Full wwPDB EM Validation Report

Apr 4, 2023 – 07:48 pm BST

PDB ID	:	8C01
EMDB ID	:	EMD-16349
Title	:	Enp1TAP_A population of yeast small ribosomal subunit precursors
Authors	:	Milkereit, P.; Poell, G.
Deposited on	:	2022-12-15
Resolution	:	2.70 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:

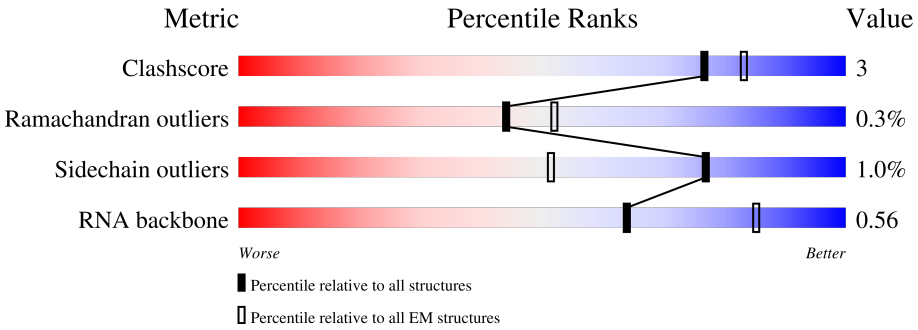
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2	1804	62% 19% 5% 14%
2	B	225	84% 6% 11%
3	C	136	44% 55%
4	E	142	5% 79% 20%
5	F	143	83% 5% 13%
6	H	146	75% 9% 16%
7	I	144	92% 6%

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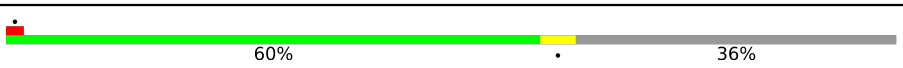
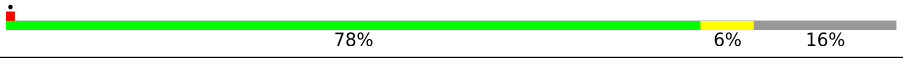
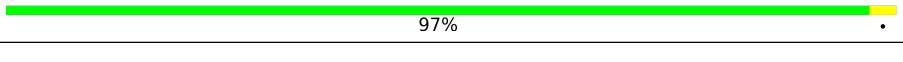
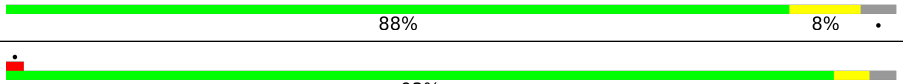
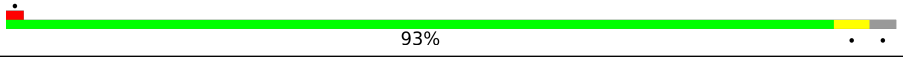
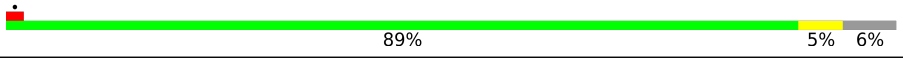
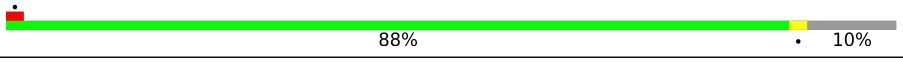
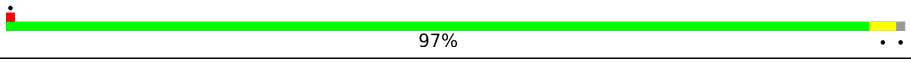
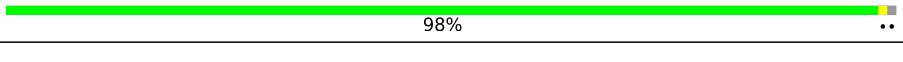
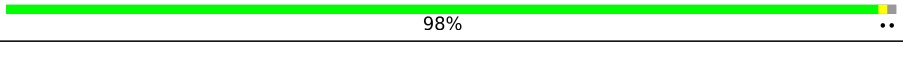
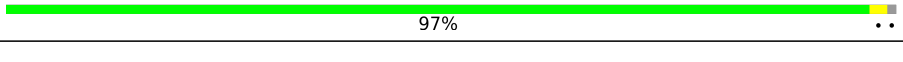
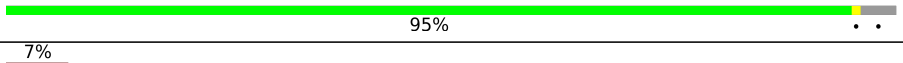
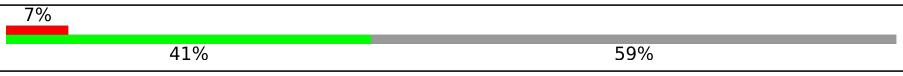
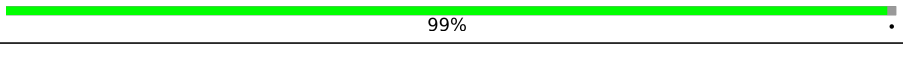
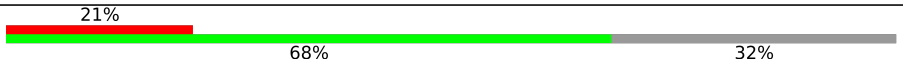
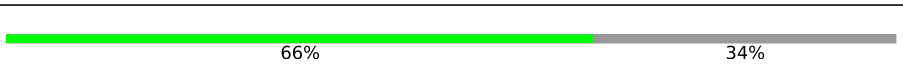
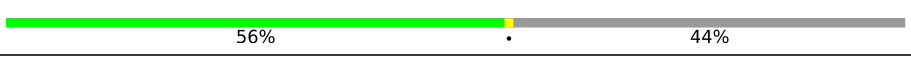
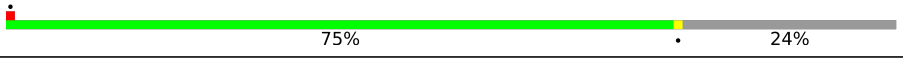
Mol	Chain	Length	Quality of chain
8	K	108	
9	L	67	
10	P	252	
11	Q	255	
12	R	254	
13	S	261	
14	T	236	
15	U	190	
16	V	200	
17	W	197	
18	X	156	
19	Y	151	
20	Z	137	
21	a	87	
22	b	130	
23	c	145	
24	d	135	
25	e	483	
26	f	82	
27	g	63	
28	o	459	
29	p	274	
30	r	425	
31	t	788	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 72685 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 rRNA precursor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1545	32971	14740	5880	10806	1545	0	0

- Molecule 2 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	201	1588	996	295	294	3	0	0

- Molecule 3 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	61	476	296	84	96	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	114	902	575	167	153	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	125	973	625	174	174	0	0

- Molecule 6 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	122	1009	636	193	178	2	0	0

- Molecule 7 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	141	Total	C	N	O	S	0	0
			1096	684	206	204	2		

- Molecule 8 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	69	Total	C	N	O	0	0
			556	356	103	97		

- Molecule 9 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	60	Total	C	N	O	S	0	0
			471	290	93	87	1		

- Molecule 10 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	206	Total	C	N	O	S	0	0
			1590	1023	281	284	2		

- Molecule 11 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	207	Total	C	N	O	S	0	0
			1557	1003	269	283	2		

- Molecule 13 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 14 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	226	Total	C	N	O	S	0	0
			1813	1137	350	323	3		

- Molecule 15 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 16 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	185	Total	C	N	O	S	0	0
			1462	907	292	261	2		

- Molecule 17 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 18 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	141	Total	C	N	O	S	0	0
			1137	730	216	188	3		

- Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 20 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	127	Total	C	N	O	S	0	0
			926	569	185	169	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	86	Total	C	N	O	S	0	0
			673	414	121	136	2		

- Molecule 22 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 23 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
24	d	130	Total	C	N	O	0	0
			1046	662	203	181		

- Molecule 25 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	e	200	Total	C	N	O	0	0
			883	476	204	203		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 27 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	36	Total	C	N	O	S	0	0
			300	191	63	45	1		

- Molecule 28 is a protein called 20S-pre-rRNA D-site endonuclease NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	o	314	Total	C	N	O	S	0	0
			2503	1574	458	462	9		

- Molecule 29 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	p	180	Total	C	N	O	S	0	0
			1425	911	257	253	4		

- Molecule 30 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	239	Total	C	N	O	S	0	0
			1818	1148	322	334	14		

- Molecule 31 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	t	598	Total	C	N	O	S	0	0
			4813	3092	838	870	13		

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

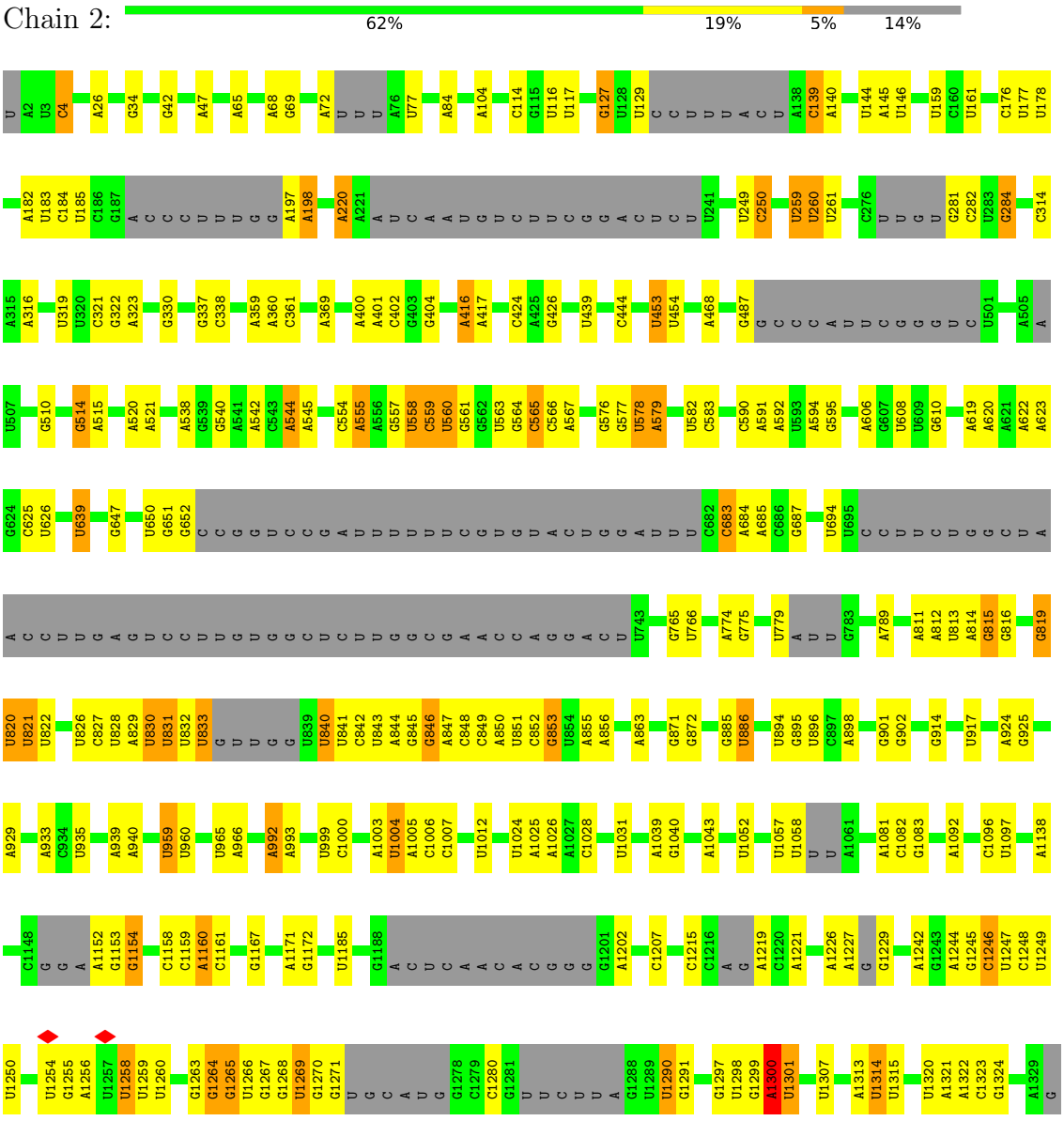
Mol	Chain	Residues	Atoms		AltConf
32	o	1	Total	Zn	0
			1	1	

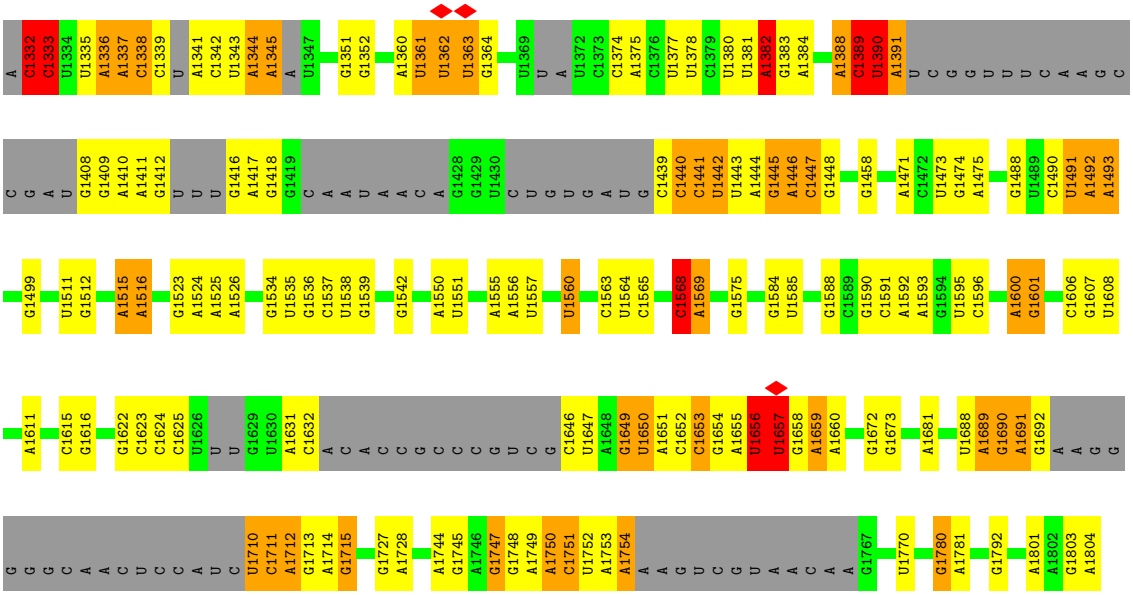
3 Residue-property plots (i)

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: 18S rRNA precursor

Chain 2:



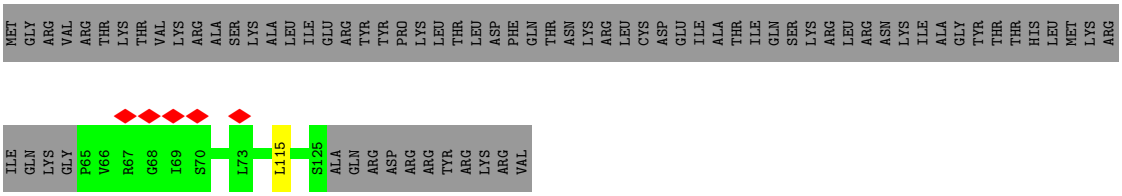


• Molecule 2: 40S ribosomal protein S5

Chain B:

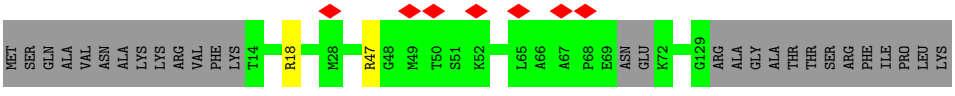
• Molecule 3: 40S ribosomal protein S17-A

Chain C:



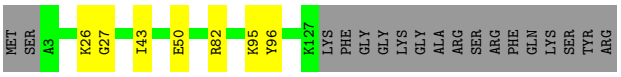
• Molecule 4: 40S ribosomal protein S15

Chain E:



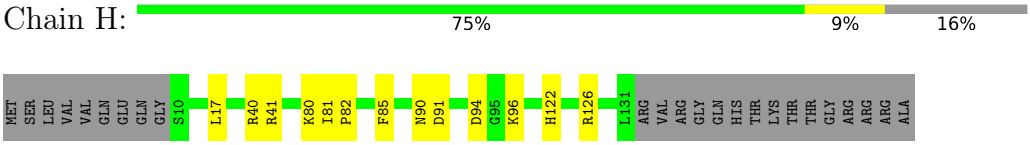
• Molecule 5: 40S ribosomal protein S16-A

Chain F:



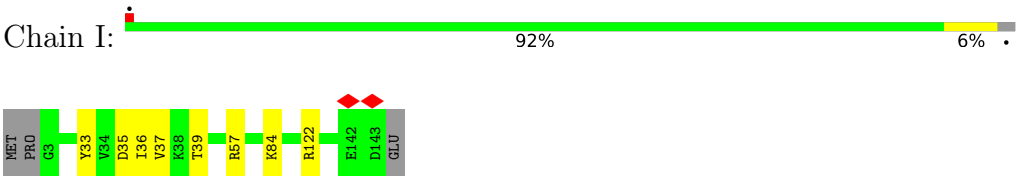
• Molecule 6: 40S ribosomal protein S18-A

Chain H:



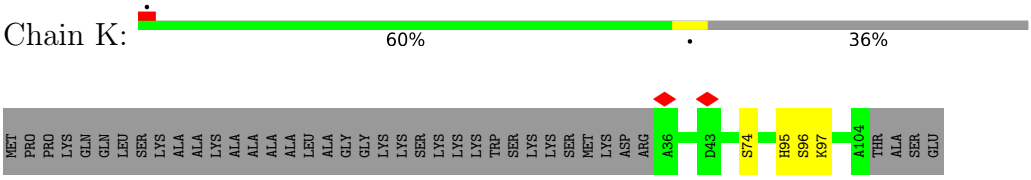
• Molecule 7: 40S ribosomal protein S19-A

Chain I:



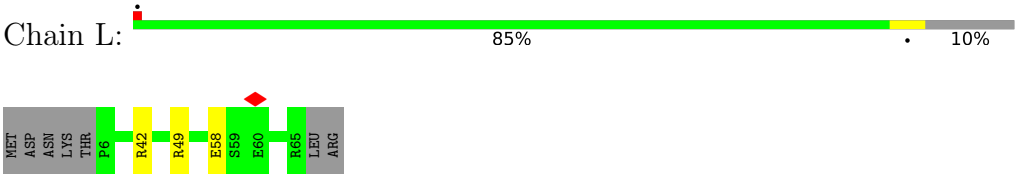
• Molecule 8: 40S ribosomal protein S25-A

Chain K:



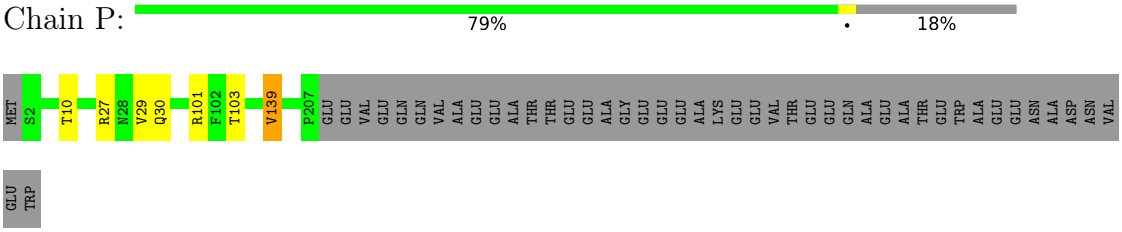
• Molecule 9: 40S ribosomal protein S28-A

Chain L:



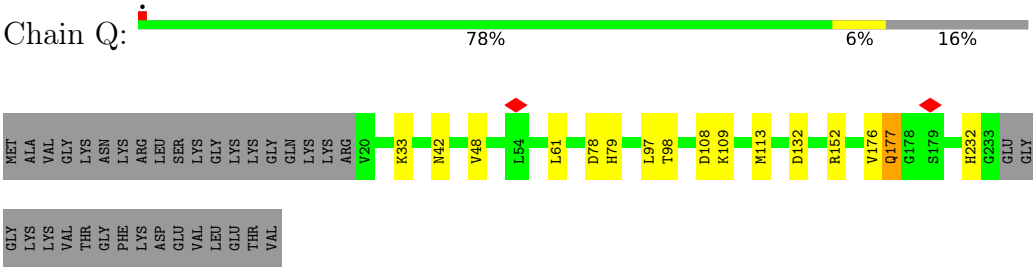
• Molecule 10: 40S ribosomal protein S0-A

Chain P:



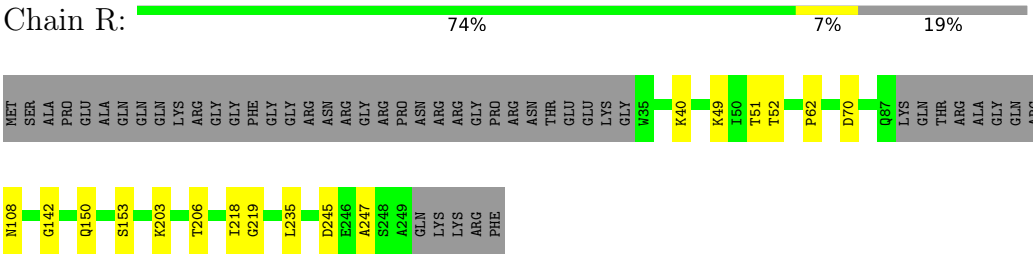
• Molecule 11: 40S ribosomal protein S1-A

Chain Q:



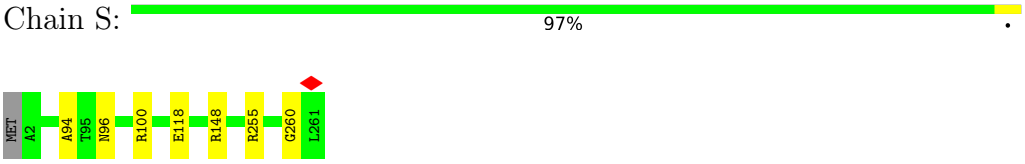
• Molecule 12: 40S ribosomal protein S2

Chain R:



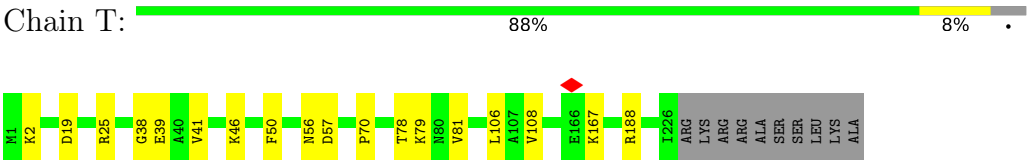
• Molecule 13: 40S ribosomal protein S4-A

Chain S:



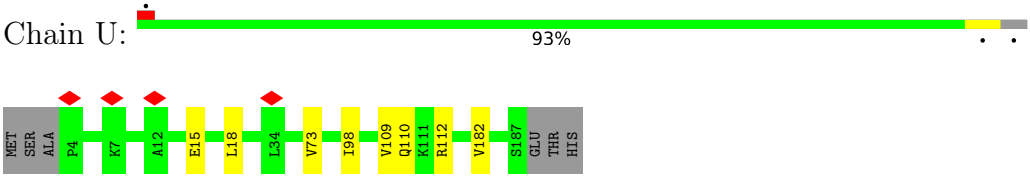
• Molecule 14: 40S ribosomal protein S6-A

Chain T:



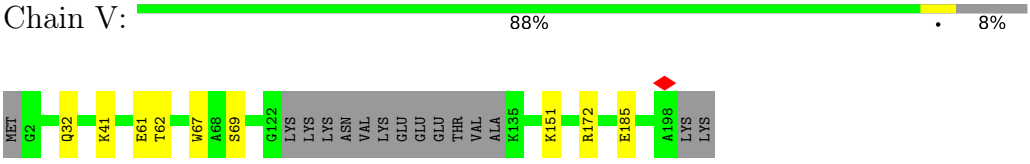
• Molecule 15: 40S ribosomal protein S7-A

Chain U:



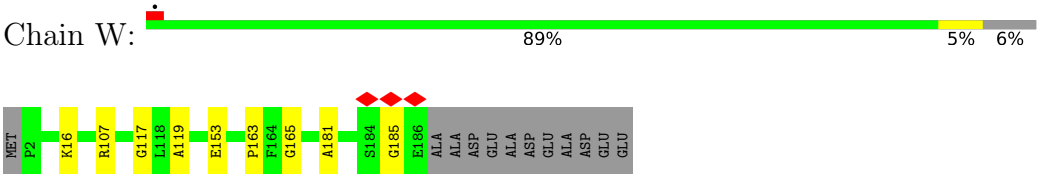
• Molecule 16: 40S ribosomal protein S8-A

Chain V:



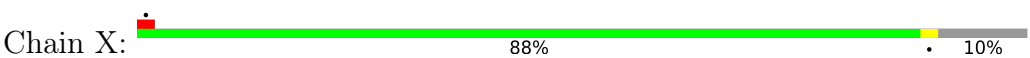
• Molecule 17: 40S ribosomal protein S9-A

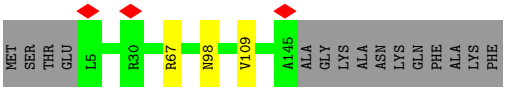
Chain W:



• Molecule 18: 40S ribosomal protein S11-A

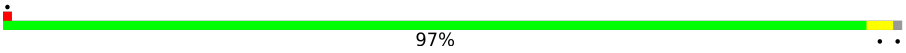
Chain X:

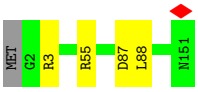




• Molecule 19: 40S ribosomal protein S13

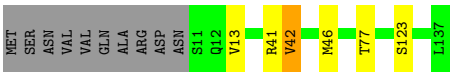
Chain Y:





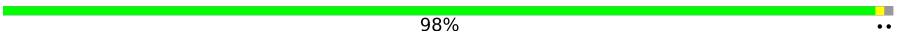
• Molecule 20: 40S ribosomal protein S14-A

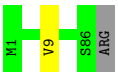
Chain Z:



• Molecule 21: 40S ribosomal protein S21-A

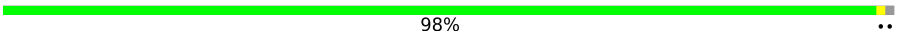
Chain a:

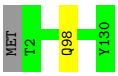




• Molecule 22: 40S ribosomal protein S22-A

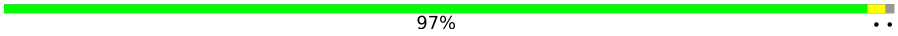
Chain b:





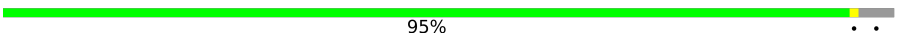
• Molecule 23: 40S ribosomal protein S23-A

Chain c:



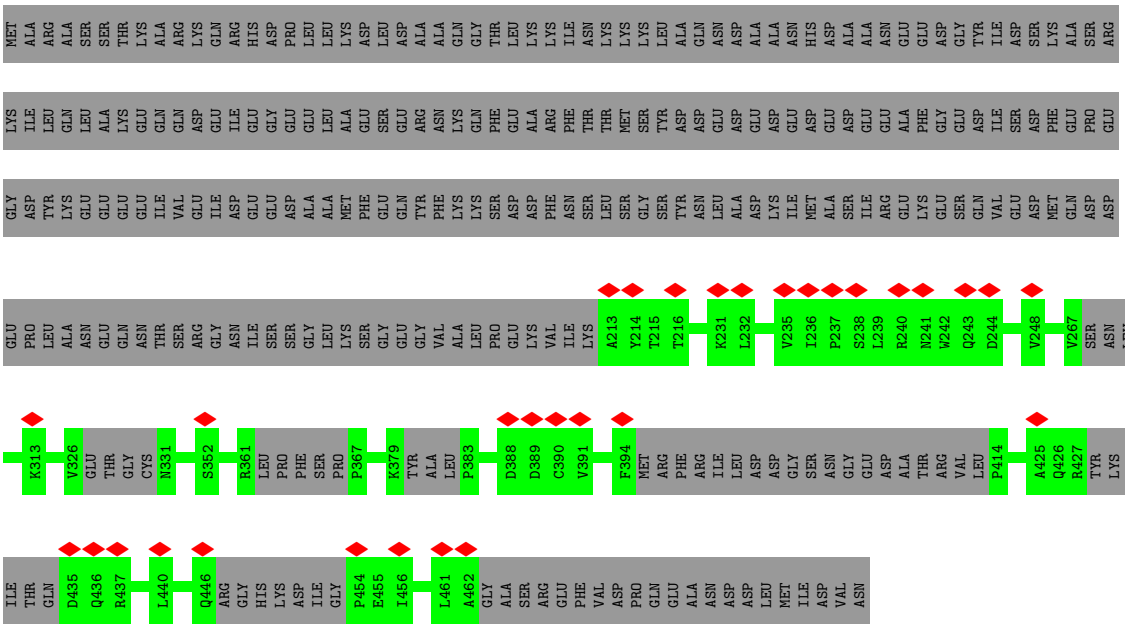
• Molecule 24: 40S ribosomal protein S24-A

Chain d:



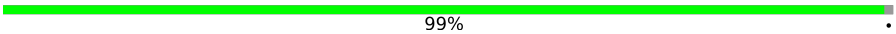
• Molecule 25: Essential nuclear protein 1

Chain e:



• Molecule 26: 40S ribosomal protein S27-A

Chain f:

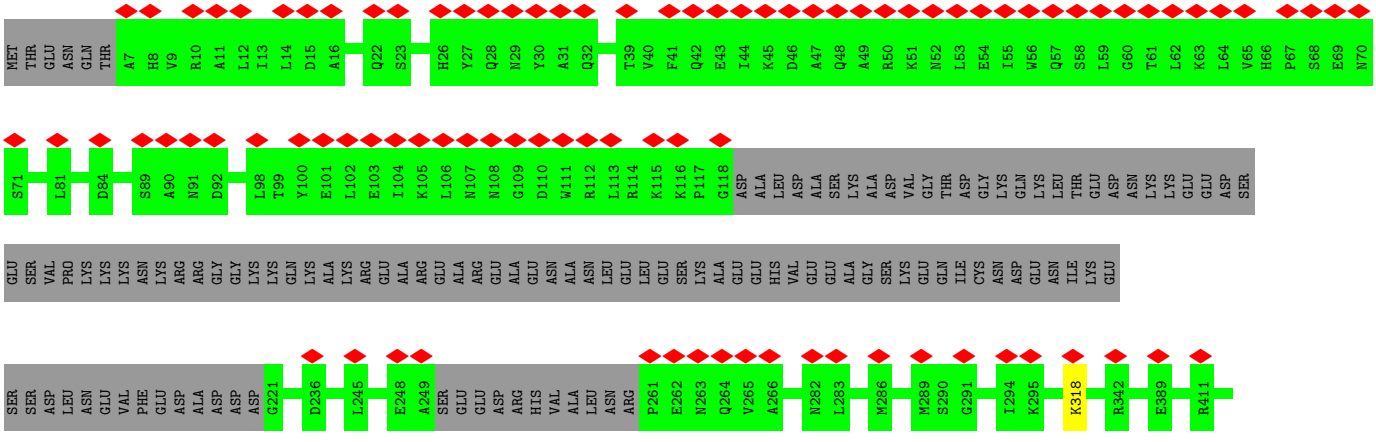


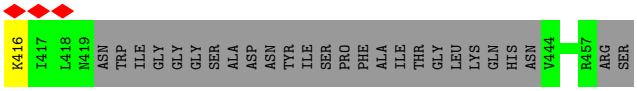
• Molecule 27: 40S ribosomal protein S30-A

Chain g:

• Molecule 28: 20S-pre-rRNA D-site endonuclease NOB1

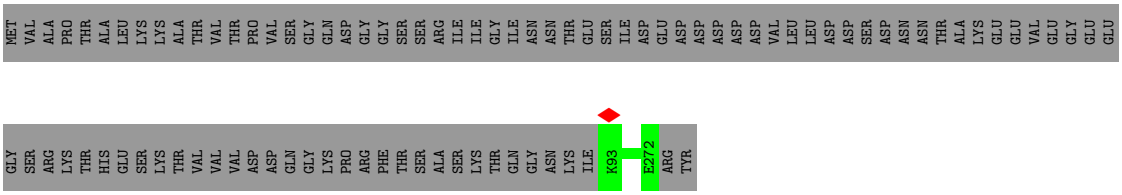
Chain o:





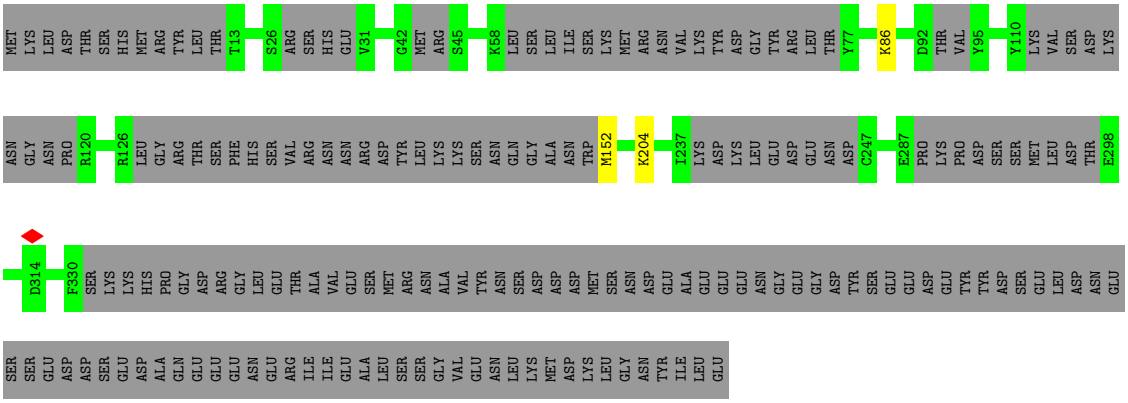
• Molecule 29: Pre-rRNA-processing protein PNO1

Chain p:



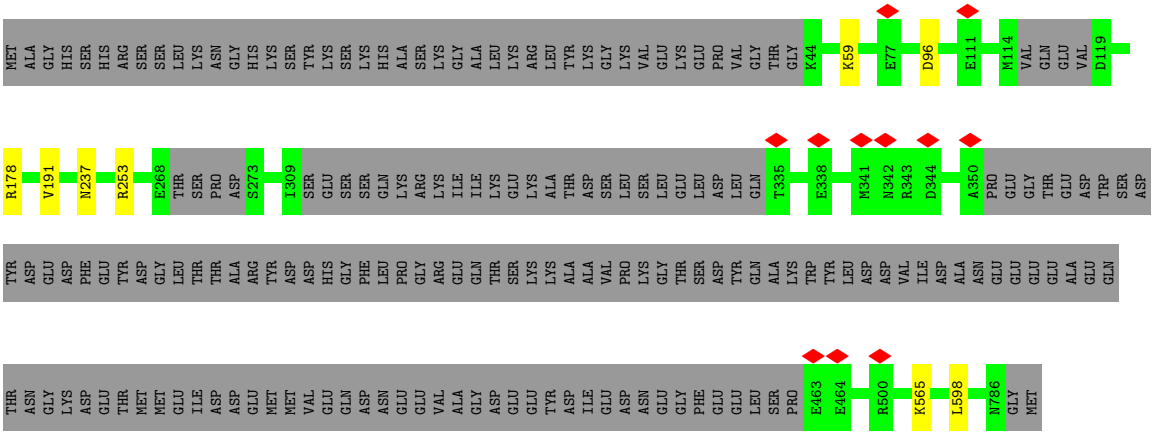
• Molecule 30: Serine/threonine-protein kinase RIO2

Chain r:



• Molecule 31: Ribosome biogenesis protein TSR1

Chain t:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180939	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	387.2, 387.2, 387.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96800005, 0.96800005, 0.96800005	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2	0.98	1/36865 (0.0%)	1.04	80/57383 (0.1%)
2	B	0.39	0/1607	0.58	0/2172
3	C	0.29	0/480	0.53	0/647
4	E	0.37	0/921	0.56	0/1236
5	F	0.41	0/990	0.57	0/1335
6	H	0.35	0/1027	0.57	0/1383
7	I	0.42	0/1113	0.59	0/1494
8	K	0.33	0/564	0.53	0/758
9	L	0.37	0/473	0.65	0/634
10	P	0.43	0/1631	0.58	0/2233
11	Q	0.40	0/1735	0.58	0/2335
12	R	0.43	0/1586	0.58	0/2158
13	S	0.49	0/2109	0.61	0/2839
14	T	0.40	0/1837	0.62	0/2455
15	U	0.38	0/1506	0.57	0/2028
16	V	0.50	0/1487	0.65	0/1988
17	W	0.50	0/1519	0.62	0/2035
18	X	0.55	0/1163	0.61	0/1568
19	Y	0.47	0/1215	0.57	0/1638
20	Z	0.40	0/937	0.63	0/1261
21	a	0.46	0/682	0.59	0/921
22	b	0.55	0/1038	0.60	0/1395
23	c	0.47	0/1139	0.61	0/1518
24	d	0.52	0/1060	0.58	0/1412
25	e	0.24	0/893	0.41	0/1130
26	f	0.41	0/620	0.54	0/838
27	g	0.47	0/306	0.65	0/407
28	o	0.31	0/2551	0.51	0/3439
29	p	0.39	0/1451	0.59	0/1955
30	r	0.34	0/1851	0.53	0/2459
31	t	0.36	0/4920	0.53	0/6644
All	All	0.74	1/77276 (0.0%)	0.85	80/111698 (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
7	I	0	1
11	Q	0	2
13	S	0	1
19	Y	0	1
31	t	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	555	A	N3-C4	-5.22	1.31	1.34

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1271	G	N3-C4-N9	-10.25	119.85	126.00
1	2	453	U	C2-N1-C1'	9.00	128.50	117.70
1	2	558	U	C2-N1-C1'	8.59	128.01	117.70
1	2	1632	C	C2-N1-C1'	8.24	127.87	118.80
1	2	555	A	N7-C8-N9	8.09	117.84	113.80
1	2	1659	A	O4'-C1'-N9	8.04	114.63	108.20
1	2	1657	U	C2-N1-C1'	7.94	127.23	117.70
1	2	830	U	C5-C4-O4	-7.89	121.17	125.90
1	2	830	U	N3-C4-O4	7.83	124.88	119.40
1	2	139	C	N1-C2-O2	7.79	123.58	118.90
1	2	1632	C	N1-C2-O2	7.77	123.56	118.90
1	2	139	C	N3-C2-O2	-7.64	116.55	121.90
1	2	558	U	N1-C2-O2	7.61	128.13	122.80
1	2	555	A	C5-N7-C8	-7.48	100.16	103.90
1	2	1653	C	C6-N1-C2	-7.47	117.31	120.30
1	2	1390	U	P-O3'-C3'	7.39	128.57	119.70
1	2	1657	U	N1-C2-O2	7.36	127.95	122.80
1	2	514	G	P-O3'-C3'	7.33	128.49	119.70
1	2	1271	G	N9-C4-C5	7.06	108.22	105.40
1	2	1447	C	C2-N1-C1'	7.02	126.52	118.80
1	2	453	U	N1-C2-O2	6.97	127.68	122.80
1	2	1632	C	C6-N1-C2	-6.89	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	453	U	N3-C2-O2	-6.86	117.39	122.20
1	2	555	A	C8-N9-C4	-6.68	103.13	105.80
1	2	1332	C	P-O3'-C3'	6.66	127.69	119.70
1	2	1271	G	C5-C6-O6	6.63	132.58	128.60
1	2	1657	U	N3-C2-O2	-6.58	117.59	122.20
1	2	1632	C	N3-C2-O2	-6.58	117.29	121.90
1	2	1271	G	N3-C4-C5	6.56	131.88	128.60
1	2	558	U	N3-C2-O2	-6.46	117.68	122.20
1	2	959	U	N3-C2-O2	-6.36	117.75	122.20
1	2	453	U	C6-N1-C1'	-6.35	112.31	121.20
1	2	610	G	C4-N9-C1'	6.29	134.67	126.50
1	2	1473	U	C2-N1-C1'	6.28	125.24	117.70
1	2	830	U	C2-N1-C1'	6.28	125.24	117.70
1	2	1473	U	N3-C2-O2	-6.24	117.83	122.20
1	2	4	C	C6-N1-C2	-6.12	117.85	120.30
1	2	1653	C	C2-N1-C1'	6.04	125.44	118.80
1	2	139	C	C6-N1-C2	-6.02	117.89	120.30
1	2	139	C	C2-N1-C1'	5.97	125.37	118.80
1	2	1271	G	C8-N9-C1'	5.96	134.75	127.00
1	2	1342	C	C2-N1-C1'	-5.95	112.25	118.80
1	2	1363	U	C2-N1-C1'	5.95	124.83	117.70
1	2	1258	U	C2-N1-C1'	5.86	124.73	117.70
1	2	1363	U	N1-C2-O2	5.83	126.88	122.80
1	2	558	U	C6-N1-C1'	-5.81	113.07	121.20
1	2	1656	U	P-O3'-C3'	5.78	126.63	119.70
1	2	1271	G	C6-C5-N7	5.77	133.86	130.40
1	2	610	G	C8-N9-C1'	-5.76	119.51	127.00
1	2	1653	C	C5-C6-N1	5.75	123.87	121.00
1	2	1389	C	N3-C2-O2	-5.68	117.92	121.90
1	2	284	G	O4'-C1'-N9	5.68	112.74	108.20
1	2	1568	C	P-O3'-C3'	5.68	126.51	119.70
1	2	1473	U	N1-C2-O2	5.66	126.76	122.80
1	2	1300	A	O4'-C1'-N9	5.65	112.72	108.20
1	2	1447	C	C6-N1-C2	-5.64	118.04	120.30
1	2	1382	A	O4'-C1'-N9	5.54	112.63	108.20
1	2	965	U	C2-N1-C1'	5.54	124.34	117.70
1	2	830	U	C5-C6-N1	5.50	125.45	122.70
1	2	281	G	O4'-C1'-N9	5.49	112.59	108.20
1	2	1333	C	C2-N1-C1'	-5.45	112.80	118.80
1	2	1632	C	C5-C6-N1	5.43	123.72	121.00
1	2	555	A	C2-N3-C4	-5.40	107.90	110.60
1	2	1363	U	N3-C2-O2	-5.37	118.44	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1439	C	C6-N1-C2	-5.35	118.16	120.30
1	2	1681	A	O4'-C1'-N9	5.32	112.46	108.20
1	2	1271	G	C4-N9-C1'	-5.29	119.62	126.50
1	2	1657	U	C6-N1-C1'	-5.27	113.83	121.20
1	2	1004	U	C2-N1-C1'	5.26	124.02	117.70
1	2	1333	C	O4'-C1'-N1	5.26	112.41	108.20
1	2	1389	C	N1-C2-O2	5.20	122.02	118.90
1	2	1632	C	C6-N1-C1'	-5.19	114.57	120.80
1	2	514	G	O4'-C1'-N9	5.16	112.33	108.20
1	2	139	C	P-O3'-C3'	5.15	125.88	119.70
1	2	1271	G	N1-C6-O6	-5.13	116.82	119.90
1	2	1332	C	O4'-C1'-N1	5.11	112.29	108.20
1	2	1440	C	N3-C2-O2	-5.09	118.33	121.90
1	2	1447	C	N1-C2-O2	5.08	121.95	118.90
1	2	558	U	C5-C6-N1	5.05	125.22	122.70
1	2	583	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	98	MET	Peptide
7	I	57	ARG	Sidechain
11	Q	132	ASP	Peptide
11	Q	152	ARG	Peptide
13	S	148	ARG	Sidechain
19	Y	3	ARG	Sidechain
31	t	178	ARG	Sidechain
31	t	253	ARG	Sidechain

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	2	32971	0	16601	245	0
2	B	1588	0	1657	5	0
3	C	476	0	491	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	902	0	934	2	0
5	F	973	0	1029	4	0
6	H	1009	0	1029	8	0
7	I	1096	0	1110	5	0
8	K	556	0	596	4	0
9	L	471	0	505	2	0
10	P	1590	0	1585	3	0
11	Q	1709	0	1784	8	0
12	R	1557	0	1641	8	0
13	S	2068	0	2154	3	0
14	T	1813	0	1905	11	0
15	U	1481	0	1572	3	0
16	V	1462	0	1486	7	0
17	W	1494	0	1573	4	0
18	X	1137	0	1207	0	0
19	Y	1192	0	1255	2	0
20	Z	926	0	950	3	0
21	a	673	0	659	0	0
22	b	1021	0	1060	0	0
23	c	1121	0	1196	0	0
24	d	1046	0	1112	0	0
25	e	883	0	322	0	0
26	f	610	0	633	0	0
27	g	300	0	331	0	0
28	o	2503	0	2513	0	0
29	p	1425	0	1502	0	0
30	r	1818	0	1678	0	0
31	t	4813	0	4773	0	0
32	o	1	0	0	0	0
All	All	72685	0	56843	305	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 3.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:284:G:H22	14:T:188:ARG:HH11	1.07	0.95
1:2:65:A:H2	1:2:84:A:H62	1.24	0.86
1:2:1690:G:H1'	1:2:1711:C:H5"	1.60	0.83
1:2:1381:U:H2'	1:2:1382:A:C8	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1291:G:H1	1:2:1324:G:H22	1.27	0.81
1:2:567:A:H62	1:2:576:G:H21	1.29	0.79
1:2:1653:C:H3'	1:2:1654:G:H8	1.49	0.77
1:2:1563:C:OP1	7:I:84:LYS:NZ	2.19	0.76
1:2:567:A:H62	1:2:576:G:N2	1.83	0.75
1:2:1264:G:N2	1:2:1266:U:OP1	2.20	0.74
2:B:94:THR:HG22	2:B:114:ILE:HG13	1.69	0.74
1:2:1749:A:C5	1:2:1750:A:H1'	2.22	0.74
1:2:901:G:H2'	1:2:902:G:C8	2.23	0.74
1:2:1300:A:O2'	1:2:1301:U:O4'	2.04	0.74
1:2:1081:A:N3	1:2:1082:C:N4	2.36	0.74
1:2:1219:A:N6	1:2:1265:G:OP1	2.21	0.73
1:2:992:A:H2	1:2:1012:U:H3	1.38	0.71
1:2:1748:G:H2'	1:2:1749:A:C8	2.25	0.71
1:2:72:A:N7	14:T:167:LYS:NZ	2.39	0.71
1:2:1752:U:H2'	1:2:1753:A:H8	1.53	0.71
1:2:1751:C:H2'	1:2:1752:U:C6	2.25	0.70
1:2:1320:U:O2'	10:P:101:ARG:NH2	2.23	0.70
1:2:1672:G:H2'	1:2:1673:G:C8	2.27	0.70
2:B:62:VAL:HG13	2:B:89:ILE:HG13	1.72	0.70
1:2:1390:U:O2'	1:2:1391:A:OP2	2.07	0.70
1:2:1215:C:O2'	1:2:1246:C:N4	2.26	0.69
1:2:284:G:H22	14:T:188:ARG:NH1	1.87	0.69
1:2:843:U:H2'	1:2:844:A:C8	2.28	0.68
1:2:843:U:H2'	1:2:844:A:H8	1.58	0.68
1:2:1752:U:H2'	1:2:1753:A:C8	2.28	0.68
1:2:1751:C:H2'	1:2:1752:U:H6	1.58	0.68
1:2:1382:A:H2'	1:2:1383:G:H8	1.60	0.67
9:L:42:ARG:NH2	9:L:58:GLU:O	2.27	0.67
1:2:846:G:H2'	1:2:847:A:C8	2.30	0.66
1:2:1383:G:H2'	1:2:1384:A:H8	1.61	0.66
1:2:1651:A:H2'	1:2:1652:C:H6	1.58	0.66
1:2:1555:A:OP2	4:E:47:ARG:NH1	2.29	0.66
1:2:1382:A:H2'	1:2:1383:G:C8	2.32	0.65
20:Z:41:ARG:O	20:Z:42:VAL:HG12	1.98	0.64
1:2:1335:U:O2	1:2:1416:G:N2	2.24	0.64
1:2:1335:U:O4	1:2:1416:G:O6	2.15	0.64
1:2:1650:U:H2'	1:2:1651:A:C8	2.34	0.63
1:2:1219:A:OP1	1:2:1445:G:N2	2.31	0.63
1:2:846:G:H2'	1:2:847:A:H8	1.64	0.63
1:2:1383:G:H2'	1:2:1384:A:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1727:G:H2'	1:2:1728:A:C8	2.34	0.63
1:2:1152:A:H2'	1:2:1153:G:C8	2.34	0.62
1:2:1215:C:HO2'	1:2:1246:C:N4	1.97	0.62
1:2:1651:A:H2'	1:2:1652:C:C6	2.34	0.62
1:2:567:A:N6	1:2:576:G:H21	1.95	0.62
1:2:1653:C:H3'	1:2:1654:G:C8	2.34	0.62
1:2:1474:G:H2'	1:2:1475:A:H8	1.65	0.61
1:2:544:A:C8	1:2:544:A:H5"	2.35	0.61
1:2:578:U:O2'	1:2:579:A:OP1	2.15	0.61
1:2:924:A:H2'	1:2:925:G:C8	2.36	0.61
4:E:18:ARG:NH1	6:H:90:ASN:OD1	2.34	0.61
1:2:554:C:H1'	1:2:555:A:H2	1.66	0.61
1:2:1291:G:H22	1:2:1324:G:N2	1.98	0.61
1:2:1344:A:O2'	1:2:1345:A:O5'	2.18	0.61
7:I:37:VAL:HG12	7:I:39:THR:H	1.65	0.61
1:2:852:C:N4	1:2:853:G:O6	2.34	0.61
11:Q:109:LYS:HE3	11:Q:113:MET:HE3	1.83	0.61
1:2:851:U:H2'	1:2:852:C:C6	2.36	0.60
1:2:1585:U:H3	1:2:1611:A:H2	1.44	0.60
1:2:650:U:H2'	1:2:651:G:C8	2.37	0.60
5:F:50:GLU:OE1	5:F:82:ARG:NH2	2.29	0.60
11:Q:33:LYS:NZ	11:Q:42:ASN:OD1	2.28	0.59
1:2:1380:U:H2'	1:2:1381:U:C6	2.37	0.59
1:2:1332:C:O2'	1:2:1333:C:OP2	2.16	0.59
1:2:885:G:H2'	1:2:886:U:C6	2.38	0.59
1:2:1655:A:H2'	1:2:1656:U:C6	2.38	0.58
1:2:566:C:H2'	1:2:567:A:C8	2.39	0.58
1:2:1474:G:H2'	1:2:1475:A:C8	2.38	0.58
1:2:1565:C:OP1	6:H:41:ARG:HD3	2.04	0.58
1:2:1381:U:H1'	1:2:1516:A:H61	1.68	0.58
1:2:1499:G:OP1	7:I:122:ARG:NH1	2.36	0.58
1:2:1652:C:H2'	1:2:1653:C:C6	2.38	0.58
1:2:1380:U:H2'	1:2:1381:U:H6	1.69	0.58
1:2:895:G:H1	1:2:917:U:H3	1.51	0.57
1:2:1727:G:H21	16:V:32:GLN:HE22	1.52	0.57
1:2:260:U:O2	16:V:41:LYS:NZ	2.24	0.57
1:2:829:A:HO2'	1:2:830:U:H6	1.52	0.57
1:2:1152:A:H2'	1:2:1153:G:H8	1.69	0.57
1:2:197:A:H2'	1:2:198:A:C8	2.38	0.57
1:2:284:G:N2	14:T:188:ARG:HD2	2.19	0.57
12:R:51:THR:HG23	12:R:52:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1750:A:H2'	1:2:1751:C:C6	2.41	0.56
1:2:1749:A:C4	1:2:1750:A:H1'	2.41	0.56
1:2:1171:A:H2'	1:2:1172:G:C8	2.41	0.56
1:2:1568:C:HO2'	1:2:1569:A:P	2.28	0.55
1:2:1656:U:C2	1:2:1658:G:C8	2.94	0.55
12:R:203:LYS:O	12:R:206:THR:HG22	2.05	0.55
1:2:1749:A:H2'	1:2:1750:A:O3'	2.06	0.55
1:2:1361:U:H4'	1:2:1362:U:OP1	2.07	0.54
1:2:821:U:H2'	1:2:822:U:C6	2.42	0.54
1:2:1381:U:H1'	1:2:1516:A:N6	2.21	0.54
1:2:1445:G:O2'	1:2:1446:A:OP2	2.25	0.54
1:2:182:A:H2'	1:2:183:U:C6	2.43	0.54
6:H:122:HIS:CE1	6:H:126:ARG:HH21	2.24	0.54
1:2:1374:C:H2'	1:2:1375:A:H8	1.73	0.53
1:2:259:U:H4'	1:2:260:U:O4	2.09	0.53
1:2:830:U:H2'	1:2:831:U:O4'	2.09	0.53
1:2:1267:G:N3	1:2:1269:U:C2	2.77	0.53
5:F:95:LYS:HE3	5:F:96:TYR:CZ	2.44	0.53
1:2:647:G:H21	1:2:687:G:H1	1.57	0.53
1:2:1300:A:O2'	1:2:1301:U:O5'	2.27	0.53
1:2:1588:G:H1	1:2:1608:U:H3	1.56	0.53
1:2:1374:C:H2'	1:2:1375:A:C8	2.44	0.52
1:2:1160:A:H2'	1:2:1161:C:C6	2.44	0.52
1:2:1727:G:H21	16:V:32:GLN:NE2	2.07	0.52
15:U:15:GLU:HA	15:U:18:LEU:HD12	1.91	0.52
1:2:1710:U:O2'	1:2:1712:A:OP2	2.27	0.52
1:2:555:A:C8	1:2:590:C:O2'	2.63	0.52
1:2:683:C:OP2	1:2:683:C:H6	1.93	0.52
1:2:1249:U:H2'	1:2:1250:U:C6	2.45	0.51
1:2:559:C:H2'	1:2:560:U:C6	2.44	0.51
1:2:1267:G:H1'	1:2:1269:U:H3	1.75	0.51
1:2:1336:A:O2'	1:2:1337:A:OP1	2.23	0.51
1:2:1542:G:N2	1:2:1569:A:OP2	2.42	0.51
1:2:1656:U:H2'	1:2:1657:U:H5'	1.93	0.50
1:2:1564:U:H2'	1:2:1565:C:C6	2.45	0.50
11:Q:176:VAL:HG12	11:Q:177:GLN:H	1.77	0.50
1:2:1154:G:H8	1:2:1154:G:OP2	1.95	0.50
11:Q:78:ASP:OD1	11:Q:79:HIS:ND1	2.42	0.50
1:2:555:A:H8	1:2:590:C:O2'	1.94	0.50
1:2:284:G:N2	14:T:188:ARG:HH11	1.92	0.49
1:2:832:U:H2'	1:2:833:U:C4'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1525:A:H2'	1:2:1526:A:C8	2.47	0.49
14:T:57:ASP:HA	14:T:106:LEU:HA	1.94	0.49
1:2:1171:A:H2'	1:2:1172:G:H8	1.77	0.49
1:2:1390:U:HO2'	1:2:1391:A:P	2.34	0.49
1:2:844:A:H2'	1:2:845:G:H8	1.77	0.49
1:2:1534:G:OP2	8:K:74:SER:OG	2.28	0.49
1:2:520:A:H2'	1:2:521:A:C8	2.47	0.49
1:2:1539:G:H4'	6:H:40:ARG:NH2	2.27	0.49
1:2:1267:G:O2'	1:2:1269:U:O2	2.25	0.49
1:2:563:U:H2'	1:2:564:G:C8	2.48	0.48
1:2:650:U:H2'	1:2:651:G:H8	1.78	0.48
1:2:832:U:H2'	1:2:833:U:H4'	1.95	0.48
1:2:819:G:C4	1:2:853:G:C2	3.00	0.48
1:2:1269:U:O2	1:2:1269:U:H5'	2.13	0.48
1:2:1441:C:H2'	1:2:1442:U:C6	2.48	0.48
1:2:828:U:H2'	1:2:829:A:C8	2.49	0.48
1:2:846:G:N3	1:2:846:G:H5'	2.29	0.48
1:2:1748:G:C6	1:2:1749:A:N6	2.82	0.48
1:2:871:G:H2'	1:2:872:G:C8	2.49	0.48
1:2:684:A:H2'	1:2:685:A:C8	2.49	0.47
12:R:245:ASP:OD1	12:R:245:ASP:N	2.47	0.47
8:K:95:HIS:CG	8:K:95:HIS:O	2.67	0.47
1:2:578:U:H3'	1:2:579:A:H5"	1.95	0.47
1:2:1564:U:H2'	1:2:1565:C:H6	1.79	0.47
1:2:1749:A:H3'	1:2:1750:A:H4'	1.95	0.47
1:2:1749:A:C3'	1:2:1750:A:H4'	2.44	0.47
17:W:107:ARG:NH2	17:W:153:GLU:OE2	2.41	0.47
1:2:591:A:H2'	1:2:592:A:C8	2.50	0.47
1:2:1332:C:C2	1:2:1333:C:C6	3.03	0.47
12:R:40:LYS:HG3	12:R:247:ALA:HB1	1.97	0.47
1:2:250:C:H6	1:2:250:C:H5'	1.80	0.47
1:2:819:G:C5	1:2:853:G:C6	3.03	0.47
1:2:1332:C:HO2'	1:2:1333:C:P	2.35	0.47
1:2:184:C:H2'	1:2:185:U:C6	2.49	0.47
1:2:1542:G:H22	1:2:1568:C:HO2'	1.63	0.47
6:H:41:ARG:NH2	7:I:36:ILE:O	2.45	0.47
1:2:1259:U:H2'	1:2:1260:U:H6	1.80	0.46
17:W:163:PRO:C	17:W:165:GLY:H	2.19	0.46
1:2:844:A:C4	1:2:845:G:C8	3.04	0.46
1:2:1266:U:C4	1:2:1267:G:C5	3.02	0.46
1:2:555:A:H8	1:2:590:C:HO2'	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:2:LYS:HB3	14:T:108:VAL:HG22	1.97	0.46
17:W:117:GLY:O	17:W:119:ALA:N	2.37	0.46
1:2:815:G:O2'	1:2:816:G:H5'	2.16	0.46
1:2:819:G:N7	1:2:853:G:C6	2.84	0.46
1:2:844:A:H2'	1:2:845:G:C8	2.51	0.46
1:2:850:A:H2'	1:2:851:U:C6	2.51	0.46
1:2:1441:C:O2'	1:2:1442:U:OP1	2.28	0.46
1:2:1747:G:C6	1:2:1748:G:C6	3.04	0.46
11:Q:108:ASP:OD1	11:Q:109:LYS:N	2.49	0.46
1:2:840:U:H2'	1:2:841:U:C6	2.51	0.46
1:2:895:G:H2'	1:2:896:U:C6	2.50	0.46
1:2:1259:U:H2'	1:2:1260:U:C6	2.52	0.45
1:2:1550:A:H2'	1:2:1551:U:C6	2.51	0.45
13:S:255:ARG:O	13:S:260:GLY:N	2.37	0.45
1:2:1202:A:H1'	1:2:1207:C:N4	2.31	0.45
1:2:1711:C:H4'	1:2:1712:A:OP2	2.16	0.45
1:2:1780:G:C8	1:2:1780:G:H5'	2.51	0.45
1:2:250:C:H5'	1:2:250:C:C6	2.51	0.45
1:2:559:C:H2'	1:2:560:U:H6	1.80	0.45
1:2:1511:U:H2'	1:2:1512:G:C8	2.52	0.45
1:2:1753:A:H2'	1:2:1754:A:C8	2.52	0.45
1:2:848:C:H2'	1:2:849:C:H6	1.82	0.45
1:2:560:U:H2'	1:2:561:G:H8	1.82	0.45
1:2:1488:G:H3'	1:2:1515:A:H61	1.82	0.45
15:U:109:VAL:HG12	15:U:110:GLN:N	2.31	0.45
1:2:220:A:N6	1:2:832:U:O4	2.50	0.45
1:2:1491:U:H1'	1:2:1492:A:OP1	2.17	0.45
19:Y:55:ARG:HG2	19:Y:55:ARG:HH11	1.83	0.44
1:2:894:U:H2'	1:2:895:G:C8	2.51	0.44
1:2:939:A:H2'	1:2:940:A:C8	2.52	0.44
14:T:39:GLU:HB3	14:T:46:LYS:HA	1.99	0.44
1:2:1388:A:H1'	1:2:1389:C:N3	2.32	0.44
12:R:142:GLY:N	12:R:153:SER:O	2.39	0.44
12:R:218:ILE:HD12	12:R:219:GLY:N	2.32	0.44
1:2:1313:A:H2'	1:2:1314:U:H5"	1.99	0.44
1:2:184:C:H2'	1:2:185:U:H6	1.82	0.44
1:2:639:U:OP1	15:U:112:ARG:NH2	2.51	0.44
1:2:1229:G:N2	1:2:1255:G:O2'	2.49	0.44
13:S:100:ARG:HH21	13:S:118:GLU:HG2	1.83	0.44
14:T:78:THR:HG22	14:T:79:LYS:N	2.33	0.44
1:2:1226:A:N3	1:2:1256:A:H2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1458:G:N3	1:2:1458:G:H2'	2.33	0.43
1:2:1382:A:C2'	1:2:1383:G:C8	3.00	0.43
8:K:95:HIS:O	8:K:96:SER:OG	2.34	0.43
2:B:183:ALA:O	2:B:186:ASN:ND2	2.32	0.43
1:2:1153:G:H2'	1:2:1154:G:O4'	2.19	0.43
1:2:1323:C:H2'	1:2:1324:G:C8	2.53	0.43
1:2:1344:A:H4'	1:2:1345:A:OP1	2.19	0.43
1:2:1646:C:H2'	1:2:1647:U:C6	2.53	0.43
1:2:116:U:H2'	1:2:117:U:C6	2.53	0.43
1:2:819:G:H5"	1:2:820:U:C4	2.54	0.43
1:2:1265:G:H4'	1:2:1266:U:O5'	2.19	0.43
6:H:91:ASP:HB3	6:H:94:ASP:O	2.17	0.43
1:2:840:U:H2'	1:2:841:U:H6	1.84	0.43
2:B:128:ASN:OD1	2:B:130:ILE:HG22	2.19	0.43
1:2:1389:C:C4	1:2:1391:A:H4'	2.54	0.43
1:2:1622:G:H2'	1:2:1623:C:C6	2.53	0.43
16:V:69:SER:OG	16:V:185:GLU:OE2	2.33	0.43
1:2:544:A:H5"	1:2:544:A:H8	1.82	0.43
1:2:1492:A:H3'	1:2:1493:A:C2	2.54	0.43
6:H:81:ILE:HA	6:H:82:PRO:HD3	1.88	0.43
10:P:29:VAL:HG12	10:P:30:GLN:O	2.19	0.43
8:K:95:HIS:O	8:K:97:LYS:N	2.45	0.42
11:Q:33:LYS:O	11:Q:98:THR:HG22	2.19	0.42
1:2:1219:A:N6	1:2:1265:G:C4	2.87	0.42
1:2:1592:A:H2'	1:2:1593:A:H8	1.84	0.42
1:2:1600:A:O2'	1:2:1601:G:OP2	2.31	0.42
12:R:106:ASP:O	12:R:108:ASN:N	2.47	0.42
1:2:841:U:H2'	1:2:842:C:H6	1.85	0.42
1:2:1160:A:H2'	1:2:1161:C:H6	1.81	0.42
1:2:1267:G:N3	1:2:1269:U:N3	2.67	0.42
1:2:1351:G:H2'	1:2:1352:G:H8	1.84	0.42
1:2:852:C:N3	1:2:853:G:C6	2.87	0.42
1:2:1388:A:N6	1:2:1408:G:H22	2.18	0.42
1:2:1752:U:C2	1:2:1753:A:N7	2.88	0.42
5:F:95:LYS:HE3	5:F:96:TYR:CE2	2.54	0.42
1:2:848:C:H2'	1:2:849:C:C6	2.54	0.42
1:2:564:G:O2'	1:2:565:C:OP2	2.30	0.42
1:2:1653:C:C4	1:2:1654:G:C6	3.08	0.42
1:2:625:C:H2'	1:2:626:U:C6	2.54	0.42
1:2:578:U:HO2'	1:2:579:A:P	2.41	0.42
14:T:78:THR:O	14:T:81:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:151:LYS:HE2	16:V:151:LYS:HA	2.02	0.42
1:2:1590:G:H2'	1:2:1591:C:C6	2.55	0.42
5:F:26:LYS:HA	5:F:26:LYS:HE2	2.00	0.42
14:T:38:GLY:O	14:T:41:VAL:HG22	2.19	0.42
1:2:1417:A:H2'	1:2:1418:G:C8	2.55	0.42
1:2:1713:G:H2'	1:2:1714:A:H8	1.85	0.42
11:Q:48:VAL:HG21	11:Q:61:LEU:HD21	2.01	0.42
1:2:1691:A:H2'	1:2:1692:G:C8	2.55	0.41
1:2:127:G:N2	1:2:178:U:O2'	2.51	0.41
1:2:182:A:H2'	1:2:183:U:H6	1.83	0.41
1:2:330:G:OP2	16:V:172:ARG:NH1	2.53	0.41
1:2:1624:C:H2'	1:2:1625:C:C6	2.55	0.41
1:2:1689:A:H2'	1:2:1690:G:H5"	2.02	0.41
1:2:1749:A:C8	1:2:1750:A:H1'	2.55	0.41
16:V:61:GLU:HG3	16:V:62:THR:HG23	2.02	0.41
1:2:1408:G:C6	1:2:1409:G:C4	3.07	0.41
1:2:1590:G:H2'	1:2:1591:C:H6	1.86	0.41
1:2:1606:C:H2'	1:2:1607:G:C8	2.55	0.41
1:2:845:G:C4	1:2:846:G:N2	2.88	0.41
1:2:1652:C:H2'	1:2:1653:C:O4'	2.20	0.41
1:2:1658:G:H5"	1:2:1659:A:H2'	2.02	0.41
1:2:319:U:H4'	1:2:323:A:C8	2.56	0.41
1:2:1649:G:H2'	1:2:1650:U:C6	2.55	0.41
19:Y:87:ASP:OD1	19:Y:88:LEU:N	2.53	0.41
1:2:1714:A:H2'	1:2:1715:G:O4'	2.20	0.41
17:W:181:ALA:O	17:W:185:GLY:N	2.41	0.41
1:2:1622:G:H2'	1:2:1623:C:H6	1.85	0.41
2:B:82:PHE:CZ	9:L:49:ARG:HG3	2.55	0.41
10:P:139:VAL:HG23	12:R:62:PRO:HG2	2.03	0.41
1:2:819:G:H1'	1:2:820:U:OP2	2.20	0.41
1:2:1248:C:C2	1:2:1249:U:C5	3.09	0.41
1:2:1254:U:H2'	1:2:1255:G:C8	2.56	0.41
1:2:1265:G:C6	1:2:1443:U:H2'	2.56	0.41
1:2:1290:U:H2'	1:2:1291:G:C8	2.56	0.41
7:I:35:ASP:C	7:I:35:ASP:OD1	2.60	0.41
1:2:554:C:H1'	1:2:555:A:C2	2.51	0.41
1:2:929:A:C8	20:Z:123:SER:O	2.74	0.41
1:2:1560:U:H5'	1:2:1560:U:O2	2.21	0.41
1:2:1713:G:H2'	1:2:1714:A:C8	2.56	0.41
1:2:826:U:H2'	1:2:827:C:C6	2.55	0.40
1:2:959:U:H2'	1:2:959:U:O2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1337:A:H2'	1:2:1338:C:C6	2.56	0.40
1:2:1360:A:H2'	1:2:1361:U:O4'	2.20	0.40
11:Q:97:LEU:HD13	11:Q:232:HIS:CD2	2.55	0.40
13:S:94:ALA:C	13:S:96:ASN:H	2.24	0.40
1:2:683:C:H2'	1:2:684:A:C8	2.57	0.40
6:H:94:ASP:O	6:H:96:LYS:N	2.54	0.40
1:2:1003:A:O2'	1:2:1004:U:O5'	2.38	0.40
1:2:1263:G:N3	1:2:1263:G:H2'	2.36	0.40
20:Z:42:VAL:HA	20:Z:46:MET:SD	2.61	0.40
1:2:416:A:H4'	1:2:417:A:OP2	2.22	0.40
1:2:829:A:H2'	1:2:830:U:C5	2.56	0.40
1:2:1341:A:N1	1:2:1384:A:C2	2.89	0.40
1:2:1592:A:H2'	1:2:1593:A:C8	2.57	0.40
1:2:1649:G:HO2'	1:2:1650:U:P	2.45	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	197/225 (88%)	187 (95%)	9 (5%)	1 (0%)	29 54
3	C	59/136 (43%)	57 (97%)	1 (2%)	1 (2%)	9 23
4	E	110/142 (78%)	103 (94%)	7 (6%)	0	100 100
5	F	123/143 (86%)	117 (95%)	5 (4%)	1 (1%)	19 43
6	H	120/146 (82%)	110 (92%)	10 (8%)	0	100 100
7	I	139/144 (96%)	133 (96%)	6 (4%)	0	100 100
8	K	67/108 (62%)	63 (94%)	4 (6%)	0	100 100
9	L	58/67 (87%)	55 (95%)	3 (5%)	0	100 100
10	P	204/252 (81%)	193 (95%)	9 (4%)	2 (1%)	15 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Q	212/255 (83%)	206 (97%)	6 (3%)	0	100	100
12	R	203/254 (80%)	192 (95%)	9 (4%)	2 (1%)	15	37
13	S	258/261 (99%)	249 (96%)	9 (4%)	0	100	100
14	T	224/236 (95%)	215 (96%)	7 (3%)	2 (1%)	17	40
15	U	182/190 (96%)	174 (96%)	7 (4%)	1 (0%)	29	54
16	V	181/200 (90%)	175 (97%)	6 (3%)	0	100	100
17	W	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
18	X	139/156 (89%)	136 (98%)	3 (2%)	0	100	100
19	Y	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
20	Z	125/137 (91%)	120 (96%)	3 (2%)	2 (2%)	9	24
21	a	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
22	b	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
23	c	142/145 (98%)	136 (96%)	5 (4%)	1 (1%)	22	46
24	d	128/135 (95%)	124 (97%)	4 (3%)	0	100	100
25	e	184/483 (38%)	181 (98%)	3 (2%)	0	100	100
26	f	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
27	g	34/63 (54%)	30 (88%)	3 (9%)	1 (3%)	4	10
28	o	306/459 (67%)	299 (98%)	7 (2%)	0	100	100
29	p	178/274 (65%)	175 (98%)	3 (2%)	0	100	100
30	r	221/425 (52%)	211 (96%)	10 (4%)	0	100	100
31	t	588/788 (75%)	567 (96%)	20 (3%)	1 (0%)	47	73
All	All	5003/6471 (77%)	4814 (96%)	174 (4%)	15 (0%)	44	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	23	VAL
5	F	27	GLY
15	U	98	ILE
20	Z	13	VAL
20	Z	42	VAL
10	P	103	THR
12	R	235	LEU
14	T	25	ARG
31	t	96	ASP

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Mol	Chain	Res	Type
3	C	115	LEU
12	R	150	GLN
10	P	139	VAL
27	g	50	VAL
14	T	70	PRO
23	c	41	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	173/191 (91%)	171 (99%)	2 (1%)	71 88
3	C	57/124 (46%)	57 (100%)	0	100 100
4	E	95/118 (80%)	95 (100%)	0	100 100
5	F	105/119 (88%)	104 (99%)	1 (1%)	76 91
6	H	109/129 (84%)	106 (97%)	3 (3%)	43 73
7	I	113/116 (97%)	112 (99%)	1 (1%)	78 92
8	K	60/89 (67%)	60 (100%)	0	100 100
9	L	53/60 (88%)	53 (100%)	0	100 100
10	P	166/210 (79%)	164 (99%)	2 (1%)	71 88
11	Q	191/224 (85%)	190 (100%)	1 (0%)	88 96
12	R	169/205 (82%)	167 (99%)	2 (1%)	71 88
13	S	221/222 (100%)	221 (100%)	0	100 100
14	T	191/201 (95%)	188 (98%)	3 (2%)	62 85
15	U	165/170 (97%)	163 (99%)	2 (1%)	71 88
16	V	147/161 (91%)	146 (99%)	1 (1%)	84 94
17	W	158/166 (95%)	157 (99%)	1 (1%)	86 95
18	X	126/137 (92%)	123 (98%)	3 (2%)	49 77
19	Y	127/128 (99%)	127 (100%)	0	100 100
20	Z	91/105 (87%)	90 (99%)	1 (1%)	73 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	a	73/74 (99%)	72 (99%)	1 (1%)	67 86
22	b	110/111 (99%)	109 (99%)	1 (1%)	78 92
23	c	119/120 (99%)	117 (98%)	2 (2%)	60 84
24	d	109/113 (96%)	107 (98%)	2 (2%)	59 83
25	e	18/424 (4%)	18 (100%)	0	100 100
26	f	70/71 (99%)	70 (100%)	0	100 100
27	g	32/54 (59%)	31 (97%)	1 (3%)	40 69
28	o	274/396 (69%)	272 (99%)	2 (1%)	84 94
29	p	157/238 (66%)	157 (100%)	0	100 100
30	r	182/384 (47%)	179 (98%)	3 (2%)	62 85
31	t	518/703 (74%)	513 (99%)	5 (1%)	76 91
All	All	4179/5563 (75%)	4139 (99%)	40 (1%)	77 91

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76	ARG
2	B	93	LEU
5	F	43	ILE
6	H	17	LEU
6	H	80	LYS
6	H	85	PHE
7	I	33	TYR
10	P	10	THR
10	P	27	ARG
11	Q	177	GLN
12	R	49	LYS
12	R	70	ASP
14	T	19	ASP
14	T	50	PHE
14	T	56	ASN
15	U	73	VAL
15	U	182	VAL
16	V	67	TRP
17	W	16	LYS
18	X	67	ARG
18	X	98	ASN
18	X	109	VAL

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Mol	Chain	Res	Type
20	Z	77	THR
21	a	9	VAL
22	b	98	GLN
23	c	27	ASN
23	c	107	PHE
24	d	121	THR
24	d	132	ARG
27	g	54	ARG
28	o	318	LYS
28	o	416	LYS
30	r	86	LYS
30	r	152	MET
30	r	204	LYS
31	t	59	LYS
31	t	191	VAL
31	t	237	ASN
31	t	565	LYS
31	t	598	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	200	ASN
6	H	78	HIS
7	I	23	GLN
7	I	77	ASN
8	K	44	GLN
8	K	95	HIS
10	P	23	HIS
11	Q	157	GLN
11	Q	211	HIS
13	S	153	ASN
13	S	258	GLN
14	T	10	ASN
15	U	29	ASN
15	U	161	GLN
16	V	32	GLN
16	V	64	ASN
17	W	48	GLN
17	W	133	HIS
23	c	27	ASN
24	d	110	GLN

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Mol	Chain	Res	Type
28	o	107	ASN
28	o	280	GLN
28	o	361	ASN
28	o	372	ASN
28	o	374	GLN
28	o	406	GLN
29	p	262	ASN
30	r	261	GLN
31	t	60	GLN
31	t	134	ASN
31	t	205	GLN
31	t	294	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1516/1804 (84%)	224 (14%)	58 (3%)

All (224) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	4	C
1	2	26	A
1	2	34	G
1	2	42	G
1	2	47	A
1	2	68	A
1	2	69	G
1	2	77	U
1	2	104	A
1	2	114	C
1	2	127	G
1	2	129	U
1	2	139	C
1	2	140	A
1	2	144	U
1	2	145	A
1	2	146	U
1	2	159	U
1	2	161	U
1	2	177	U

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Mol	Chain	Res	Type
1	2	198	A
1	2	220	A
1	2	249	U
1	2	250	C
1	2	259	U
1	2	260	U
1	2	261	U
1	2	282	C
1	2	314	C
1	2	316	A
1	2	321	C
1	2	322	G
1	2	337	G
1	2	338	C
1	2	359	A
1	2	360	A
1	2	361	C
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	424	C
1	2	426	G
1	2	439	U
1	2	444	C
1	2	453	U
1	2	454	U
1	2	487	G
1	2	515	A
1	2	538	A
1	2	540	G
1	2	542	A
1	2	544	A
1	2	545	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	560	U
1	2	565	C
1	2	577	G
1	2	578	U

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Mol	Chain	Res	Type
1	2	579	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	608	U
1	2	619	A
1	2	620	A
1	2	623	A
1	2	639	U
1	2	652	G
1	2	683	C
1	2	694	U
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	779	U
1	2	789	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	819	G
1	2	820	U
1	2	821	U
1	2	831	U
1	2	833	U
1	2	840	U
1	2	846	G
1	2	853	G
1	2	856	A
1	2	863	A
1	2	886	U
1	2	898	A
1	2	914	G
1	2	933	A
1	2	935	U
1	2	960	U
1	2	966	A
1	2	992	A
1	2	993	A

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Mol	Chain	Res	Type
1	2	1000	C
1	2	1005	A
1	2	1006	C
1	2	1007	C
1	2	1025	A
1	2	1026	A
1	2	1028	C
1	2	1031	U
1	2	1039	A
1	2	1040	G
1	2	1043	A
1	2	1052	U
1	2	1057	U
1	2	1058	U
1	2	1083	G
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1138	A
1	2	1154	G
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1167	G
1	2	1185	U
1	2	1221	A
1	2	1227	A
1	2	1242	A
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1247	U
1	2	1258	U
1	2	1264	G
1	2	1265	G
1	2	1269	U
1	2	1270	G
1	2	1290	U
1	2	1298	U
1	2	1299	G
1	2	1300	A
1	2	1301	U

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Mol	Chain	Res	Type
1	2	1307	U
1	2	1315	U
1	2	1321	A
1	2	1322	A
1	2	1333	C
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1343	U
1	2	1344	A
1	2	1345	A
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1377	U
1	2	1378	U
1	2	1382	A
1	2	1388	A
1	2	1389	C
1	2	1390	U
1	2	1391	A
1	2	1410	A
1	2	1411	A
1	2	1412	G
1	2	1440	C
1	2	1442	U
1	2	1444	A
1	2	1445	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1471	A
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1515	A
1	2	1516	A
1	2	1523	G
1	2	1524	A
1	2	1535	U
1	2	1536	G

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Mol	Chain	Res	Type
1	2	1537	C
1	2	1538	U
1	2	1556	A
1	2	1557	U
1	2	1560	U
1	2	1568	C
1	2	1569	A
1	2	1575	G
1	2	1584	G
1	2	1595	U
1	2	1596	C
1	2	1601	G
1	2	1616	G
1	2	1631	A
1	2	1650	U
1	2	1657	U
1	2	1660	A
1	2	1688	U
1	2	1689	A
1	2	1690	G
1	2	1691	A
1	2	1711	C
1	2	1712	A
1	2	1715	G
1	2	1745	G
1	2	1747	G
1	2	1750	A
1	2	1751	C
1	2	1754	A
1	2	1770	U
1	2	1780	G
1	2	1781	A
1	2	1792	G
1	2	1801	A
1	2	1803	G
1	2	1804	A

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	47	A
1	2	139	C

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Mol	Chain	Res	Type
1	2	140	A
1	2	176	C
1	2	249	U
1	2	321	C
1	2	322	G
1	2	369	A
1	2	400	A
1	2	453	U
1	2	468	A
1	2	510	G
1	2	514	G
1	2	544	A
1	2	558	U
1	2	582	U
1	2	606	A
1	2	622	A
1	2	765	G
1	2	811	A
1	2	814	A
1	2	819	G
1	2	855	A
1	2	999	U
1	2	1024	U
1	2	1158	C
1	2	1245	G
1	2	1268	G
1	2	1280	C
1	2	1297	G
1	2	1298	U
1	2	1314	U
1	2	1321	A
1	2	1332	C
1	2	1336	A
1	2	1343	U
1	2	1344	A
1	2	1361	U
1	2	1362	U
1	2	1377	U
1	2	1390	U
1	2	1441	C
1	2	1444	A
1	2	1491	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1492	A
1	2	1556	A
1	2	1568	C
1	2	1595	U
1	2	1600	A
1	2	1615	C
1	2	1631	A
1	2	1649	G
1	2	1656	U
1	2	1710	U
1	2	1711	C
1	2	1744	A
1	2	1750	A
1	2	1780	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

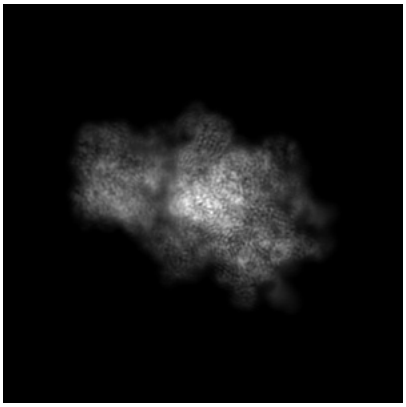
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16349. These allow visual inspection of the internal detail of the map and identification of artifacts.

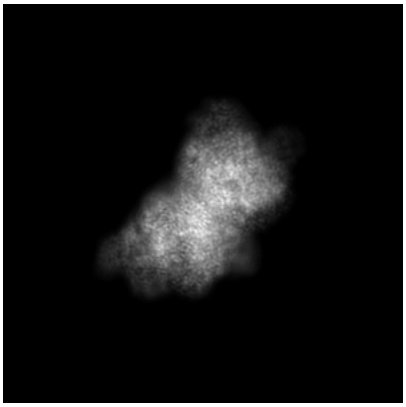
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

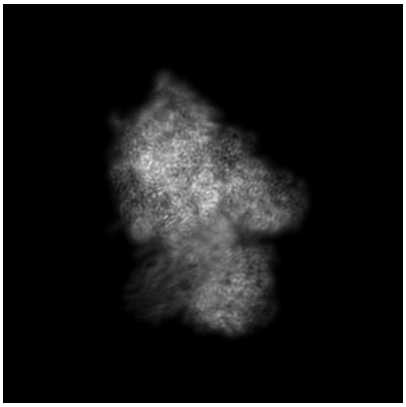
6.1.1 Primary map



X



Y

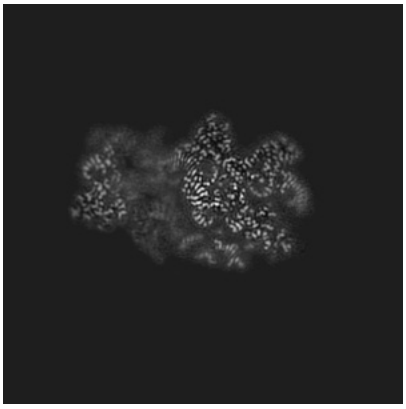


Z

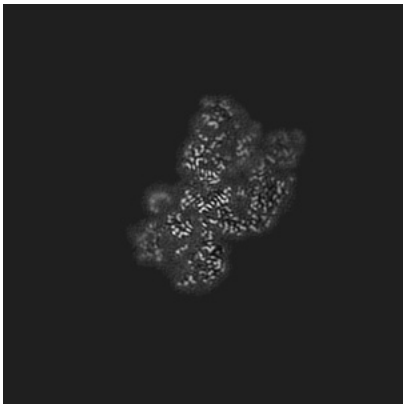
The images above show the map projected in three orthogonal directions.

6.2 Central slices

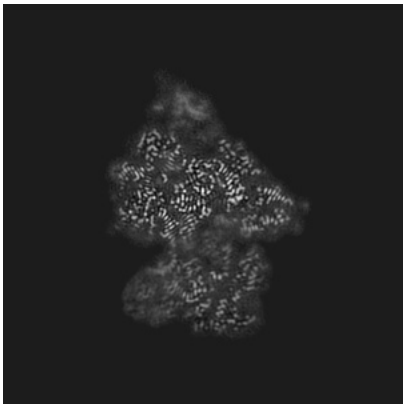
6.2.1 Primary map



X Index: 200



Y Index: 200

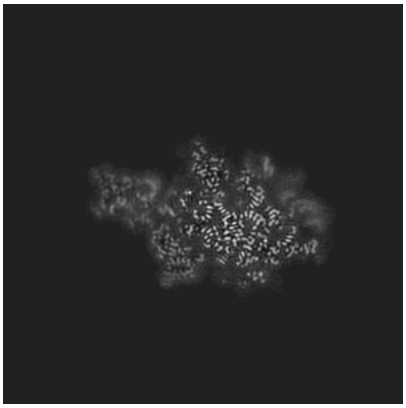


Z Index: 200

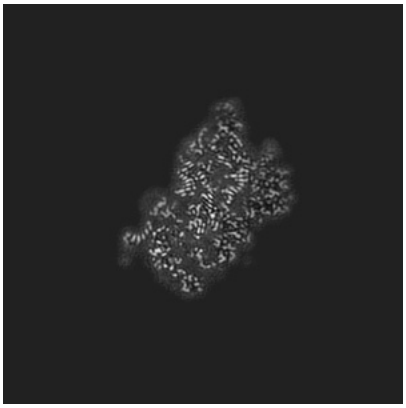
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

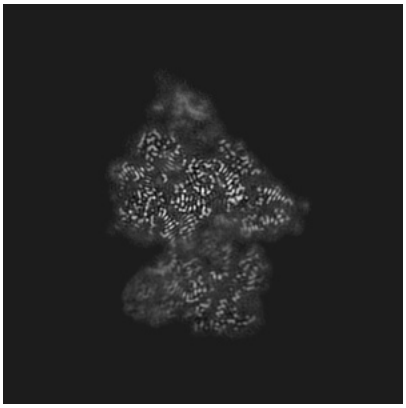
6.3.1 Primary map



X Index: 173



Y Index: 217

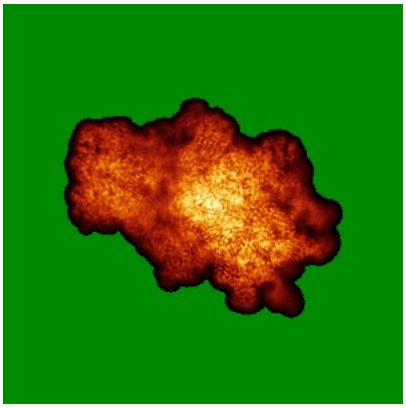


Z Index: 200

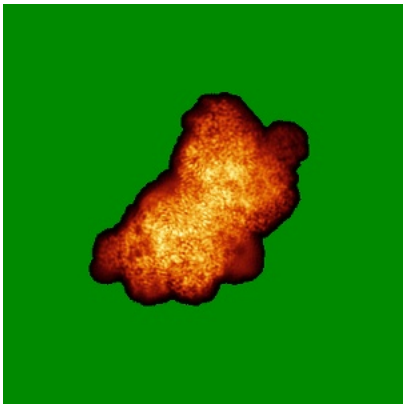
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

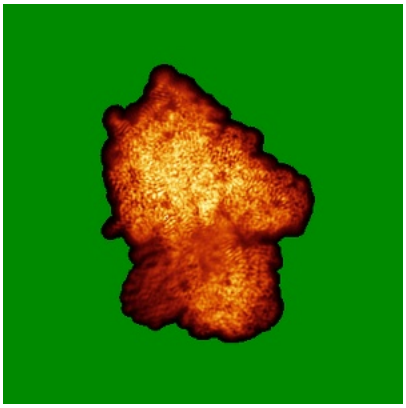
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

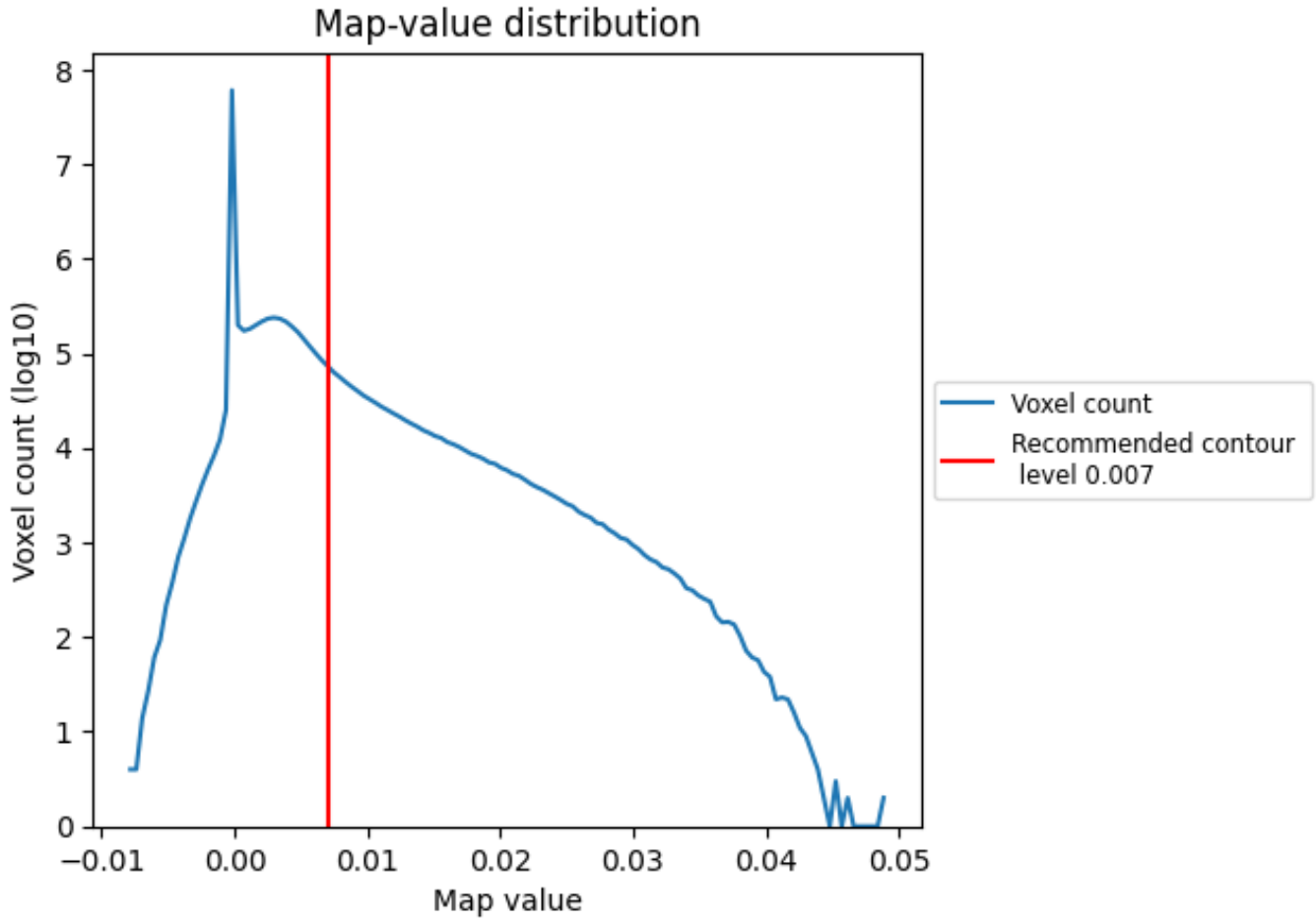
6.6 Mask visualisation (i)

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

7 Map analysis

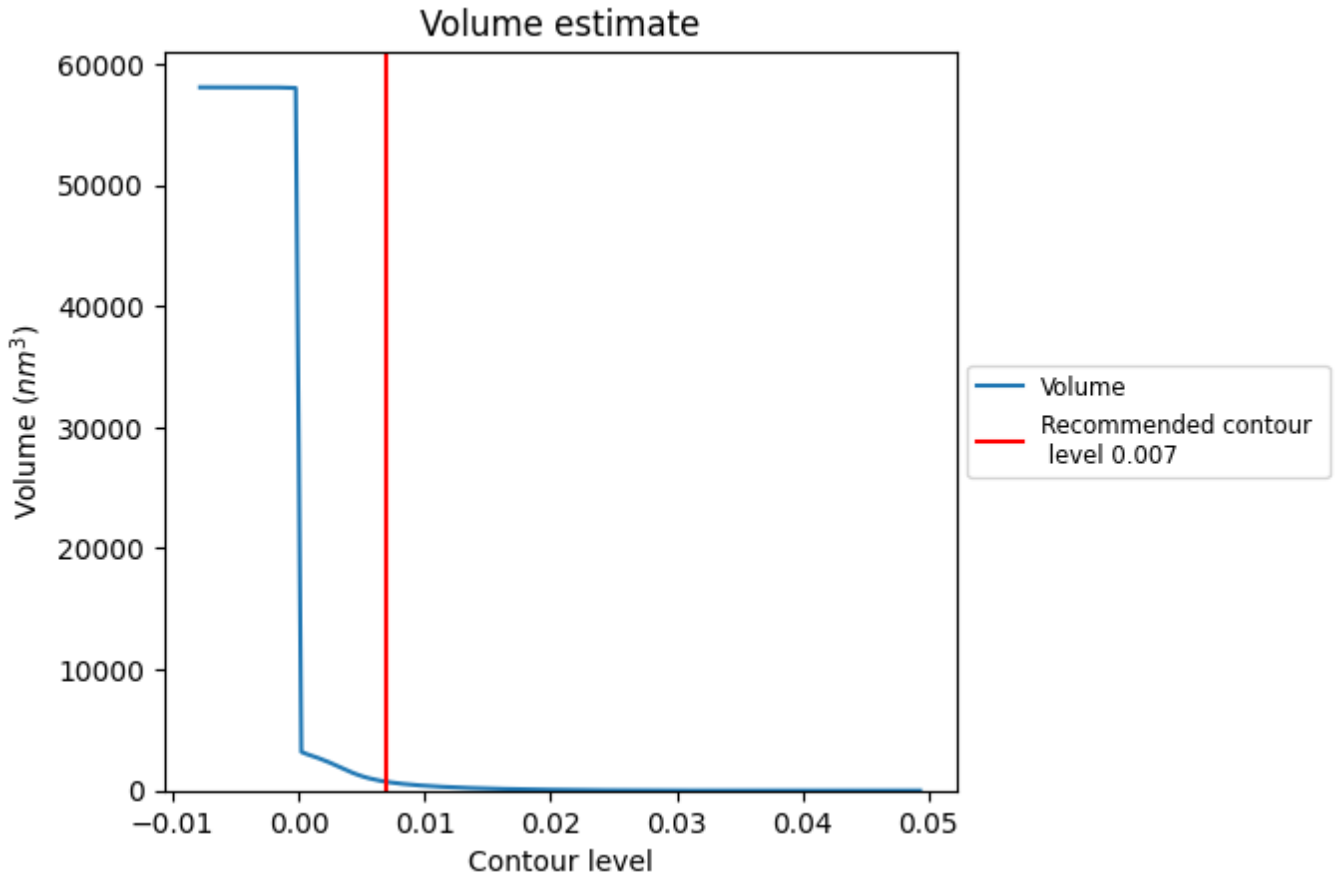
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

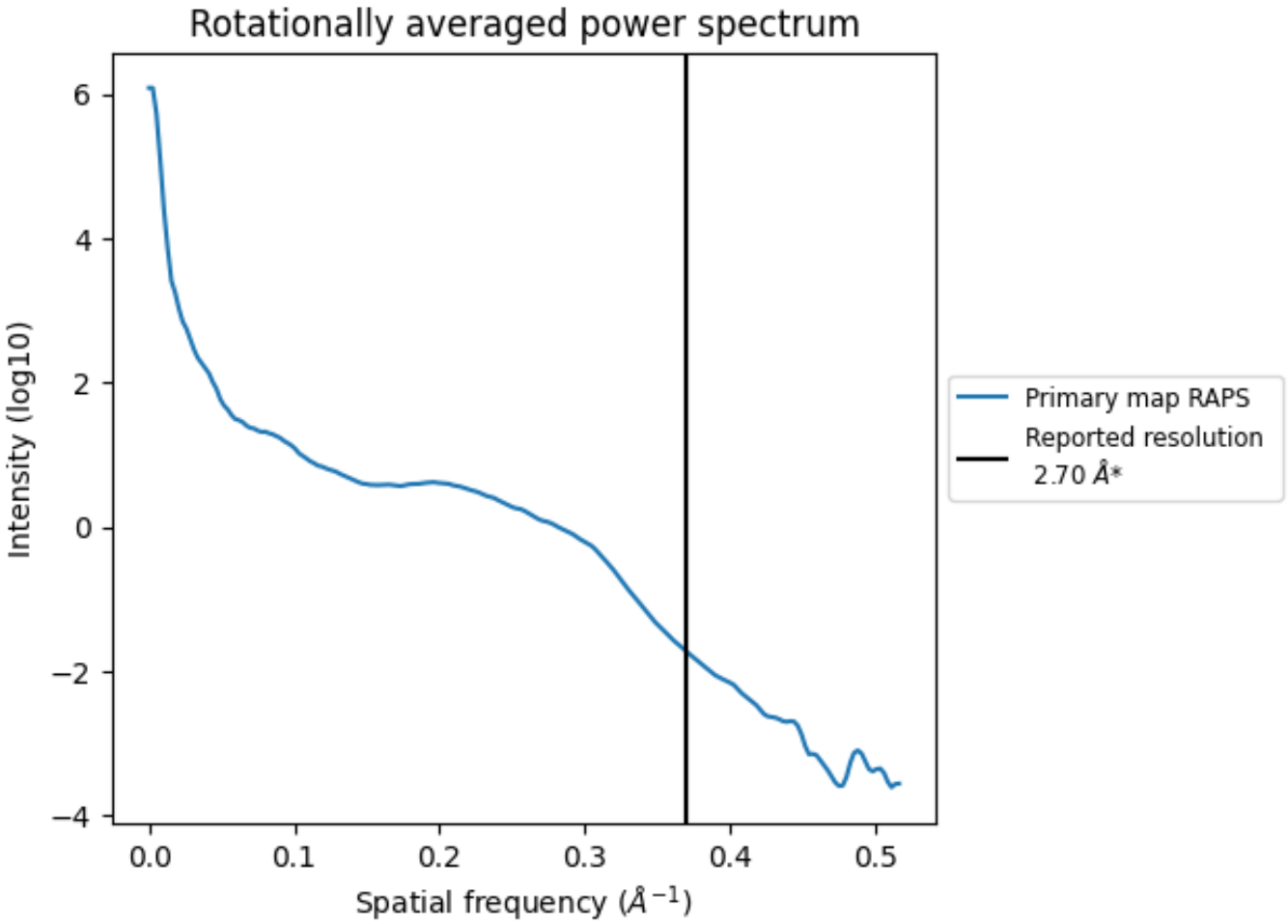
7.2 Volume estimate



The volume at the recommended contour level is 719 nm^3; this corresponds to an approximate mass of 650 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 (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

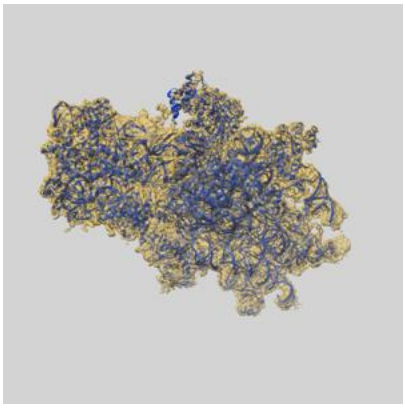
8 Fourier-Shell correlation (i)

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

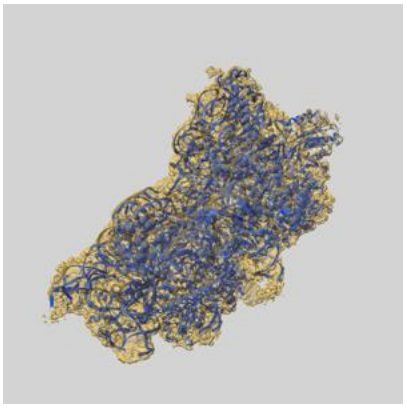
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16349 and PDB model 8C01. Per-residue inclusion information can be found in section 3 on page 9.

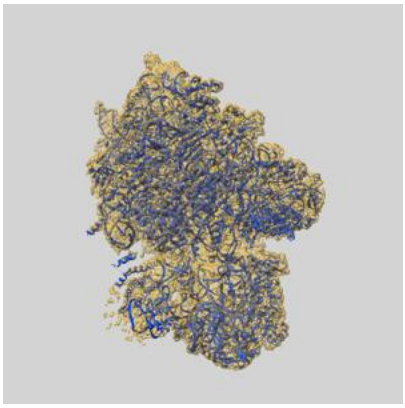
9.1 Map-model overlay



X



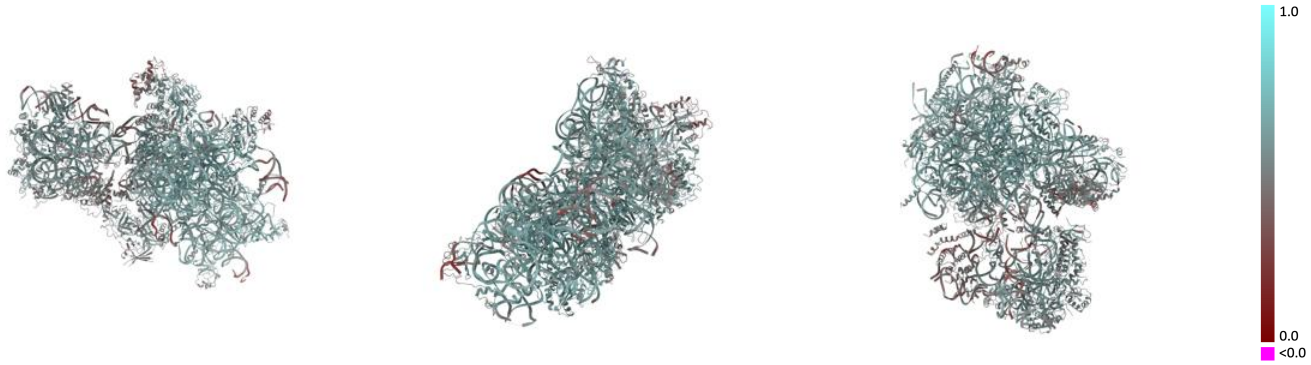
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

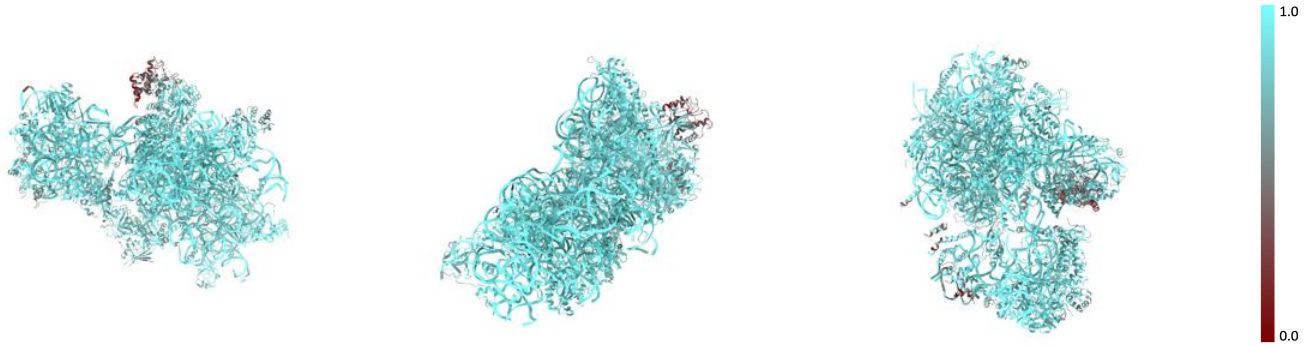
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

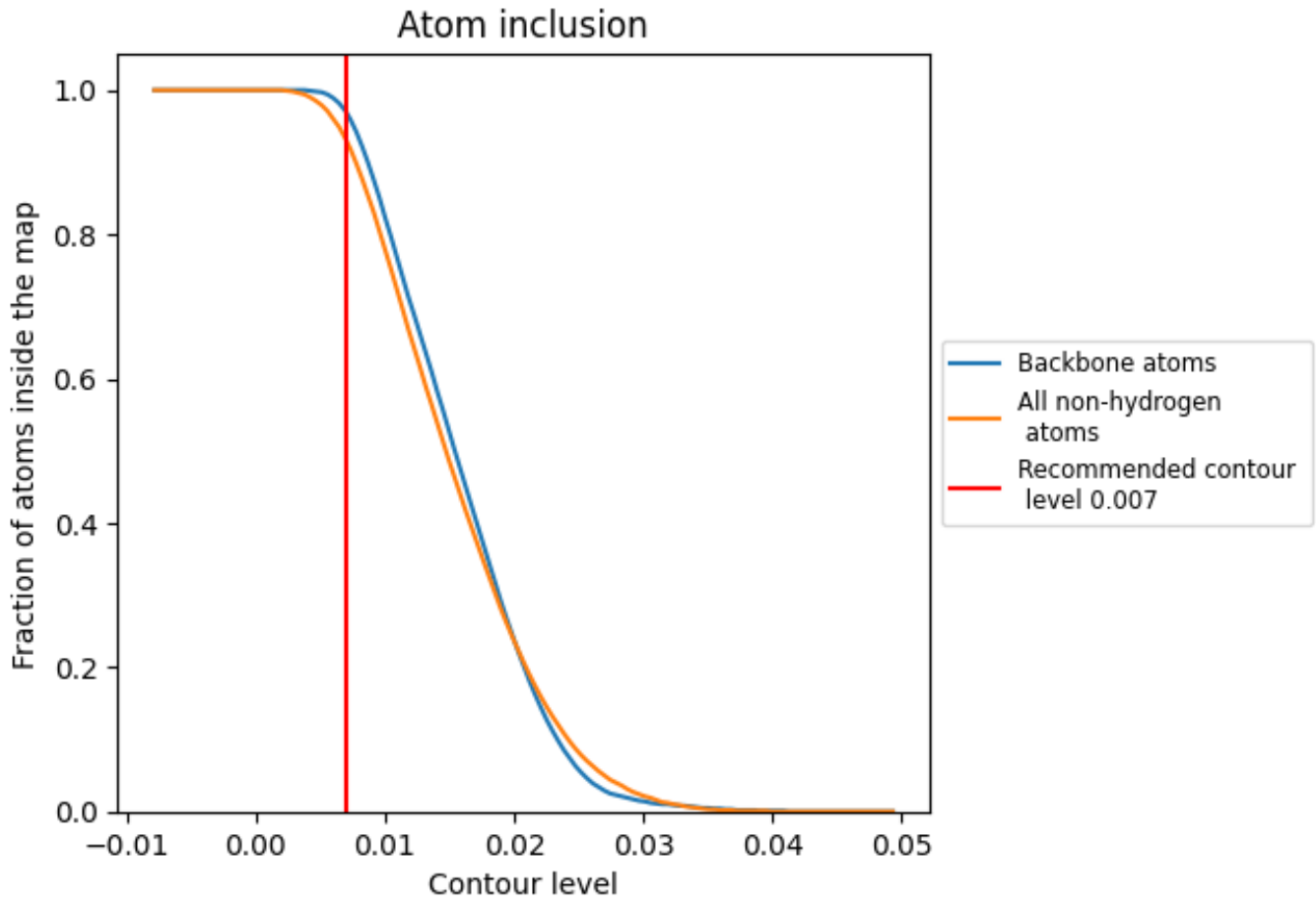
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.5690
2	0.9840	0.5780
B	0.9110	0.5480
C	0.7090	0.5270
E	0.7980	0.5260
F	0.9090	0.5470
H	0.8390	0.5330
I	0.9300	0.5540
K	0.7740	0.5380
L	0.8720	0.5310
P	0.9650	0.6030
Q	0.9140	0.5680
R	0.9540	0.6120
S	0.9590	0.6130
T	0.9100	0.5600
U	0.8380	0.5370
V	0.9670	0.6160
W	0.9420	0.6120
X	0.9560	0.6210
Y	0.9410	0.5990
Z	0.9570	0.5810
a	0.9250	0.6040
b	0.9790	0.6320
c	0.9630	0.6110
d	0.9490	0.6050
e	0.7310	0.4460
f	0.9420	0.5950
g	0.8990	0.5730
o	0.6000	0.4940
p	0.9120	0.5450
r	0.8490	0.4620
t	0.8740	0.5310