:HD11	2:B:200:GLN:HG3	1.92	0.52
3:C:202:LEU:HD23	3:C:203:TRP:N	2.25	0.52
12:L:107:HIS:N	12:L:108:PRO:CD	2.73	0.52
2:B:66:TYR:HE1	2:B:88:CYS:SG	2.33	0.51
24:X:28:LEU:HD13	24:X:32:GLU:HB2	1.91	0.51
19:S:33:THR:O	19:S:38:ILE:HG23	2.09	0.51
5:E:106:GLU:HA	5:E:111:THR:HG21	1.91	0.51
11:K:14:ILE:CG1	11:K:27:ILE:HD11	2.40	0.51
33:7:1:G:N2	33:7:70:A:C2	2.79	0.51
1:A:413:A:H2'	1:A:414:C:C6	2.45	0.51
7:G:149:ILE:HD12	7:G:227:PHE:CZ	2.44	0.51
9:I:61:GLU:O	9:I:64:VAL:HG22	2.10	0.51
1:A:529:U:O2'	27:1:61:PHE:O	2.27	0.51
10:J:36:LYS:HG2	10:J:37:THR:HG23	1.92	0.51
10:J:71:THR:HG23	10:J:72:TYR:CD2	2.45	0.51
16:P:56:ILE:HG13	16:P:81:VAL:HG23	1.93	0.51
17:Q:96:ILE:HG22	17:Q:127:VAL:HG11	1.92	0.51
19:S:38:ILE:O	19:S:38:ILE:CG2	2.58	0.51
2:B:178:LYS:O	2:B:179:VAL:HG13	2.10	0.51
6:F:228:ILE:HD11	6:F:236:ILE:HD11	1.92	0.51
1:A:1850:G:O6	24:X:43:ARG:NH2	2.44	0.51
33:7:15:G:C6	33:7:46:G:N2	2.79	0.51
1:A:1811:A:O2'	1:A:1813:U:OP2	2.24	0.51
9:I:67:MET:HE3	9:I:67:MET:HA	1.92	0.51
1:A:932:U:O2	1:A:932:U:O4'	2.27	0.50
11:K:83:LEU:HD22	11:K:120:HIS:O	2.12	0.50
1:A:981:U:H4'	1:A:982:A:OP2	2.11	0.50
22:V:40:LYS:O	22:V:41:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:C:OP1	6:F:29:PRO:O	2.30	0.50
7:G:168:MET:SD	7:G:168:MET:N	2.84	0.50
16:P:56:ILE:O	16:P:56:ILE:HG22	2.11	0.50
12:L:57:ALA:HB2	12:L:193:GLY:HA2	1.94	0.50
2:B:175:GLU:HG3	2:B:193:ILE:HD12	1.93	0.50
27:1:97:LEU:HB3	27:1:98:ILE:HD13	1.94	0.50
3:C:168:GLU:HB3	3:C:202:LEU:HD11	1.94	0.50
17:Q:22:GLN:O	17:Q:23:ARG:C	2.54	0.50
2:B:125:THR:HG22	2:B:172:MET:HE3	1.94	0.50
1:A:331:G:OP1	22:V:137:THR:HG22	2.12	0.50
1:A:433:C:H2'	1:A:434:A:O4'	2.11	0.50
22:V:128:VAL:HG12	22:V:142:VAL:HA	1.94	0.50
1:A:1059:U:H2'	1:A:1060:G:O4'	2.12	0.49
6:F:186:GLY:O	6:F:188:SER:N	2.44	0.49
3:C:63:ILE:HG22	26:Z:36:VAL:HG22	1.94	0.49
1:A:2029:A:O2'	1:A:2030:U:H5'	2.12	0.49
6:F:45:VAL:HG23	6:F:80:CYS:O	2.11	0.49
20:T:27:ALA:HB1	20:T:38:ARG:HD2	1.94	0.49
1:A:644:U:O2	10:J:115:ARG:NH2	2.44	0.49
19:S:29:ILE:O	19:S:33:THR:HG23	2.12	0.49
25:Y:162:ILE:O	25:Y:166:VAL:HG13	2.11	0.49
11:K:78:ARG:CD	11:K:126:LEU:HD23	2.42	0.49
22:V:99:LYS:HG2	22:V:100:TYR:CE2	2.48	0.49
29:3:23:CYS:SG	29:3:74:CYS:HB3	2.52	0.49
2:B:34:ALA:HB2	2:B:43:PHE:CE2	2.46	0.49
7:G:168:MET:HB2	11:K:95:PRO:HB2	1.94	0.49
1:A:5:U:O2'	1:A:560:G:O3'	2.24	0.49
3:C:74:VAL:HG13	3:C:118:PRO:HB3	1.95	0.49
1:A:822:G:OP1	6:F:22:LYS:NZ	2.46	0.49
10:J:76:ILE:HD12	10:J:76:ILE:O	2.12	0.49
16:P:106:LYS:CE	16:P:135:ILE:HG22	2.43	0.49
23:W:41:ILE:HG23	23:W:46:MET:HE3	1.95	0.49
1:A:970:G:N1	1:A:971:G:C6	2.81	0.49
1:A:1409:U:O2	1:A:1409:U:O4'	2.29	0.49
2:B:204:ILE:HD13	2:B:205:TYR:HB2	1.95	0.48
21:U:33:ILE:HG21	21:U:66:VAL:HG11	1.95	0.48
27:1:100:LYS:HB2	27:1:102:THR:HG23	1.95	0.48
1:A:1022:A:H2'	1:A:1023:A:C8	2.48	0.48
1:A:1281:C:H2'	1:A:1282:U:O4'	2.14	0.48
1:A:1980:A:N6	1:A:2011:G:C6	2.81	0.48
1:A:619:U:OP2	17:Q:5:LYS:HE3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:U:O2	1:A:1788:U:O4'	2.29	0.48
14:N:103:ILE:O	14:N:103:ILE:HG22	2.13	0.48
23:W:13:ALA:O	23:W:16:ILE:O	2.31	0.48
1:A:338:U:OP1	12:L:31:ARG:NE	2.45	0.48
1:A:575:G:H4'	17:Q:90:ASP:HA	1.95	0.48
1:A:999:A:OP1	29:3:32:LYS:NZ	2.42	0.48
1:A:1186:G:OP1	7:G:178:ARG:NH1	2.47	0.48
1:A:2053:U:O2	1:A:2053:U:O5'	2.31	0.48
19:S:15:LEU:HD11	19:S:66:ILE:HD11	1.94	0.48
1:A:1234:A:H2'	1:A:1235:G:O4'	2.14	0.48
1:A:1047:A:H2'	1:A:1048:A:O4'	2.14	0.48
1:A:1404:U:H2'	1:A:1405:U:O4'	2.13	0.48
8:H:142:ARG:O	8:H:146:ASN:N	2.46	0.48
24:X:21:ASP:O	24:X:25:LEU:HD13	2.13	0.48
27:1:119:VAL:HG13	27:1:119:VAL:O	2.13	0.48
8:H:52:ILE:HD12	8:H:109:LEU:HD21	1.96	0.48
10:J:39:ALA:HA	10:J:42:ILE:HG22	1.96	0.48
10:J:100:ILE:C	10:J:101:LEU:HD12	2.39	0.48
16:P:36:SER:O	16:P:37:PHE:HB2	2.14	0.48
24:X:93:ILE:HG22	24:X:106:GLU:HA	1.94	0.48
1:A:301:A:H4'	6:F:130:LEU:HD21	1.94	0.47
10:J:61:LEU:CD1	10:J:175:VAL:HG23	2.44	0.47
11:K:7:LEU:C	11:K:7:LEU:HD23	2.38	0.47
11:K:90:ILE:HG22	11:K:102:LEU:HG	1.95	0.47
20:T:28:ILE:HA	20:T:37:CYS:HA	1.96	0.47
6:F:43:PRO:HG2	6:F:46:ILE:HG12	1.96	0.47
26:Z:72:MET:HB2	26:Z:78:LEU:HD22	1.96	0.47
3:C:172:LEU:C	3:C:172:LEU:HD13	2.40	0.47
8:H:57:ASP:HA	8:H:106:LEU:HA	1.95	0.47
1:A:2045:A:H2'	1:A:2046:G:O4'	2.14	0.47
4:D:124:LEU:HD11	4:D:153:PHE:HB3	1.97	0.47
8:H:57:ASP:OD1	8:H:61:PHE:N	2.47	0.47
1:A:1171:U:O2'	30:4:16:LYS:O	2.32	0.47
1:A:1635:C:H4'	23:W:49:LYS:HA	1.95	0.47
30:4:44:LEU:HD21	30:4:52:VAL:HG21	1.96	0.47
1:A:95:A:C6	1:A:404:G:C6	3.03	0.47
11:K:41:MET:HG2	11:K:46:TYR:HB2	1.96	0.47
25:Y:163:ASN:O	25:Y:166:VAL:HG22	2.14	0.47
1:A:995:A:H2'	1:A:996:C:O4'	2.15	0.47
1:A:1100:U:H3'	1:A:1101:G:H5'	1.97	0.47
1:A:2088:C:N4	29:3:93:ARG:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:LEU:CD2	9:I:108:GLN:HA	2.45	0.47
10:J:28:GLU:HB2	10:J:39:ALA:HB3	1.96	0.47
10:J:126:ILE:O	10:J:130:ILE:HG23	2.14	0.47
14:N:23:LEU:HB3	14:N:31:ILE:HD11	1.96	0.47
15:O:22:ILE:HD11	15:O:48:VAL:HG11	1.96	0.47
16:P:106:LYS:HE2	16:P:135:ILE:HG22	1.96	0.47
19:S:17:ILE:CG2	19:S:35:ILE:HD11	2.45	0.47
1:A:114:A:O2'	22:V:70:ARG:NE	2.48	0.47
1:A:54:C:O2'	1:A:465:G:N7	2.43	0.47
11:K:8:ALA:HB1	11:K:74:VAL:HG11	1.97	0.47
23:W:7:LYS:HE3	23:W:8:THR:HG23	1.97	0.47
1:A:375:U:O2	1:A:375:U:O4'	2.32	0.47
1:A:1270:G:O2'	1:A:1873:A:N6	2.48	0.47
4:D:106:LEU:HD21	4:D:123:VAL:HG11	1.96	0.47
7:G:179:ILE:HD11	7:G:181:LEU:CD1	2.45	0.47
1:A:19:A:H2'	1:A:20:G:O4'	2.15	0.46
1:A:161:U:O2	1:A:161:U:O4'	2.31	0.46
1:A:1388:A:N1	1:A:1430:G:O2'	2.36	0.46
14:N:108:VAL:HG12	14:N:109:VAL:HG23	1.95	0.46
1:A:823:C:OP1	6:F:21:ASN:HB3	2.15	0.46
1:A:1857:U:O2	1:A:1857:U:O4'	2.31	0.46
15:O:37:ASP:HB3	15:O:40:ILE:HD13	1.97	0.46
2:B:171:ILE:HD11	2:B:200:GLN:CG	2.45	0.46
7:G:165:THR:HG23	7:G:166:VAL:O	2.16	0.46
9:I:26:LEU:HD22	9:I:108:GLN:HG3	1.96	0.46
11:K:9:ASP:OD1	11:K:9:ASP:C	2.58	0.46
21:U:129:TYR:CB	21:U:135:LEU:HD13	2.45	0.46
25:Y:29:ILE:HG21	25:Y:155:ILE:CG2	2.46	0.46
1:A:2063:U:H2'	1:A:2064:C:O4'	2.15	0.46
1:A:818:C:H1'	5:E:143:ILE:HG13	1.96	0.46
1:A:1704:G:N3	1:A:1704:G:H2'	2.31	0.46
1:A:1888:U:H2'	1:A:1889:G:H8	1.81	0.46
13:M:98:VAL:HG12	13:M:99:ASP:H	1.81	0.46
3:C:119:ARG:HD2	7:G:252:TYR:HB3	1.96	0.46
14:N:57:VAL:HG23	14:N:57:VAL:O	2.16	0.46
4:D:106:LEU:CD2	4:D:123:VAL:HG21	2.39	0.46
8:H:25:LEU:HB3	8:H:26:PRO:HD3	1.98	0.46
8:H:63:MET:HE1	8:H:102:VAL:HG12	1.98	0.46
12:L:56:ARG:NH1	12:L:190:GLY:O	2.49	0.46
1:A:2061:U:O2	16:P:150:ARG:HD2	2.15	0.46
1:A:528:A:H2'	1:A:529:U:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:95:HIS:NE2	18:R:111:ILE:HD13	2.32	0.45
22:V:87:ILE:HD12	22:V:114:CYS:SG	2.55	0.45
1:A:2027:C:H2'	1:A:2028:U:H6	1.81	0.45
3:C:60:ALA:HB2	3:C:160:ILE:HD11	1.96	0.45
8:H:106:LEU:HD11	8:H:109:LEU:HD12	1.97	0.45
21:U:71:ILE:HD13	21:U:71:ILE:C	2.41	0.45
1:A:3:C:O2	5:E:17:ARG:NH2	2.47	0.45
6:F:125:LYS:HA	6:F:159:THR:HA	1.98	0.45
13:M:32:LEU:HD23	13:M:68:ILE:HB	1.99	0.45
30:4:65:THR:HG22	30:4:69:CYS:HA	1.98	0.45
8:H:75:LEU:HD21	8:H:97:VAL:HG22	1.99	0.45
9:I:171:CYS:HA	9:I:181:ILE:HD11	1.99	0.45
1:A:1447:A:HO2'	1:A:1450:A:N6	2.14	0.45
2:B:121:ILE:HD13	2:B:164:ILE:HG21	1.98	0.45
12:L:25:ARG:O	12:L:27:TYR:N	2.48	0.45
1:A:1091:C:O2'	1:A:1226:A:N1	2.44	0.45
1:A:1264:A:N6	1:A:1265:G:C6	2.85	0.45
1:A:1951:G:C6	1:A:2037:A:C6	3.05	0.45
15:O:74:HIS:HB2	15:O:76:TYR:CE2	2.51	0.45
21:U:129:TYR:HB3	21:U:135:LEU:HD13	1.98	0.45
1:A:1076:C:O3'	16:P:149:ARG:NH2	2.50	0.45
1:A:1679:G:O2'	20:T:24:ASN:OD1	2.32	0.45
2:B:70:LEU:HD12	2:B:84:ILE:HD11	1.99	0.45
4:D:163:GLU:N	4:D:164:PRO:CD	2.80	0.45
21:U:63:VAL:HG21	21:U:71:ILE:HB	1.99	0.45
25:Y:83:ILE:HD11	25:Y:123:LEU:HD12	1.98	0.45
1:A:167:A:H5'	8:H:176:GLN:HG2	1.99	0.45
1:A:998:A:N7	16:P:137:THR:HG23	2.32	0.45
1:A:1027:C:O2'	21:U:55:ARG:NH2	2.50	0.45
7:G:211:SER:OG	7:G:212:SER:N	2.49	0.45
25:Y:29:ILE:HG21	25:Y:155:ILE:HG23	1.99	0.45
1:A:1108:A:O2'	1:A:1109:G:OP2	2.29	0.45
1:A:1869:G:N3	1:A:1869:G:H2'	2.31	0.45
7:G:117:GLY:HA3	7:G:202:PHE:HB3	1.98	0.45
29:3:79:ILE:HG22	29:3:84:VAL:HG23	1.98	0.45
1:A:525:G:C2'	1:A:526:G:O5'	2.65	0.44
1:A:1413:U:O2'	1:A:1415:A:N7	2.43	0.44
1:A:1626:U:O2'	1:A:1812:A:N1	2.45	0.44
5:E:6:ARG:NH1	6:F:23:MET:SD	2.89	0.44
1:A:832:A:N3	1:A:832:A:C2'	2.80	0.44
1:A:1702:C:O2	1:A:1702:C:O4'	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ALA:HB2	2:B:43:PHE:HE2	1.80	0.44
3:C:155:HIS:O	26:Z:59:ARG:NH1	2.50	0.44
10:J:126:ILE:CD1	10:J:179:ILE:HG21	2.47	0.44
14:N:35:CYS:SG	14:N:36:SER:N	2.89	0.44
19:S:33:THR:O	19:S:38:ILE:CG2	2.65	0.44
19:S:34:ALA:O	19:S:38:ILE:HD11	2.17	0.44
32:6:23:LYS:O	32:6:24:LEU:CB	2.65	0.44
1:A:1215:G:O2'	1:A:1231:G:O6	2.33	0.44
2:B:208:GLN:O	2:B:209:ASN:C	2.60	0.44
1:A:1431:A:OP1	4:D:161:THR:HG21	2.17	0.44
2:B:69:ASN:O	2:B:71:ALA:N	2.51	0.44
4:D:126:HIS:O	4:D:129:GLU:HG3	2.17	0.44
1:A:269:A:OP1	8:H:176:GLN:NE2	2.49	0.44
1:A:2027:C:H2'	1:A:2028:U:C6	2.52	0.44
1:A:618:U:H5''	17:Q:15:LEU:HD22	2.00	0.44
10:J:41:GLU:HB3	10:J:72:TYR:CD2	2.53	0.44
1:A:90:U:H4'	1:A:169:A:O4'	2.18	0.44
1:A:1881:G:N1	1:A:1907:G:O2'	2.36	0.44
3:C:73:VAL:O	3:C:73:VAL:HG12	2.17	0.44
5:E:142:ASP:O	5:E:142:ASP:CG	2.61	0.44
17:Q:92:CYS:HB3	17:Q:132:LEU:HD11	1.99	0.44
29:3:21:LEU:C	29:3:21:LEU:HD12	2.43	0.44
1:A:118:U:O2'	1:A:339:A:N3	2.39	0.44
1:A:141:G:N7	8:H:177:ARG:NH2	2.65	0.44
1:A:1743:A:C2	1:A:1787:U:O4	2.71	0.44
4:D:137:VAL:HG22	4:D:187:VAL:HG23	2.00	0.44
8:H:158:ILE:HD13	8:H:158:ILE:H	1.82	0.44
19:S:33:THR:O	19:S:38:ILE:CB	2.65	0.44
19:S:100:VAL:HG13	19:S:105:LEU:HB2	2.00	0.44
27:1:112:LEU:HD12	27:1:112:LEU:C	2.42	0.44
2:B:160:GLN:HB3	2:B:204:ILE:HD11	1.98	0.44
9:I:64:VAL:HG12	9:I:84:VAL:HG11	2.00	0.44
22:V:38:TRP:CE2	22:V:52:LYS:HG2	2.53	0.44
1:A:65:A:C2	1:A:86:A:N7	2.86	0.43
1:A:810:A:C2	1:A:854:A:C2	3.06	0.43
1:A:1302:G:C2	1:A:1897:A:C2	3.06	0.43
1:A:2027:C:C4	1:A:2028:U:C5	3.06	0.43
10:J:81:ILE:CD1	10:J:94:LEU:HD22	2.46	0.43
12:L:101:ILE:HG13	12:L:200:ILE:HD12	2.00	0.43
13:M:41:GLU:HB3	13:M:42:PRO:HD3	2.00	0.43
1:A:378:A:C5	1:A:379:G:H1'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:LEU:HB2	5:E:104:LEU:CD1	2.48	0.43
22:V:78:VAL:HG12	22:V:89:ILE:HG22	2.01	0.43
1:A:752:U:O2'	1:A:753:U:O5'	2.36	0.43
10:J:126:ILE:HD13	10:J:179:ILE:HG21	2.00	0.43
14:N:21:ILE:HB	14:N:88:ILE:HG23	1.99	0.43
16:P:126:ILE:HG21	29:3:53:ILE:HD11	2.01	0.43
17:Q:102:VAL:HG22	17:Q:127:VAL:CG1	2.46	0.43
1:A:28:A:H2'	1:A:29:U:O4'	2.17	0.43
2:B:179:VAL:HB	2:B:180:LEU:HG	2.01	0.43
5:E:116:LEU:O	5:E:118:LEU:HD13	2.18	0.43
6:F:38:LEU:HD12	6:F:38:LEU:O	2.18	0.43
6:F:222:LEU:HD23	6:F:222:LEU:C	2.43	0.43
8:H:28:MET:HA	8:H:102:VAL:HG23	2.00	0.43
9:I:94:MET:HE2	28:2:58:VAL:HG12	2.01	0.43
22:V:130:GLN:O	22:V:131:CYS:CB	2.66	0.43
1:A:1108:A:N6	1:A:1192:A:C8	2.87	0.43
21:U:30:PRO:O	21:U:34:GLU:HG2	2.18	0.43
21:U:71:ILE:O	21:U:74:ILE:HG12	2.18	0.43
25:Y:90:HIS:CB	25:Y:93:ILE:HD11	2.49	0.43
1:A:1008:A:H2'	1:A:1009:A:C8	2.53	0.43
1:A:1266:G:C6	1:A:1267:C:C4	3.06	0.43
10:J:52:VAL:HG11	10:J:170:ILE:CG2	2.48	0.43
14:N:90:LEU:HD22	14:N:97:VAL:HG12	1.99	0.43
21:U:80:ILE:HG22	21:U:80:ILE:O	2.18	0.43
1:A:364:U:H2'	1:A:366:A:H5''	2.00	0.43
1:A:622:A:O2'	1:A:628:A:N1	2.44	0.43
1:A:1704:G:C2	1:A:1705:C:C5	3.07	0.43
1:A:1821:A:H2'	1:A:1822:A:C8	2.53	0.43
14:N:59:THR:HG22	14:N:82:ARG:HB3	2.01	0.43
16:P:44:VAL:CG1	16:P:54:VAL:HG23	2.48	0.43
16:P:55:ARG:O	16:P:56:ILE:HD13	2.18	0.43
17:Q:102:VAL:HG12	17:Q:104:VAL:HG12	2.00	0.43
12:L:104:ILE:HG22	12:L:105:ASP:C	2.43	0.43
19:S:91:ASP:O	19:S:93:LYS:N	2.51	0.43
33:7:39:A:C2	33:7:40:U:C2	3.07	0.43
1:A:832:A:N3	1:A:832:A:H2'	2.33	0.43
1:A:1823:U:H3'	1:A:1824:A:H5''	2.01	0.43
2:B:34:ALA:HB1	2:B:35:PRO:HD2	2.01	0.43
6:F:47:LEU:HD11	6:F:101:LEU:HD21	2.00	0.43
8:H:2:LYS:O	8:H:3:LEU:HD12	2.19	0.43
21:U:37:ILE:HD11	21:U:63:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:92:ILE:HD11	21:U:139:TRP:HH2	1.84	0.43
22:V:114:CYS:O	22:V:115:SER:OG	2.37	0.43
1:A:1100:U:H3'	1:A:1101:G:C5'	2.49	0.43
5:E:52:ILE:HG23	5:E:76:LEU:HD11	2.01	0.43
6:F:18:TRP:CH2	6:F:42:ILE:HA	2.54	0.43
19:S:30:ILE:O	19:S:33:THR:OG1	2.29	0.43
1:A:14:U:OP2	7:G:218:THR:HG21	2.18	0.42
1:A:364:U:H2'	1:A:366:A:C5'	2.49	0.42
4:D:72:LEU:HD11	15:O:78:ILE:HD11	2.00	0.42
22:V:67:VAL:HG21	22:V:141:ASN:HD21	1.84	0.42
1:A:109:C:H5''	1:A:389:G:O2'	2.18	0.42
1:A:1095:A:N7	1:A:2064:C:O2'	2.46	0.42
5:E:121:SER:OG	5:E:122:VAL:N	2.51	0.42
6:F:138:ILE:HD12	6:F:146:SER:HB3	2.01	0.42
24:X:28:LEU:HD12	24:X:33:LEU:HD22	2.01	0.42
27:1:77:TYR:CG	27:1:83:VAL:HG22	2.54	0.42
1:A:2049:G:C2	1:A:2050:U:C6	3.07	0.42
5:E:53:ARG:HB3	5:E:53:ARG:CZ	2.49	0.42
19:S:42:MET:O	19:S:45:VAL:HG22	2.19	0.42
1:A:105:A:H5'	1:A:107:A:C4	2.55	0.42
1:A:336:G:O2'	12:L:33:PRO:HB3	2.20	0.42
1:A:1448:U:OP2	1:A:1450:A:N6	2.45	0.42
1:A:2083:A:N7	29:3:34:LYS:NZ	2.67	0.42
2:B:229:MET:HE3	2:B:229:MET:HA	2.01	0.42
3:C:184:LEU:O	26:Z:45:TYR:N	2.44	0.42
6:F:183:VAL:HG11	6:F:188:SER:O	2.19	0.42
13:M:56:ILE:HD13	13:M:90:ILE:HG21	2.01	0.42
21:U:101:HIS:CE1	21:U:105:ASN:HD22	2.36	0.42
31:5:9:VAL:HG13	31:5:25:VAL:HG13	2.00	0.42
32:6:27:LYS:O	32:6:28:LYS:C	2.62	0.42
1:A:167:A:OP2	8:H:137:ARG:NH1	2.52	0.42
1:A:804:U:H3'	1:A:805:A:H5'	2.01	0.42
9:I:134:PRO:O	9:I:137:ARG:HG2	2.20	0.42
9:I:135:LEU:HD23	31:5:47:PRO:HG2	2.00	0.42
11:K:10:CYS:SG	11:K:27:ILE:HG23	2.60	0.42
1:A:1714:U:H2'	1:A:1715:A:O4'	2.19	0.42
15:O:26:LEU:HG	15:O:32:ILE:HD12	2.02	0.42
1:A:923:U:N3	1:A:925:C:O2	2.53	0.42
1:A:954:G:H2'	1:A:955:U:C6	2.55	0.42
11:K:9:ASP:OD1	11:K:10:CYS:N	2.53	0.42
12:L:13:LEU:HD23	12:L:14:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:96:ILE:CG2	17:Q:127:VAL:HG11	2.50	0.42
23:W:31:ASN:O	23:W:35:THR:HG23	2.20	0.42
1:A:250:A:H4'	1:A:251:U:OP1	2.19	0.42
1:A:485:C:O2	1:A:517:G:N2	2.53	0.42
1:A:1061:A:H2	1:A:1081:U:O4	2.02	0.42
1:A:1882:U:C5	1:A:1907:G:N2	2.88	0.42
1:A:1882:U:O4	1:A:1908:A:C2	2.73	0.42
2:B:140:ILE:HG23	2:B:213:ARG:HD3	2.00	0.42
5:E:145:SER:O	5:E:146:PHE:C	2.62	0.42
19:S:28:VAL:HG12	19:S:61:LEU:HD11	2.02	0.42
25:Y:102:PHE:O	25:Y:118:ALA:HB2	2.19	0.42
1:A:936:A:H2'	1:A:937:G:O4'	2.19	0.42
1:A:1450:A:H2'	1:A:1451:G:O4'	2.20	0.42
1:A:1888:U:H2'	1:A:1889:G:C8	2.54	0.42
1:A:989:C:H2'	1:A:990:U:C6	2.55	0.41
1:A:1447:A:HO2'	1:A:1450:A:H62	1.67	0.41
1:A:1679:G:N9	20:T:39:GLN:HG3	2.35	0.41
17:Q:102:VAL:CG2	17:Q:127:VAL:HG12	2.47	0.41
27:1:77:TYR:CD2	27:1:83:VAL:HG22	2.55	0.41
1:A:87:A:OP1	27:1:120:ARG:NH2	2.53	0.41
1:A:525:G:H2'	1:A:526:G:O5'	2.20	0.41
25:Y:29:ILE:HD11	25:Y:88:TYR:HB3	2.02	0.41
2:B:123:GLY:HA2	2:B:165:ARG:HD2	2.03	0.41
21:U:38:ILE:HD12	21:U:42:LYS:HE2	2.03	0.41
21:U:55:ARG:HA	21:U:60:ILE:O	2.20	0.41
27:1:5:PHE:O	27:1:43:ARG:NH1	2.48	0.41
29:3:74:CYS:SG	29:3:75:VAL:N	2.92	0.41
1:A:981:U:O2'	1:A:982:A:P	2.78	0.41
1:A:1235:G:H2'	1:A:1236:U:O4'	2.20	0.41
2:B:37:MET:HE3	2:B:231:LEU:HD11	2.02	0.41
3:C:62:ARG:HA	3:C:184:LEU:HD13	2.02	0.41
6:F:48:LEU:HD13	6:F:48:LEU:HA	1.98	0.41
7:G:168:MET:HE2	7:G:170:VAL:HG13	2.02	0.41
8:H:66:GLY:O	8:H:67:VAL:C	2.62	0.41
13:M:51:GLU:N	13:M:52:PRO:HD2	2.35	0.41
18:R:65:GLU:C	18:R:67:ALA:H	2.29	0.41
25:Y:93:ILE:N	25:Y:93:ILE:HD12	2.36	0.41
30:4:45:PHE:O	30:4:48:ALA:HB2	2.21	0.41
1:A:1108:A:O2'	1:A:1109:G:P	2.78	0.41
1:A:1821:A:C6	1:A:1822:A:C6	3.08	0.41
4:D:28:ILE:HG21	4:D:69:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:84:ILE:HD12	21:U:149:LEU:HD12	2.03	0.41
22:V:114:CYS:HA	22:V:142:VAL:HG12	2.03	0.41
1:A:586:A:H2'	1:A:586:A:N3	2.35	0.41
2:B:177:SER:O	2:B:178:LYS:C	2.63	0.41
4:D:143:LEU:CD2	4:D:151:MET:HE2	2.46	0.41
8:H:76:LEU:HA	8:H:94:ARG:HA	2.01	0.41
1:A:338:U:OP1	12:L:56:ARG:NH2	2.53	0.41
1:A:486:A:C2	1:A:516:G:C2	3.09	0.41
1:A:1243:A:H2'	1:A:1244:A:O4'	2.19	0.41
5:E:83:GLN:CB	5:E:85:LEU:HD23	2.50	0.41
16:P:64:ALA:O	16:P:66:ARG:N	2.54	0.41
21:U:87:ASP:OD1	21:U:87:ASP:N	2.53	0.41
1:A:1185:A:H2'	1:A:1186:G:O4'	2.21	0.41
1:A:1261:A:H2'	1:A:1262:C:C6	2.56	0.41
1:A:15:U:H2'	1:A:16:G:O4'	2.21	0.41
1:A:542:C:H3'	1:A:543:A:H5''	2.03	0.41
1:A:831:U:C3'	1:A:832:A:H5'	2.51	0.41
1:A:872:A:H2'	1:A:873:A:O4'	2.21	0.41
1:A:1453:G:C2'	1:A:1454:G:H5'	2.50	0.41
7:G:165:THR:OG1	7:G:183:PRO:HA	2.21	0.41
16:P:107:THR:HG23	29:3:42:ARG:NH1	2.36	0.41
29:3:23:CYS:SG	29:3:74:CYS:N	2.94	0.41
2:B:91:ILE:HD12	2:B:91:ILE:C	2.46	0.41
2:B:135:LEU:HD12	2:B:217:ILE:HG22	2.03	0.41
4:D:24:PHE:HZ	4:D:72:LEU:HD13	1.86	0.41
6:F:86:LEU:HD13	6:F:103:TYR:CD2	2.55	0.41
10:J:27:ILE:C	10:J:27:ILE:HD12	2.45	0.41
22:V:135:SER:HB3	22:V:138:VAL:HG12	2.03	0.41
1:A:1277:G:N3	1:A:1296:C:O2'	2.43	0.40
1:A:1976:G:C6	1:A:1977:G:N1	2.89	0.40
2:B:92:ILE:O	2:B:94:ARG:N	2.55	0.40
11:K:2:VAL:HG22	11:K:3:ARG:N	2.36	0.40
16:P:146:ARG:O	16:P:147:ARG:CG	2.69	0.40
22:V:112:CYS:SG	22:V:128:VAL:HG11	2.61	0.40
1:A:981:U:O2	1:A:983:G:N1	2.54	0.40
4:D:70:THR:O	4:D:73:VAL:HG22	2.21	0.40
8:H:78:LYS:HD3	8:H:81:MET:HE3	2.03	0.40
10:J:180:THR:O	10:J:180:THR:OG1	2.37	0.40
12:L:48:GLY:O	12:L:49:ARG:C	2.63	0.40
19:S:45:VAL:HG11	19:S:85:PHE:CZ	2.56	0.40
1:A:87:A:H2'	1:A:88:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:A:OP1	32:6:15:LYS:NZ	2.53	0.40
1:A:1636:A:N7	23:W:3:ARG:NH2	2.69	0.40
1:A:359:A:C6	1:A:360:C:C2	3.10	0.40
1:A:533:A:OP2	27:1:94:ARG:NH1	2.55	0.40
1:A:836:C:HO2'	1:A:837:A:C5'	2.33	0.40
1:A:1003:C:N4	1:A:1178:C:H4'	2.37	0.40
1:A:1253:A:O3'	29:3:85:ARG:NH2	2.54	0.40
1:A:1900:U:H2'	1:A:1901:U:O4'	2.22	0.40
6:F:158:ASP:HB2	6:F:173:LEU:O	2.21	0.40
7:G:149:ILE:HD12	7:G:227:PHE:CE2	2.55	0.40
7:G:168:MET:HE2	7:G:170:VAL:CG1	2.52	0.40
9:I:81:ILE:O	9:I:84:VAL:HG22	2.21	0.40
19:S:35:ILE:O	19:S:38:ILE:HG12	1.98	0.40
1:A:958:U:H4'	1:A:1058:G:OP1	2.21	0.40
1:A:1034:U:H3'	1:A:1034:U:O2	2.22	0.40
1:A:1846:U:C5	24:X:39:ALA:HB3	2.57	0.40
6:F:69:ILE:HB	6:F:93:THR:HG22	2.03	0.40
11:K:119:LYS:O	11:K:120:HIS:HB2	2.22	0.40
24:X:93:ILE:HG22	24:X:106:GLU:CA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	208/262 (79%)	168 (81%)	28 (14%)	12 (6%)	1	10
3	C	193/263 (73%)	163 (84%)	22 (11%)	8 (4%)	2	17
4	D	149/221 (67%)	129 (87%)	17 (11%)	3 (2%)	6	31
5	E	183/189 (97%)	159 (87%)	19 (10%)	5 (3%)	4	25
6	F	255/261 (98%)	217 (85%)	31 (12%)	7 (3%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	222/272 (82%)	195 (88%)	20 (9%)	7 (3%)	3	21
8	H	200/306 (65%)	173 (86%)	19 (10%)	8 (4%)	2	17
9	I	176/195 (90%)	153 (87%)	14 (8%)	9 (5%)	1	13
10	J	186/194 (96%)	160 (86%)	17 (9%)	9 (5%)	2	14
11	K	127/130 (98%)	104 (82%)	16 (13%)	7 (6%)	1	11
12	L	166/218 (76%)	134 (81%)	23 (14%)	9 (5%)	1	12
13	M	136/144 (94%)	116 (85%)	13 (10%)	7 (5%)	1	13
14	N	96/118 (81%)	83 (86%)	8 (8%)	5 (5%)	1	12
15	O	77/137 (56%)	66 (86%)	10 (13%)	1 (1%)	9	40
16	P	125/151 (83%)	103 (82%)	18 (14%)	4 (3%)	3	21
17	Q	142/145 (98%)	128 (90%)	13 (9%)	1 (1%)	18	52
18	R	92/141 (65%)	73 (79%)	13 (14%)	6 (6%)	1	8
19	S	126/156 (81%)	100 (79%)	17 (14%)	9 (7%)	1	6
20	T	46/54 (85%)	43 (94%)	2 (4%)	1 (2%)	5	29
21	U	147/151 (97%)	133 (90%)	10 (7%)	4 (3%)	4	25
22	V	142/161 (88%)	123 (87%)	9 (6%)	10 (7%)	1	6
23	W	91/137 (66%)	80 (88%)	7 (8%)	4 (4%)	2	15
24	X	92/145 (63%)	82 (89%)	6 (6%)	4 (4%)	2	16
25	Y	152/170 (89%)	134 (88%)	12 (8%)	6 (4%)	2	18
26	Z	70/82 (85%)	62 (89%)	3 (4%)	5 (7%)	1	6
27	1	118/133 (89%)	104 (88%)	9 (8%)	5 (4%)	2	16
28	2	35/105 (33%)	30 (86%)	5 (14%)	0	100	100
29	3	93/107 (87%)	80 (86%)	10 (11%)	3 (3%)	3	21
30	4	74/82 (90%)	48 (65%)	21 (28%)	5 (7%)	1	7
31	5	54/67 (81%)	50 (93%)	4 (7%)	0	100	100
32	6	41/58 (71%)	34 (83%)	4 (10%)	3 (7%)	1	6
All	All	4014/4955 (81%)	3427 (85%)	420 (10%)	167 (4%)	3	16

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	84	ILE
2	B	93	ASN

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Mol	Chain	Res	Type
2	B	147	GLN
2	B	179	VAL
3	C	20	CYS
3	C	95	ALA
4	D	149	LYS
5	E	16	LYS
8	H	39	ASP
8	H	67	VAL
9	I	71	GLY
9	I	157	ILE
9	I	159	SER
10	J	57	LYS
10	J	132	SER
11	K	23	ARG
11	K	77	PRO
12	L	23	LYS
12	L	49	ARG
12	L	168	ILE
13	M	17	ALA
14	N	74	ASN
14	N	105	ILE
14	N	108	VAL
18	R	42	ILE
18	R	51	SER
18	R	65	GLU
18	R	66	PRO
18	R	86	VAL
19	S	133	VAL
21	U	146	ALA
22	V	41	VAL
25	Y	54	PRO
25	Y	67	LYS
25	Y	145	ARG
26	Z	30	GLY
30	4	19	LEU
30	4	81	ILE
32	6	24	LEU
3	C	199	ASP
5	E	134	ILE
5	E	137	GLY
5	E	146	PHE
6	F	187	HIS

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Mol	Chain	Res	Type
6	F	231	ASN
8	H	66	GLY
9	I	42	HIS
9	I	174	GLU
10	J	4	VAL
10	J	157	SER
10	J	181	ARG
11	K	120	HIS
12	L	22	LYS
12	L	165	SER
13	M	40	VAL
13	M	41	GLU
13	M	139	TYR
14	N	102	SER
16	P	138	ASP
19	S	14	ILE
19	S	92	LEU
19	S	94	GLU
19	S	101	ILE
22	V	16	GLN
22	V	24	SER
22	V	101	ASN
22	V	130	GLN
23	W	17	VAL
23	W	67	ARG
23	W	69	ILE
24	X	112	ILE
25	Y	91	PRO
25	Y	109	GLY
26	Z	75	LYS
27	1	64	LEU
27	1	117	LYS
29	3	11	SER
29	3	60	SER
2	B	107	ARG
3	C	115	PHE
5	E	15	PRO
6	F	3	LYS
6	F	185	ALA
6	F	195	ILE
6	F	232	THR
7	G	120	ASN

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Mol	Chain	Res	Type
7	G	148	LEU
8	H	110	ASN
9	I	70	HIS
9	I	158	LYS
10	J	105	GLN
10	J	112	ILE
11	K	4	MET
11	K	29	PRO
12	L	8	ARG
12	L	61	ASP
19	S	19	ASN
22	V	131	CYS
25	Y	142	LYS
27	1	34	SER
27	1	49	LYS
29	3	46	ASP
30	4	56	SER
2	B	82	LYS
3	C	30	GLU
3	C	99	ALA
7	G	162	ASP
8	H	179	VAL
9	I	16	TYR
9	I	68	MET
10	J	15	ASP
10	J	110	PHE
13	M	33	ASN
14	N	67	SER
15	O	35	GLU
16	P	139	SER
19	S	40	LYS
21	U	132	LYS
21	U	141	TYR
22	V	56	TYR
22	V	115	SER
26	Z	23	LEU
30	4	58	ASN
32	6	23	LYS
32	6	28	LYS
2	B	70	LEU
2	B	116	LYS
2	B	138	PHE

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Mol	Chain	Res	Type
2	B	146	ARG
2	B	209	ASN
3	C	116	THR
3	C	143	VAL
4	D	143	LEU
6	F	30	LYS
7	G	212	SER
7	G	215	LYS
8	H	16	ILE
13	M	30	ILE
13	M	116	SER
16	P	65	ASP
18	R	122	PHE
19	S	28	VAL
20	T	9	PRO
21	U	61	PRO
22	V	155	ARG
23	W	26	LEU
24	X	49	ILE
24	X	87	PRO
24	X	116	LEU
26	Z	80	PHE
27	1	31	ASN
2	B	98	THR
7	G	157	GLY
16	P	144	SER
22	V	54	GLY
26	Z	81	GLN
30	4	69	CYS
8	H	25	LEU
11	K	52	ILE
11	K	107	PRO
12	L	170	PRO
17	Q	88	PRO
7	G	160	ILE
8	H	121	ILE
4	D	36	GLY
12	L	202	GLY
19	S	24	GLY

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	
2	B	195/238 (82%)	161 (83%)	34 (17%)	2	10
3	C	167/227 (74%)	141 (84%)	26 (16%)	2	13
4	D	132/188 (70%)	115 (87%)	17 (13%)	4	20
5	E	160/167 (96%)	136 (85%)	24 (15%)	3	15
6	F	233/237 (98%)	185 (79%)	48 (21%)	1	7
7	G	191/222 (86%)	154 (81%)	37 (19%)	1	8
8	H	181/279 (65%)	152 (84%)	29 (16%)	2	13
9	I	154/165 (93%)	126 (82%)	28 (18%)	2	9
10	J	177/183 (97%)	152 (86%)	25 (14%)	3	17
11	K	115/116 (99%)	91 (79%)	24 (21%)	1	6
12	L	152/193 (79%)	134 (88%)	18 (12%)	5	23
13	M	116/122 (95%)	110 (95%)	6 (5%)	21	54
14	N	91/109 (84%)	70 (77%)	21 (23%)	1	5
15	O	76/129 (59%)	63 (83%)	13 (17%)	2	11
16	P	99/119 (83%)	84 (85%)	15 (15%)	3	14
17	Q	120/121 (99%)	104 (87%)	16 (13%)	4	19
18	R	83/121 (69%)	81 (98%)	2 (2%)	43	70
19	S	113/136 (83%)	96 (85%)	17 (15%)	3	15
20	T	43/48 (90%)	39 (91%)	4 (9%)	8	33
21	U	132/133 (99%)	110 (83%)	22 (17%)	2	11
22	V	131/144 (91%)	107 (82%)	24 (18%)	2	9
23	W	86/127 (68%)	74 (86%)	12 (14%)	3	17
24	X	88/130 (68%)	77 (88%)	11 (12%)	4	21
25	Y	137/151 (91%)	113 (82%)	24 (18%)	2	10
26	Z	60/70 (86%)	48 (80%)	12 (20%)	1	7
27	1	103/115 (90%)	89 (86%)	14 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	2	35/88 (40%)	31 (89%)	4 (11%)	5	24
29	3	87/98 (89%)	77 (88%)	10 (12%)	5	24
30	4	70/76 (92%)	58 (83%)	12 (17%)	2	11
31	5	46/54 (85%)	43 (94%)	3 (6%)	15	47
32	6	36/47 (77%)	32 (89%)	4 (11%)	6	25
All	All	3609/4353 (83%)	3053 (85%)	556 (15%)	5	14

All (556) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	42	ASN
2	B	46	THR
2	B	49	THR
2	B	55	LYS
2	B	91	ILE
2	B	93	ASN
2	B	98	THR
2	B	104	SER
2	B	107	ARG
2	B	108	ASP
2	B	112	SER
2	B	115	ARG
2	B	120	LEU
2	B	127	VAL
2	B	129	THR
2	B	135	LEU
2	B	144	LYS
2	B	146	ARG
2	B	158	THR
2	B	163	LYS
2	B	165	ARG
2	B	173	THR
2	B	178	LYS
2	B	179	VAL
2	B	182	LYS
2	B	199	LYS
2	B	203	LYS
2	B	204	ILE
2	B	210	VAL
2	B	218	LEU

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Mol	Chain	Res	Type
2	B	219	LYS
2	B	222	LYS
2	B	229	MET
2	B	233	THR
3	C	16	LYS
3	C	20	CYS
3	C	29	LEU
3	C	40	ARG
3	C	50	LEU
3	C	58	GLN
3	C	63	ILE
3	C	65	VAL
3	C	67	ILE
3	C	79	ARG
3	C	81	PHE
3	C	88	LYS
3	C	111	ILE
3	C	114	LYS
3	C	117	GLU
3	C	123	VAL
3	C	133	VAL
3	C	140	ASN
3	C	168	GLU
3	C	169	SER
3	C	170	ILE
3	C	172	LEU
3	C	180	GLU
3	C	181	VAL
3	C	188	ILE
3	C	200	MET
4	D	5	ILE
4	D	12	ILE
4	D	16	VAL
4	D	22	ASN
4	D	25	LEU
4	D	76	ARG
4	D	107	ARG
4	D	128	MET
4	D	129	GLU
4	D	133	LYS
4	D	138	ILE
4	D	158	LEU

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Mol	Chain	Res	Type
4	D	163	GLU
4	D	169	VAL
4	D	178	LEU
4	D	182	VAL
4	D	188	LYS
5	E	7	ASN
5	E	16	LYS
5	E	22	GLU
5	E	37	LYS
5	E	46	GLN
5	E	62	LEU
5	E	65	LYS
5	E	68	LYS
5	E	72	GLN
5	E	81	VAL
5	E	102	PRO
5	E	112	LYS
5	E	127	VAL
5	E	128	LEU
5	E	135	ARG
5	E	141	VAL
5	E	142	ASP
5	E	143	ILE
5	E	148	VAL
5	E	161	THR
5	E	177	LEU
5	E	178	LYS
5	E	181	LYS
5	E	184	THR
6	F	3	LYS
6	F	5	ILE
6	F	7	LYS
6	F	9	LEU
6	F	18	TRP
6	F	38	LEU
6	F	39	LEU
6	F	44	LEU
6	F	47	LEU
6	F	52	LEU
6	F	59	ASP
6	F	65	LEU
6	F	72	VAL

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Mol	Chain	Res	Type
6	F	75	LYS
6	F	80	CYS
6	F	92	ILE
6	F	93	THR
6	F	102	LEU
6	F	108	ARG
6	F	114	ILE
6	F	117	GLU
6	F	118	GLU
6	F	126	VAL
6	F	130	LEU
6	F	132	ARG
6	F	133	LYS
6	F	138	ILE
6	F	156	VAL
6	F	159	THR
6	F	160	VAL
6	F	161	ARG
6	F	166	THR
6	F	168	LYS
6	F	169	VAL
6	F	171	GLU
6	F	173	LEU
6	F	180	LEU
6	F	181	VAL
6	F	184	THR
6	F	191	ARG
6	F	204	THR
6	F	208	ILE
6	F	220	THR
6	F	225	VAL
6	F	228	ILE
6	F	231	ASN
6	F	252	ARG
6	F	254	ASN
7	G	41	TRP
7	G	52	LYS
7	G	53	GLU
7	G	76	ASP
7	G	84	CYS
7	G	95	ILE
7	G	98	VAL

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Mol	Chain	Res	Type
7	G	101	GLN
7	G	103	ARG
7	G	106	GLN
7	G	123	CYS
7	G	132	GLU
7	G	146	LEU
7	G	147	SER
7	G	149	ILE
7	G	151	VAL
7	G	159	LYS
7	G	160	ILE
7	G	168	MET
7	G	173	LYS
7	G	177	VAL
7	G	178	ARG
7	G	179	ILE
7	G	181	LEU
7	G	182	VAL
7	G	190	ILE
7	G	196	THR
7	G	199	MET
7	G	200	LEU
7	G	206	LYS
7	G	211	SER
7	G	217	LYS
7	G	224	ARG
7	G	230	LEU
7	G	242	TRP
7	G	244	VAL
7	G	253	GLU
8	H	1	MET
8	H	15	SER
8	H	23	LYS
8	H	29	GLU
8	H	36	VAL
8	H	40	SER
8	H	41	ILE
8	H	67	VAL
8	H	73	VAL
8	H	75	LEU
8	H	76	LEU
8	H	78	LYS

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Mol	Chain	Res	Type
8	H	82	LYS
8	H	94	ARG
8	H	95	LYS
8	H	97	VAL
8	H	109	LEU
8	H	111	LEU
8	H	113	LEU
8	H	114	VAL
8	H	121	ILE
8	H	131	LYS
8	H	137	ARG
8	H	158	ILE
8	H	178	LEU
8	H	180	THR
8	H	184	LEU
8	H	206	LYS
8	H	212	LEU
9	I	10	LEU
9	I	12	LYS
9	I	16	TYR
9	I	21	ILE
9	I	29	CYS
9	I	35	LYS
9	I	50	LYS
9	I	54	LYS
9	I	63	LEU
9	I	72	ARG
9	I	79	LYS
9	I	100	LEU
9	I	107	VAL
9	I	108	GLN
9	I	109	LYS
9	I	117	THR
9	I	118	ARG
9	I	128	GLN
9	I	137	ARG
9	I	138	VAL
9	I	157	ILE
9	I	158	LYS
9	I	164	LEU
9	I	179	TYR
9	I	181	ILE

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Mol	Chain	Res	Type
9	I	182	LYS
9	I	189	ARG
9	I	190	VAL
10	J	4	VAL
10	J	9	LEU
10	J	17	GLU
10	J	27	ILE
10	J	31	SER
10	J	42	ILE
10	J	47	CYS
10	J	52	VAL
10	J	57	LYS
10	J	67	LYS
10	J	74	ARG
10	J	94	LEU
10	J	112	ILE
10	J	113	ILE
10	J	119	LEU
10	J	132	SER
10	J	136	ILE
10	J	139	LYS
10	J	155	LEU
10	J	159	GLU
10	J	166	GLU
10	J	178	LYS
10	J	180	THR
10	J	181	ARG
10	J	188	LEU
11	K	2	VAL
11	K	9	ASP
11	K	12	LYS
11	K	13	THR
11	K	14	ILE
11	K	19	LYS
11	K	25	VAL
11	K	32	LYS
11	K	34	VAL
11	K	41	MET
11	K	47	ILE
11	K	52	ILE
11	K	53	VAL
11	K	62	VAL

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Mol	Chain	Res	Type
11	K	63	VAL
11	K	70	ASN
11	K	75	ILE
11	K	81	VAL
11	K	110	ILE
11	K	111	MET
11	K	115	GLU
11	K	120	HIS
11	K	125	VAL
11	K	130	PHE
12	L	8	ARG
12	L	10	LYS
12	L	13	LEU
12	L	21	HIS
12	L	28	GLU
12	L	43	VAL
12	L	49	ARG
12	L	59	LYS
12	L	72	ILE
12	L	76	THR
12	L	98	LYS
12	L	106	SER
12	L	112	TRP
12	L	172	LEU
12	L	177	LYS
12	L	188	ARG
12	L	205	LEU
12	L	216	LYS
13	M	75	GLN
13	M	79	ILE
13	M	83	ARG
13	M	98	VAL
13	M	105	GLU
13	M	128	LYS
14	N	27	ASN
14	N	28	LEU
14	N	31	ILE
14	N	35	CYS
14	N	39	MET
14	N	40	LYS
14	N	43	LYS
14	N	53	VAL

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Mol	Chain	Res	Type
14	N	54	ARG
14	N	60	LEU
14	N	67	SER
14	N	73	THR
14	N	74	ASN
14	N	78	ARG
14	N	81	LEU
14	N	86	ARG
14	N	90	LEU
14	N	99	GLN
14	N	105	ILE
14	N	108	VAL
14	N	115	ILE
15	O	21	LEU
15	O	32	ILE
15	O	34	VAL
15	O	36	LYS
15	O	42	ARG
15	O	46	LEU
15	O	53	ILE
15	O	61	LYS
15	O	63	ARG
15	O	69	LYS
15	O	72	TRP
15	O	73	LYS
15	O	85	GLU
16	P	44	VAL
16	P	54	VAL
16	P	63	LYS
16	P	65	ASP
16	P	70	SER
16	P	81	VAL
16	P	85	LEU
16	P	93	ILE
16	P	98	ARG
16	P	103	THR
16	P	104	LYS
16	P	129	ILE
16	P	138	ASP
16	P	141	ARG
16	P	143	LYS
17	Q	5	LYS

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Mol	Chain	Res	Type
17	Q	9	LEU
17	Q	19	ARG
17	Q	74	VAL
17	Q	81	LYS
17	Q	84	THR
17	Q	93	LEU
17	Q	94	ASN
17	Q	96	ILE
17	Q	102	VAL
17	Q	104	VAL
17	Q	120	VAL
17	Q	124	VAL
17	Q	126	LYS
17	Q	132	LEU
17	Q	135	LEU
18	R	42	ILE
18	R	96	TRP
19	S	21	ASN
19	S	22	VAL
19	S	27	LYS
19	S	32	LEU
19	S	41	ARG
19	S	45	VAL
19	S	72	ILE
19	S	79	PHE
19	S	81	ILE
19	S	89	ARG
19	S	98	ILE
19	S	109	LEU
19	S	111	GLU
19	S	115	ARG
19	S	117	LYS
19	S	129	TRP
19	S	132	ARG
20	T	17	ARG
20	T	28	ILE
20	T	30	ARG
20	T	39	GLN
21	U	3	ARG
21	U	11	ILE
21	U	16	LEU
21	U	22	GLN

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Mol	Chain	Res	Type
21	U	27	LYS
21	U	33	ILE
21	U	38	ILE
21	U	54	LEU
21	U	65	SER
21	U	67	THR
21	U	71	ILE
21	U	72	LEU
21	U	74	ILE
21	U	75	LEU
21	U	88	LEU
21	U	91	LEU
21	U	106	LYS
21	U	119	GLU
21	U	121	LYS
21	U	127	ARG
21	U	133	LYS
21	U	149	LEU
22	V	17	GLU
22	V	39	LYS
22	V	64	THR
22	V	70	ARG
22	V	74	LEU
22	V	81	ASN
22	V	83	MET
22	V	85	ARG
22	V	87	ILE
22	V	90	ARG
22	V	97	VAL
22	V	101	ASN
22	V	102	ARG
22	V	114	CYS
22	V	121	LYS
22	V	125	ILE
22	V	127	THR
22	V	130	GLN
22	V	141	ASN
22	V	142	VAL
22	V	147	LYS
22	V	150	ILE
22	V	155	ARG
22	V	160	LEU

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Mol	Chain	Res	Type
23	W	4	VAL
23	W	7	LYS
23	W	14	ARG
23	W	49	LYS
23	W	50	VAL
23	W	54	VAL
23	W	55	THR
23	W	57	LEU
23	W	61	ILE
23	W	78	ARG
23	W	81	ARG
23	W	82	LEU
24	X	33	LEU
24	X	40	ARG
24	X	42	ARG
24	X	46	GLN
24	X	52	LYS
24	X	60	ILE
24	X	72	LYS
24	X	76	VAL
24	X	80	LEU
24	X	107	ILE
24	X	108	LYS
25	Y	17	LEU
25	Y	36	LEU
25	Y	47	LEU
25	Y	48	HIS
25	Y	50	LYS
25	Y	52	THR
25	Y	62	THR
25	Y	67	LYS
25	Y	68	LEU
25	Y	78	ILE
25	Y	79	ARG
25	Y	84	LEU
25	Y	85	ARG
25	Y	87	LEU
25	Y	90	HIS
25	Y	98	LEU
25	Y	99	ARG
25	Y	101	GLN
25	Y	127	LEU

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Mol	Chain	Res	Type
25	Y	129	GLN
25	Y	143	LYS
25	Y	148	THR
25	Y	150	LYS
25	Y	160	ARG
26	Z	11	ILE
26	Z	12	TYR
26	Z	15	ARG
26	Z	16	LYS
26	Z	23	LEU
26	Z	28	GLU
26	Z	48	LYS
26	Z	63	GLU
26	Z	68	LEU
26	Z	70	ARG
26	Z	76	LYS
26	Z	78	LEU
27	1	7	ILE
27	1	11	LYS
27	1	19	ARG
27	1	50	LEU
27	1	54	ASN
27	1	55	THR
27	1	81	ASP
27	1	86	PHE
27	1	98	ILE
27	1	107	ARG
27	1	112	LEU
27	1	113	LYS
27	1	117	LYS
27	1	120	ARG
28	2	36	LEU
28	2	70	VAL
28	2	97	SER
28	2	98	GLN
29	3	10	ARG
29	3	26	CYS
29	3	30	VAL
29	3	50	GLN
29	3	62	PHE
29	3	64	LEU
29	3	74	CYS

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Mol	Chain	Res	Type
29	3	79	ILE
29	3	88	SER
29	3	93	ARG
30	4	15	LYS
30	4	17	HIS
30	4	18	LYS
30	4	19	LEU
30	4	20	LYS
30	4	34	LYS
30	4	41	ILE
30	4	60	MET
30	4	61	LEU
30	4	71	LEU
30	4	81	ILE
30	4	82	GLU
31	5	23	ILE
31	5	24	GLN
31	5	48	VAL
32	6	14	VAL
32	6	33	ARG
32	6	36	LYS
32	6	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	HIS
2	B	132	ASN
2	B	209	ASN
3	C	23	HIS
3	C	113	GLN
3	C	140	ASN
3	C	164	ASN
4	D	13	ASN
4	D	102	GLN
4	D	126	HIS
4	D	170	ASN
5	E	26	GLN
6	F	13	ASN
6	F	36	HIS
6	F	116	ASN
7	G	65	HIS

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Mol	Chain	Res	Type
7	G	73	GLN
7	G	82	ASN
7	G	122	HIS
7	G	189	GLN
8	H	11	ASN
8	H	13	GLN
8	H	70	ASN
8	H	119	ASN
9	I	42	HIS
9	I	48	GLN
9	I	194	ASN
10	J	107	ASN
11	K	24	GLN
11	K	64	ASN
12	L	167	ASN
13	M	75	GLN
15	O	80	ASN
16	P	94	HIS
17	Q	94	ASN
18	R	88	ASN
19	S	49	GLN
19	S	97	ASN
19	S	127	HIS
19	S	137	HIS
21	U	57	ASN
21	U	62	GLN
21	U	105	ASN
21	U	123	HIS
23	W	31	ASN
25	Y	128	GLN
25	Y	138	GLN
25	Y	157	ASN
26	Z	33	GLN
27	1	54	ASN
29	3	14	ASN
29	3	17	HIS
29	3	40	ASN
30	4	7	ASN
32	6	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1587/2092 (75%)	479 (30%)	71 (4%)
33	7	73/74 (98%)	30 (41%)	3 (4%)
All	All	1660/2166 (76%)	509 (30%)	74 (4%)

All (509) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	C
1	A	5	U
1	A	17	C
1	A	25	C
1	A	26	A
1	A	27	U
1	A	34	G
1	A	35	U
1	A	39	A
1	A	40	A
1	A	42	G
1	A	44	U
1	A	45	U
1	A	47	A
1	A	50	C
1	A	57	G
1	A	59	G
1	A	60	A
1	A	61	A
1	A	67	A
1	A	71	A
1	A	81	U
1	A	82	G
1	A	103	U
1	A	106	A
1	A	116	A
1	A	117	G
1	A	125	G
1	A	127	C
1	A	128	A
1	A	129	U
1	A	130	U
1	A	138	U
1	A	139	A
1	A	142	G

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Mol	Chain	Res	Type
1	A	143	A
1	A	144	U
1	A	151	G
1	A	157	G
1	A	159	U
1	A	165	U
1	A	166	A
1	A	169	A
1	A	174	C
1	A	182	U
1	A	183	C
1	A	186	U
1	A	206	A
1	A	207	G
1	A	208	U
1	A	209	A
1	A	217	G
1	A	247	G
1	A	249	A
1	A	250	A
1	A	251	U
1	A	252	U
1	A	255	A
1	A	258	A
1	A	260	A
1	A	262	A
1	A	264	G
1	A	266	A
1	A	267	A
1	A	268	C
1	A	272	U
1	A	274	A
1	A	292	G
1	A	305	G
1	A	316	C
1	A	320	C
1	A	322	G
1	A	323	C
1	A	326	U
1	A	327	U
1	A	335	G
1	A	339	A

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Mol	Chain	Res	Type
1	A	343	G
1	A	344	C
1	A	345	C
1	A	350	A
1	A	357	U
1	A	358	G
1	A	359	A
1	A	360	C
1	A	361	G
1	A	365	A
1	A	366	A
1	A	367	C
1	A	375	U
1	A	376	A
1	A	379	G
1	A	396	G
1	A	399	C
1	A	405	A
1	A	406	A
1	A	407	A
1	A	408	U
1	A	409	A
1	A	410	G
1	A	422	A
1	A	423	A
1	A	424	G
1	A	425	G
1	A	428	G
1	A	430	C
1	A	431	A
1	A	432	G
1	A	434	A
1	A	440	G
1	A	443	A
1	A	445	U
1	A	446	U
1	A	450	C
1	A	451	A
1	A	454	U
1	A	458	A
1	A	459	A
1	A	460	G

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Mol	Chain	Res	Type
1	A	461	A
1	A	465	G
1	A	466	A
1	A	467	G
1	A	470	A
1	A	481	A
1	A	483	A
1	A	488	U
1	A	494	G
1	A	513	A
1	A	515	U
1	A	516	G
1	A	521	G
1	A	526	G
1	A	527	A
1	A	534	A
1	A	543	A
1	A	545	A
1	A	546	G
1	A	547	U
1	A	548	A
1	A	549	A
1	A	562	A
1	A	564	G
1	A	565	U
1	A	566	C
1	A	568	G
1	A	572	C
1	A	574	A
1	A	575	G
1	A	579	C
1	A	584	G
1	A	585	U
1	A	586	A
1	A	587	A
1	A	589	U
1	A	592	A
1	A	601	A
1	A	602	G
1	A	603	C
1	A	612	A
1	A	613	A

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Mol	Chain	Res	Type
1	A	616	U
1	A	617	G
1	A	618	U
1	A	626	A
1	A	627	A
1	A	629	A
1	A	630	C
1	A	631	G
1	A	641	G
1	A	642	A
1	A	645	U
1	A	646	U
1	A	648	A
1	A	651	G
1	A	753	U
1	A	756	A
1	A	757	A
1	A	758	U
1	A	760	C
1	A	792	U
1	A	793	G
1	A	794	U
1	A	801	G
1	A	804	U
1	A	805	A
1	A	806	A
1	A	815	G
1	A	816	U
1	A	821	A
1	A	824	A
1	A	828	A
1	A	829	G
1	A	830	U
1	A	832	A
1	A	833	A
1	A	837	A
1	A	845	U
1	A	846	G
1	A	849	U
1	A	851	A
1	A	852	A
1	A	856	U

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Mol	Chain	Res	Type
1	A	857	A
1	A	858	U
1	A	859	A
1	A	866	A
1	A	869	A
1	A	870	A
1	A	873	A
1	A	874	A
1	A	875	A
1	A	876	U
1	A	877	U
1	A	878	G
1	A	880	A
1	A	881	C
1	A	882	A
1	A	886	U
1	A	887	A
1	A	888	A
1	A	889	A
1	A	915	G
1	A	917	C
1	A	920	A
1	A	921	G
1	A	923	U
1	A	924	A
1	A	925	C
1	A	927	A
1	A	928	U
1	A	929	U
1	A	930	A
1	A	931	A
1	A	941	C
1	A	942	U
1	A	945	G
1	A	955	U
1	A	967	A
1	A	972	U
1	A	978	U
1	A	981	U
1	A	982	A
1	A	983	G
1	A	984	A

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Mol	Chain	Res	Type
1	A	990	U
1	A	998	A
1	A	1002	A
1	A	1003	C
1	A	1004	U
1	A	1011	G
1	A	1013	A
1	A	1021	A
1	A	1029	U
1	A	1035	A
1	A	1036	A
1	A	1051	U
1	A	1054	G
1	A	1057	A
1	A	1061	A
1	A	1062	A
1	A	1065	C
1	A	1073	U
1	A	1074	A
1	A	1076	C
1	A	1079	C
1	A	1081	U
1	A	1090	C
1	A	1092	A
1	A	1093	U
1	A	1095	A
1	A	1097	C
1	A	1101	G
1	A	1108	A
1	A	1109	G
1	A	1112	G
1	A	1116	G
1	A	1119	G
1	A	1168	U
1	A	1175	G
1	A	1177	A
1	A	1183	U
1	A	1187	A
1	A	1192	A
1	A	1193	A
1	A	1194	A
1	A	1195	G

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Mol	Chain	Res	Type
1	A	1197	C
1	A	1198	U
1	A	1199	U
1	A	1200	U
1	A	1209	G
1	A	1210	G
1	A	1227	G
1	A	1230	A
1	A	1239	A
1	A	1244	A
1	A	1247	G
1	A	1251	G
1	A	1254	G
1	A	1255	G
1	A	1259	C
1	A	1260	C
1	A	1261	A
1	A	1265	G
1	A	1268	G
1	A	1286	U
1	A	1291	C
1	A	1293	C
1	A	1294	A
1	A	1295	A
1	A	1297	A
1	A	1300	G
1	A	1301	G
1	A	1302	G
1	A	1303	A
1	A	1304	A
1	A	1305	A
1	A	1308	C
1	A	1318	A
1	A	1319	G
1	A	1322	A
1	A	1366	A
1	A	1367	U
1	A	1374	G
1	A	1375	C
1	A	1381	C
1	A	1382	G
1	A	1383	U

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Mol	Chain	Res	Type
1	A	1384	U
1	A	1385	U
1	A	1386	U
1	A	1387	U
1	A	1388	A
1	A	1409	U
1	A	1415	A
1	A	1416	U
1	A	1422	U
1	A	1423	A
1	A	1431	A
1	A	1437	U
1	A	1441	C
1	A	1442	U
1	A	1443	G
1	A	1444	C
1	A	1445	U
1	A	1448	U
1	A	1450	A
1	A	1451	G
1	A	1453	G
1	A	1454	G
1	A	1456	G
1	A	1459	U
1	A	1607	U
1	A	1623	U
1	A	1625	C
1	A	1626	U
1	A	1635	C
1	A	1636	A
1	A	1644	U
1	A	1645	C
1	A	1646	U
1	A	1648	A
1	A	1649	C
1	A	1659	U
1	A	1660	U
1	A	1661	U
1	A	1664	G
1	A	1668	A
1	A	1673	A
1	A	1674	G

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Mol	Chain	Res	Type
1	A	1677	C
1	A	1678	U
1	A	1679	G
1	A	1692	A
1	A	1693	U
1	A	1702	C
1	A	1705	C
1	A	1706	A
1	A	1715	A
1	A	1717	A
1	A	1718	C
1	A	1719	U
1	A	1720	G
1	A	1721	A
1	A	1723	A
1	A	1727	A
1	A	1728	U
1	A	1732	G
1	A	1735	U
1	A	1749	C
1	A	1787	U
1	A	1790	C
1	A	1792	U
1	A	1795	G
1	A	1796	C
1	A	1802	G
1	A	1806	U
1	A	1811	A
1	A	1812	A
1	A	1813	U
1	A	1814	C
1	A	1817	U
1	A	1818	A
1	A	1819	U
1	A	1820	C
1	A	1824	A
1	A	1830	C
1	A	1832	U
1	A	1833	G
1	A	1834	A
1	A	1835	U
1	A	1836	G

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Mol	Chain	Res	Type
1	A	1837	G
1	A	1845	U
1	A	1854	U
1	A	1855	U
1	A	1856	A
1	A	1861	U
1	A	1866	A
1	A	1868	C
1	A	1870	A
1	A	1871	G
1	A	1873	A
1	A	1881	G
1	A	1882	U
1	A	1887	A
1	A	1892	U
1	A	1898	G
1	A	1899	A
1	A	1902	G
1	A	1904	G
1	A	1907	G
1	A	1908	A
1	A	1911	A
1	A	1913	G
1	A	1916	C
1	A	1927	U
1	A	1928	A
1	A	1929	C
1	A	1937	C
1	A	1954	U
1	A	1955	G
1	A	1961	U
1	A	1962	A
1	A	1976	G
1	A	1977	G
1	A	1978	A
1	A	1979	C
1	A	1980	A
1	A	1981	A
1	A	1982	G
1	A	1987	A
1	A	2008	U
1	A	2012	G

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Mol	Chain	Res	Type
1	A	2019	C
1	A	2020	G
1	A	2021	U
1	A	2028	U
1	A	2029	A
1	A	2034	U
1	A	2042	A
1	A	2045	A
1	A	2048	A
1	A	2049	G
1	A	2052	G
1	A	2054	A
1	A	2058	A
1	A	2060	G
1	A	2061	U
1	A	2065	C
1	A	2072	G
1	A	2074	A
1	A	2075	C
1	A	2084	G
1	A	2085	G
1	A	2086	A
1	A	2088	C
33	7	2	G
33	7	8	U
33	7	9	G
33	7	10	G
33	7	12	G
33	7	16	U
33	7	17	U
33	7	18	G
33	7	20	U
33	7	21	U
33	7	22	A
33	7	29	G
33	7	31	G
33	7	32	U
33	7	33	C
33	7	34	U
33	7	44	G
33	7	45	A
33	7	46	G

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Mol	Chain	Res	Type
33	7	49	C
33	7	50	G
33	7	51	U
33	7	53	A
33	7	55	U
33	7	56	U
33	7	57	C
33	7	58	G
33	7	69	U
33	7	72	C
33	7	74	A

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	25	C
1	A	39	A
1	A	44	U
1	A	60	A
1	A	105	A
1	A	116	A
1	A	127	C
1	A	138	U
1	A	142	G
1	A	156	A
1	A	206	A
1	A	246	A
1	A	250	A
1	A	251	U
1	A	267	A
1	A	291	A
1	A	358	G
1	A	406	A
1	A	423	A
1	A	427	A
1	A	431	A
1	A	544	G
1	A	546	G
1	A	614	A
1	A	752	U
1	A	793	G
1	A	805	A

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Mol	Chain	Res	Type
1	A	815	G
1	A	844	G
1	A	850	G
1	A	858	U
1	A	877	U
1	A	919	U
1	A	923	U
1	A	930	A
1	A	981	U
1	A	983	G
1	A	1028	U
1	A	1100	U
1	A	1182	A
1	A	1183	U
1	A	1209	G
1	A	1259	C
1	A	1318	A
1	A	1381	C
1	A	1386	U
1	A	1423	A
1	A	1447	A
1	A	1448	U
1	A	1455	C
1	A	1645	C
1	A	1660	U
1	A	1672	C
1	A	1673	A
1	A	1692	A
1	A	1703	U
1	A	1786	U
1	A	1813	U
1	A	1818	A
1	A	1819	U
1	A	1834	A
1	A	1855	U
1	A	1865	G
1	A	1869	G
1	A	1870	A
1	A	1897	A
1	A	1898	G
1	A	1912	C
1	A	1976	G

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Mol	Chain	Res	Type
1	A	1977	G
1	A	2053	U
33	7	9	G
33	7	17	U
33	7	20	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 68 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
35	34G	A	2168	-	39,39,39	2.75	8 (20%)	51,56,56	1.89	10 (19%)

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
35	34G	A	2168	-	-	10/14/49/49	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	2168	34G	CBC-CBG	-9.18	1.43	1.52
35	A	2168	34G	CAM-CAX	-7.80	1.38	1.51
35	A	2168	34G	CAL-CAW	-5.72	1.41	1.51
35	A	2168	34G	CBD-CBH	-5.64	1.43	1.52
35	A	2168	34G	CAP-CBH	-5.07	1.48	1.53
35	A	2168	34G	CAO-CBG	4.69	1.58	1.53
35	A	2168	34G	CAK-CAL	3.27	1.58	1.50
35	A	2168	34G	CAQ-NBI	2.71	1.51	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	2168	34G	CAW-CBC-CBG	-6.34	113.78	121.38
35	A	2168	34G	CAQ-NBI-CBH	5.03	117.45	110.12
35	A	2168	34G	CBF-CAP-CBH	-4.76	102.90	111.76
35	A	2168	34G	CAP-CBF-CBE	-3.90	104.18	110.57
35	A	2168	34G	CAH-CBC-CBG	2.84	126.62	120.67
35	A	2168	34G	CAE-OAV-CBB	-2.56	113.76	117.51
35	A	2168	34G	CAL-CAK-NAR	2.35	112.21	109.02
35	A	2168	34G	OAS-CAY-CBA	2.24	118.45	115.40
35	A	2168	34G	CBF-CAO-CBG	-2.12	106.68	113.47
35	A	2168	34G	CAC-OAT-CAZ	-2.00	114.57	117.51

There are no chirality outliers.

All (10) torsion outliers are listed below:

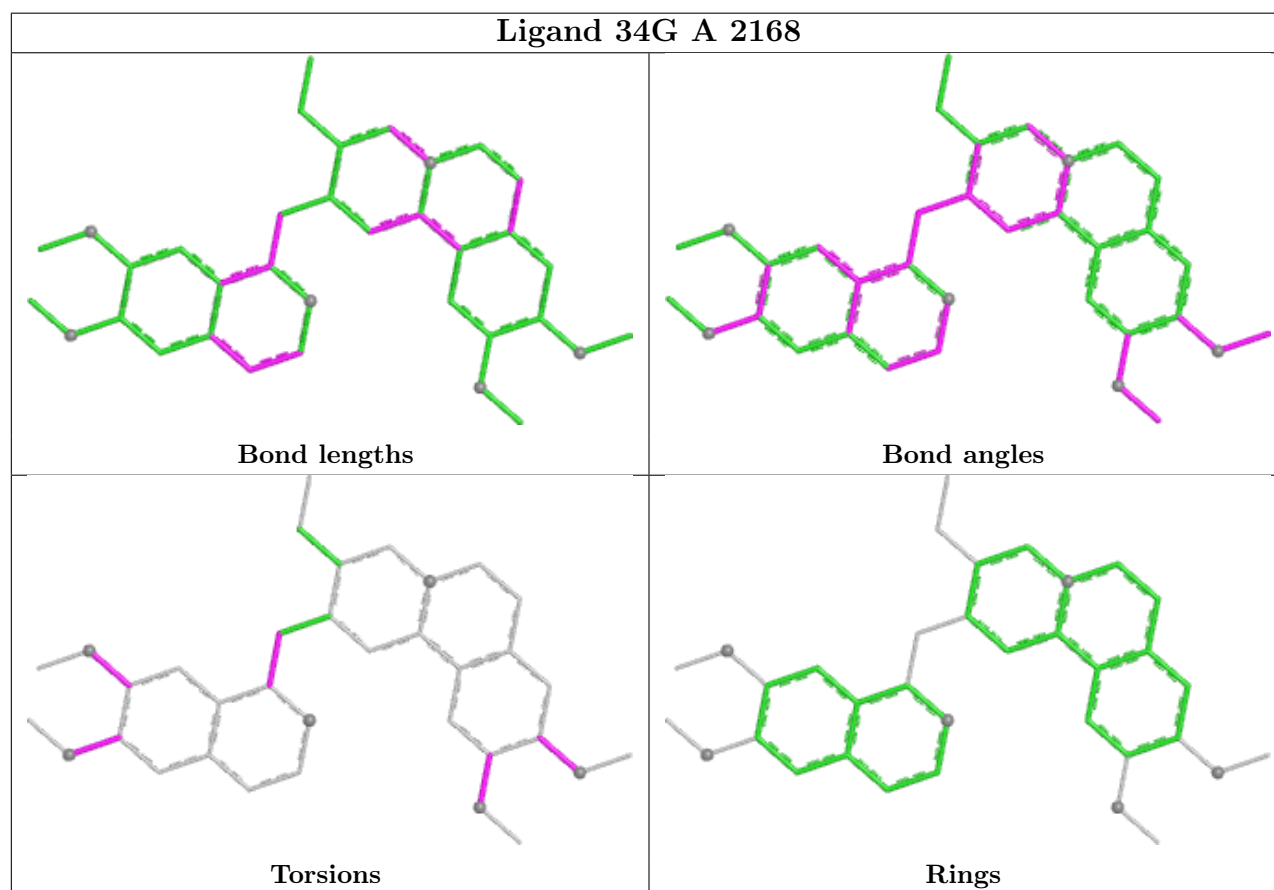
Mol	Chain	Res	Type	Atoms
35	A	2168	34G	CBF-CAO-CBG-NAR
35	A	2168	34G	CBF-CAO-CBG-CBC
35	A	2168	34G	CAZ-CBB-OAV-CAE
35	A	2168	34G	CBA-CAY-OAS-CAB
35	A	2168	34G	CAI-CBB-OAV-CAE
35	A	2168	34G	CAF-CAY-OAS-CAB
35	A	2168	34G	CAG-CAZ-OAT-CAC
35	A	2168	34G	CAY-CBA-OAU-CAD
35	A	2168	34G	CBB-CAZ-OAT-CAC
35	A	2168	34G	CAH-CBA-OAU-CAD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	2168	34G	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

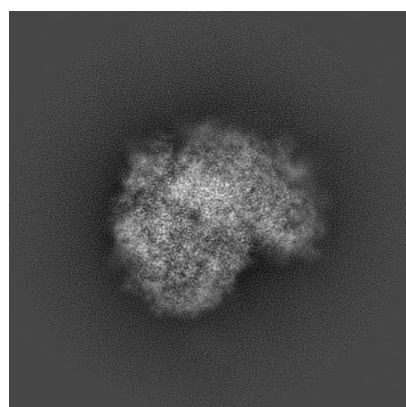
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2660. These allow visual inspection of the internal detail of the map and identification of artifacts.

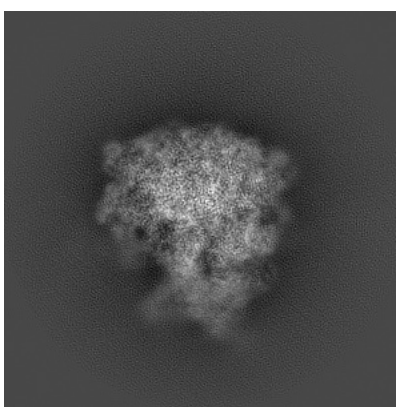
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

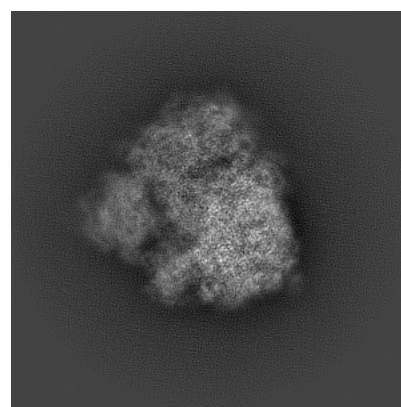
6.1.1 Primary map



X



Y

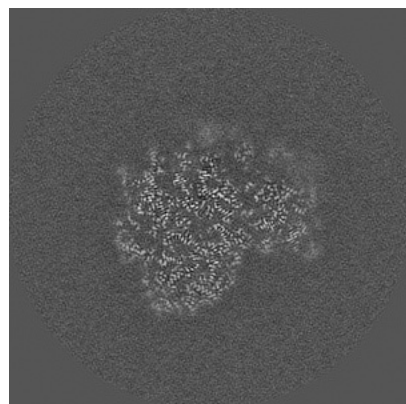


Z

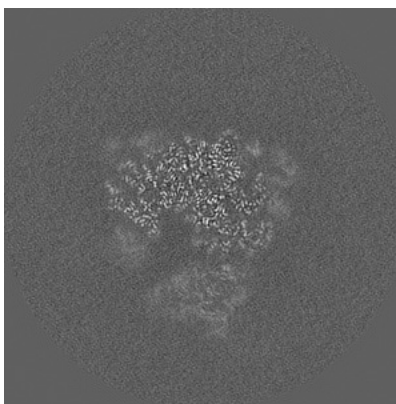
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

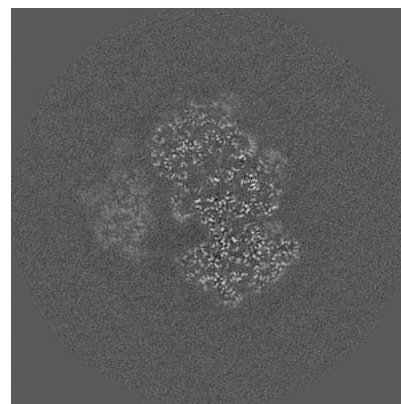
6.2.1 Primary map



X Index: 180



Y Index: 180

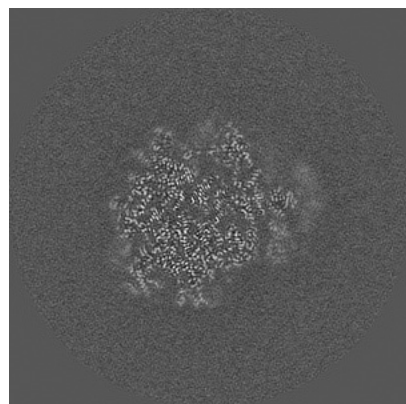


Z Index: 180

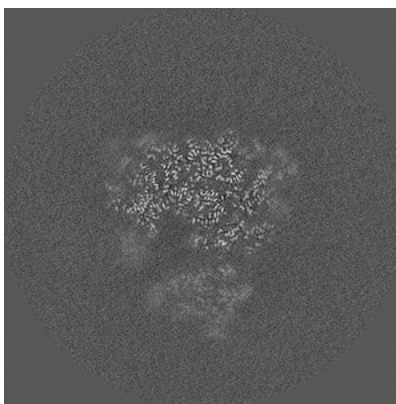
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

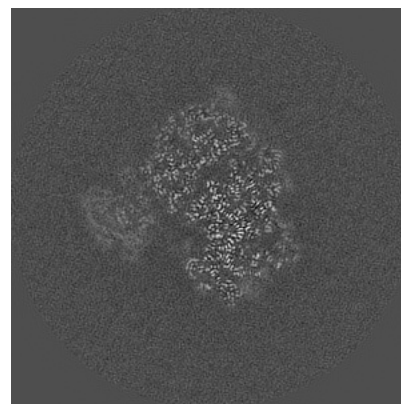
6.3.1 Primary map



X Index: 201



Y Index: 183

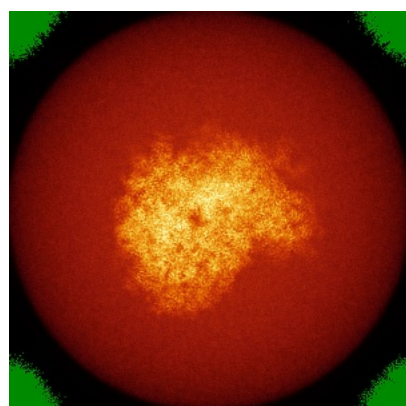


Z Index: 187

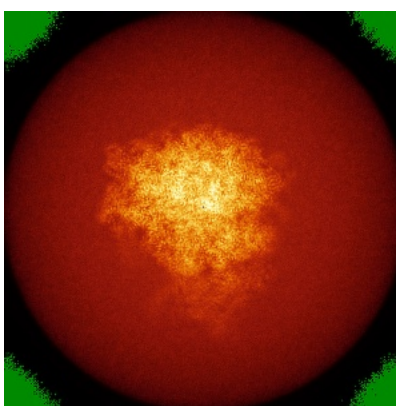
The images above show the largest variance slices of the map in three orthogonal directions.

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

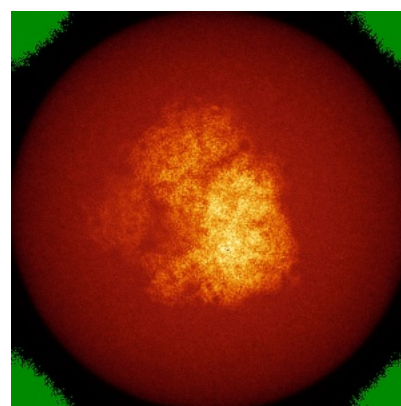
6.4.1 Primary map



X



Y

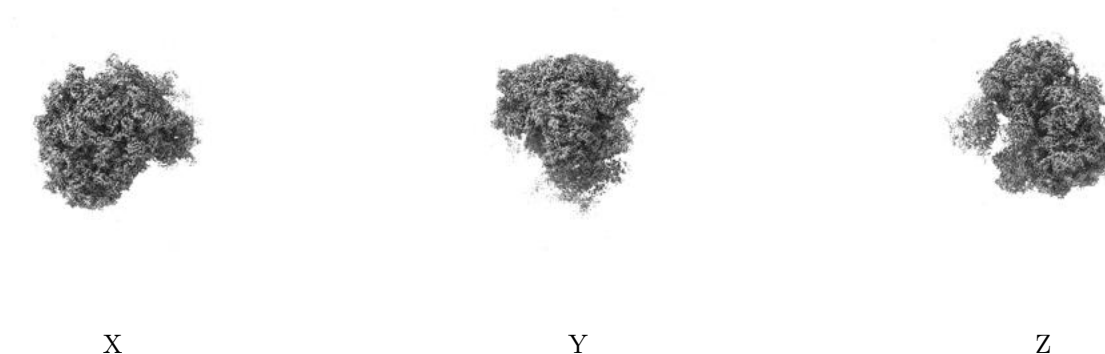


Z

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

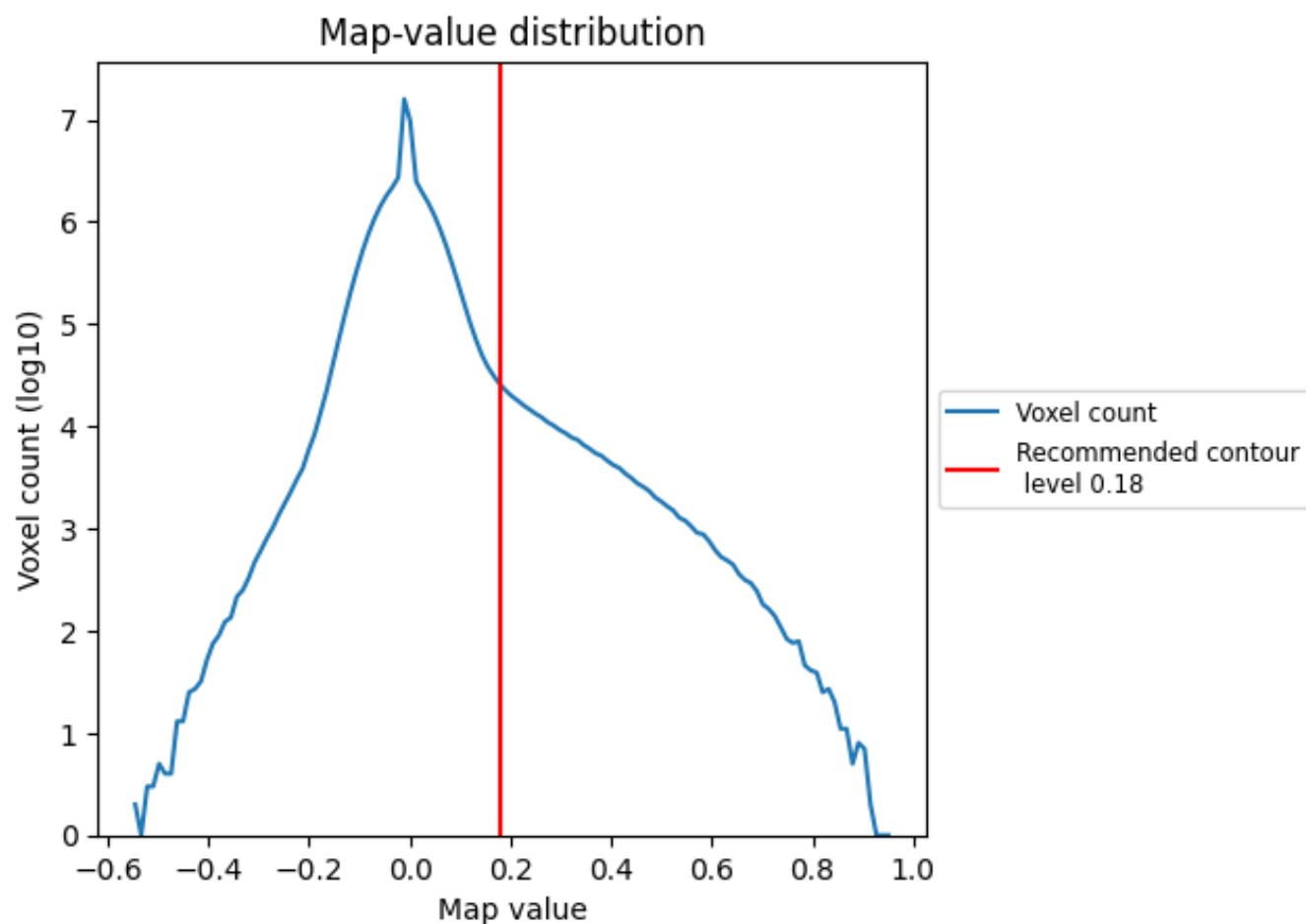
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

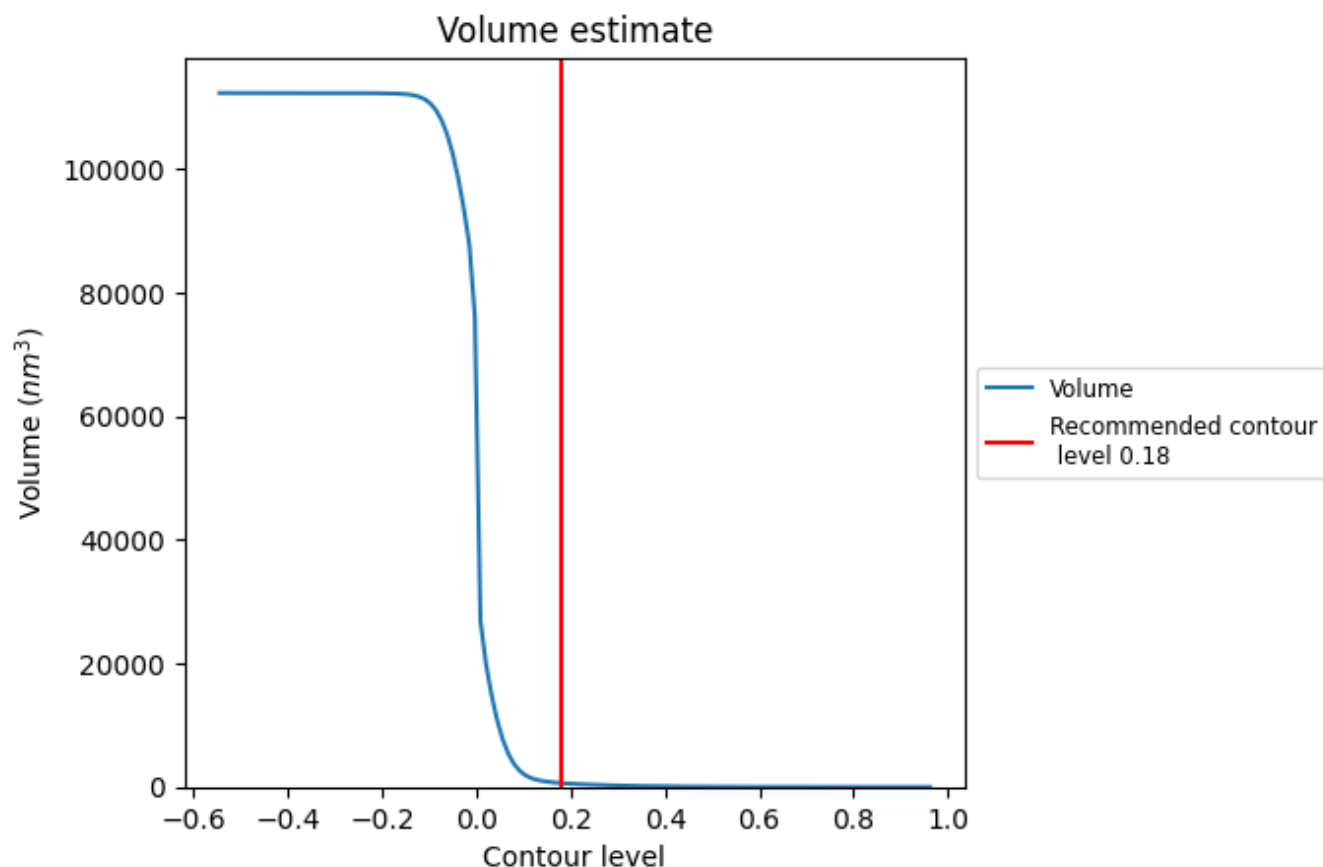
This section contains the results of statistical analysis of the map.

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.

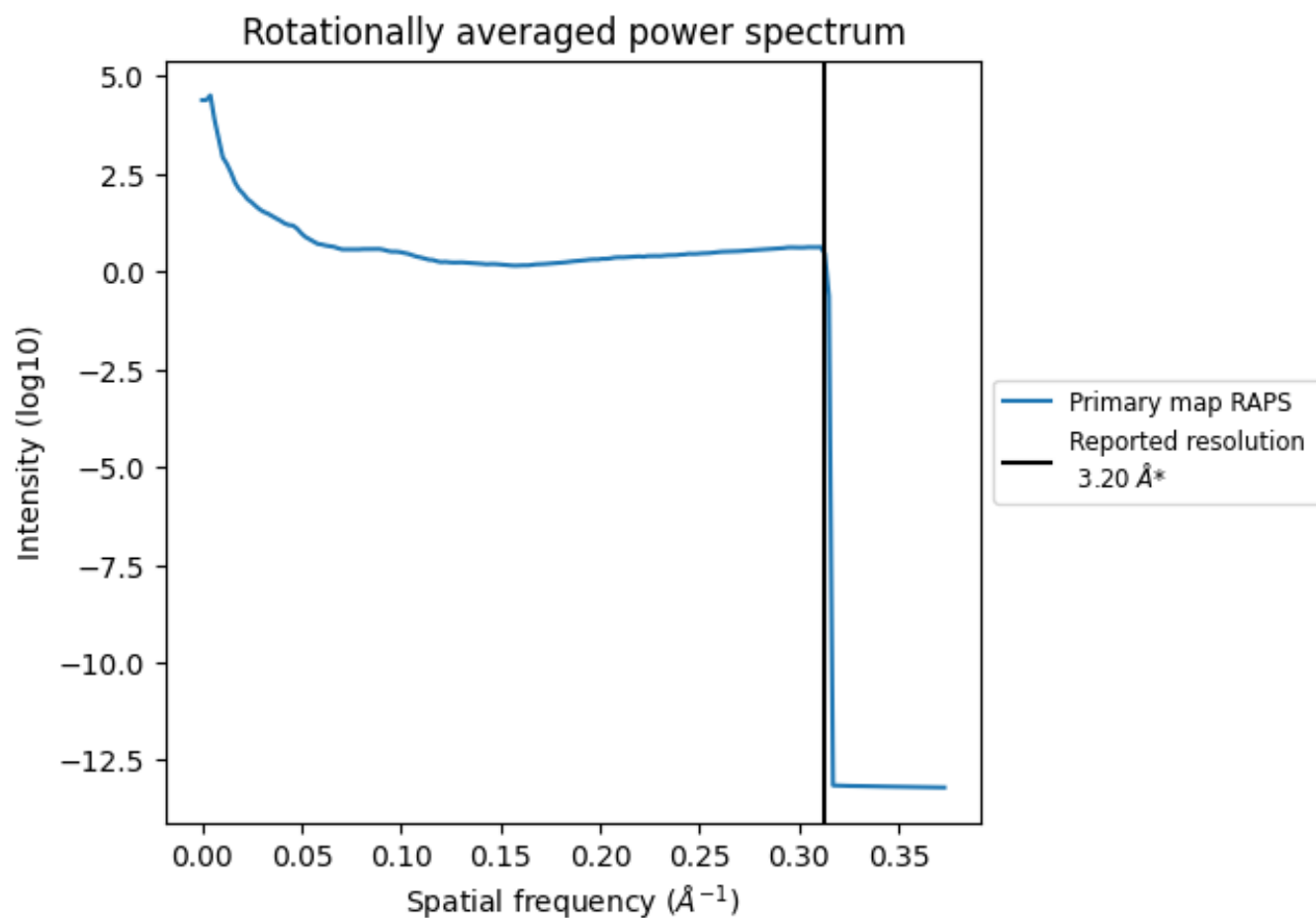
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 628 nm^3 ; this corresponds to an approximate mass of 567 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 0.312 Å⁻¹

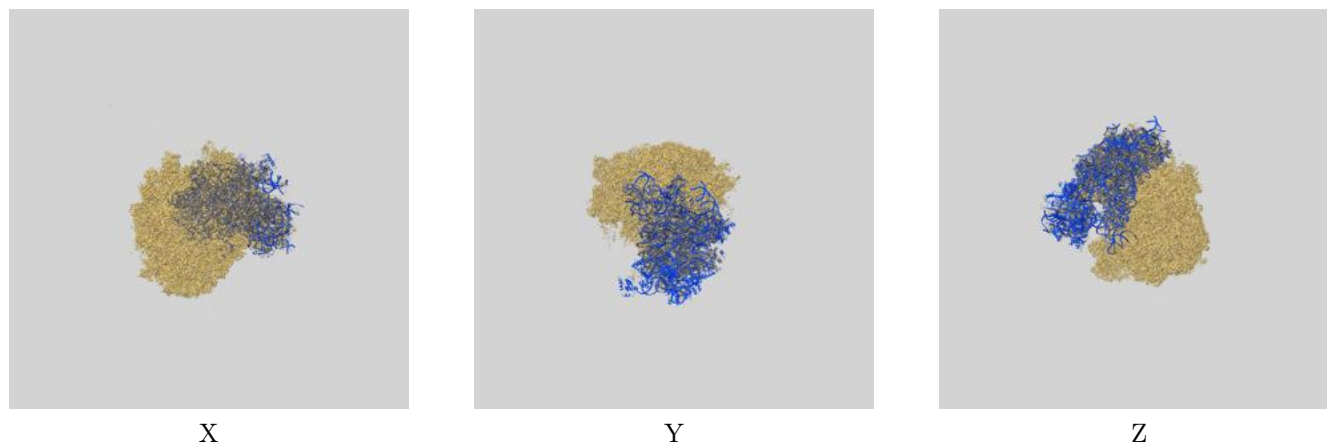
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

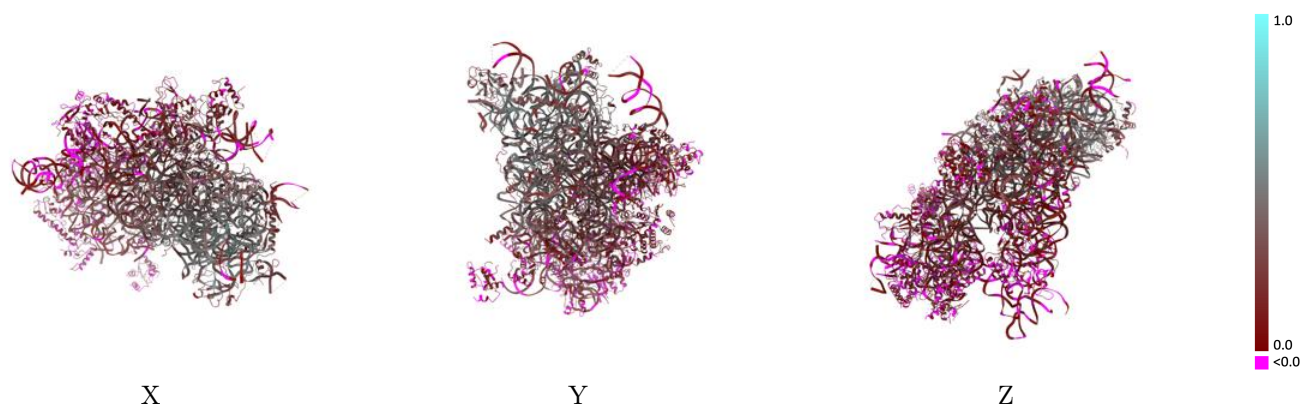
This section contains information regarding the fit between EMDB map EMD-2660 and PDB model 3J7A. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



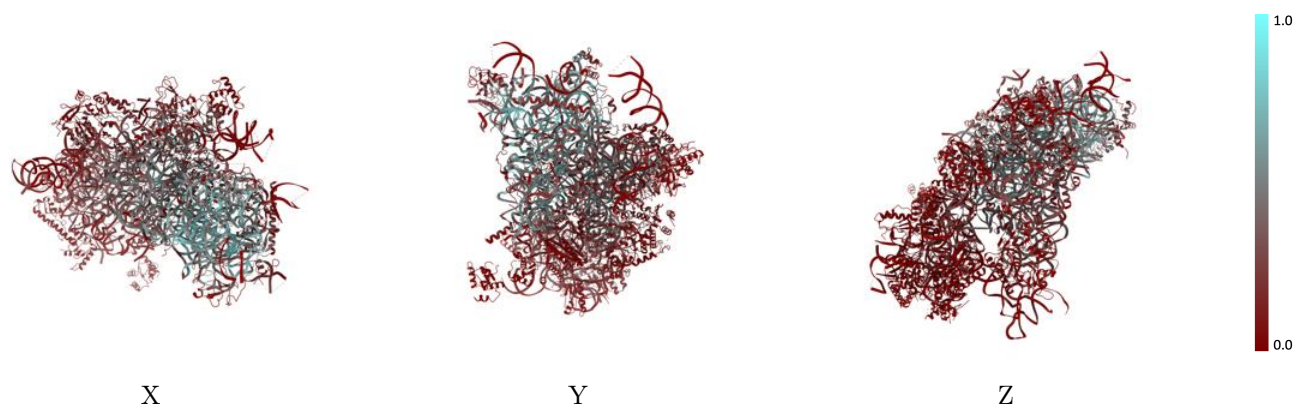
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



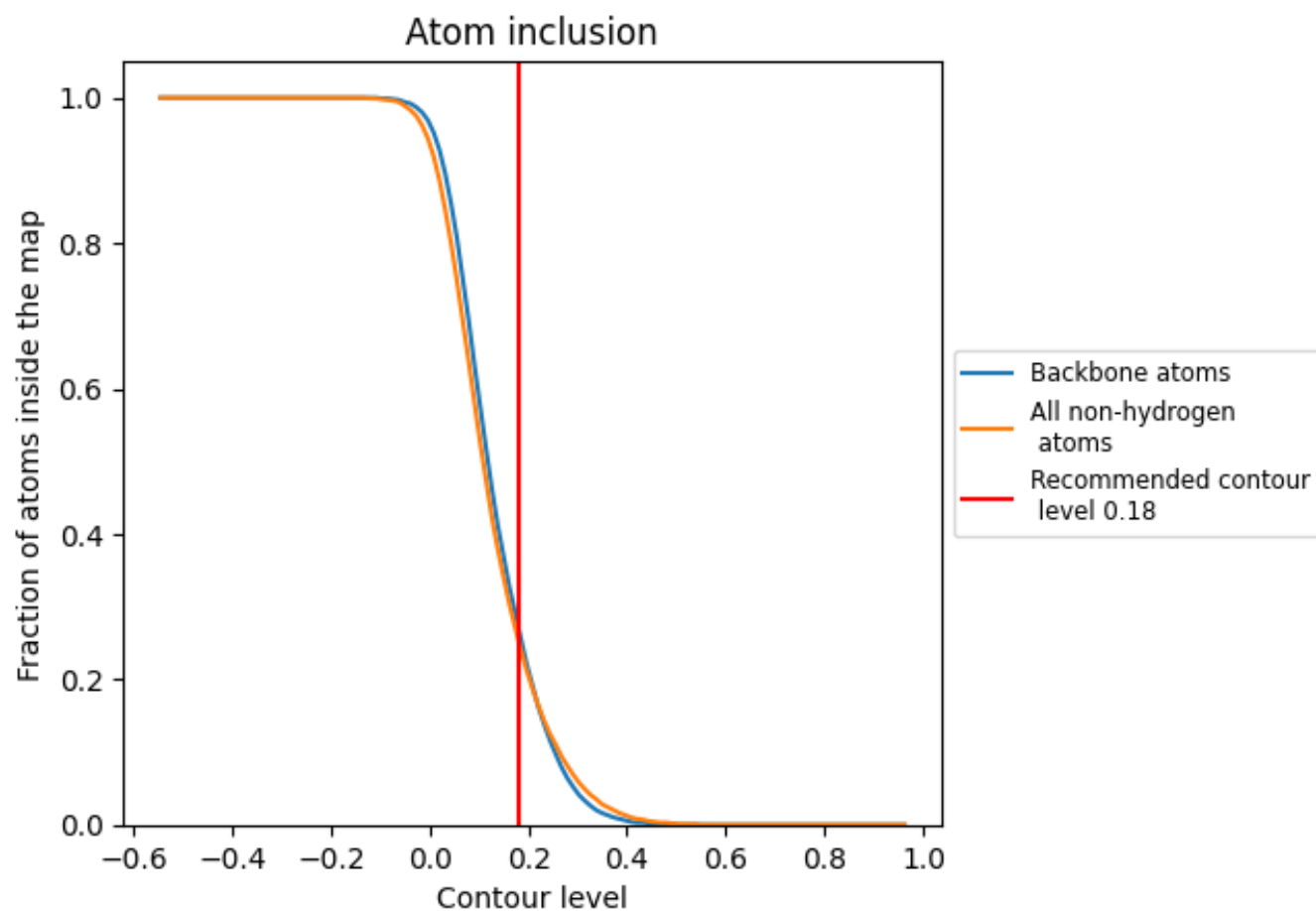
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 27% of all backbone atoms, 25% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2530	 0.2310
1	 0.3220	 0.3510
2	 0.0090	 0.0410
3	 0.1660	 0.1200
4	 0.1120	 0.1360
5	 0.0050	 0.0840
6	 0.2530	 0.3130
7	 0.0640	 0.0450
A	 0.3410	 0.2730
B	 0.1220	 0.0800
C	 0.1160	 0.1470
D	 0.0210	 0.1460
E	 0.3260	 0.3110
F	 0.3490	 0.3730
G	 0.2440	 0.2420
H	 0.2490	 0.3400
I	 0.0110	 0.0680
J	 0.0960	 0.1600
K	 0.2870	 0.2510
L	 0.4140	 0.3770
M	 0.0090	 0.0430
N	 0.0150	 0.1240
O	 0.0060	 0.1150
P	 0.1210	 0.0660
Q	 0.3490	 0.3620
R	 0.0000	 0.0290
S	 0.0120	 0.0870
T	 0.0280	 0.1650
U	 0.2120	 0.1940
V	 0.3940	 0.3640
W	 0.0170	 0.1050
X	 0.0050	 0.0480
Y	 0.0220	 0.0770
Z	 0.1490	 0.1730

