



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:58 PM EST

PDB ID : 7JQB
EMDB ID : EMD-22432
Title : SARS-CoV-2 Nsp1 and rabbit 40S ribosome complex
Authors : Yuan, S.; Xiong, Y.
Deposited on : 2020-08-10
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.dev43
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) : 2.31.2

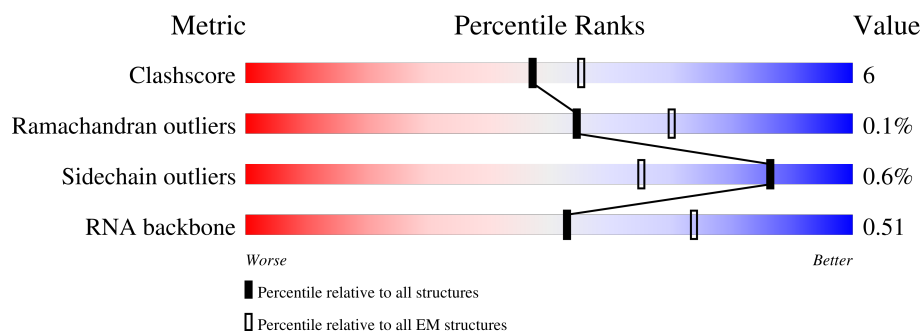
1 Overall quality at a glance

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 $\leq 5\%$. 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	1869	
2	a	125	
3	B	295	
4	b	115	
5	C	264	
6	D	293	
7	d	69	

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Mol	Chain	Length	Quality of chain
8	E	243	
9	f	133	
10	G	204	
11	g	156	
12	H	249	
13	h	317	
14	I	194	
15	J	208	
16	K	194	
17	L	165	
18	N	132	
19	Q	145	
20	R	146	
21	S	135	
22	T	152	
23	U	145	
24	V	119	
25	W	83	
26	Z	130	
27	F	36	
28	M	263	
29	O	158	
30	P	151	
31	X	168	
32	Y	130	

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Mol	Chain	Length	Quality of chain
33	c	143	<div><div></div><div>97%</div><div></div></div>
34	e	84	<div><div>5%</div><div>98%</div><div></div></div>

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 74976 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 2 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8
b	109	ARG	PRO	conflict	UNP G1TFE8

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 7 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 9 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 10 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 11 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 12 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 13 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 14 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 15 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 16 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 17 is a protein called S10_pectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 18 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 20 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 23 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	36	Total	C	N	O	S	0	0
			280	171	50	58	1		

- Molecule 28 is a protein called 40S ribosomal protein S4.

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

- Molecule 29 is a protein called uS17.

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

- Molecule 30 is a protein called uS15.

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

- Molecule 31 is a protein called Uncharacterized protein.

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

- Molecule 32 is a protein called uS8.

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

- Molecule 33 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	142	Total	C	N	O	S	0	0
			1106	698	220	184	4		

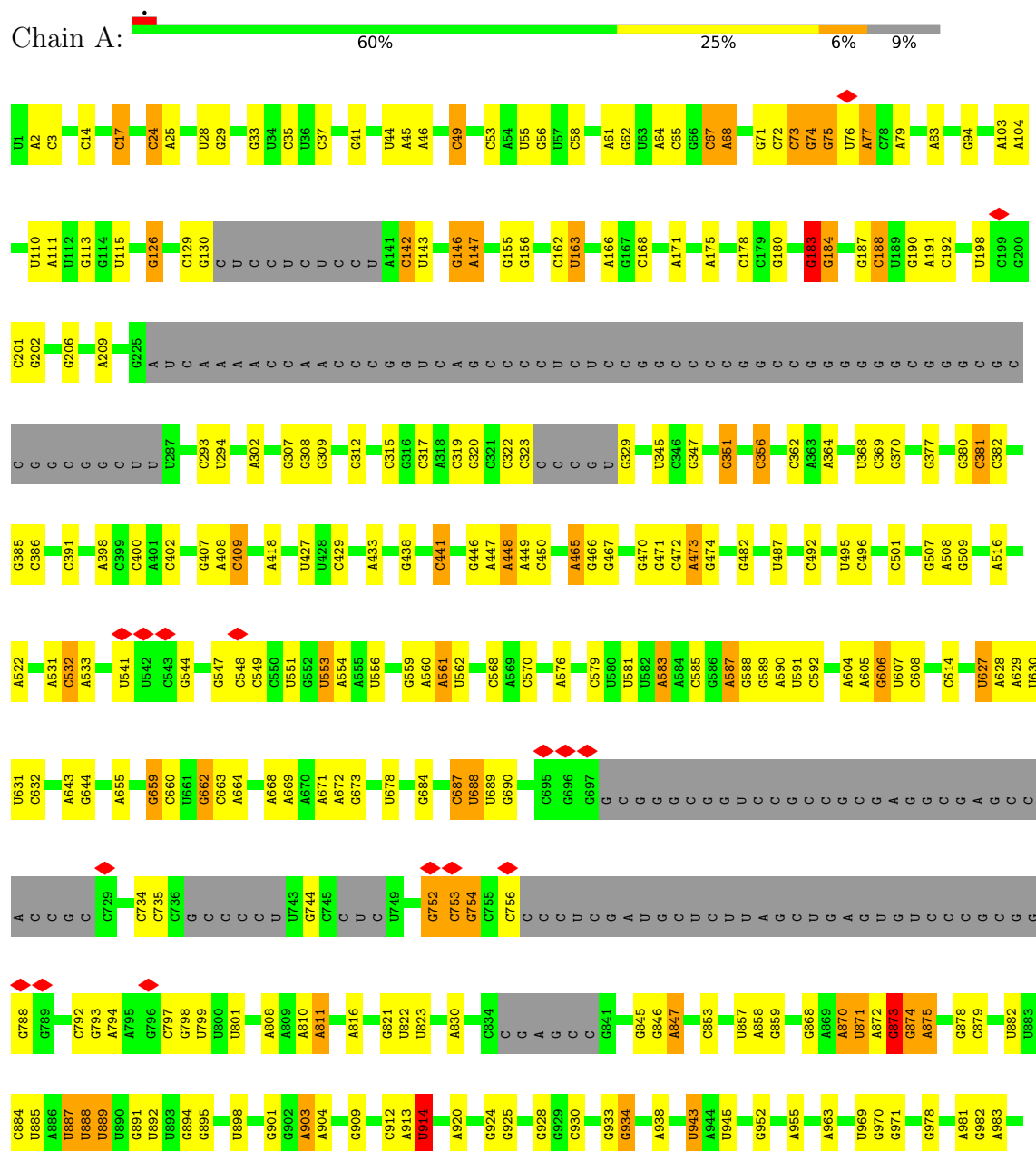
- Molecule 34 is a protein called eS27.

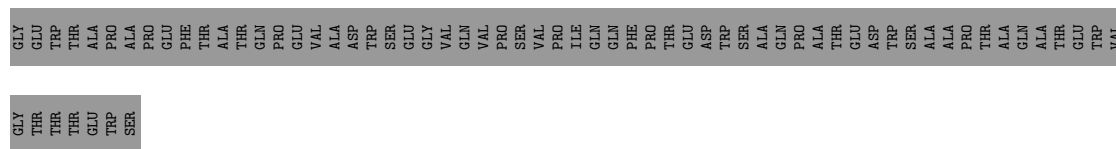
Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	84	Total	C	N	O	S	0	0
			659	413	122	116	8		

3 Residue-property plots

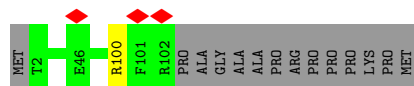
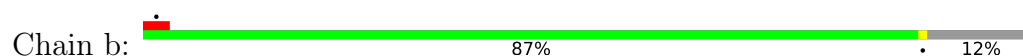
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: rRNA

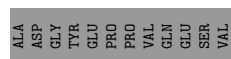




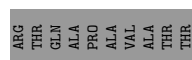
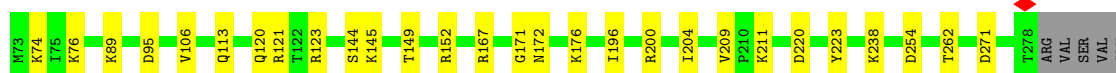
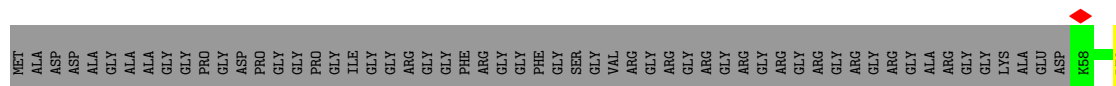
- Molecule 4: 40S ribosomal protein S26



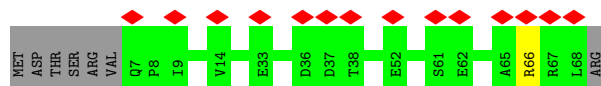
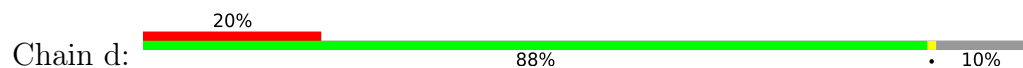
- Molecule 5: eS1



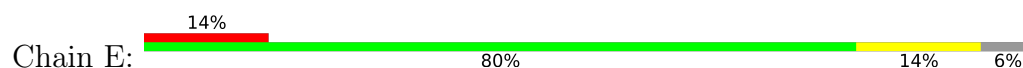
- Molecule 6: uS5

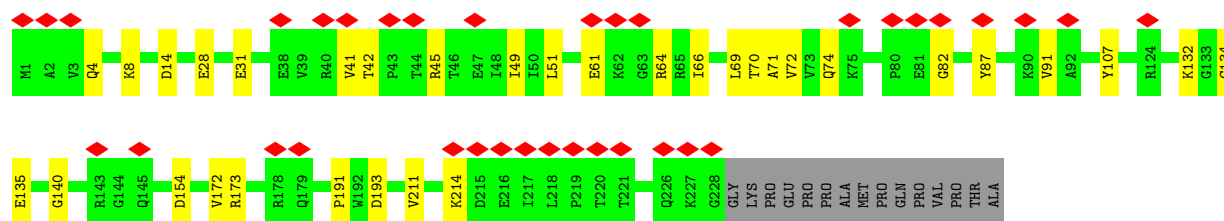


- Molecule 7: eS28

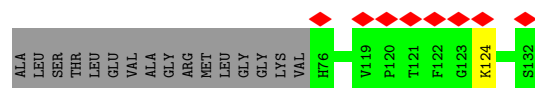
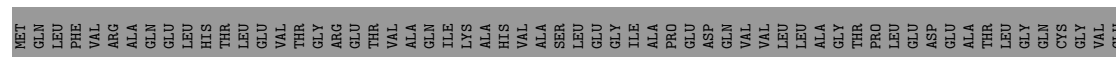


- Molecule 8: Ribosomal protein S3

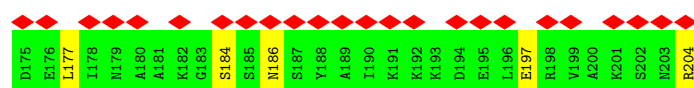
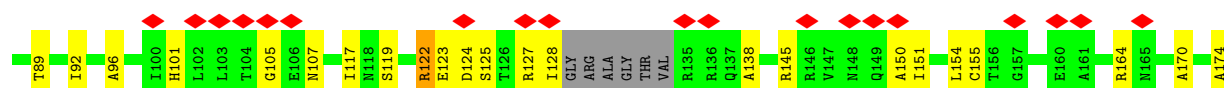
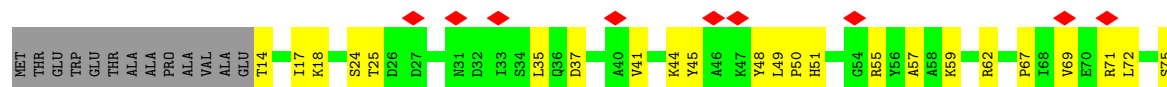




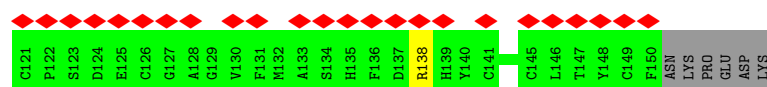
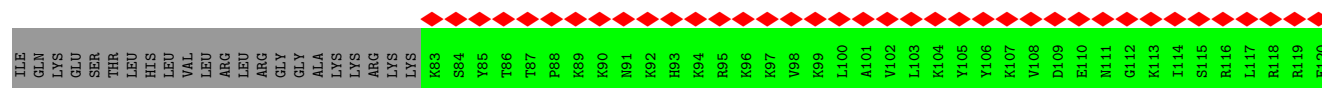
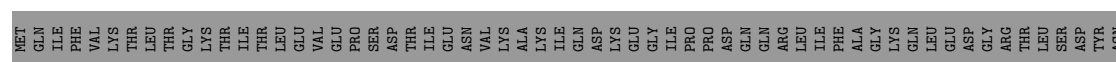
• Molecule 9: eS30



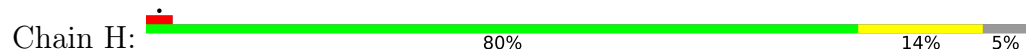
• Molecule 10: uS7

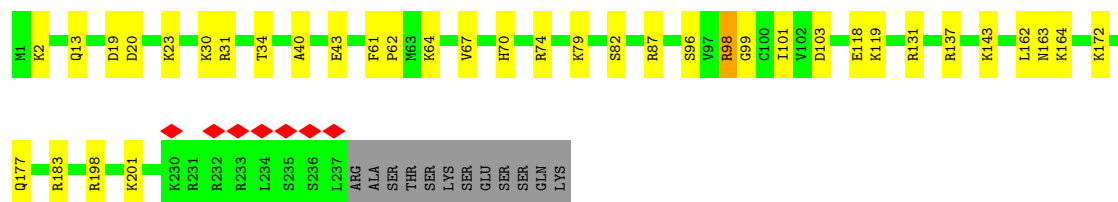


• Molecule 11: eS31

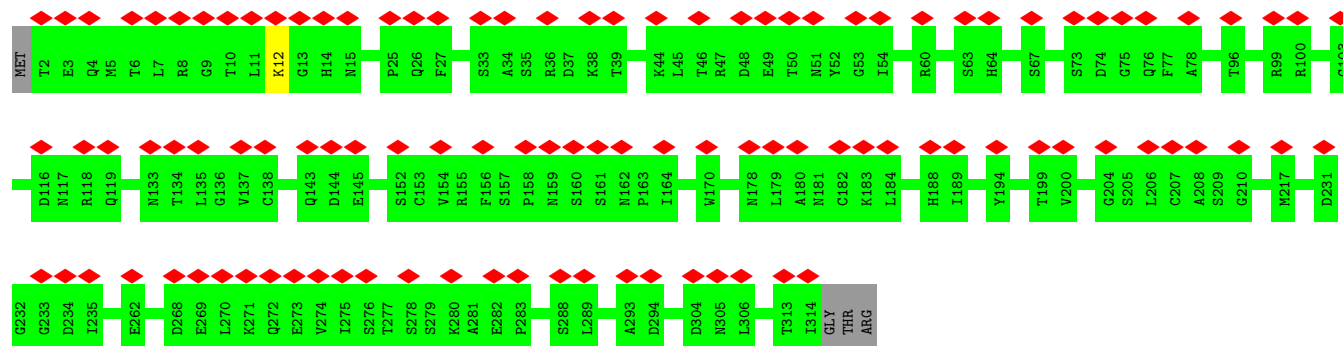


• Molecule 12: eS6

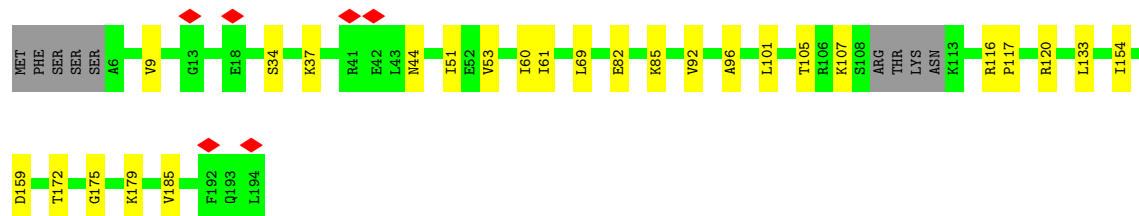
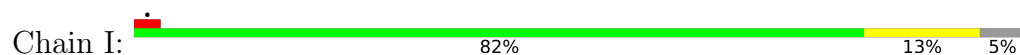




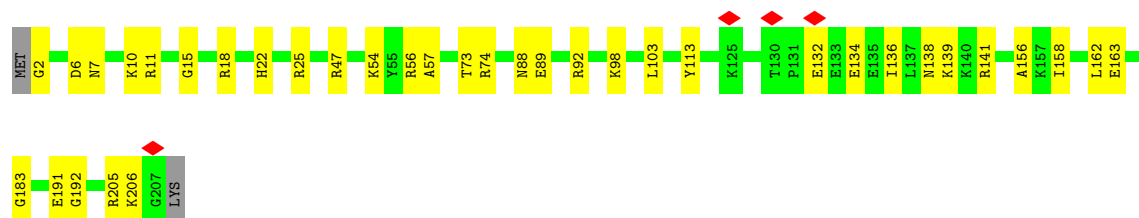
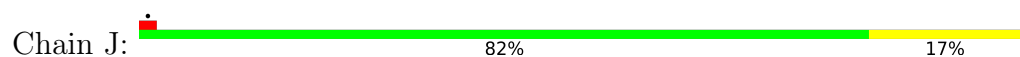
• Molecule 13: RACK1



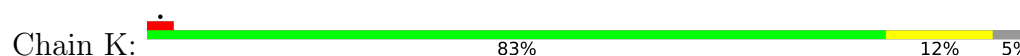
• Molecule 14: eS7



• Molecule 15: eS8

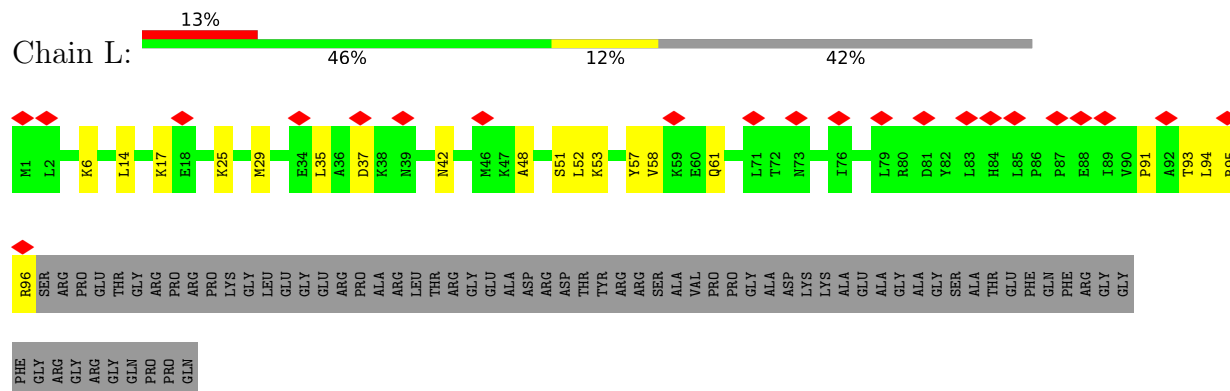


• Molecule 16: uS4

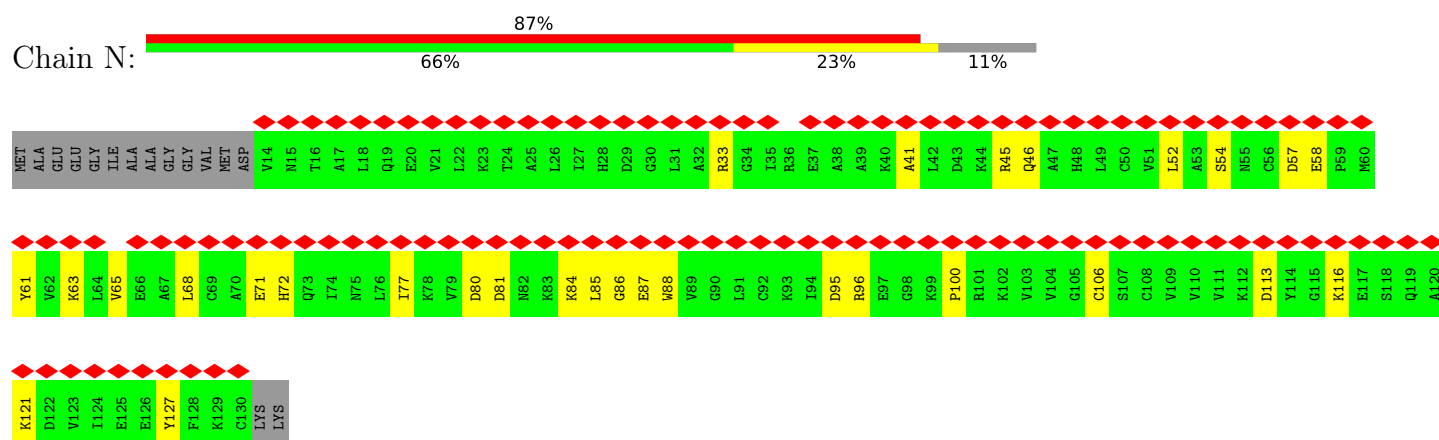


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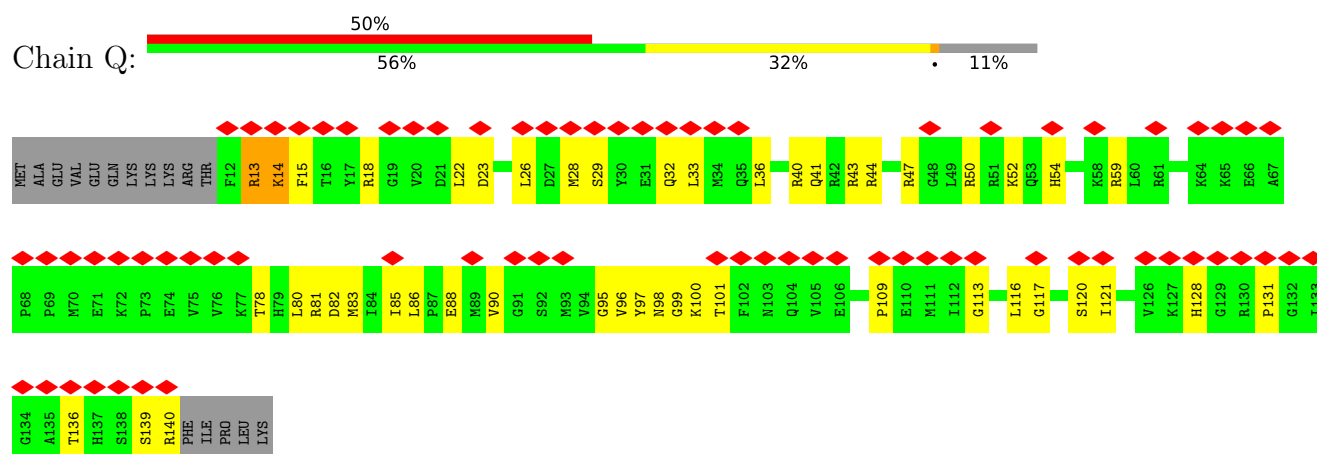
- Molecule 17: S10_pectin domain-containing protein



- Molecule 18: eS12

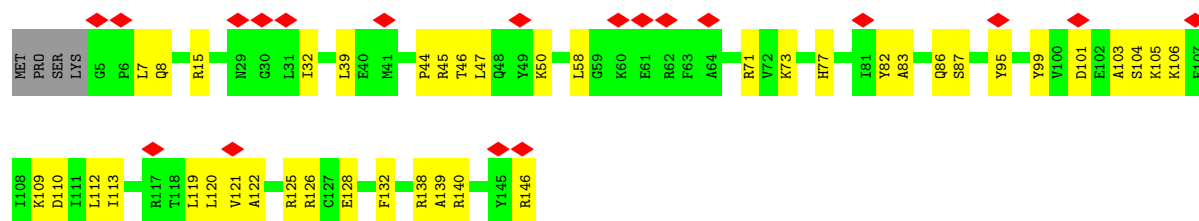


- Molecule 19: uS19

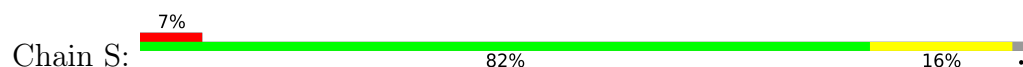


- Molecule 20: Uncharacterized protein

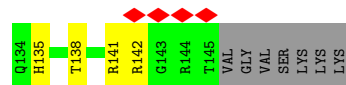
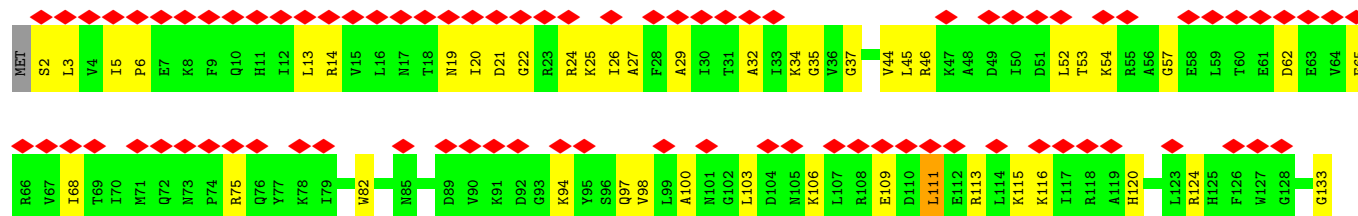




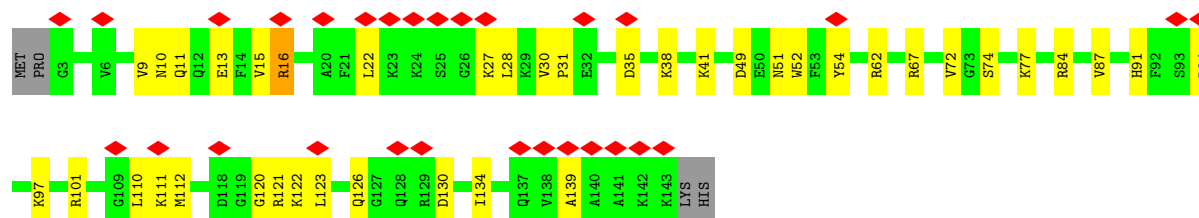
- Molecule 21: eS17



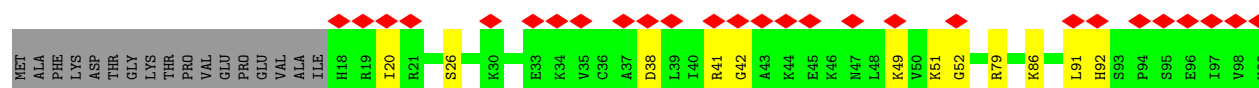
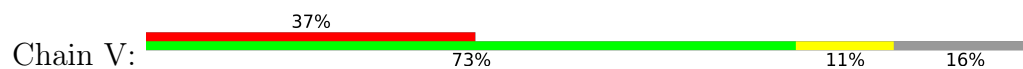
- Molecule 22: uS13

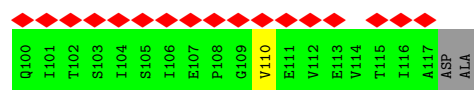


- Molecule 23: Uncharacterized protein

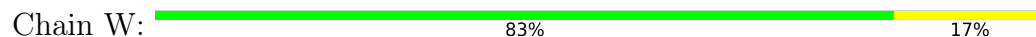


- Molecule 24: uS10

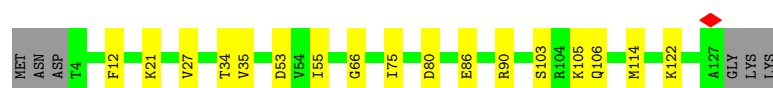
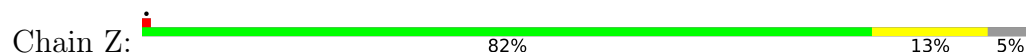




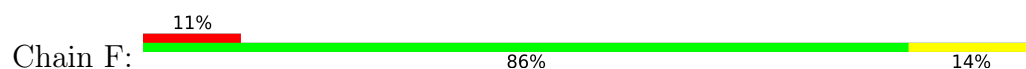
- Molecule 25: 40S ribosomal protein S21



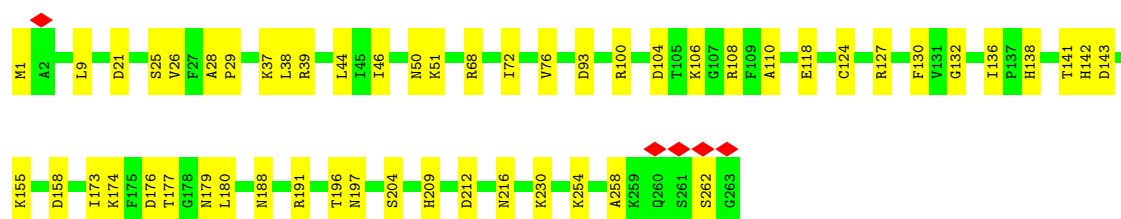
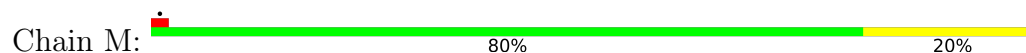
- Molecule 26: 40S ribosomal protein S24



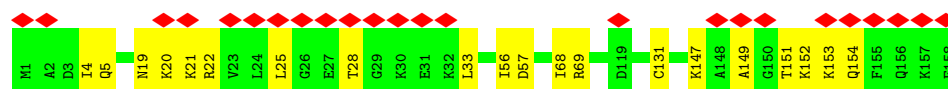
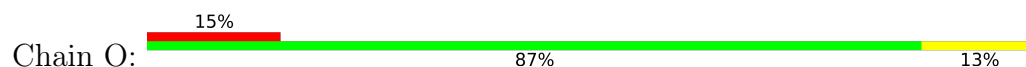
- Molecule 27: Host translation inhibitor nsp1



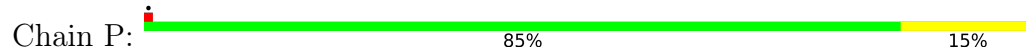
- Molecule 28: 40S ribosomal protein S4

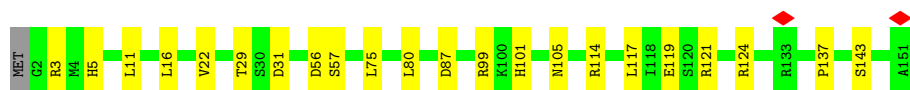


- Molecule 29: uS17



- Molecule 30: uS15

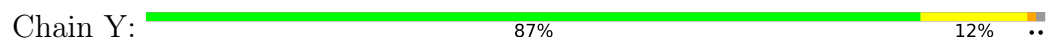




- Molecule 31: Uncharacterized protein



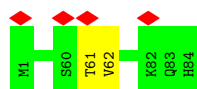
- Molecule 32: uS8



- Molecule 33: Uncharacterized protein



- Molecule 34: eS27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	353927	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.392	Depositor
Minimum map value	-2.806	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	341.75998, 341.75998, 341.75998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.83	0/40509	1.04	175/63128 (0.3%)
2	a	0.29	0/604	0.60	0/810
3	B	0.42	0/1747	0.50	0/2374
4	b	0.45	0/828	0.51	0/1109
5	C	0.40	0/1756	0.51	0/2350
6	D	0.47	0/1753	0.51	0/2369
7	d	0.27	0/490	0.49	0/656
8	E	0.33	0/1796	0.52	0/2417
9	f	0.39	0/462	0.49	0/607
10	G	0.28	0/1492	0.50	0/2005
11	g	0.28	0/567	0.54	0/753
12	H	0.36	0/1946	0.49	0/2590
13	h	0.28	0/2493	0.54	0/3394
14	I	0.36	0/1510	0.55	0/2022
15	J	0.44	0/1715	0.52	0/2287
16	K	0.44	0/1550	0.49	0/2069
17	L	0.28	0/834	0.48	0/1125
18	N	0.30	0/918	0.61	0/1233
19	Q	0.28	0/1079	0.50	0/1441
20	R	0.29	0/1146	0.52	0/1534
21	S	0.32	0/1082	0.51	0/1452
22	T	0.31	0/1208	0.59	1/1618 (0.1%)
23	U	0.27	0/1115	0.50	1/1493 (0.1%)
24	V	0.27	0/805	0.50	0/1081
25	W	0.41	0/643	0.49	0/860
26	Z	0.43	0/1028	0.51	0/1366
27	F	0.37	0/285	0.44	0/384
28	M	0.45	0/2125	0.60	0/2856
29	O	0.48	0/1319	0.63	1/1761 (0.1%)
30	P	0.42	0/1232	0.59	2/1656 (0.1%)
31	X	0.38	0/1029	0.66	0/1380
32	Y	0.49	0/1051	0.56	0/1406
33	c	0.45	0/1124	0.61	1/1500 (0.1%)
34	e	0.43	0/673	0.63	0/902

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.65	0/79914	0.85	181/115988 (0.2%)

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
3	B	0	1
5	C	0	1
8	E	0	1
28	M	0	1
29	O	0	2
30	P	0	1
31	X	0	3
33	c	0	1
34	e	0	2
All	All	0	13

There are no bond length outliers.

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	C	N1-C2-O2	13.71	127.12	118.90
1	A	501	C	C2-N1-C1'	13.53	133.69	118.80
1	A	1453	C	C2-N1-C1'	12.78	132.85	118.80
1	A	1453	C	N1-C2-O2	12.09	126.16	118.90
1	A	293	C	N1-C2-O2	10.97	125.48	118.90
1	A	501	C	N3-C2-O2	-10.57	114.50	121.90
1	A	1453	C	C6-N1-C2	-10.24	116.20	120.30
1	A	1453	C	C5-C6-N1	10.18	126.09	121.00
1	A	501	C	C6-N1-C1'	-9.91	108.91	120.80
1	A	356	C	N1-C2-O2	9.79	124.78	118.90
1	A	293	C	N3-C2-O2	-9.32	115.37	121.90
1	A	356	C	C2-N1-C1'	9.29	129.02	118.80
1	A	55	U	C2-N1-C1'	9.29	128.85	117.70
1	A	1139	C	N3-C2-O2	-9.23	115.44	121.90
1	A	853	C	C2-N1-C1'	9.22	128.95	118.80
1	A	853	C	N1-C2-O2	9.20	124.42	118.90
1	A	853	C	N3-C2-O2	-8.93	115.65	121.90
1	A	55	U	N1-C2-O2	8.78	128.95	122.80
1	A	1139	C	C2-N1-C1'	8.62	128.28	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	C	C2-N1-C1'	8.60	128.26	118.80
1	A	55	U	N3-C2-O2	-8.50	116.25	122.20
1	A	1453	C	N3-C2-O2	-8.40	116.02	121.90
1	A	73	C	N1-C2-O2	8.35	123.91	118.90
1	A	1364	U	N1-C2-O2	8.30	128.61	122.80
1	A	1453	C	C6-N1-C1'	-8.22	110.94	120.80
1	A	1624	U	C2-N1-C1'	8.18	127.52	117.70
1	A	1364	U	C2-N1-C1'	8.04	127.34	117.70
1	A	1139	C	N1-C2-O2	7.97	123.68	118.90
1	A	1453	C	C2-N3-C4	7.91	123.86	119.90
1	A	356	C	N3-C2-O2	-7.68	116.52	121.90
1	A	1520	G	C4-N9-C1'	7.68	136.49	126.50
1	A	427	U	C2-N1-C1'	7.67	126.90	117.70
1	A	1057	C	C2-N1-C1'	7.65	127.22	118.80
1	A	1303	C	C2-N1-C1'	7.55	127.10	118.80
1	A	630	U	C2-N1-C1'	7.46	126.66	117.70
1	A	501	C	C6-N1-C2	-7.37	117.35	120.30
1	A	1364	U	N3-C2-O2	-7.35	117.05	122.20
1	A	1551	U	C2-N1-C1'	7.34	126.51	117.70
1	A	1314	U	C2-N1-C1'	7.32	126.48	117.70
1	A	1520	G	N3-C4-N9	7.30	130.38	126.00
1	A	823	U	C2-N1-C1'	7.30	126.46	117.70
1	A	823	U	N3-C2-O2	-7.30	117.09	122.20
1	A	1518	C	N3-C2-O2	-7.29	116.80	121.90
1	A	75	G	N3-C4-C5	-7.19	125.00	128.60
1	A	1314	U	N1-C2-O2	7.15	127.80	122.80
1	A	1314	U	N3-C2-O2	-7.14	117.20	122.20
1	A	1139	C	C6-N1-C2	-7.02	117.49	120.30
1	A	688	U	P-O3'-C3'	7.00	128.10	119.70
1	A	49	C	N1-C2-O2	6.94	123.06	118.90
1	A	427	U	N3-C2-O2	-6.92	117.36	122.20
1	A	853	C	C6-N1-C2	-6.91	117.54	120.30
1	A	887	U	C2-N1-C1'	6.88	125.95	117.70
1	A	75	G	C2-N3-C4	6.87	115.34	111.90
1	A	1834	A	N7-C8-N9	6.87	117.23	113.80
1	A	1624	U	N1-C2-O2	6.85	127.60	122.80
1	A	1518	C	N1-C2-O2	6.84	123.00	118.90
1	A	73	C	N3-C2-O2	-6.80	117.14	121.90
1	A	356	C	C6-N1-C1'	-6.78	112.66	120.80
1	A	427	U	N1-C2-O2	6.77	127.54	122.80
1	A	1520	G	N3-C4-C5	-6.75	125.23	128.60
1	A	627	U	P-O3'-C3'	6.73	127.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	G	C4-N9-C1'	6.70	135.21	126.50
1	A	178	C	N1-C2-O2	6.68	122.91	118.90
1	A	1551	U	N1-C2-O2	6.68	127.48	122.80
1	A	752	G	P-O3'-C3'	6.67	127.70	119.70
1	A	553	U	P-O3'-C3'	6.59	127.60	119.70
1	A	501	C	C5-C6-N1	6.58	124.29	121.00
1	A	1022	U	C2-N1-C1'	6.57	125.59	117.70
1	A	402	C	C5-C6-N1	6.54	124.27	121.00
1	A	1057	C	N1-C2-O2	6.54	122.82	118.90
1	A	630	U	N1-C2-O2	6.51	127.36	122.80
1	A	1520	G	C8-N9-C1'	-6.51	118.54	127.00
1	A	1022	U	N3-C2-O2	-6.40	117.72	122.20
1	A	1022	U	N1-C2-O2	6.39	127.27	122.80
1	A	188	C	N1-C2-O2	6.38	122.72	118.90
1	A	1303	C	N1-C2-O2	6.38	122.73	118.90
30	P	11	LEU	CA-CB-CG	6.36	129.94	115.30
1	A	73	C	C2-N1-C1'	6.36	125.80	118.80
1	A	606	G	C4-N9-C1'	6.36	134.77	126.50
1	A	1660	C	C2-N1-C1'	6.31	125.74	118.80
1	A	1518	C	C2-N1-C1'	6.29	125.72	118.80
1	A	55	U	C6-N1-C1'	-6.28	112.40	121.20
1	A	75	G	N3-C4-N9	6.26	129.76	126.00
1	A	1551	U	N3-C2-O2	-6.24	117.83	122.20
1	A	659	G	C4-N9-C1'	6.23	134.60	126.50
1	A	606	G	N3-C4-N9	6.19	129.71	126.00
1	A	1834	A	C5-N7-C8	-6.18	100.81	103.90
1	A	735	C	C5-C6-N1	6.18	124.09	121.00
1	A	1852	C	N1-C2-O2	6.14	122.59	118.90
23	U	87	VAL	C-N-CA	6.14	137.04	121.70
1	A	1862	G	OP1-P-O3'	6.10	118.63	105.20
1	A	1624	U	N3-C2-O2	-6.09	117.93	122.20
1	A	1646	C	P-O3'-C3'	6.09	127.01	119.70
1	A	853	C	C6-N1-C1'	-6.07	113.52	120.80
1	A	1752	C	N1-C2-O2	6.02	122.51	118.90
1	A	402	C	C6-N1-C2	-5.99	117.90	120.30
1	A	1057	C	C6-N1-C1'	-5.91	113.71	120.80
1	A	293	C	C6-N1-C1'	-5.90	113.72	120.80
1	A	887	U	N1-C2-O2	5.89	126.92	122.80
1	A	1118	C	C2-N1-C1'	5.88	125.27	118.80
1	A	1081	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1057	C	N3-C2-O2	-5.86	117.80	121.90
1	A	1742	C	N1-C2-O2	5.86	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	G	N3-C4-C5	-5.83	125.68	128.60
1	A	659	G	C8-N9-C1'	-5.83	119.42	127.00
1	A	1660	C	N1-C2-O2	5.83	122.40	118.90
1	A	73	C	C6-N1-C2	-5.82	117.97	120.30
1	A	630	U	N3-C2-O2	-5.79	118.14	122.20
1	A	687	C	N1-C2-O2	5.79	122.38	118.90
1	A	1331	C	N1-C2-O2	5.77	122.36	118.90
1	A	823	U	N1-C2-O2	5.75	126.83	122.80
1	A	465	A	P-O3'-C3'	5.72	126.57	119.70
1	A	293	C	C6-N1-C2	-5.71	118.02	120.30
1	A	1118	C	C6-N1-C2	-5.70	118.02	120.30
1	A	1123	C	N1-C2-O2	5.69	122.31	118.90
1	A	870	A	P-O3'-C3'	5.69	126.53	119.70
1	A	183	G	C4-N9-C1'	5.68	133.89	126.50
1	A	606	G	C6-C5-N7	-5.67	127.00	130.40
1	A	1362	U	N3-C2-O2	-5.65	118.25	122.20
1	A	606	G	N3-C4-C5	-5.63	125.79	128.60
1	A	1624	U	C6-N1-C1'	-5.61	113.34	121.20
1	A	49	C	N3-C2-O2	-5.58	117.99	121.90
1	A	1518	C	C6-N1-C2	-5.56	118.08	120.30
1	A	632	C	C6-N1-C2	-5.54	118.08	120.30
1	A	606	G	C4-C5-N7	5.54	113.02	110.80
1	A	1303	C	N3-C2-O2	-5.54	118.03	121.90
1	A	183	G	N3-C4-N9	5.52	129.31	126.00
1	A	322	C	N1-C2-O2	5.51	122.21	118.90
1	A	1535	U	N1-C2-O2	5.51	126.66	122.80
30	P	22	VAL	C-N-CD	-5.51	108.48	120.60
1	A	532	C	O5'-P-OP1	5.50	117.30	110.70
1	A	914	U	N3-C2-O2	-5.48	118.36	122.20
1	A	1139	C	C6-N1-C1'	-5.48	114.22	120.80
1	A	1624	U	O4'-C1'-N1	5.47	112.58	108.20
1	A	1303	C	C6-N1-C2	-5.46	118.11	120.30
1	A	37	C	N1-C2-O2	5.45	122.17	118.90
1	A	1535	U	C2-N1-C1'	5.45	124.23	117.70
33	c	91	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	532	C	P-O3'-C3'	5.43	126.22	119.70
1	A	1865	C	C6-N1-C2	-5.43	118.13	120.30
1	A	873	G	N3-C4-C5	-5.42	125.89	128.60
1	A	188	C	N3-C2-O2	-5.41	118.11	121.90
1	A	75	G	C8-N9-C1'	-5.41	119.97	127.00
1	A	1060	A	O4'-C1'-N9	5.40	112.52	108.20
1	A	1852	C	N3-C2-O2	-5.37	118.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1364	U	C6-N1-C1'	-5.34	113.72	121.20
1	A	178	C	N3-C2-O2	-5.33	118.17	121.90
1	A	1834	A	C4-C5-N7	5.33	113.37	110.70
29	O	33	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	391	C	N1-C2-O2	5.30	122.08	118.90
1	A	191	A	OP1-P-O3'	5.29	116.85	105.20
1	A	142	C	N1-C2-O2	5.29	122.08	118.90
22	T	111	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	659	G	N3-C4-N9	5.28	129.17	126.00
1	A	427	U	C6-N1-C1'	-5.27	113.82	121.20
1	A	1842	C	C6-N1-C2	-5.27	118.19	120.30
1	A	1865	C	C2-N1-C1'	5.27	124.59	118.80
1	A	1752	C	N3-C2-O2	-5.21	118.25	121.90
1	A	1261	C	N1-C2-O2	5.20	122.02	118.90
1	A	1016	U	N3-C2-O2	-5.18	118.58	122.20
1	A	1123	C	N3-C2-O2	-5.16	118.29	121.90
1	A	49	C	C2-N1-C1'	5.15	124.46	118.80
1	A	1271	C	N1-C2-O2	5.15	121.99	118.90
1	A	1599	U	N3-C2-O2	-5.14	118.60	122.20
1	A	1067	C	N1-C2-O2	5.12	121.97	118.90
1	A	1242	U	N1-C2-O2	5.12	126.38	122.80
1	A	24	C	P-O3'-C3'	5.10	125.83	119.70
1	A	1785	C	N1-C2-O2	5.10	121.96	118.90
1	A	37	C	N3-C2-O2	-5.09	118.34	121.90
1	A	879	C	N1-C2-O2	5.09	121.95	118.90
1	A	1865	C	N3-C2-O2	-5.09	118.34	121.90
1	A	630	U	C6-N1-C1'	-5.09	114.08	121.20
1	A	14	C	N3-C2-O2	-5.07	118.35	121.90
1	A	1016	U	N1-C2-O2	5.06	126.34	122.80
1	A	930	C	N1-C2-O2	5.05	121.93	118.90
1	A	585	C	N1-C2-O2	5.05	121.93	118.90
1	A	823	U	C6-N1-C1'	-5.04	114.14	121.20
1	A	1303	C	C6-N1-C1'	-5.04	114.75	120.80
1	A	1865	C	N1-C2-O2	5.04	121.92	118.90
1	A	409	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1148	A	C2-N3-C4	-5.02	108.09	110.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	43	SER	Peptide

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Mol	Chain	Res	Type	Group
5	C	189	ILE	Peptide
8	E	41	VAL	Peptide
28	M	204	SER	Peptide
29	O	147	LYS	Peptide
29	O	4	ILE	Peptide
30	P	137	PRO	Peptide
31	X	127	GLY	Peptide
31	X	137	SER	Peptide
31	X	55	ARG	Peptide
33	c	86	PRO	Peptide
34	e	61	THR	Peptide
34	e	62	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36229	0	18300	208	0
2	a	598	0	656	0	0
3	B	1710	0	1708	13	0
4	b	814	0	867	0	0
5	C	1729	0	1803	29	0
6	D	1716	0	1806	19	0
7	d	488	0	514	0	0
8	E	1768	0	1866	21	0
9	f	457	0	502	0	0
10	G	1471	0	1522	37	0
11	g	555	0	567	0	0
12	H	1923	0	2089	29	0
13	h	2436	0	2393	0	0
14	I	1488	0	1582	15	0
15	J	1686	0	1772	23	0
16	K	1525	0	1640	20	0
17	L	810	0	836	13	0
18	N	908	0	939	18	0
19	Q	1058	0	1104	36	0
20	R	1128	0	1195	29	0
21	S	1068	0	1121	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	1190	0	1249	33	0
23	U	1097	0	1132	31	0
24	V	795	0	862	9	0
25	W	636	0	637	10	0
26	Z	1011	0	1083	13	0
27	F	280	0	250	4	0
28	M	2083	0	2189	35	0
29	O	1296	0	1374	9	0
30	P	1208	0	1294	14	0
31	X	1016	0	1039	16	0
32	Y	1034	0	1080	11	0
33	c	1106	0	1179	0	0
34	e	659	0	683	0	0
All	All	74976	0	58833	594	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 6.

All (594) 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:A:1091:C:HO2'	32:Y:2:VAL:N	1.78	0.82
1:A:925:G:H1	1:A:1017:U:H3	1.34	0.76
1:A:928:G:H1	1:A:1013:U:H3	1.38	0.72
1:A:1286:G:H21	1:A:1313:A:H62	1.44	0.65
5:C:149:GLN:HE22	5:C:154:SER:HB3	1.61	0.64
19:Q:98:ASN:ND2	19:Q:121:ILE:O	2.31	0.63
1:A:1497:G:N7	17:L:25:LYS:NZ	2.46	0.63
8:E:49:ILE:HG12	8:E:87:TYR:HB2	1.80	0.63
1:A:1547:C:H1'	1:A:1670:C:H4'	1.81	0.63
6:D:196:ILE:HB	6:D:223:TYR:HB2	1.81	0.62
14:I:53:VAL:HG21	14:I:172:THR:HA	1.81	0.62
5:C:224:GLU:HG3	5:C:227:LYS:H	1.64	0.62
1:A:1693:G:H21	1:A:1834:A:H8	1.48	0.61
10:G:72:LEU:HD11	10:G:154:LEU:HD11	1.82	0.61
16:K:121:LYS:H	16:K:125:HIS:HD2	1.46	0.61
21:S:31:ASN:OD1	21:S:31:ASN:N	2.34	0.60
1:A:1834:A:H2	1:A:1837:G:H1	1.50	0.60
29:O:25:LEU:H	29:O:28:THR:HG23	1.67	0.60
21:S:31:ASN:HA	21:S:34:VAL:HB	1.83	0.59
1:A:64:A:H2	1:A:83:A:H62	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:G:N7	23:U:101:ARG:NH2	2.50	0.59
12:H:98:ARG:NH2	12:H:103:ASP:OD1	2.34	0.59
29:O:149:ALA:HB1	29:O:152:LYS:HE3	1.85	0.59
1:A:1450:G:H5''	21:S:33:ARG:HH22	1.68	0.59
28:M:100:ARG:NH2	28:M:118:GLU:O	2.36	0.59
1:A:1473:G:H2'	1:A:1475:G:H22	1.67	0.59
1:A:94:G:OP2	28:M:1:MET:N	2.32	0.59
1:A:583:A:OP1	16:K:162:ARG:NH2	2.36	0.59
31:X:34:PHE:HB3	31:X:41:PHE:HB2	1.85	0.59
1:A:1024:A:OP2	30:P:124:ARG:NH2	2.33	0.58
3:B:77:ILE:HG12	3:B:99:ILE:HB	1.85	0.58
20:R:132:PHE:O	20:R:140:ARG:NH2	2.36	0.58
17:L:91:PRO:HD2	17:L:94:LEU:HD12	1.85	0.58
8:E:28:GLU:HG2	17:L:61:GLN:HG2	1.86	0.58
1:A:1605:G:OP1	23:U:84:ARG:NH2	2.37	0.58
23:U:13:GLU:HA	23:U:16:ARG:HE	1.67	0.58
28:M:21:ASP:N	28:M:21:ASP:OD1	2.37	0.58
1:A:1259:A:N6	1:A:1519:U:OP1	2.34	0.58
10:G:92:ILE:HG23	10:G:170:ALA:HA	1.85	0.58
17:L:29:MET:SD	17:L:42:ASN:ND2	2.77	0.58
6:D:171:GLY:O	32:Y:98:GLN:NE2	2.37	0.58
1:A:1674:G:OP1	10:G:51:HIS:NE2	2.37	0.57
1:A:1543:U:OP2	23:U:62:ARG:NH1	2.33	0.57
19:Q:44:ARG:NH1	19:Q:82:ASP:O	2.37	0.57
1:A:659:G:HO2'	1:A:662:G:HO2'	1.53	0.57
18:N:95:ASP:HB3	18:N:100:PRO:HA	1.86	0.57
1:A:1568:C:O2	1:A:1627:C:O2'	2.23	0.57
1:A:1005:G:OP2	5:C:162:ARG:NH1	2.38	0.57
1:A:1414:A:N6	1:A:1425:G:O6	2.38	0.57
1:A:1658:G:OP2	1:A:1660:C:N4	2.38	0.57
26:Z:21:LYS:HD2	26:Z:75:ILE:HD11	1.87	0.57
1:A:1299:A:OP2	19:Q:59:ARG:NH2	2.38	0.56
19:Q:18:ARG:NH1	19:Q:36:LEU:O	2.38	0.56
1:A:1587:G:H1	23:U:74:SER:HG	1.52	0.56
3:B:13:GLU:HA	3:B:16:LEU:HD12	1.87	0.56
20:R:110:ASP:HA	20:R:113:ILE:HB	1.88	0.56
1:A:1515:G:N2	19:Q:99:GLY:O	2.36	0.56
14:I:51:ILE:HG21	14:I:179:LYS:HG2	1.87	0.56
5:C:60:ASP:OD1	5:C:60:ASP:N	2.38	0.56
28:M:173:ILE:HG23	28:M:230:LYS:HE3	1.86	0.56
1:A:1261:C:OP1	1:A:1518:C:N4	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:G:N2	1:A:1569:A:OP2	2.35	0.56
14:I:34:SER:O	14:I:37:LYS:NZ	2.38	0.56
8:E:134:CYS:SG	8:E:135:GLU:N	2.79	0.56
10:G:50:PRO:HB3	10:G:69:VAL:HG13	1.87	0.56
24:V:38:ASP:HB2	24:V:41:ARG:HH21	1.70	0.56
28:M:158:ASP:OD1	28:M:158:ASP:N	2.38	0.56
15:J:89:GLU:OE2	15:J:92:ARG:NH2	2.38	0.56
28:M:197:ASN:HB3	28:M:209:HIS:HB2	1.86	0.56
8:E:45:ARG:NH2	8:E:82:GLY:O	2.38	0.56
19:Q:81:ARG:NH2	19:Q:117:GLY:O	2.39	0.56
5:C:33:VAL:HG13	5:C:44:ILE:HB	1.88	0.55
5:C:150:ILE:HD13	21:S:129:LYS:HB2	1.88	0.55
30:P:5:HIS:HD2	30:P:121:ARG:HE	1.54	0.55
14:I:117:PRO:HG2	14:I:120:ARG:HD3	1.89	0.55
22:T:35:GLY:O	22:T:97:GLN:NE2	2.39	0.55
1:A:126:G:OP1	12:H:198:ARG:NH2	2.39	0.55
19:Q:41:GLN:NE2	19:Q:113:GLY:O	2.39	0.55
19:Q:81:ARG:NH1	19:Q:97:TYR:O	2.37	0.55
1:A:1646:C:O5'	20:R:138:ARG:NH1	2.39	0.55
23:U:72:VAL:HG21	23:U:101:ARG:HG3	1.89	0.55
23:U:111:LYS:HB2	23:U:126:GLN:HE21	1.72	0.55
19:Q:136:THR:H	19:Q:139:SER:HB2	1.72	0.55
22:T:25:LYS:HE3	22:T:53:THR:HA	1.89	0.55
1:A:146:G:OP1	12:H:143:LYS:NZ	2.39	0.55
1:A:1628:C:OP1	23:U:38:LYS:NZ	2.40	0.55
1:A:1678:A:H62	10:G:57:ALA:HB1	1.72	0.55
25:W:74:LYS:O	25:W:81:LYS:NZ	2.39	0.55
8:E:154:ASP:OD1	8:E:154:ASP:N	2.40	0.54
21:S:99:ASP:OD1	21:S:99:ASP:N	2.36	0.54
22:T:138:THR:HA	22:T:141:ARG:HH21	1.70	0.54
1:A:952:G:H21	31:X:52:THR:HG21	1.71	0.54
1:A:1647:A:OP1	20:R:138:ARG:NH2	2.40	0.54
22:T:75:ARG:HH22	22:T:94:LYS:HB3	1.72	0.54
1:A:1719:A:N6	1:A:1814:G:O2'	2.40	0.54
5:C:182:LYS:O	5:C:186:ASN:ND2	2.40	0.54
19:Q:100:LYS:HG3	19:Q:101:THR:HG23	1.90	0.54
22:T:2:SER:OG	22:T:3:LEU:N	2.39	0.54
17:L:53:LYS:HB3	17:L:58:VAL:HG23	1.90	0.54
19:Q:23:ASP:HA	19:Q:26:LEU:HD23	1.88	0.54
22:T:98:VAL:HB	22:T:103:LEU:HD13	1.90	0.54
1:A:561:A:H5'	16:K:171:GLY:HA3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:211:GLU:HA	3:B:214:GLU:HB2	1.89	0.54
12:H:118:GLU:HG2	12:H:119:LYS:HG3	1.90	0.54
19:Q:28:MET:SD	19:Q:32:GLN:NE2	2.81	0.54
10:G:24:SER:O	10:G:107:ASN:ND2	2.41	0.54
1:A:587:A:H5'	1:A:592:C:H41	1.72	0.54
8:E:172:VAL:O	8:E:173:ARG:NH1	2.41	0.53
10:G:25:THR:OG1	10:G:41:VAL:O	2.26	0.53
22:T:13:LEU:HB2	22:T:20:ILE:HG13	1.90	0.53
1:A:1678:A:N6	10:G:57:ALA:O	2.42	0.53
20:R:101:ASP:OD2	20:R:104:SER:N	2.42	0.53
27:F:171:ARG:NH2	27:F:172:GLU:OE2	2.41	0.53
31:X:30:VAL:HG12	31:X:94:HIS:HB2	1.90	0.53
1:A:1455:A:H4'	21:S:28:PHE:HB2	1.89	0.53
1:A:1808:U:H2'	1:A:1809:A:H8	1.73	0.53
8:E:132:LYS:HE3	8:E:191:PRO:HA	1.89	0.53
28:M:127:ARG:HD3	28:M:142:HIS:HA	1.90	0.53
28:M:176:ASP:OD1	28:M:179:ASN:ND2	2.40	0.53
1:A:1521:C:OP1	22:T:124:ARG:NH1	2.39	0.53
10:G:127:ARG:NH2	10:G:128:ILE:O	2.41	0.53
22:T:22:GLY:O	22:T:57:GLY:N	2.41	0.53
1:A:847:A:O2'	28:M:106:LYS:NZ	2.41	0.53
10:G:89:THR:HA	10:G:92:ILE:HD12	1.91	0.53
22:T:27:ALA:HB2	22:T:52:LEU:HB3	1.91	0.53
1:A:351:G:OP1	15:J:7:ASN:ND2	2.40	0.53
1:A:1115:U:H1'	1:A:1116:C:H2'	1.90	0.53
19:Q:13:ARG:NH1	19:Q:14:LYS:O	2.41	0.53
30:P:29:THR:OG1	30:P:31:ASP:OD1	2.27	0.53
3:B:85:ARG:NH1	3:B:203:PHE:O	2.42	0.53
15:J:134:GLU:O	15:J:138:ASN:ND2	2.40	0.53
1:A:1334:G:H5'	8:E:140:GLY:HA2	1.90	0.52
23:U:122:LYS:NZ	23:U:123:LEU:O	2.38	0.52
30:P:87:ASP:OD1	30:P:87:ASP:N	2.41	0.52
1:A:1564:C:OP1	23:U:121:ARG:NH1	2.43	0.52
1:A:1545:A:N6	1:A:1655:C:O2'	2.42	0.52
14:I:53:VAL:HG23	14:I:175:GLY:HA3	1.91	0.52
18:N:113:ASP:OD2	18:N:113:ASP:N	2.41	0.52
19:Q:33:LEU:HA	19:Q:36:LEU:HB2	1.92	0.52
1:A:433:A:H5''	15:J:22:HIS:HB3	1.91	0.52
1:A:1358:U:OP2	6:D:123:ARG:NH1	2.43	0.52
1:A:1461:G:H3'	1:A:1463:U:H3	1.75	0.52
18:N:58:GLU:HB3	18:N:61:TYR:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:8:GLN:HB3	20:R:95:TYR:HE1	1.74	0.52
31:X:103:ASN:ND2	31:X:140:THR:O	2.42	0.52
14:I:60:ILE:HB	14:I:92:VAL:HG12	1.91	0.52
26:Z:114:MET:O	26:Z:122:LYS:NZ	2.42	0.52
3:B:142:LEU:O	25:W:60:ARG:NH2	2.43	0.52
1:A:888:U:H2'	1:A:889:U:H4'	1.91	0.52
1:A:1506:A:H4'	1:A:1507:G:H3'	1.90	0.52
1:A:1678:A:OP1	10:G:145:ARG:NH1	2.43	0.52
21:S:77:GLU:O	21:S:81:ARG:NH2	2.42	0.52
28:M:177:THR:HG23	28:M:196:THR:HA	1.92	0.52
15:J:88:ASN:HB3	15:J:205:ARG:HH21	1.75	0.51
16:K:95:ASP:OD2	16:K:95:ASP:N	2.43	0.51
10:G:75:SER:HG	10:G:155:CYS:HG	1.58	0.51
15:J:139:LYS:O	15:J:141:ARG:NH2	2.44	0.51
3:B:76:VAL:HG12	3:B:123:VAL:HB	1.93	0.51
23:U:22:LEU:HD13	23:U:28:LEU:HD21	1.92	0.51
26:Z:80:ASP:OD1	26:Z:80:ASP:N	2.40	0.51
1:A:522:A:OP2	16:K:45:ARG:NH2	2.39	0.51
18:N:81:ASP:O	18:N:84:LYS:NZ	2.42	0.51
23:U:77:LYS:HE2	23:U:94:ARG:HH22	1.76	0.51
1:A:1552:G:OP1	1:A:1578:U:N3	2.44	0.51
6:D:95:ASP:OD1	6:D:95:ASP:N	2.39	0.51
10:G:37:ASP:OD1	10:G:44:LYS:NZ	2.42	0.51
1:A:1252:C:N4	20:R:146:ARG:OXT	2.44	0.51
18:N:85:LEU:HA	18:N:88:TRP:HB2	1.92	0.51
1:A:1753:C:H2'	1:A:1754:G:H8	1.75	0.51
16:K:136:ARG:HD3	16:K:160:SER:HA	1.93	0.51
1:A:1285:G:N1	18:N:57:ASP:O	2.41	0.51
1:A:1299:A:O2'	1:A:1301:A:OP1	2.28	0.51
17:L:91:PRO:HB2	17:L:93:THR:HG22	1.91	0.51
26:Z:86:GLU:OE2	26:Z:90:ARG:NH1	2.43	0.51
8:E:61:GLU:H	8:E:64:ARG:HB3	1.76	0.51
10:G:55:ARG:O	10:G:62:ARG:NH1	2.44	0.51
12:H:23:LYS:NZ	12:H:40:ALA:O	2.44	0.51
3:B:36:GLN:O	3:B:53:ARG:NH1	2.44	0.50
17:L:37:ASP:N	17:L:37:ASP:OD1	2.44	0.50
18:N:87:GLU:OE1	18:N:96:ARG:NH2	2.43	0.50
19:Q:96:VAL:HB	19:Q:116:LEU:HD12	1.93	0.50
1:A:1236:G:O2'	19:Q:131:PRO:O	2.23	0.50
1:A:1355:C:O3'	6:D:238:LYS:NZ	2.44	0.50
1:A:1555:U:H4'	1:A:1556:A:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:176:LYS:O	6:D:200:ARG:NH1	2.40	0.50
14:I:69:LEU:HD22	14:I:96:ALA:HB2	1.92	0.50
1:A:507:G:O6	26:Z:105:LYS:NZ	2.43	0.50
1:A:924:G:OP2	30:P:3:ARG:NH1	2.45	0.50
15:J:73:THR:O	15:J:74:ARG:NH1	2.43	0.50
17:L:95:ARG:HH11	17:L:96:ARG:HG2	1.76	0.50
28:M:130:PHE:HB2	28:M:138:HIS:HB2	1.91	0.50
1:A:1259:A:O2'	1:A:1263:U:N3	2.44	0.50
1:A:1622:U:OP1	22:T:120:HIS:ND1	2.33	0.50
15:J:11:ARG:NH1	15:J:15:GLY:O	2.44	0.50
22:T:103:LEU:HA	22:T:106:LYS:HB2	1.93	0.50
8:E:31:GLU:HA	8:E:107:TYR:HE2	1.76	0.50
10:G:14:THR:HG1	10:G:48:TYR:HH	1.58	0.50
10:G:123:GLU:OE1	10:G:204:ARG:NH1	2.45	0.50
12:H:43:GLU:OE2	12:H:119:LYS:NZ	2.45	0.50
1:A:1665:G:OP1	23:U:91:HIS:NE2	2.40	0.50
12:H:19:ASP:OD1	12:H:19:ASP:N	2.38	0.50
8:E:51:LEU:HB3	8:E:91:VAL:HG12	1.94	0.50
10:G:51:HIS:O	20:R:82:TYR:OH	2.30	0.50
22:T:65:GLU:HA	22:T:68:ILE:HG12	1.93	0.50
28:M:176:ASP:OD1	28:M:176:ASP:N	2.45	0.50
10:G:18:LYS:HB2	10:G:24:SER:HA	1.93	0.50
24:V:49:LYS:NZ	24:V:92:HIS:O	2.44	0.50
25:W:71:ARG:HH12	32:Y:23:ARG:HH21	1.58	0.50
22:T:46:ARG:HB3	23:U:35:ASP:HB2	1.93	0.49
28:M:104:ASP:HB3	28:M:110:ALA:HB2	1.93	0.49
18:N:116:LYS:HA	18:N:121:LYS:HE3	1.94	0.49
31:X:131:ASP:OD2	31:X:131:ASP:N	2.45	0.49
1:A:1283:C:O2'	1:A:1313:A:N1	2.39	0.49
22:T:109:GLU:HG3	22:T:113:ARG:HH21	1.78	0.49
31:X:20:GLN:NE2	31:X:21:VAL:O	2.45	0.49
1:A:446:G:OP2	15:J:47:ARG:NH1	2.41	0.49
1:A:1444:U:OP1	20:R:15:ARG:NH2	2.46	0.49
16:K:136:ARG:NH1	16:K:159:PHE:O	2.44	0.49
30:P:31:ASP:OD1	30:P:31:ASP:N	2.40	0.49
1:A:1232:U:H2'	1:A:1233:G:H8	1.78	0.49
8:E:42:THR:HG23	8:E:45:ARG:HB3	1.95	0.49
12:H:30:LYS:HG2	12:H:34:THR:HG21	1.94	0.49
1:A:945:U:H1'	31:X:140:THR:HG21	1.94	0.49
3:B:63:ARG:NH1	25:W:37:ALA:O	2.46	0.49
5:C:52:THR:HG23	5:C:57:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:72:ASP:O	6:D:74:LYS:NZ	2.46	0.49
20:R:45:ARG:NH2	23:U:10:ASN:OD1	2.45	0.49
1:A:496:C:H5'	28:M:29:PRO:HA	1.94	0.49
14:I:82:GLU:HA	14:I:85:LYS:HG2	1.94	0.49
18:N:52:LEU:HD13	18:N:65:VAL:HG11	1.95	0.49
22:T:34:LYS:HB3	22:T:100:ALA:HA	1.95	0.49
1:A:560:A:H5'	16:K:174:LYS:HB2	1.95	0.49
1:A:570:C:O2'	26:Z:34:THR:O	2.27	0.49
12:H:74:ARG:NH1	12:H:96:SER:OG	2.45	0.49
30:P:75:LEU:HD12	30:P:80:LEU:HB2	1.94	0.49
5:C:63:LYS:HE2	5:C:90:ASP:HA	1.95	0.49
6:D:106:VAL:H	27:F:178:ASN:HD21	1.61	0.49
22:T:26:ILE:HD12	22:T:29:ALA:HB3	1.95	0.49
29:O:19:ASN:OD1	29:O:22:ARG:NH2	2.41	0.49
1:A:495:U:H4'	28:M:25:SER:HB2	1.93	0.48
1:A:1013:U:OP1	1:A:1129:G:O2'	2.31	0.48
32:Y:66:THR:OG1	32:Y:67:GLY:N	2.46	0.48
1:A:1550:G:H3'	1:A:1579:A:H61	1.77	0.48
1:A:1628:C:O2'	22:T:82:TRP:O	2.26	0.48
19:Q:50:ARG:O	19:Q:54:HIS:ND1	2.44	0.48
28:M:46:ILE:HA	28:M:50:ASN:HD22	1.78	0.48
1:A:183:G:O2'	1:A:184:G:O4'	2.31	0.48
1:A:1623:A:H5''	22:T:133:GLY:HA3	1.95	0.48
5:C:33:VAL:HG22	5:C:44:ILE:HD12	1.94	0.48
5:C:129:THR:OG1	5:C:131:ASP:O	2.30	0.48
24:V:26:SER:HB2	24:V:110:VAL:HA	1.95	0.48
6:D:144:SER:OG	6:D:145:LYS:N	2.45	0.48
1:A:142:C:N4	1:A:329:G:OP2	2.47	0.48
1:A:1616:U:OP2	19:Q:43:ARG:NH2	2.46	0.48
15:J:6:ASP:OD1	15:J:6:ASP:N	2.44	0.48
20:R:113:ILE:HD11	20:R:120:LEU:HD12	1.95	0.48
1:A:17:C:O2'	1:A:1194:A:N1	2.40	0.48
1:A:1580:A:OP1	24:V:86:LYS:NZ	2.40	0.48
8:E:69:LEU:HA	8:E:72:VAL:HG22	1.95	0.48
1:A:1275:G:O2'	1:A:1321:G:N2	2.46	0.48
1:A:1553:C:O2'	1:A:1554:C:O4'	2.30	0.48
6:D:271:ASP:OD2	6:D:271:ASP:N	2.44	0.48
8:E:66:ILE:O	8:E:70:THR:OG1	2.25	0.48
15:J:158:ILE:HD11	15:J:163:GLU:HB3	1.95	0.48
1:A:1542:C:H4'	23:U:11:GLN:HB2	1.95	0.48
3:B:126:ASP:OD1	3:B:165:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:P:99:ARG:HH12	30:P:143:SER:HB3	1.79	0.48
1:A:377:G:H5'	15:J:98:LYS:HB3	1.96	0.48
1:A:1533:A:OP2	10:G:164:ARG:NH2	2.40	0.48
32:Y:86:LEU:HD21	32:Y:113:HIS:HB2	1.96	0.48
15:J:113:TYR:OH	15:J:156:ALA:O	2.30	0.47
1:A:1524:G:OP2	22:T:141:ARG:NH1	2.45	0.47
1:A:441:C:OP2	15:J:2:GLY:N	2.47	0.47
1:A:744:G:N2	1:A:797:C:O2	2.42	0.47
1:A:1139:C:H5	1:A:1149:A:H62	1.61	0.47
19:Q:136:THR:OG1	19:Q:139:SER:N	2.48	0.47
29:O:152:LYS:HG2	29:O:154:GLN:HE21	1.78	0.47
1:A:1401:A:H4'	24:V:52:GLY:HA3	1.97	0.47
1:A:1617:G:N1	1:A:1620:A:OP2	2.47	0.47
8:E:211:VAL:H	21:S:39:ALA:HA	1.80	0.47
15:J:57:ALA:HB2	15:J:183:GLY:HA2	1.96	0.47
18:N:41:ALA:O	18:N:46:GLN:NE2	2.48	0.47
20:R:106:LYS:HA	20:R:109:LYS:HB3	1.96	0.47
28:M:124:CYS:HB3	28:M:141:THR:HB	1.96	0.47
10:G:14:THR:HB	10:G:17:ILE:HG23	1.97	0.47
1:A:1560:U:O2'	1:A:1583:C:O2'	2.32	0.47
1:A:1617:G:N7	19:Q:47:ARG:NH1	2.58	0.47
6:D:113:GLN:NE2	6:D:120:GLN:OE1	2.48	0.47
6:D:220:ASP:OD1	6:D:220:ASP:N	2.44	0.47
12:H:162:LEU:HD21	12:H:172:LYS:HD2	1.97	0.47
1:A:156:G:OP1	12:H:2:LYS:NZ	2.40	0.47
1:A:1649:U:OP1	20:R:128:GLU:N	2.47	0.47
5:C:34:LYS:O	5:C:98:THR:OG1	2.31	0.47
10:G:45:TYR:HB3	10:G:67:PRO:HD3	1.95	0.47
17:L:93:THR:HG23	17:L:94:LEU:HG	1.97	0.47
19:Q:29:SER:HB3	19:Q:32:GLN:HG2	1.95	0.47
1:A:317:C:OP2	12:H:183:ARG:NH2	2.47	0.47
1:A:1324:G:O2'	1:A:1510:G:O2'	2.22	0.47
1:A:1477:U:H5'	21:S:3:ARG:HH21	1.79	0.47
1:A:1237:C:O2'	19:Q:128:HIS:ND1	2.36	0.47
21:S:47:ARG:HA	21:S:50:ILE:HB	1.97	0.47
1:A:1255:G:OP1	1:A:1256:G:O2'	2.32	0.46
12:H:31:ARG:HB3	12:H:101:ILE:HD13	1.97	0.46
17:L:14:LEU:HA	17:L:17:LYS:HB3	1.97	0.46
23:U:49:ASP:HB3	23:U:52:TRP:HB3	1.96	0.46
25:W:15:ARG:NH1	25:W:33:GLN:OE1	2.46	0.46
1:A:53:C:O2'	1:A:507:G:N7	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:G:O2'	1:A:77:A:OP1	2.34	0.46
1:A:983:A:H2	31:X:139:SER:HB2	1.80	0.46
14:I:154:ILE:HB	14:I:185:VAL:HG23	1.97	0.46
15:J:162:LEU:HD11	15:J:191:GLU:HG2	1.96	0.46
18:N:77:ILE:HD13	18:N:127:TYR:HE2	1.78	0.46
23:U:22:LEU:HD22	23:U:28:LEU:HD11	1.97	0.46
24:V:20:ILE:HB	24:V:91:LEU:HB2	1.98	0.46
26:Z:55:ILE:HG23	26:Z:75:ILE:HG22	1.97	0.46
28:M:174:LYS:O	28:M:179:ASN:ND2	2.48	0.46
14:I:159:ASP:OD1	14:I:159:ASP:N	2.45	0.46
20:R:58:LEU:HD21	20:R:112:LEU:HG	1.97	0.46
25:W:73:ALA:HB1	25:W:78:ILE:HB	1.97	0.46
1:A:1519:U:O2	22:T:135:HIS:NE2	2.46	0.46
18:N:81:ASP:HB3	18:N:84:LYS:HG2	1.97	0.46
20:R:112:LEU:HD13	20:R:119:LEU:HD13	1.96	0.46
1:A:1560:U:HO2'	1:A:1583:C:HO2'	1.63	0.46
1:A:1562:C:H4'	23:U:120:GLY:H	1.80	0.46
1:A:1707:U:O2	1:A:1849:G:N2	2.47	0.46
15:J:132:GLU:O	15:J:136:ILE:N	2.44	0.46
1:A:1649:U:H2'	1:A:1650:A:C8	2.51	0.46
20:R:44:PRO:HB2	20:R:46:THR:HG22	1.97	0.46
21:S:101:ASP:OD2	21:S:101:ASP:N	2.47	0.46
1:A:168:C:OP1	12:H:131:ARG:NE	2.43	0.46
5:C:146:ARG:HH11	5:C:206:PRO:HG3	1.81	0.46
28:M:38:LEU:HD23	28:M:39:ARG:HD3	1.98	0.46
31:X:86:LYS:NZ	31:X:122:SER:O	2.47	0.46
1:A:1465:A:OP1	21:S:60:ARG:NH1	2.49	0.46
17:L:52:LEU:HG	17:L:57:TYR:HB2	1.98	0.46
16:K:121:LYS:H	16:K:125:HIS:CD2	2.32	0.45
21:S:43:SER:HB3	21:S:46:LEU:HB2	1.97	0.45
32:Y:27:ILE:HG12	32:Y:61:ILE:HB	1.98	0.45
1:A:1529:C:H1'	1:A:1665:G:H21	1.81	0.45
10:G:35:LEU:HD12	10:G:117:ILE:HG12	1.99	0.45
28:M:9:LEU:HB3	28:M:28:ALA:HB3	1.98	0.45
1:A:1645:C:H5'	20:R:139:ALA:HA	1.98	0.45
6:D:121:ARG:HH12	6:D:123:ARG:HD3	1.82	0.45
10:G:154:LEU:HD13	10:G:177:LEU:HD21	1.98	0.45
31:X:23:GLU:H	31:X:23:GLU:HG3	1.63	0.45
31:X:36:SER:OG	31:X:37:PHE:N	2.49	0.45
3:B:37:TYR:OH	3:B:57:LYS:NZ	2.44	0.45
5:C:123:ALA:HB2	5:C:165:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:204:ILE:O	6:D:211:LYS:NZ	2.46	0.45
20:R:7:LEU:O	20:R:99:TYR:OH	2.28	0.45
1:A:146:G:O2'	1:A:147:A:O5'	2.34	0.45
10:G:14:THR:O	10:G:18:LYS:NZ	2.48	0.45
22:T:20:ILE:HB	22:T:24:ARG:HH22	1.81	0.45
23:U:9:VAL:HG22	23:U:139:ALA:HB2	1.98	0.45
24:V:38:ASP:O	24:V:42:GLY:N	2.47	0.45
30:P:56:ASP:OD1	30:P:57:SER:N	2.50	0.45
1:A:1298:G:H4'	19:Q:78:THR:HA	1.98	0.45
16:K:107:GLU:O	16:K:113:GLN:NE2	2.49	0.45
1:A:104:A:H62	1:A:356:C:H5	1.65	0.45
1:A:581:U:H4'	26:Z:66:GLY:HA3	1.98	0.45
1:A:934:G:H22	1:A:1008:A:H2	1.64	0.45
12:H:20:ASP:OD2	12:H:23:LYS:N	2.45	0.45
22:T:21:ASP:O	22:T:24:ARG:NH2	2.49	0.45
1:A:1566:G:H1	23:U:97:LYS:HE3	1.82	0.45
1:A:1585:U:O2'	1:A:1587:G:OP2	2.34	0.45
16:K:179:LYS:O	16:K:183:GLY:N	2.40	0.45
1:A:1627:C:H5''	23:U:41:LYS:HZ3	1.81	0.45
10:G:122:ARG:N	10:G:197:GLU:OE2	2.48	0.45
32:Y:112:ASP:OD1	32:Y:112:ASP:N	2.50	0.45
1:A:198:U:O2'	1:A:201:C:N4	2.51	0.44
5:C:107:ARG:NH1	31:X:133:THR:O	2.50	0.44
16:K:67:ASP:OD2	16:K:70:ARG:N	2.45	0.44
26:Z:27:VAL:HG11	26:Z:35:VAL:HG11	2.00	0.44
1:A:816:A:OP2	16:K:10:ARG:NH2	2.51	0.44
1:A:495:U:O2'	28:M:25:SER:OG	2.30	0.44
1:A:1786:U:H2'	1:A:1787:G:H8	1.82	0.44
5:C:139:CYS:SG	5:C:140:VAL:N	2.90	0.44
18:N:86:GLY:HA2	18:N:106:CYS:H	1.83	0.44
31:X:63:LYS:HA	31:X:63:LYS:HD3	1.81	0.44
1:A:72:C:O2'	1:A:74:G:OP2	2.35	0.44
5:C:128:LYS:HE2	5:C:132:GLY:HA2	2.00	0.44
5:C:129:THR:OG1	5:C:131:ASP:OD1	2.29	0.44
6:D:149:THR:HG22	6:D:152:ARG:HH12	1.83	0.44
12:H:64:LYS:HZ3	12:H:82:SER:HB3	1.83	0.44
18:N:45:ARG:HA	18:N:45:ARG:HD3	1.88	0.44
10:G:71:ARG:HH11	10:G:151:ILE:HD12	1.83	0.44
23:U:38:LYS:HE3	23:U:38:LYS:HB2	1.77	0.44
29:O:151:THR:HG23	29:O:153:LYS:HE2	1.98	0.44
1:A:1808:U:H2'	1:A:1809:A:C8	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:24:LEU:HD12	21:S:24:LEU:HA	1.88	0.44
1:A:67:C:H41	12:H:163:ASN:HA	1.83	0.44
1:A:792:C:H2'	1:A:793:G:C8	2.53	0.44
1:A:1565:C:H2'	1:A:1566:G:H8	1.82	0.44
10:G:14:THR:O	10:G:48:TYR:OH	2.36	0.44
20:R:83:ALA:O	20:R:87:SER:OG	2.29	0.44
22:T:14:ARG:HH21	22:T:19:ASN:HD21	1.66	0.44
1:A:380:G:P	15:J:56:ARG:HH22	2.41	0.43
1:A:1734:G:O2'	1:A:1800:A:N6	2.50	0.43
20:R:86:GLN:HE22	20:R:122:ALA:HB2	1.82	0.43
1:A:381:C:OP2	15:J:54:LYS:NZ	2.39	0.43
1:A:874:G:H2'	1:A:875:A:C8	2.53	0.43
1:A:1114:U:H3	1:A:1119:A:H61	1.66	0.43
1:A:1513:C:H2'	1:A:1514:G:H8	1.83	0.43
18:N:54:SER:HB2	18:N:80:ASP:HA	2.00	0.43
21:S:31:ASN:ND2	21:S:55:THR:OG1	2.51	0.43
28:M:258:ALA:O	28:M:262:SER:OG	2.37	0.43
1:A:1294:G:H2'	1:A:1295:A:H8	1.84	0.43
1:A:1719:A:N6	1:A:1720:U:O2	2.50	0.43
3:B:205:ARG:NH2	21:S:81:ARG:O	2.51	0.43
8:E:214:LYS:HD2	8:E:214:LYS:HA	1.81	0.43
28:M:44:LEU:HD13	28:M:72:ILE:HD11	2.01	0.43
1:A:996:A:OP1	30:P:114:ARG:NH1	2.51	0.43
1:A:1549:U:OP2	8:E:8:LYS:NZ	2.50	0.43
15:J:103:LEU:HD23	15:J:103:LEU:HA	1.90	0.43
17:L:14:LEU:HD22	17:L:35:LEU:HD21	2.01	0.43
19:Q:15:PHE:HB3	19:Q:22:LEU:HD21	1.99	0.43
26:Z:103:SER:H	26:Z:106:GLN:HE21	1.67	0.43
1:A:560:A:OP1	16:K:174:LYS:NZ	2.52	0.43
1:A:1590:C:H42	20:R:77:HIS:HE1	1.67	0.43
10:G:184:SER:OG	10:G:186:ASN:OD1	2.34	0.43
1:A:1624:U:H3	19:Q:40:ARG:HH22	1.66	0.43
1:A:1649:U:H2'	1:A:1650:A:H8	1.84	0.43
25:W:14:PRO:HG2	25:W:23:ILE:HD12	2.01	0.43
10:G:124:ASP:N	10:G:124:ASP:OD1	4.15	0.43
18:N:68:LEU:HB2	18:N:71:GLU:HG2	2.00	0.43
22:T:20:ILE:HG22	22:T:32:ALA:HB3	2.00	0.43
24:V:51:LYS:HA	24:V:51:LYS:HD3	1.74	0.43
31:X:85:CYS:SG	31:X:86:LYS:N	2.92	0.43
1:A:448:A:H5''	15:J:25:ARG:HA	2.01	0.43
1:A:753:C:O2'	1:A:754:G:O4'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:C:H2'	1:A:1526:G:H8	1.84	0.43
5:C:144:LYS:HD3	5:C:208:HIS:HB3	2.00	0.43
10:G:49:LEU:HD13	20:R:47:LEU:HA	2.01	0.43
22:T:111:LEU:O	22:T:115:LYS:N	2.52	0.43
30:P:5:HIS:HB3	30:P:117:LEU:HD13	2.00	0.43
1:A:793:G:H2'	1:A:794:A:H8	1.83	0.43
1:A:1033:G:N1	1:A:1080:A:O2'	2.43	0.43
28:M:143:ASP:OD1	28:M:143:ASP:N	2.45	0.43
1:A:756:C:O2	1:A:788:G:N2	2.51	0.42
8:E:14:ASP:OD2	8:E:14:ASP:N	2.52	0.42
14:I:101:LEU:O	14:I:116:ARG:NH1	2.52	0.42
23:U:134:ILE:HD13	23:U:134:ILE:HA	1.88	0.42
26:Z:53:ASP:OD1	26:Z:53:ASP:N	2.51	0.42
1:A:1514:G:H2'	1:A:1515:G:H8	1.84	0.42
10:G:72:LEU:HD12	10:G:151:ILE:HG23	2.01	0.42
14:I:133:LEU:HD23	14:I:133:LEU:HA	1.85	0.42
30:P:101:HIS:CE1	30:P:105:ASN:HD22	2.36	0.42
1:A:1302:G:H1	1:A:1307:U:H3	1.66	0.42
1:A:1488:C:O2'	1:A:1490:G:OP2	2.28	0.42
5:C:57:ILE:HG22	5:C:59:SER:H	1.84	0.42
6:D:172:ASN:ND2	16:K:95:ASP:OD1	2.52	0.42
21:S:36:GLU:HG3	21:S:47:ARG:HG2	2.01	0.42
26:Z:12:PHE:HZ	26:Z:21:LYS:HD3	1.85	0.42
28:M:68:ARG:HD2	28:M:76:VAL:HG11	2.01	0.42
29:O:56:ILE:HG23	29:O:57:ASP:H	1.83	0.42
32:Y:35:VAL:O	32:Y:39:THR:OG1	2.32	0.42
3:B:102:ARG:HD2	3:B:102:ARG:HA	1.80	0.42
8:E:193:ASP:N	8:E:193:ASP:OD1	2.51	0.42
10:G:125:SER:HA	10:G:138:ALA:HA	2.02	0.42
20:R:103:ALA:HA	20:R:106:LYS:HG2	2.01	0.42
28:M:155:LYS:HA	28:M:155:LYS:HD3	1.72	0.42
1:A:1578:U:H2'	8:E:4:GLN:HB3	2.02	0.42
5:C:40:ASN:ND2	5:C:75:GLN:OE1	2.52	0.42
12:H:67:VAL:HG23	12:H:99:GLY:HA2	2.00	0.42
23:U:51:ASN:HB2	23:U:54:TYR:HD2	1.84	0.42
1:A:35:C:H5''	1:A:579:C:H5''	2.02	0.42
1:A:1299:A:H5'	19:Q:52:LYS:HE3	2.02	0.42
1:A:1598:G:N2	1:A:1599:U:O4	2.45	0.42
1:A:1630:A:H5''	22:T:37:GLY:H	1.84	0.42
14:I:9:VAL:HB	14:I:44:ASN:HD21	1.83	0.42
19:Q:121:ILE:HD12	19:Q:121:ILE:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:126:ARG:HD3	20:R:126:ARG:HA	1.87	0.42
22:T:106:LYS:HD2	22:T:106:LYS:HA	1.76	0.42
22:T:142:ARG:HD3	22:T:142:ARG:HA	1.76	0.42
1:A:1294:G:H1	1:A:1305:C:H42	1.68	0.42
16:K:180:LYS:HD2	16:K:180:LYS:HA	1.80	0.42
15:J:10:LYS:O	15:J:18:ARG:NH1	2.53	0.42
21:S:16:ILE:O	21:S:20:TYR:N	2.50	0.42
23:U:110:LEU:HB3	23:U:112:MET:HG2	2.02	0.42
30:P:16:LEU:HD23	30:P:16:LEU:HA	1.93	0.42
1:A:163:U:OP2	12:H:87:ARG:NH1	2.36	0.42
1:A:912:C:C2	1:A:914:U:H1'	2.55	0.42
3:B:109:THR:O	6:D:89:LYS:NZ	2.50	0.42
29:O:68:ILE:HD13	29:O:131:CYS:HB3	2.01	0.42
32:Y:85:ASP:OD2	32:Y:85:ASP:N	2.46	0.42
1:A:201:C:H3'	1:A:202:G:H8	1.84	0.41
1:A:969:U:OP1	1:A:970:G:O2'	2.29	0.41
14:I:51:ILE:HG12	14:I:61:ILE:HD11	2.00	0.41
31:X:101:GLY:HA2	31:X:106:LYS:HB3	2.02	0.41
1:A:68:A:OP2	12:H:164:LYS:NZ	2.53	0.41
1:A:345:U:OP1	28:M:37:LYS:NZ	2.50	0.41
5:C:77:ASP:OD1	5:C:77:ASP:N	2.52	0.41
21:S:77:GLU:HB3	21:S:81:ARG:HH22	1.85	0.41
29:O:21:LYS:HD2	29:O:21:LYS:HA	1.76	0.41
1:A:857:U:H2'	1:A:858:A:C8	2.56	0.41
1:A:882:U:H3	1:A:904:A:H61	1.68	0.41
1:A:1101:U:H2'	1:A:1102:G:C8	2.56	0.41
16:K:151:LEU:HD23	16:K:151:LEU:HA	1.89	0.41
19:Q:52:LYS:HG3	19:Q:80:LEU:HD11	2.01	0.41
20:R:73:LYS:HB2	20:R:73:LYS:HE2	1.88	0.41
27:F:162:ASN:OD1	27:F:162:ASN:N	2.51	0.41
1:A:981:A:H2'	1:A:982:G:C8	2.55	0.41
1:A:1226:G:N1	1:A:1639:G:OP2	2.40	0.41
1:A:1392:U:H2'	1:A:1393:G:C8	2.55	0.41
1:A:1823:A:H3'	1:A:1824:A:H8	1.85	0.41
5:C:29:ASP:N	5:C:49:VAL:O	2.53	0.41
6:D:76:LYS:HA	6:D:76:LYS:HD3	1.87	0.41
10:G:55:ARG:HG3	20:R:125:ARG:HD3	2.02	0.41
16:K:50:LEU:HD13	16:K:105:PHE:HE2	1.85	0.41
19:Q:81:ARG:NH1	19:Q:120:SER:OG	2.54	0.41
19:Q:85:ILE:HD11	19:Q:116:LEU:HB3	2.01	0.41
25:W:27:LYS:HD3	25:W:27:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:C:N4	1:A:473:A:OP2	2.43	0.41
1:A:64:A:OP1	12:H:177:GLN:NE2	2.53	0.41
1:A:871:U:H2'	1:A:873:G:H22	1.85	0.41
1:A:1010:G:H2'	1:A:1011:A:C8	2.55	0.41
12:H:79:LYS:HE3	12:H:79:LYS:HB2	1.87	0.41
19:Q:81:ARG:HB3	19:Q:117:GLY:HA3	2.02	0.41
22:T:54:LYS:HE3	22:T:54:LYS:HB3	1.96	0.41
1:A:687:C:OP2	32:Y:32:LYS:NZ	2.41	0.41
1:A:1270:G:O2'	1:A:1299:A:N6	2.54	0.41
1:A:1541:G:H4'	23:U:15:VAL:HG21	2.02	0.41
5:C:103:MET:HG3	5:C:215:VAL:HB	2.02	0.41
16:K:19:PRO:O	16:K:24:ARG:NH2	2.53	0.41
19:Q:29:SER:H	19:Q:32:GLN:HE21	1.67	0.41
19:Q:90:VAL:HG11	19:Q:109:PRO:HG3	2.02	0.41
25:W:4:ASP:OD2	25:W:4:ASP:N	2.54	0.41
28:M:180:LEU:HD23	28:M:180:LEU:HA	1.93	0.41
5:C:33:VAL:HA	5:C:96:CYS:HB2	2.02	0.41
8:E:71:ALA:HA	8:E:74:GLN:HE21	1.86	0.41
10:G:14:THR:OG1	10:G:48:TYR:OH	2.35	0.41
10:G:119:SER:HB2	10:G:150:ALA:HB1	2.02	0.41
18:N:121:LYS:HB2	18:N:121:LYS:HE2	1.84	0.41
20:R:50:LYS:HB3	20:R:50:LYS:HE3	1.84	0.41
22:T:62:ASP:N	22:T:62:ASP:OD1	2.52	0.41
23:U:130:ASP:O	23:U:134:ILE:N	2.47	0.41
28:M:51:LYS:HD3	28:M:51:LYS:HA	1.81	0.41
30:P:99:ARG:NH2	30:P:119:GLU:OE2	2.54	0.41
1:A:1205:C:O2'	1:A:1834:A:N6	2.53	0.41
5:C:137:LEU:HG	5:C:215:VAL:HG22	2.01	0.41
6:D:254:ASP:N	6:D:254:ASP:OD1	2.51	0.41
1:A:28:U:H2'	1:A:29:G:H8	1.85	0.41
1:A:166:A:H1'	12:H:13:GLN:HE21	1.85	0.41
1:A:522:A:H5''	16:K:145:PRO:HD2	2.02	0.41
1:A:982:G:H2'	1:A:983:A:H8	1.86	0.41
1:A:1453:C:H2'	1:A:1454:A:H4'	2.02	0.41
10:G:101:HIS:O	10:G:105:GLY:N	2.51	0.41
12:H:70:HIS:HA	12:H:98:ARG:HH12	1.85	0.41
18:N:71:GLU:OE1	18:N:72:HIS:ND1	2.44	0.41
19:Q:86:LEU:HB3	19:Q:88:GLU:HG2	2.03	0.41
25:W:22:ARG:HE	25:W:22:ARG:HB3	1.60	0.41
27:F:156:ASP:OD1	27:F:156:ASP:N	2.53	0.41
28:M:25:SER:OG	28:M:26:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:M:132:GLY:N	28:M:136:ILE:O	2.43	0.41
32:Y:31:SER:H	32:Y:34:ILE:HD12	1.85	0.41
1:A:744:G:H22	1:A:797:C:H1'	1.86	0.41
1:A:1643:U:H2'	1:A:1644:C:C6	2.56	0.41
17:L:48:ALA:O	17:L:51:SER:OG	2.37	0.41
20:R:32:ILE:HG21	20:R:39:LEU:HD22	2.02	0.41
23:U:30:VAL:HA	23:U:31:PRO:HD3	1.96	0.41
1:A:171:A:OP2	12:H:137:ARG:NH2	2.46	0.40
1:A:846:G:OP2	28:M:108:ARG:NH2	2.44	0.40
1:A:1115:U:O2	1:A:1116:C:O2'	2.34	0.40
1:A:1480:A:O2'	24:V:79:ARG:NH2	2.55	0.40
1:A:1513:C:H2'	1:A:1514:G:C8	2.56	0.40
12:H:61:PHE:HA	12:H:62:PRO:HD3	1.93	0.40
14:I:105:THR:HG23	14:I:107:LYS:H	1.86	0.40
19:Q:78:THR:N	19:Q:95:GLY:O	2.39	0.40
19:Q:83:MET:HB3	19:Q:116:LEU:HD21	2.03	0.40
22:T:44:VAL:HG23	22:T:45:LEU:HD12	2.03	0.40
23:U:67:ARG:HE	23:U:67:ARG:HB3	1.58	0.40
1:A:903:A:H1'	1:A:904:A:C8	2.56	0.40
1:A:1474:A:H4'	20:R:121:VAL:HG11	2.03	0.40
1:A:1647:A:N1	1:A:1675:A:H5''	2.36	0.40
12:H:103:ASP:OD1	12:H:103:ASP:N	2.54	0.40
15:J:192:GLY:HA2	29:O:20:LYS:HD2	2.03	0.40
23:U:27:LYS:HG3	23:U:110:LEU:HG	2.04	0.40
28:M:212:ASP:OD1	28:M:216:ASN:N	2.54	0.40
1:A:61:A:HO2'	1:A:315:C:HO2'	1.68	0.40
1:A:943:U:OP1	5:C:214:LYS:NZ	2.39	0.40
5:C:131:ASP:OD1	5:C:131:ASP:N	2.55	0.40
5:C:147:ASN:OD1	5:C:147:ASN:N	2.46	0.40
12:H:201:LYS:HE3	12:H:201:LYS:HB3	1.90	0.40
22:T:5:ILE:HD12	22:T:6:PRO:HD2	2.03	0.40
26:Z:103:SER:HB3	26:Z:106:GLN:HG2	2.02	0.40
28:M:93:ASP:N	28:M:93:ASP:OD1	2.51	0.40
28:M:188:ASN:HB3	28:M:191:ARG:HD3	2.04	0.40
1:A:429:C:O2'	1:A:811:A:N1	2.46	0.40
1:A:1550:G:O2'	1:A:1558:C:O2	2.32	0.40
1:A:1577:G:O2'	1:A:1579:A:N3	2.41	0.40
1:A:166:A:N3	12:H:13:GLN:NE2	2.68	0.40
1:A:1692:U:H2'	1:A:1693:G:C8	2.57	0.40
10:G:96:ALA:HA	10:G:174:ALA:HB2	2.02	0.40
31:X:85:CYS:HB2	31:X:90:ILE:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	a	73/125 (58%)	66 (90%)	7 (10%)	0	100	100
3	B	215/295 (73%)	209 (97%)	6 (3%)	0	100	100
4	b	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
5	C	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
6	D	219/293 (75%)	216 (99%)	3 (1%)	0	100	100
7	d	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
8	E	226/243 (93%)	212 (94%)	14 (6%)	0	100	100
9	f	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
10	G	181/204 (89%)	170 (94%)	11 (6%)	0	100	100
11	g	66/156 (42%)	56 (85%)	10 (15%)	0	100	100
12	H	235/249 (94%)	226 (96%)	9 (4%)	0	100	100
13	h	311/317 (98%)	281 (90%)	30 (10%)	0	100	100
14	I	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
15	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
16	K	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
17	L	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
18	N	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
19	Q	127/145 (88%)	115 (91%)	12 (9%)	0	100	100
20	R	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
21	S	130/135 (96%)	117 (90%)	13 (10%)	0	100	100
22	T	142/152 (93%)	127 (89%)	15 (11%)	0	100	100
23	U	139/145 (96%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	V	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
25	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
26	Z	122/130 (94%)	121 (99%)	1 (1%)	0	100	100
27	F	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
28	M	261/263 (99%)	237 (91%)	24 (9%)	0	100	100
29	O	156/158 (99%)	137 (88%)	18 (12%)	1 (1%)	25	50
30	P	148/151 (98%)	137 (93%)	11 (7%)	0	100	100
31	X	134/168 (80%)	108 (81%)	26 (19%)	0	100	100
32	Y	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	19	43
33	c	140/143 (98%)	128 (91%)	11 (8%)	1 (1%)	22	46
34	e	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
All	All	4789/5544 (86%)	4455 (93%)	331 (7%)	3 (0%)	54	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	O	5	GLN
33	c	130	LEU
32	Y	67	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	a	66/103 (64%)	65 (98%)	1 (2%)	65	86
3	B	180/245 (74%)	179 (99%)	1 (1%)	86	95
4	b	88/98 (90%)	87 (99%)	1 (1%)	73	90
5	C	194/231 (84%)	194 (100%)	0	100	100
6	D	187/225 (83%)	184 (98%)	3 (2%)	62	85
7	d	55/62 (89%)	54 (98%)	1 (2%)	59	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	190/202 (94%)	190 (100%)	0	100	100
9	f	47/106 (44%)	46 (98%)	1 (2%)	53	80
10	G	158/170 (93%)	156 (99%)	2 (1%)	69	87
11	g	61/140 (44%)	60 (98%)	1 (2%)	62	85
12	H	207/218 (95%)	206 (100%)	1 (0%)	88	96
13	h	272/275 (99%)	271 (100%)	1 (0%)	91	97
14	I	165/174 (95%)	165 (100%)	0	100	100
15	J	178/180 (99%)	177 (99%)	1 (1%)	86	95
16	K	161/168 (96%)	161 (100%)	0	100	100
17	L	87/136 (64%)	86 (99%)	1 (1%)	73	90
18	N	99/108 (92%)	97 (98%)	2 (2%)	55	81
19	Q	115/130 (88%)	112 (97%)	3 (3%)	46	75
20	R	117/121 (97%)	115 (98%)	2 (2%)	60	84
21	S	119/121 (98%)	119 (100%)	0	100	100
22	T	125/132 (95%)	124 (99%)	1 (1%)	81	93
23	U	111/115 (96%)	110 (99%)	1 (1%)	78	92
24	V	92/107 (86%)	92 (100%)	0	100	100
25	W	67/67 (100%)	67 (100%)	0	100	100
26	Z	107/112 (96%)	107 (100%)	0	100	100
27	F	29/31 (94%)	29 (100%)	0	100	100
28	M	225/225 (100%)	224 (100%)	1 (0%)	91	97
29	O	142/142 (100%)	141 (99%)	1 (1%)	84	94
30	P	130/131 (99%)	130 (100%)	0	100	100
31	X	106/130 (82%)	106 (100%)	0	100	100
32	Y	112/113 (99%)	112 (100%)	0	100	100
33	c	114/115 (99%)	114 (100%)	0	100	100
34	e	76/76 (100%)	76 (100%)	0	100	100
All	All	4182/4709 (89%)	4156 (99%)	26 (1%)	86	95

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	113	THR

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Mol	Chain	Res	Type
3	B	104	THR
4	b	100	ARG
6	D	167	ARG
6	D	209	VAL
6	D	262	THR
7	d	66	ARG
9	f	124	LYS
10	G	59	LYS
10	G	122	ARG
11	g	138	ARG
12	H	98	ARG
13	h	12	LYS
15	J	206	LYS
17	L	6	LYS
18	N	33	ARG
18	N	63	LYS
19	Q	13	ARG
19	Q	14	LYS
19	Q	140	ARG
20	R	71	ARG
20	R	105	LYS
22	T	116	LYS
23	U	16	ARG
28	M	254	LYS
29	O	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	64	ASN
2	a	112	ASN
3	B	141	ASN
4	b	17	HIS
5	C	149	GLN
5	C	158	HIS
6	D	272	HIS
7	d	29	GLN
9	f	88	GLN
9	f	117	ASN
10	G	31	ASN
10	G	110	GLN
11	g	135	HIS

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Mol	Chain	Res	Type
12	H	177	GLN
13	h	26	GLN
13	h	187	ASN
13	h	226	HIS
13	h	305	ASN
15	J	64	ASN
16	K	124	HIS
16	K	125	HIS
17	L	39	ASN
18	N	48	HIS
19	Q	32	GLN
19	Q	53	GLN
20	R	77	HIS
20	R	97	GLN
21	S	83	ASN
22	T	17	ASN
22	T	19	ASN
23	U	137	GLN
25	W	35	ASN
26	Z	106	GLN
27	F	178	ASN
28	M	50	ASN
29	O	112	HIS
29	O	154	GLN
30	P	5	HIS
30	P	105	ASN
32	Y	24	GLN
33	c	77	ASN
33	c	92	ASN
34	e	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1685/1869 (90%)	354 (21%)	15 (0%)

All (354) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	C

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Mol	Chain	Res	Type
1	A	17	C
1	A	25	A
1	A	33	G
1	A	41	G
1	A	44	U
1	A	45	A
1	A	46	A
1	A	56	G
1	A	58	C
1	A	62	G
1	A	65	C
1	A	67	C
1	A	68	A
1	A	71	G
1	A	73	C
1	A	74	G
1	A	76	U
1	A	77	A
1	A	79	A
1	A	103	A
1	A	111	A
1	A	113	G
1	A	115	U
1	A	126	G
1	A	129	C
1	A	130	G
1	A	143	U
1	A	146	G
1	A	147	A
1	A	155	G
1	A	162	C
1	A	163	U
1	A	175	A
1	A	180	G
1	A	183	G
1	A	184	G
1	A	187	G
1	A	188	C
1	A	190	G
1	A	192	C
1	A	206	G
1	A	209	A

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Mol	Chain	Res	Type
1	A	294	U
1	A	302	A
1	A	307	G
1	A	308	G
1	A	309	G
1	A	312	G
1	A	319	C
1	A	320	G
1	A	323	C
1	A	347	G
1	A	351	G
1	A	362	C
1	A	364	A
1	A	368	U
1	A	369	C
1	A	370	G
1	A	381	C
1	A	382	C
1	A	385	G
1	A	386	C
1	A	398	A
1	A	400	C
1	A	407	G
1	A	408	A
1	A	409	C
1	A	418	A
1	A	438	G
1	A	441	C
1	A	447	A
1	A	448	A
1	A	449	A
1	A	450	C
1	A	465	A
1	A	466	G
1	A	467	G
1	A	470	G
1	A	471	G
1	A	472	C
1	A	473	A
1	A	474	G
1	A	482	G
1	A	487	U

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Mol	Chain	Res	Type
1	A	492	C
1	A	508	A
1	A	509	G
1	A	516	A
1	A	531	A
1	A	532	C
1	A	533	A
1	A	541	U
1	A	544	G
1	A	547	G
1	A	548	C
1	A	549	C
1	A	551	U
1	A	554	A
1	A	556	U
1	A	559	G
1	A	561	A
1	A	562	U
1	A	568	C
1	A	576	A
1	A	583	A
1	A	587	A
1	A	588	G
1	A	589	G
1	A	590	A
1	A	591	U
1	A	604	A
1	A	605	A
1	A	606	G
1	A	607	U
1	A	608	C
1	A	614	C
1	A	627	U
1	A	628	A
1	A	629	A
1	A	631	U
1	A	643	A
1	A	644	G
1	A	655	A
1	A	660	C
1	A	662	G
1	A	663	C

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Mol	Chain	Res	Type
1	A	664	A
1	A	668	A
1	A	669	A
1	A	671	A
1	A	672	A
1	A	673	G
1	A	678	U
1	A	684	G
1	A	689	U
1	A	690	G
1	A	734	C
1	A	752	G
1	A	753	C
1	A	754	G
1	A	798	G
1	A	799	U
1	A	801	U
1	A	808	A
1	A	810	A
1	A	811	A
1	A	821	G
1	A	822	U
1	A	830	A
1	A	845	G
1	A	847	A
1	A	859	G
1	A	868	G
1	A	870	A
1	A	871	U
1	A	872	A
1	A	873	G
1	A	874	G
1	A	875	A
1	A	878	G
1	A	884	C
1	A	885	U
1	A	887	U
1	A	888	U
1	A	889	U
1	A	891	G
1	A	892	U
1	A	894	G

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Mol	Chain	Res	Type
1	A	895	G
1	A	898	U
1	A	901	G
1	A	903	A
1	A	909	G
1	A	913	A
1	A	914	U
1	A	920	A
1	A	933	G
1	A	934	G
1	A	938	A
1	A	943	U
1	A	955	A
1	A	963	A
1	A	971	G
1	A	978	G
1	A	990	A
1	A	992	A
1	A	999	G
1	A	1017	U
1	A	1023	A
1	A	1050	A
1	A	1060	A
1	A	1062	A
1	A	1080	A
1	A	1083	A
1	A	1085	C
1	A	1115	U
1	A	1116	C
1	A	1117	C
1	A	1118	C
1	A	1121	G
1	A	1133	A
1	A	1138	C
1	A	1143	A
1	A	1148	A
1	A	1149	A
1	A	1153	C
1	A	1154	U
1	A	1168	G
1	A	1195	A
1	A	1203	G

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Mol	Chain	Res	Type
1	A	1207	G
1	A	1208	A
1	A	1215	C
1	A	1221	G
1	A	1224	G
1	A	1242	U
1	A	1248	U
1	A	1251	A
1	A	1253	A
1	A	1256	G
1	A	1257	G
1	A	1258	A
1	A	1264	C
1	A	1273	C
1	A	1274	G
1	A	1275	G
1	A	1282	A
1	A	1284	A
1	A	1285	G
1	A	1286	G
1	A	1287	A
1	A	1295	A
1	A	1298	G
1	A	1301	A
1	A	1302	G
1	A	1303	C
1	A	1308	U
1	A	1309	C
1	A	1311	C
1	A	1320	G
1	A	1330	G
1	A	1332	A
1	A	1333	U
1	A	1341	C
1	A	1342	U
1	A	1343	U
1	A	1348	G
1	A	1354	G
1	A	1371	U
1	A	1372	U
1	A	1378	A
1	A	1382	A

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Mol	Chain	Res	Type
1	A	1396	A
1	A	1397	U
1	A	1398	G
1	A	1401	A
1	A	1402	A
1	A	1404	U
1	A	1424	G
1	A	1428	G
1	A	1431	G
1	A	1432	U
1	A	1449	G
1	A	1452	A
1	A	1454	A
1	A	1455	A
1	A	1463	U
1	A	1464	C
1	A	1466	G
1	A	1480	A
1	A	1484	A
1	A	1489	A
1	A	1490	G
1	A	1494	U
1	A	1498	A
1	A	1506	A
1	A	1507	G
1	A	1508	A
1	A	1510	G
1	A	1519	U
1	A	1520	G
1	A	1521	C
1	A	1522	A
1	A	1523	C
1	A	1533	A
1	A	1536	G
1	A	1547	C
1	A	1548	G
1	A	1552	G
1	A	1553	C
1	A	1554	C
1	A	1555	U
1	A	1556	A
1	A	1557	C

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Mol	Chain	Res	Type
1	A	1560	U
1	A	1570	G
1	A	1574	C
1	A	1578	U
1	A	1580	A
1	A	1582	C
1	A	1584	G
1	A	1585	U
1	A	1587	G
1	A	1588	A
1	A	1601	A
1	A	1602	U
1	A	1605	G
1	A	1606	G
1	A	1621	U
1	A	1622	U
1	A	1623	A
1	A	1637	A
1	A	1638	G
1	A	1646	C
1	A	1647	A
1	A	1648	G
1	A	1654	G
1	A	1663	A
1	A	1665	G
1	A	1671	G
1	A	1686	G
1	A	1698	C
1	A	1699	A
1	A	1701	C
1	A	1702	G
1	A	1715	A
1	A	1721	U
1	A	1722	G
1	A	1726	G
1	A	1744	G
1	A	1753	C
1	A	1757	G
1	A	1779	G
1	A	1780	G
1	A	1783	C
1	A	1784	G

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Mol	Chain	Res	Type
1	A	1785	C
1	A	1800	A
1	A	1801	A
1	A	1823	A
1	A	1825	A
1	A	1835	A
1	A	1836	G
1	A	1838	U
1	A	1849	G
1	A	1851	A
1	A	1861	G
1	A	1862	G
1	A	1863	A
1	A	1865	C
1	A	1867	U
1	A	1869	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	24	C
1	A	110	U
1	A	369	C
1	A	465	A
1	A	532	C
1	A	553	U
1	A	561	A
1	A	627	U
1	A	688	U
1	A	752	G
1	A	870	A
1	A	874	G
1	A	1137	U
1	A	1395	C
1	A	1646	C

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

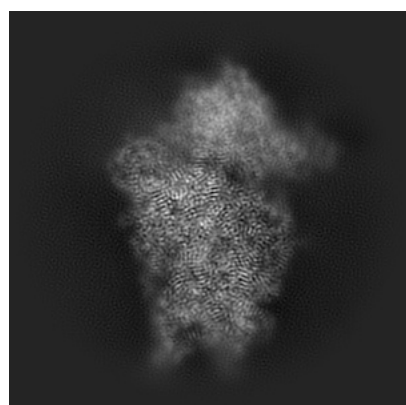
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22432. These allow visual inspection of the internal detail of the map and identification of artifacts.

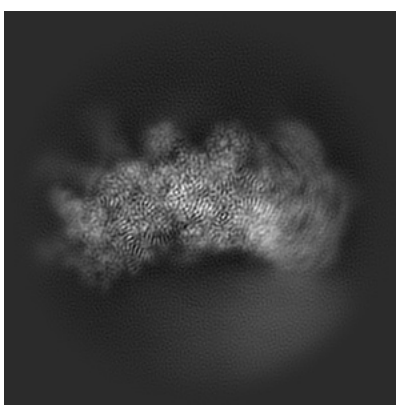
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

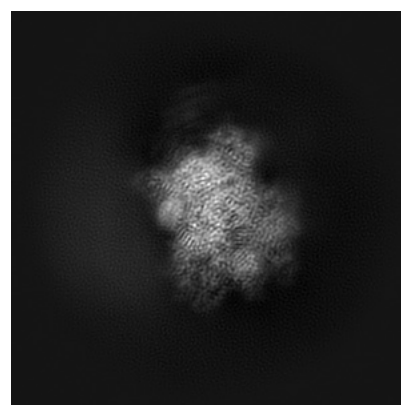
6.1.1 Primary map



X



Y

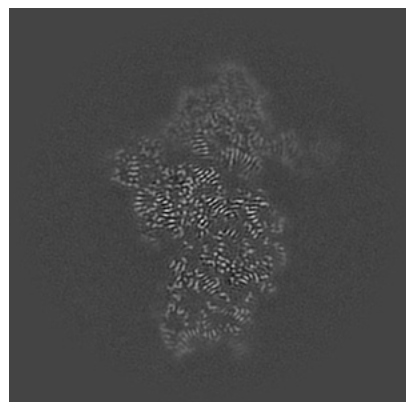


Z

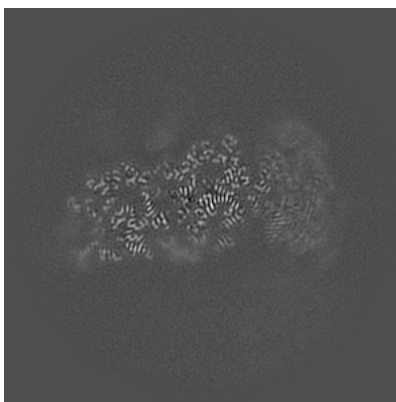
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

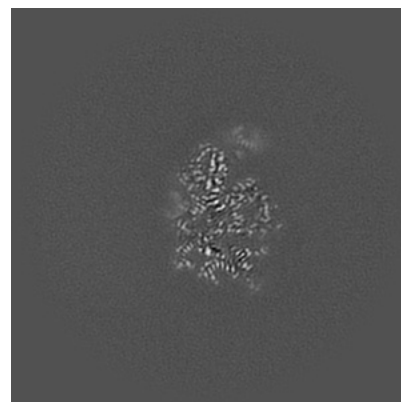
6.2.1 Primary map



X Index: 160



Y Index: 160

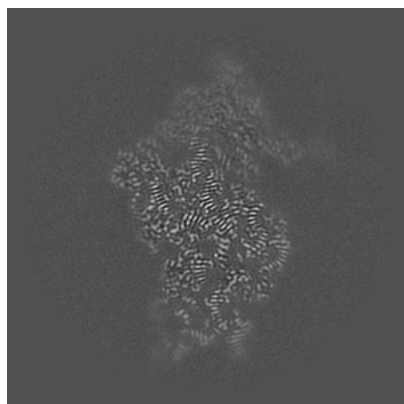


Z Index: 160

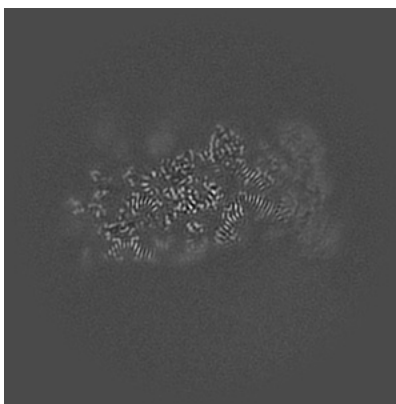
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

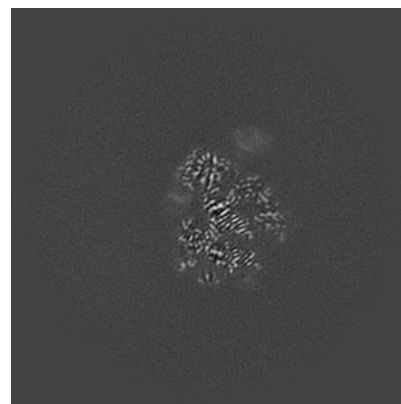
6.3.1 Primary map



X Index: 165



Y Index: 154

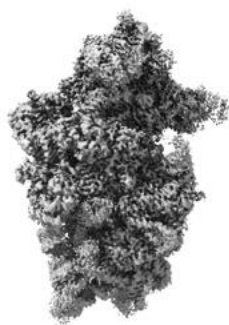


Z Index: 165

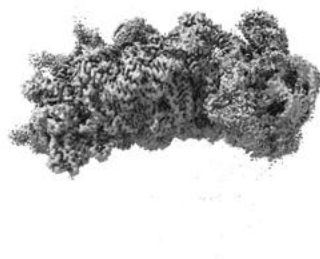
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

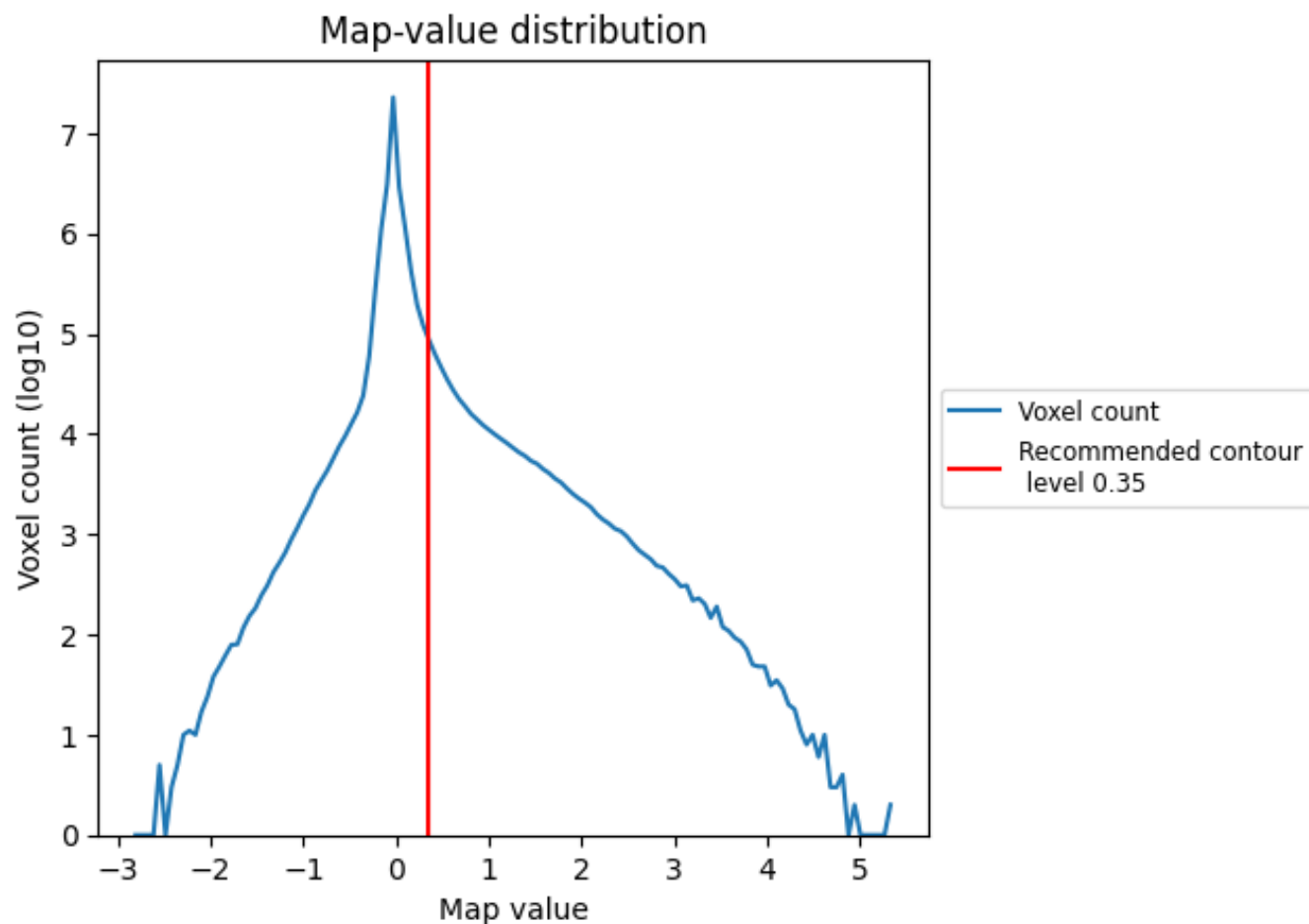
6.5 Mask visualisation

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

7 Map analysis [i](#)

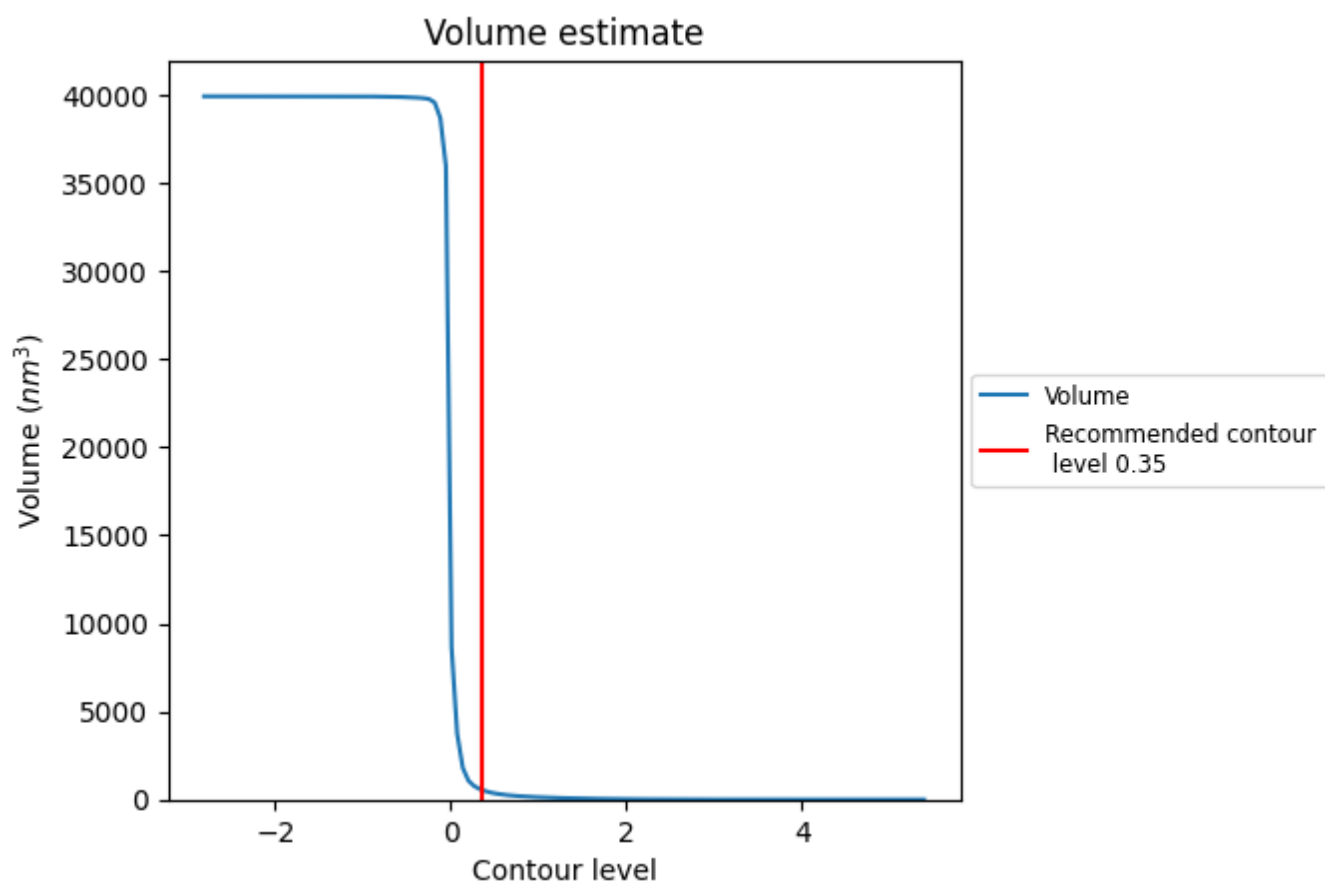
This section contains the results of statistical analysis of the map.

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.

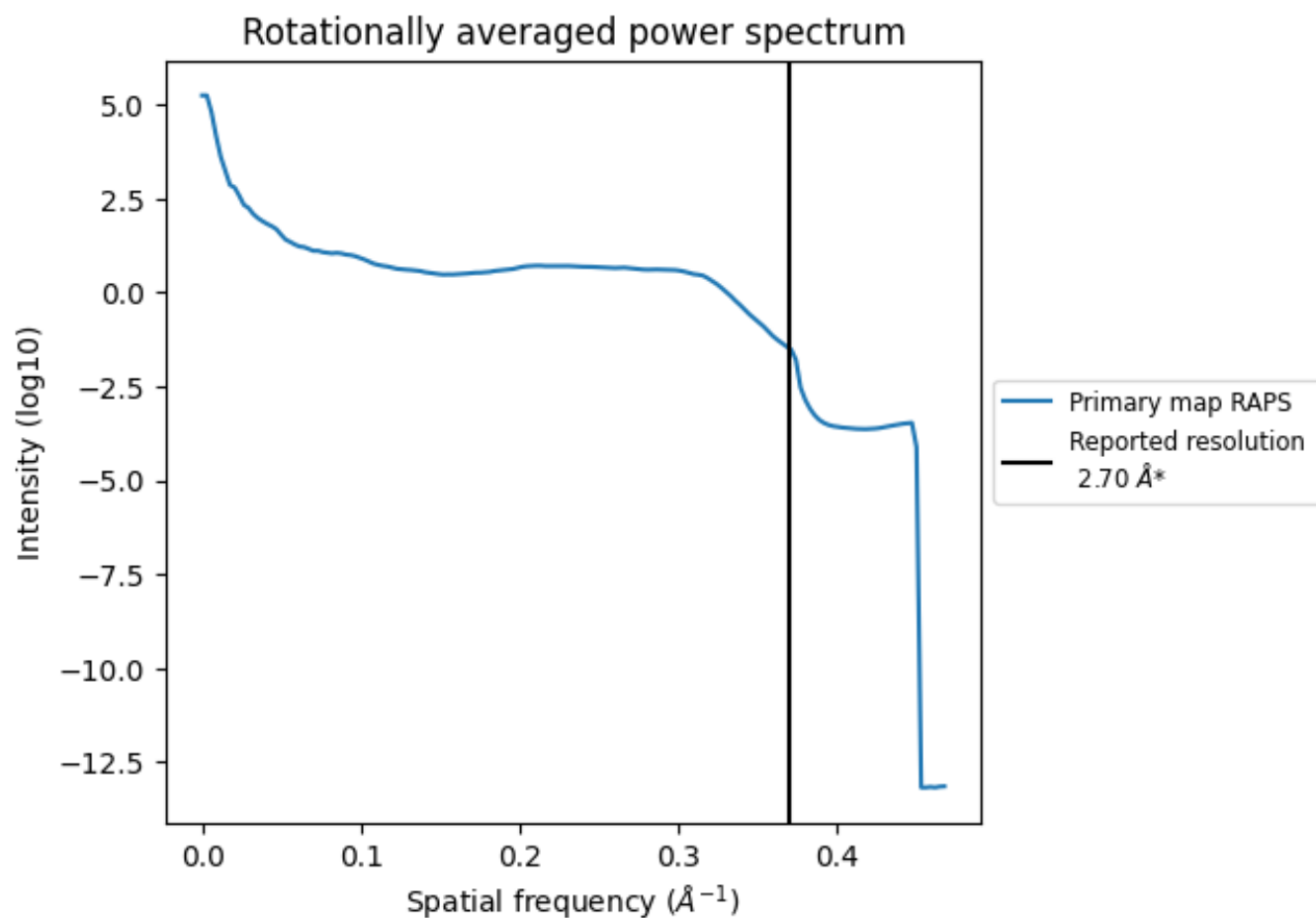
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 567 nm³; this corresponds to an approximate mass of 512 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 0.370 Å⁻¹

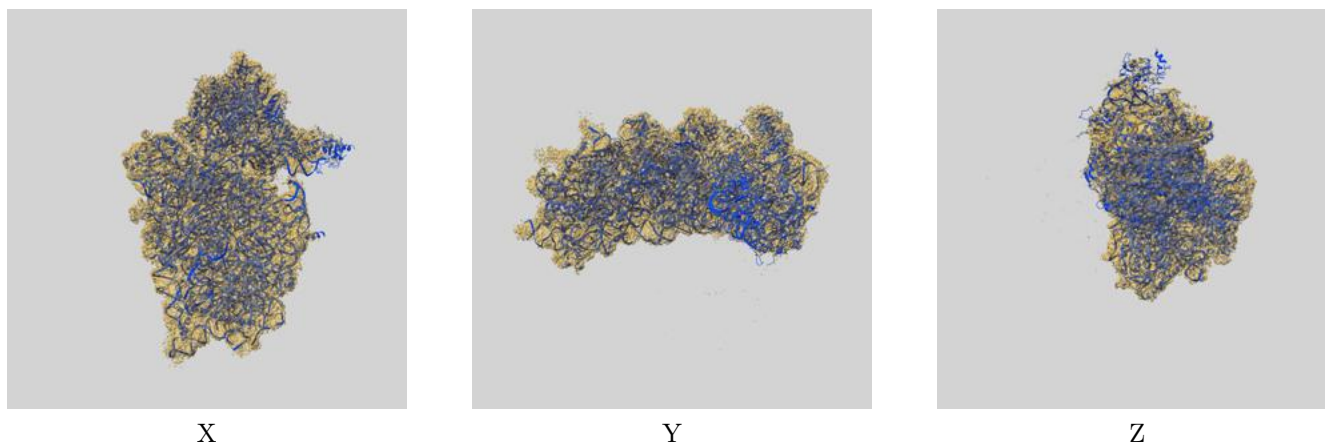
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

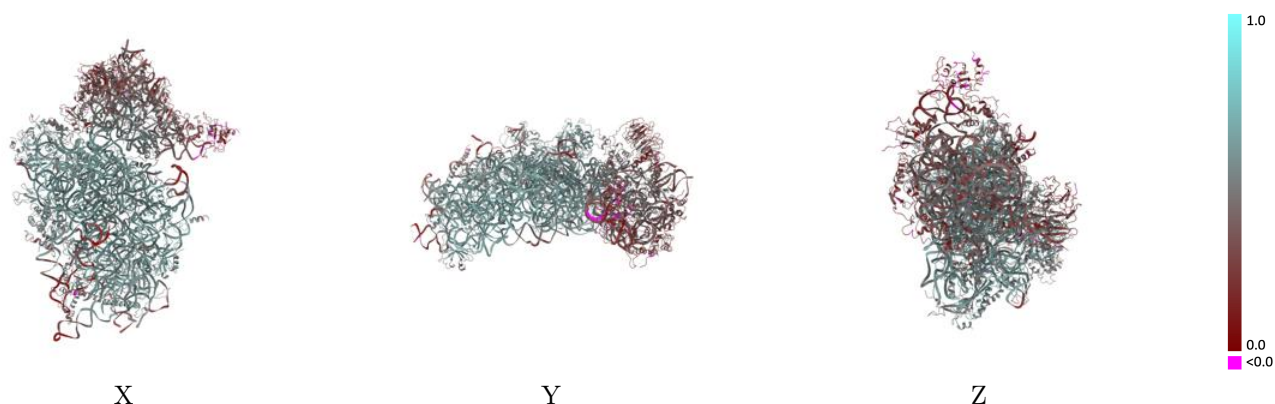
This section contains information regarding the fit between EMDB map EMD-22432 and PDB model 7JQB. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



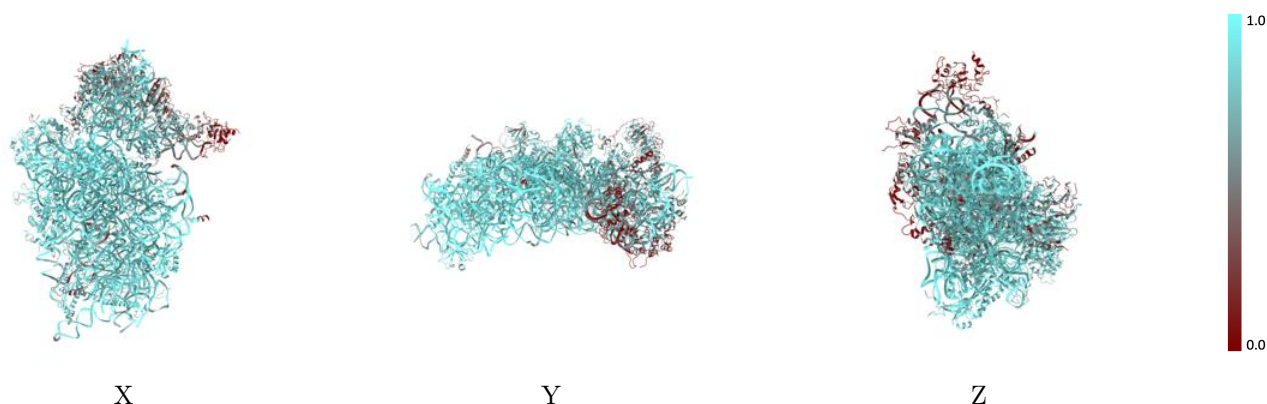
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



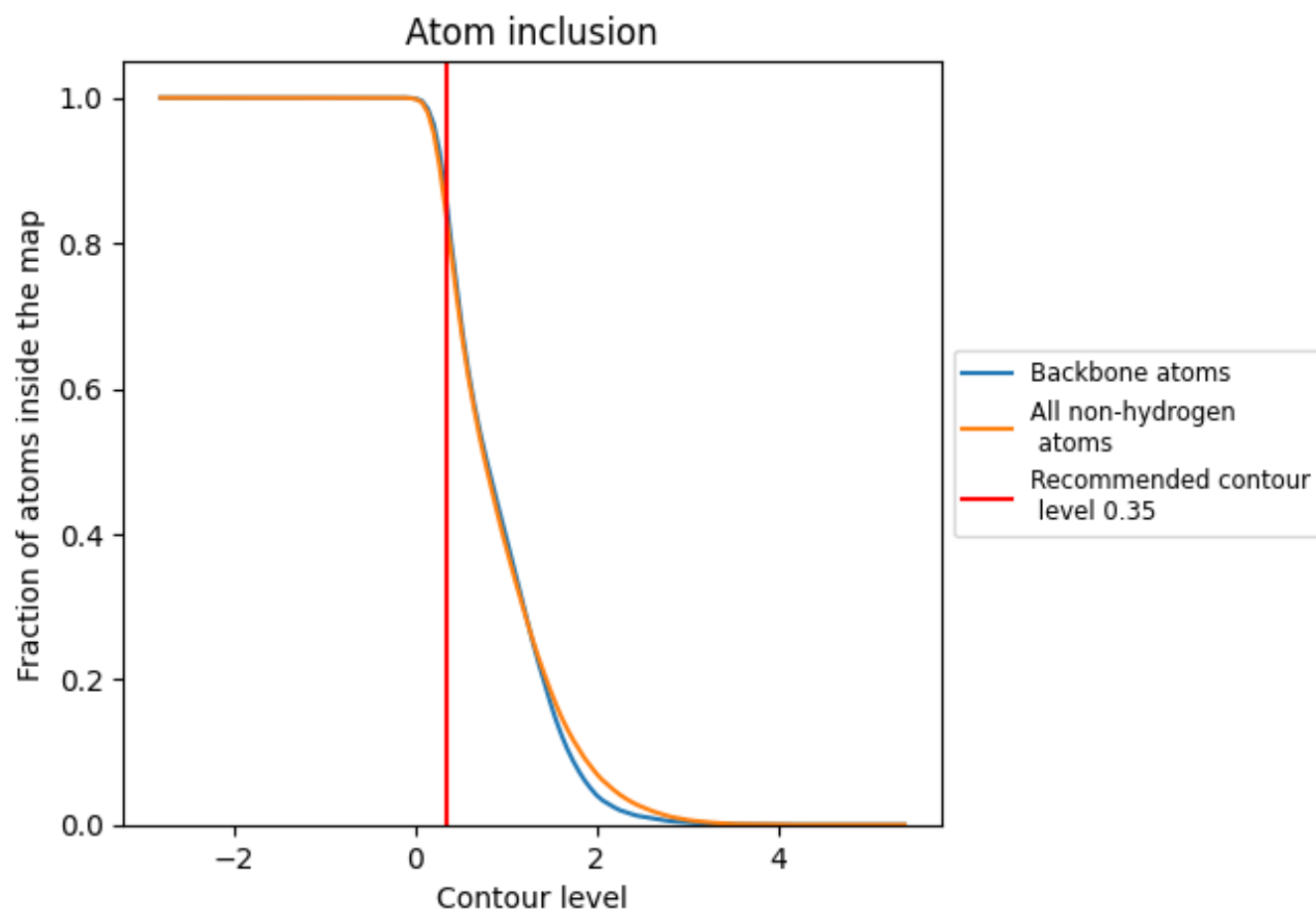
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8311	 0.4980
A	 0.9220	 0.5290
B	 0.9143	 0.5770
C	 0.9111	 0.5630
D	 0.9198	 0.5920
E	 0.6707	 0.4240
F	 0.8321	 0.5460
G	 0.5908	 0.3590
H	 0.8755	 0.5270
I	 0.8248	 0.5130
J	 0.8888	 0.5500
K	 0.9044	 0.5820
L	 0.6114	 0.3500
M	 0.9051	 0.5650
N	 0.0425	 0.1560
O	 0.7970	 0.5210
P	 0.8985	 0.5590
Q	 0.3633	 0.2950
R	 0.6886	 0.3670
S	 0.7601	 0.4550
T	 0.4044	 0.3270
U	 0.6514	 0.3590
V	 0.4780	 0.3560
W	 0.9244	 0.5800
X	 0.8582	 0.5090
Y	 0.9465	 0.6010
Z	 0.9307	 0.5800
a	 0.3671	 0.2860
b	 0.8963	 0.5660
c	 0.9184	 0.5810
d	 0.6085	 0.3920
e	 0.8501	 0.5320
f	 0.8159	 0.5310
g	 0.1019	 0.1760
h	 0.5391	 0.2980

