



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 01:46 AM EST

PDB ID : 6P4G  
EMDB ID : EMD-20248  
Title : Structure of a mammalian small ribosomal subunit in complex with the Israeli Acute Paralysis Virus IRES (Class 1)  
Authors : Acosta-Reyes, F.J.; Neupane, R.; Frank, J.; Fernandez, I.S.  
Deposited on : 2019-05-27  
Resolution : 3.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

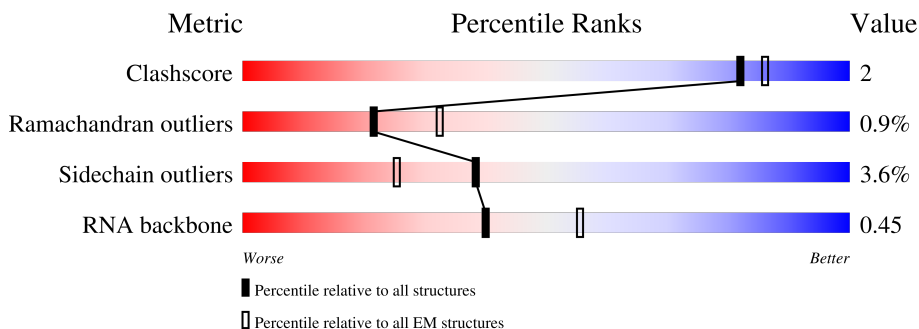
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.










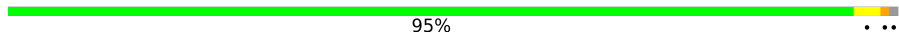













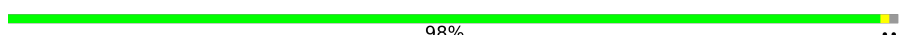

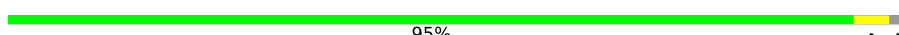

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	1869	
2	B	295	
3	C	264	
4	D	255	
5	E	281	
6	F	263	
7	G	204	


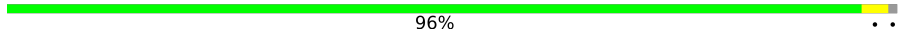
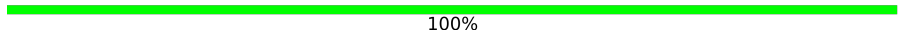
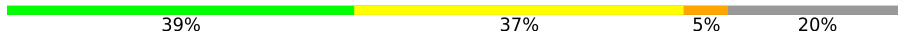
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Mol	Chain	Length	Quality of chain
8	H	249	90%  . . 5%
9	I	194	85%  10% 5%
10	J	208	89%  9% ..
11	K	194	88%  7% . 5%
12	L	149	61%  .. 36%
13	M	158	77%  11% . 9%
14	N	132	85%  . 11%
15	O	151	95%  ..
16	P	151	81%  7% .. 10%
17	Q	145	65%  15% . 18%
18	R	172	74%  7% . 17%
19	S	135	85%  12% ..
20	T	152	82%  11% 7%
21	U	145	88%  9% .
22	V	119	77%  7% 16%
23	W	83	73%  23% .
24	X	130	88%  9% ..
25	Y	143	90%  7% ..
26	Z	134	89%  . 7%
27	a	125	56%  44%
28	b	115	77%  9% 15%
29	c	84	98%  ..
30	d	69	87%  . 10%
31	e	56	95%  ..
32	f	133	41%  . 57%

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Mol	Chain	Length	Quality of chain
33	g	156	 43% 56%
34	h	317	 96%
35	n	25	 100%
36	1	253	 39% 37% 5% 20%

## 2 Entry composition i

There are 36 unique types of molecules in this entry. The entry contains 79374 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1697	36229	16171	6507	11855	1696	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	217	1706	1085	295	317	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	PRO	LEU	conflict	UNP G1TWL4

- Molecule 3 is a protein called eS1.

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

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	221	1712	1107	296	299	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- Molecule 5 is a protein called uS3.

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

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	262	2073	1323	384	357	9	0	0

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	184	1462	915	276	264	7	0	0

- Molecule 8 is a protein called eS6.

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

- Molecule 9 is a protein called eS7.

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

- Molecule 10 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 11 is a protein called uS4.

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

- Molecule 12 is a protein called eS10.

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

- Molecule 13 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called eS12.

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

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

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

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	119	Total	C	N	O	S	0	0
			990	630	186	167	7		

- Molecule 18 is a protein called uS9.

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

- Molecule 19 is a protein called eS17.

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

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	141	Total	C	N	O	S	0	0
			1168	734	235	198	1		

- Molecule 21 is a protein called eS19.

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

- Molecule 22 is a protein called uS10.

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

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	83	Total	C	N	O	S	0	0
			630	387	118	120	5		

- Molecule 24 is a protein called uS8.

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

- Molecule 25 is a protein called uS12.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	141	1098	693	219	183	3	0	0

- Molecule 26 is a protein called eS24.

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

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	70	557	358	101	97	1	0	0

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	98	778	485	158	129	6	0	0

- Molecule 29 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	83	651	408	121	115	7	0	0

- Molecule 30 is a protein called eS28.

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

- Molecule 31 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e	55	459	286	94	74	5	0	0

- Molecule 32 is a protein called eS30.

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

- Molecule 33 is a protein called eS31.

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

- Molecule 34 is a protein called RACK1.

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

- Molecule 35 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

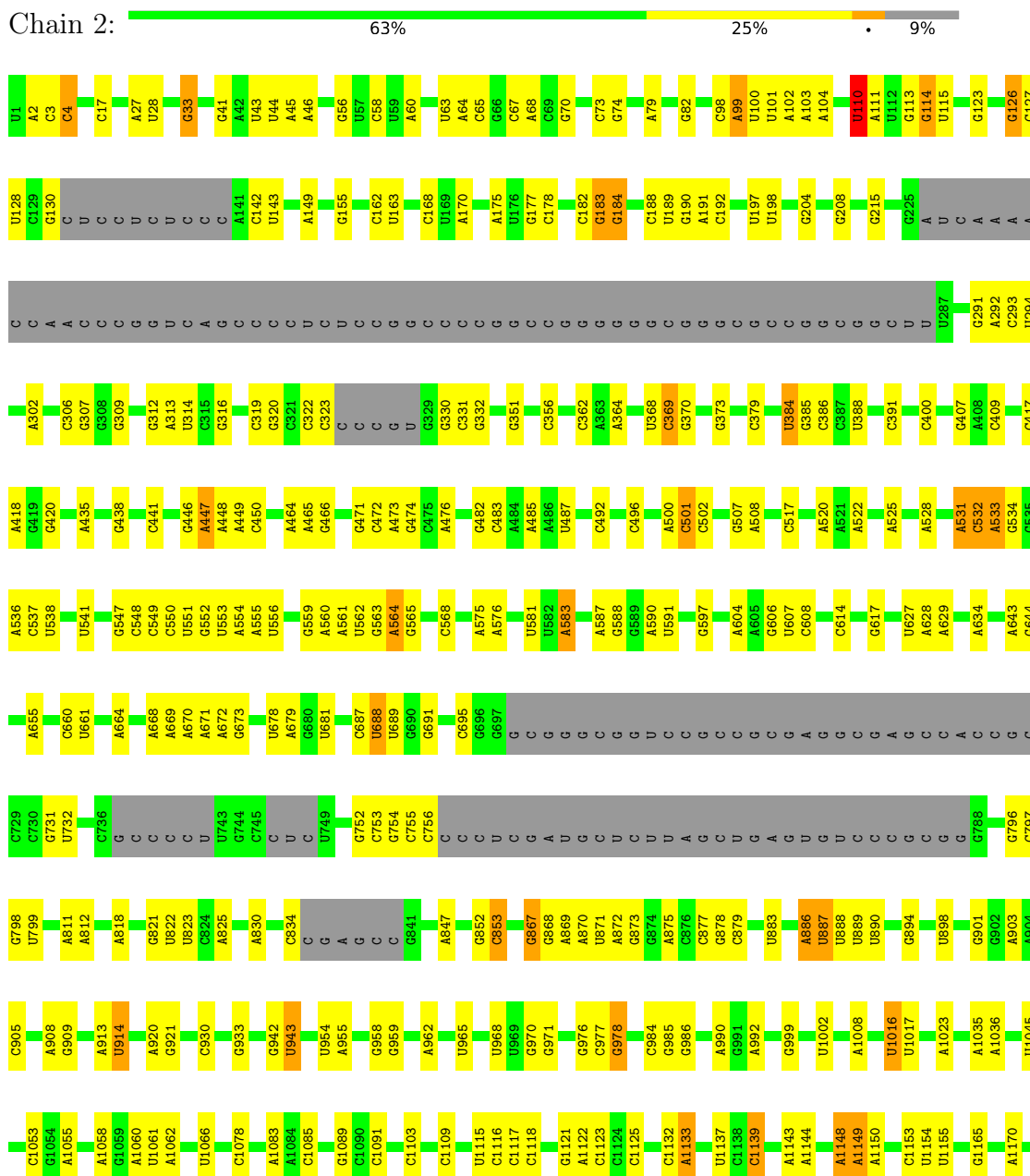
- Molecule 36 is a RNA chain called IAPV-IRES.

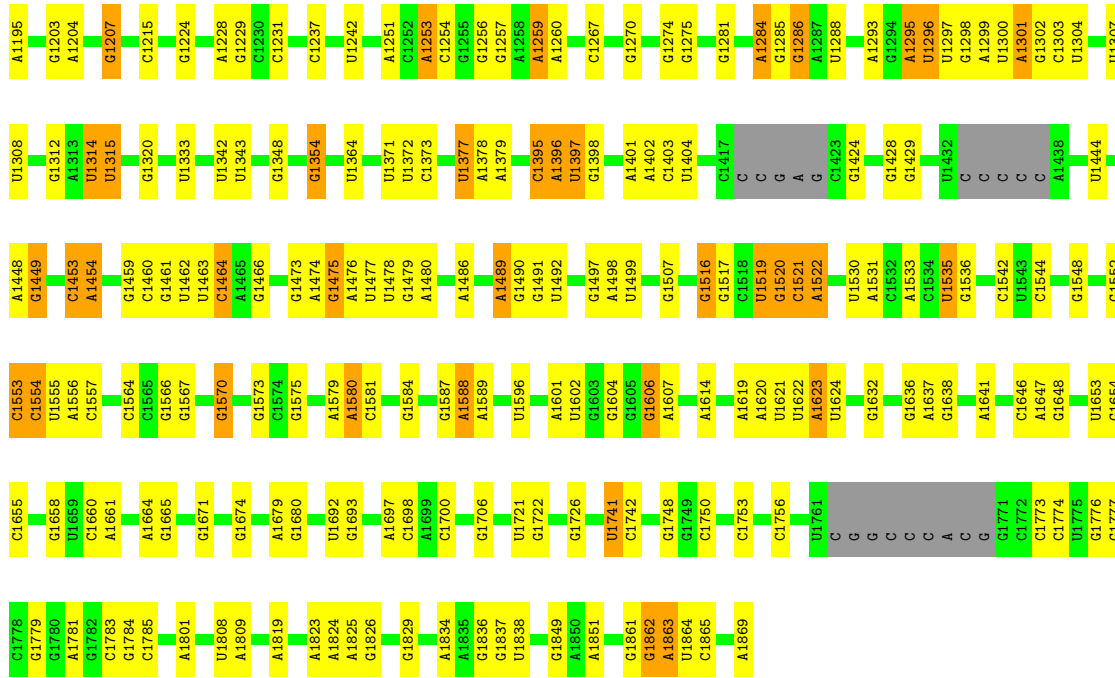
Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	203	Total	C	N	O	P	0	0
			4323	1932	767	1421	203		

### 3 Residue-property plots

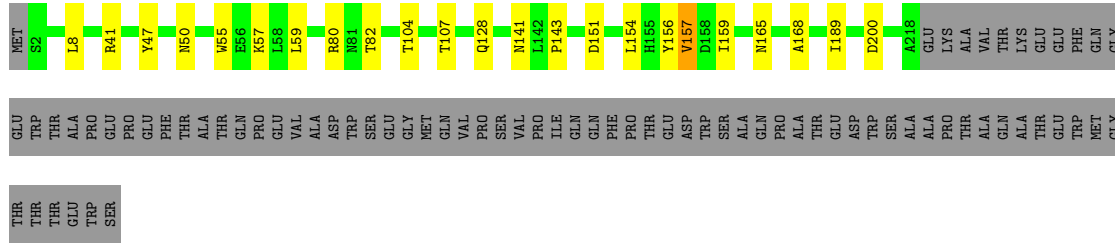
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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

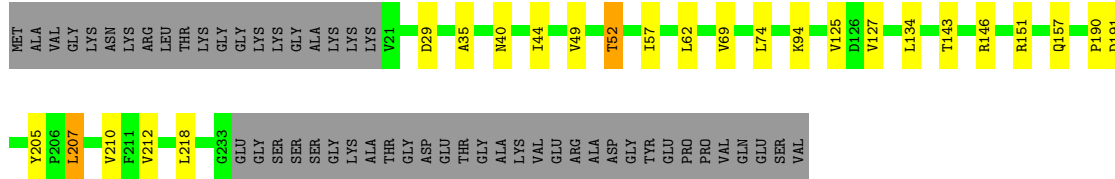




● Molecule 2: uS2

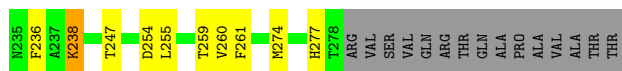


● Molecule 3: eS1

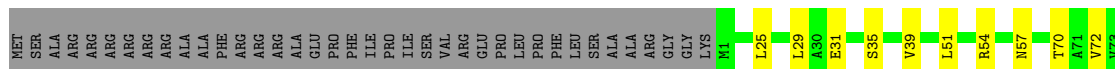


● Molecule 4: uS5





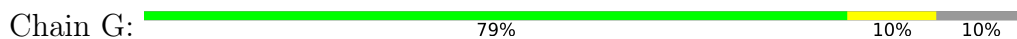
• Molecule 5: uS3



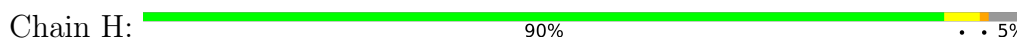
• Molecule 6: eS4



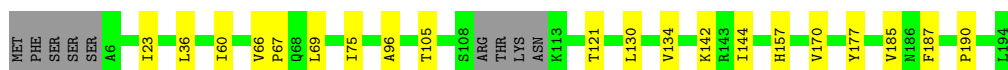
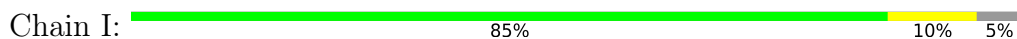
• Molecule 7: uS7



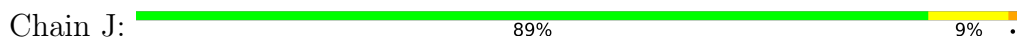
• Molecule 8: eS6




• Molecule 9: eS7



• Molecule 10: eS8



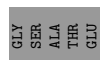
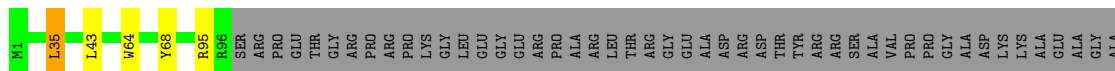
• Molecule 11: uS4

Chain K:  88% 7% • 5%



• Molecule 12: eS10

Chain L:  61% •• 36%




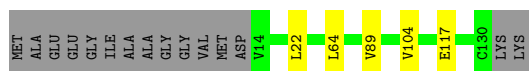
• Molecule 13: uS17

Chain M:  77% 11% • 9%



• Molecule 14: eS12

Chain N:  85% • 11%




• Molecule 15: uS15

Chain O:  95% ••



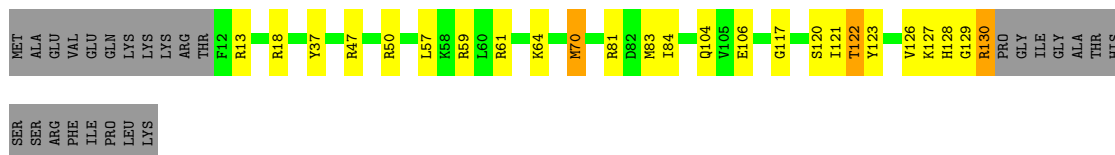
• Molecule 16: uS11

Chain P:  81% 7% •• 10%

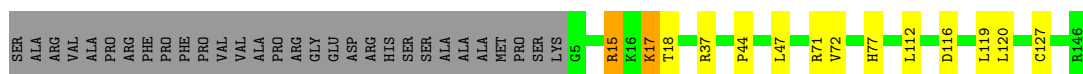


• Molecule 17: uS19

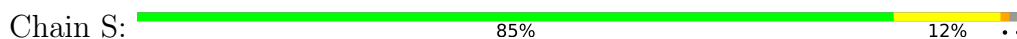
Chain Q:  65% 15% • 18%



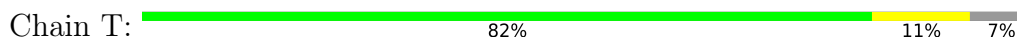
• Molecule 18: uS9



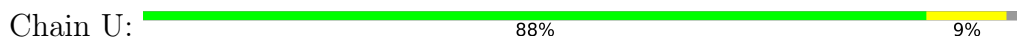
• Molecule 19: eS17



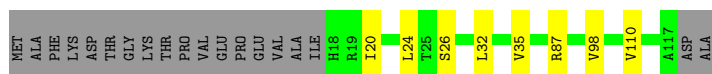
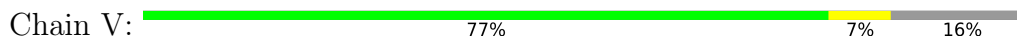
• Molecule 20: uS13



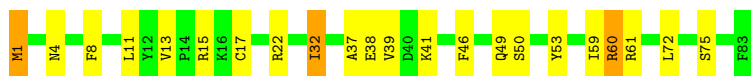
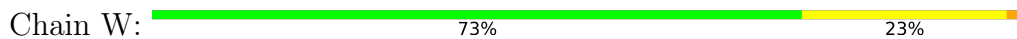
• Molecule 21: eS19



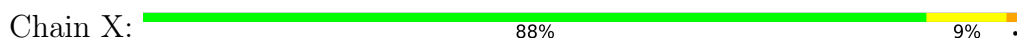
• Molecule 22: uS10

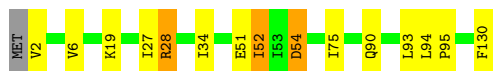


• Molecule 23: eS21

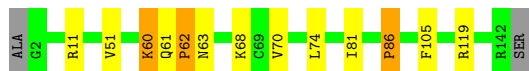
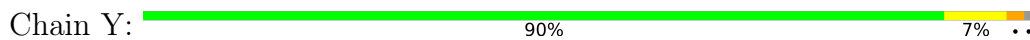


• Molecule 24: uS8

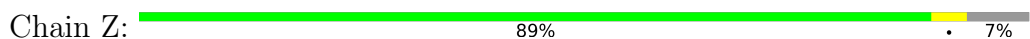




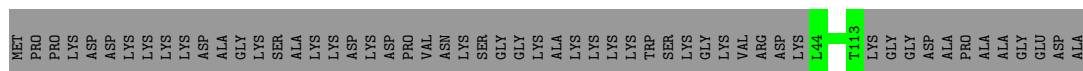
• Molecule 25: uS12



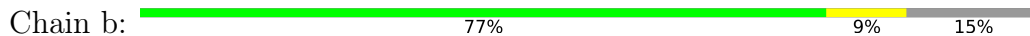
• Molecule 26: eS24



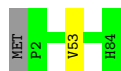
• Molecule 27: eS25



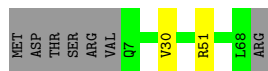
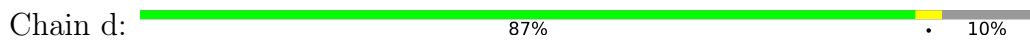
• Molecule 28: eS26



• Molecule 29: eS27



• Molecule 30: eS28



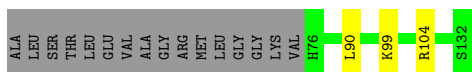
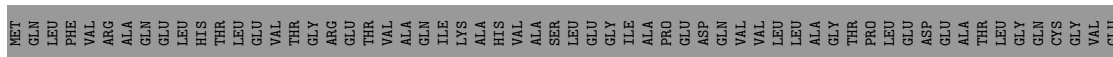
• Molecule 31: eS29



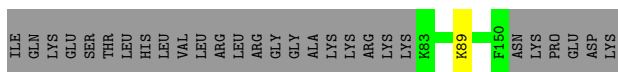
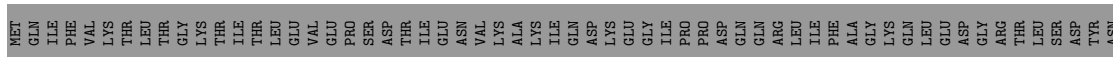




• Molecule 32: eS30



• Molecule 33: eS31



• Molecule 34: RACK1



• Molecule 35: eL41



There are no outlier residues recorded for this chain.

• Molecule 36: IAPV-IRES



06610	06618
C6611	G
A6612	C
I6613	G
	A
	U
	G

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	2	0.27	0/40509	0.70	7/63128 (0.0%)
2	B	0.65	0/1744	0.78	0/2371
3	C	0.66	0/1756	0.80	0/2350
4	D	0.65	0/1748	0.82	0/2362
5	E	0.68	0/1796	0.82	0/2417
6	F	0.65	0/2115	0.81	0/2843
7	G	0.67	0/1482	0.82	0/1990
8	H	0.67	0/1946	0.84	0/2590
9	I	0.68	0/1510	0.81	0/2022
10	J	0.65	0/1715	0.83	0/2287
11	K	0.65	0/1550	0.84	0/2069
12	L	0.64	0/834	0.76	0/1125
13	M	0.64	0/1195	0.83	0/1597
14	N	0.71	0/918	0.80	0/1233
15	O	0.66	0/1226	0.77	0/1649
16	P	0.67	0/1029	0.89	1/1380 (0.1%)
17	Q	0.66	0/1009	0.82	0/1346
18	R	0.66	0/1146	0.83	0/1534
19	S	0.68	0/1082	0.83	0/1452
20	T	0.67	0/1186	0.82	0/1589
21	U	0.67	0/1115	0.83	0/1493
22	V	0.68	0/805	0.82	0/1081
23	W	0.68	0/638	0.84	0/855
24	X	0.64	0/1051	0.82	0/1406
25	Y	0.66	0/1116	0.84	0/1490
26	Z	0.65	0/1028	0.79	0/1366
27	a	0.68	0/563	0.80	0/758
28	b	0.65	0/791	0.88	1/1062 (0.1%)
29	c	0.66	0/665	0.81	0/891
30	d	0.68	0/490	0.85	0/656
31	e	0.65	0/470	0.84	1/623 (0.2%)
32	f	0.66	0/462	0.82	0/607
33	g	0.67	0/567	0.80	0/753
34	h	0.68	0/2493	0.80	0/3394

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	n	0.60	0/240	0.86	0/305
36	1	0.24	0/4833	0.72	1/7529 (0.0%)
All	All	0.49	0/84823	0.76	11/123603 (0.0%)

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
7	G	0	3
8	H	0	1
9	I	0	1
10	J	0	1
18	R	0	1
24	X	0	3
25	Y	0	1
34	h	0	1
All	All	0	12

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	138	ASP	CB-CA-C	9.31	129.02	110.40
28	b	74	CYS	CA-CB-SG	6.51	125.73	114.00
1	2	1741	U	C2'-C3'-O3'	6.43	123.99	113.70
1	2	688	U	C2'-C3'-O3'	6.42	123.97	113.70
1	2	110	U	C2'-C3'-O3'	6.01	123.32	113.70
1	2	1489	A	C2'-C3'-O3'	5.99	123.28	113.70
1	2	1377	U	C4'-C3'-O3'	5.46	123.91	113.00
36	1	6541	A	C2'-C3'-O3'	5.32	122.21	113.70
1	2	1314	U	C2'-C3'-O3'	5.06	121.79	113.70
31	e	39	CYS	CA-CB-SG	5.04	123.08	114.00
1	2	501	C	N1-C1'-C2'	5.03	120.54	114.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	135	ARG	Peptide

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Mol	Chain	Res	Type	Group
7	G	18	LYS	Peptide
7	G	59	LYS	Peptide
8	H	121	ILE	Peptide
9	I	134	VAL	Peptide
10	J	29	LEU	Peptide
18	R	15	ARG	Peptide
24	X	27	ILE	Peptide
24	X	28	ARG	Peptide
24	X	54	ASP	Peptide
25	Y	86	PRO	Peptide
34	h	36	ARG	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	36229	0	18300	132	0
2	B	1706	0	1697	11	0
3	C	1729	0	1803	10	0
4	D	1712	0	1808	14	0
5	E	1768	0	1866	8	0
6	F	2073	0	2173	7	0
7	G	1462	0	1510	7	0
8	H	1923	0	2089	6	0
9	I	1488	0	1582	11	0
10	J	1686	0	1772	20	0
11	K	1525	0	1640	8	0
12	L	810	0	836	2	0
13	M	1175	0	1249	11	0
14	N	908	0	939	2	0
15	O	1202	0	1289	2	0
16	P	1016	0	1039	6	0
17	Q	990	0	1038	19	0
18	R	1128	0	1195	6	0
19	S	1068	0	1121	10	0
20	T	1168	0	1226	6	0
21	U	1097	0	1130	7	0
22	V	795	0	862	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	W	630	0	631	13	0
24	X	1034	0	1080	9	0
25	Y	1098	0	1167	4	0
26	Z	1011	0	1083	3	0
27	a	557	0	610	0	0
28	b	778	0	824	0	0
29	c	651	0	672	0	0
30	d	488	0	514	0	0
31	e	459	0	448	0	0
32	f	457	0	502	0	0
33	g	555	0	567	0	0
34	h	2436	0	2393	0	0
35	n	239	0	289	0	0
36	1	4323	0	2182	6	0
All	All	79374	0	61126	286	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 2.

All (286) 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)
10:J:202:ILE:HG23	10:J:206:LYS:CE	1.67	1.24
10:J:202:ILE:CG2	10:J:206:LYS:HE3	1.67	1.21
10:J:202:ILE:CG2	10:J:206:LYS:CE	2.26	1.10
10:J:202:ILE:CG2	10:J:206:LYS:NZ	2.37	0.86
1:2:531:A:H3'	1:2:532:C:H5''	1.62	0.82
10:J:202:ILE:HG23	10:J:206:LYS:HE3	0.82	0.78
10:J:202:ILE:HG21	10:J:206:LYS:NZ	2.02	0.75
10:J:202:ILE:O	10:J:206:LYS:HG3	1.94	0.66
1:2:293:C:O2	1:2:293:C:H2'	1.99	0.63
1:2:447:A:H4'	6:F:3:ARG:HB2	1.80	0.63
23:W:32:ILE:CG2	23:W:60:ARG:HD2	2.30	0.62
1:2:501:C:O2	1:2:501:C:H2'	2.02	0.60
1:2:984:C:O2'	16:P:138:ASP:HB3	2.02	0.59
9:I:36:LEU:HB2	9:I:75:ILE:HD11	1.85	0.59
9:I:144:ILE:N	24:X:51:GLU:OE2	2.36	0.59
1:2:1521:C:H5'	17:Q:126:VAL:CG1	2.33	0.58
1:2:1700:C:C2	1:2:1834:A:N6	2.72	0.58
10:J:202:ILE:CG2	10:J:206:LYS:HZ2	2.15	0.58
21:U:75:MET:HA	21:U:78:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ILE:HD11	13:M:68:ILE:HG13	1.85	0.57
4:D:200:ARG:O	11:K:54:ARG:NH1	2.38	0.56
22:V:24:LEU:HB3	22:V:32:LEU:HD11	1.88	0.56
4:D:234:GLY:O	4:D:238:LYS:HG3	2.06	0.56
4:D:141:LEU:HD11	4:D:238:LYS:HD3	1.88	0.56
13:M:68:ILE:HD13	13:M:131:CYS:HB3	1.87	0.56
17:Q:81:ARG:HB3	17:Q:117:GLY:HA3	1.88	0.56
17:Q:81:ARG:HH11	17:Q:81:ARG:HG2	1.71	0.56
1:2:1521:C:H5'	17:Q:126:VAL:HG13	1.87	0.55
2:B:82:THR:HG23	2:B:168:ALA:HA	1.89	0.55
1:2:1016:U:H2'	1:2:1016:U:O2	2.07	0.55
19:S:102:THR:HA	19:S:105:MET:HG2	1.89	0.55
1:2:4:C:O2'	11:K:18:ARG:NH1	2.39	0.54
1:2:853:C:O4'	1:2:853:C:O2	2.25	0.54
1:2:1516:G:C8	1:2:1516:G:H5''	2.42	0.54
1:2:1117:C:O2	1:2:1117:C:O4'	2.25	0.54
13:M:99:TYR:O	13:M:101:ARG:HD3	2.07	0.54
10:J:202:ILE:HG22	10:J:206:LYS:CE	2.32	0.54
21:U:40:ALA:HB3	21:U:43:LYS:HG2	1.90	0.54
1:2:114:G:OP1	13:M:69:ARG:NH1	2.41	0.53
2:B:154:LEU:HD22	2:B:157:VAL:HG21	1.90	0.53
14:N:22:LEU:HD11	14:N:89:VAL:HA	1.91	0.53
1:2:1520:G:N3	1:2:1520:G:H2'	2.23	0.53
1:2:887:U:HO2'	1:2:889:U:H5	1.56	0.53
1:2:314:U:OP2	8:H:191:ARG:NH2	2.42	0.53
1:2:369:C:O2	1:2:369:C:O4'	2.25	0.53
1:2:1091:C:HO2'	24:X:2:VAL:N	2.06	0.52
5:E:126:ILE:HD11	5:E:134:CYS:SG	2.49	0.52
1:2:1118:C:O4'	1:2:1118:C:O2	2.26	0.52
6:F:19:MET:HE1	6:F:108:ARG:CZ	2.39	0.52
1:2:110:U:H3	1:2:351:G:H1	1.58	0.52
1:2:942:G:H21	16:P:137:SER:HB2	1.75	0.52
9:I:170:VAL:HG13	9:I:187:PHE:HB2	1.91	0.52
36:1:6603:C:H2'	36:1:6605:A:OP2	2.09	0.52
1:2:583:A:OP1	11:K:162:ARG:NH2	2.43	0.51
22:V:20:ILE:HG21	22:V:98:VAL:HG21	1.92	0.51
22:V:26:SER:HB2	22:V:32:LEU:HD13	1.93	0.51
36:1:6544:G:O2'	36:1:6545:G:O5'	2.28	0.51
1:2:1535:U:O2'	7:G:82:ASN:OD1	2.29	0.51
1:2:867:G:H4'	13:M:149:ALA:HB1	1.93	0.51
1:2:1444:U:O2'	1:2:1580:A:N1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:501:C:O2	1:2:501:C:C2'	2.59	0.50
1:2:1364:U:O4'	1:2:1364:U:O2	2.28	0.50
1:2:962:A:N1	1:2:1055:A:O2'	2.44	0.50
1:2:943:U:C5'	1:2:943:U:H6	2.25	0.50
1:2:1606:G:O2'	1:2:1632:G:N2	2.45	0.50
2:B:104:THR:O	2:B:107:THR:HG23	2.11	0.50
1:2:1473:G:O2'	1:2:1475:G:N2	2.44	0.50
5:E:72:VAL:HG22	12:L:68:TYR:HD1	1.77	0.50
13:M:111:VAL:HG11	13:M:128:VAL:HG11	1.94	0.50
13:M:131:CYS:SG	13:M:134:LEU:HD21	2.52	0.50
1:2:914:U:O2	1:2:914:U:O4'	2.29	0.49
1:2:507:G:O6	26:Z:105:LYS:NZ	2.46	0.49
25:Y:61:GLN:HB3	25:Y:62:PRO:HD3	1.93	0.49
1:2:4:C:H4'	4:D:207:ALA:HB2	1.93	0.49
25:Y:74:LEU:HD11	25:Y:81:ILE:HD12	1.93	0.49
13:M:126:VAL:HG23	13:M:145:VAL:HG22	1.94	0.49
19:S:74:GLN:HG3	19:S:78:ARG:HD2	1.92	0.49
1:2:1623:A:H5''	20:T:133:GLY:HA3	1.94	0.49
1:2:1862:G:H4'	1:2:1863:A:OP1	2.12	0.49
1:2:1587:G:C6	21:U:67:ARG:HD3	2.48	0.49
1:2:1530:U:H2'	1:2:1531:A:O4'	2.13	0.49
36:1:6589:C:H4'	36:1:6590:A:H5'	1.95	0.49
2:B:143:PRO:HA	23:W:32:ILE:HG13	1.95	0.48
23:W:32:ILE:HD13	23:W:32:ILE:O	2.12	0.48
1:2:1231:C:O2'	1:2:1253:A:N6	2.45	0.48
11:K:170:PRO:O	11:K:175:ARG:NH1	2.46	0.48
17:Q:57:LEU:HG	17:Q:83:MET:SD	2.53	0.48
17:Q:123:TYR:CD1	17:Q:123:TYR:C	2.86	0.48
19:S:71:ILE:HG22	19:S:72:LYS:H	1.79	0.48
6:F:128:LYS:HA	6:F:156:MET:HG3	1.96	0.48
1:2:191:A:N6	1:2:208:G:O2'	2.46	0.48
1:2:1396:A:H2'	1:2:1398:G:N7	2.29	0.48
1:2:1303:C:O2	1:2:1303:C:O4'	2.29	0.48
24:X:6:VAL:HG12	24:X:34:ILE:HD11	1.96	0.48
1:2:1522:A:C5	17:Q:128:HIS:HB3	2.49	0.48
20:T:80:PRO:HB2	20:T:82:TRP:CD1	2.49	0.48
1:2:1587:G:N2	1:2:1587:G:OP1	2.44	0.48
23:W:53:TYR:OH	23:W:72:LEU:O	2.23	0.48
1:2:384:U:O4	10:J:5:ARG:NH2	2.47	0.48
10:J:202:ILE:HG22	10:J:206:LYS:HD2	1.96	0.48
19:S:107:LYS:HA	19:S:112:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:823:U:O2	1:2:823:U:O4'	2.32	0.47
1:2:1584:G:OP1	21:U:77:LYS:NZ	2.45	0.47
1:2:420:G:HI'	1:2:661:U:O2	2.13	0.47
17:Q:61:ARG:HA	17:Q:64:LYS:HE3	1.96	0.47
1:2:522:A:OP2	11:K:45:ARG:NH1	2.47	0.47
1:2:1260:A:C6	1:2:1619:A:C6	3.03	0.47
1:2:1589:A:N3	1:2:1653:U:O2'	2.36	0.47
1:2:887:U:O2'	1:2:889:U:H5	1.96	0.47
1:2:955:A:N1	1:2:968:U:O2'	2.42	0.47
9:I:144:ILE:HB	24:X:52:ILE:HG23	1.96	0.47
1:2:563:G:HO2'	1:2:564:A:H8	1.62	0.47
5:E:74:GLN:HB3	5:E:84:VAL:HG11	1.96	0.47
19:S:74:GLN:N	19:S:75:GLU:HA	2.29	0.47
1:2:64:A:C2	1:2:82:G:C2	3.03	0.47
1:2:183:G:O2'	1:2:184:G:O4'	2.30	0.47
1:2:887:U:O2	1:2:887:U:C2'	2.63	0.47
1:2:1137:U:O2'	1:2:1139:C:OP2	2.31	0.47
1:2:1237:C:H4'	17:Q:129:GLY:O	2.15	0.47
1:2:1297:U:O4	17:Q:59:ARG:NH1	2.48	0.47
1:2:1499:U:C5'	5:E:176:LEU:HD21	2.45	0.47
5:E:70:THR:HA	5:E:86:LEU:HD13	1.95	0.47
13:M:38:LYS:NZ	13:M:64:GLY:O	2.46	0.47
1:2:27:A:H2'	1:2:28:U:O4'	2.15	0.47
1:2:1624:U:O2	1:2:1624:U:O4'	2.33	0.47
8:H:121:ILE:HG23	8:H:124:LEU:HB2	1.97	0.47
7:G:87:LEU:HD21	18:R:47:LEU:HD11	1.97	0.47
8:H:5:ILE:HD12	8:H:16:ILE:HD13	1.97	0.47
1:2:823:U:C5	11:K:144:ILE:HD12	2.50	0.47
22:V:35:VAL:HG21	22:V:110:VAL:HG21	1.97	0.47
25:Y:62:PRO:HB2	25:Y:63:ASN:H	1.53	0.47
20:T:121:ARG:HG3	20:T:131:VAL:HG21	1.97	0.46
1:2:1397:U:O2	1:2:1397:U:O4'	2.30	0.46
4:D:259:THR:HG21	23:W:15:ARG:HA	1.97	0.46
17:Q:129:GLY:O	17:Q:130:ARG:C	2.54	0.46
1:2:1658:G:OP2	1:2:1660:C:N4	2.49	0.46
4:D:101:ALA:O	4:D:103:LYS:HG3	2.15	0.46
7:G:39:ILE:HG23	7:G:68:ILE:HD13	1.97	0.46
10:J:202:ILE:HG21	10:J:206:LYS:HZ1	1.78	0.46
23:W:22:ARG:NH2	24:X:19:LYS:O	2.49	0.46
1:2:1270:G:O2'	1:2:1301:A:N7	2.48	0.46
1:2:379:C:O2	10:J:5:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1454:A:C8	19:S:3:ARG:HD2	2.51	0.46
1:2:1636:G:N3	1:2:1636:G:H2'	2.31	0.46
9:I:130:LEU:HD23	9:I:142:LYS:HE3	1.98	0.46
10:J:36:THR:HG23	10:J:96:LEU:HB2	1.96	0.46
1:2:1622:U:C4	17:Q:122:THR:HG23	2.51	0.46
24:X:90:GLN:HB2	24:X:94:LEU:HD12	1.97	0.46
3:C:52:THR:HG23	3:C:57:ILE:HA	1.98	0.45
4:D:132:ASP:O	4:D:216:MET:O	2.34	0.45
6:F:44:LEU:HD11	6:F:70:ILE:HG21	1.98	0.45
1:2:1300:U:OP1	17:Q:59:ARG:NE	2.48	0.45
1:2:1395:C:H1'	1:2:1474:A:C4	2.52	0.45
1:2:293:C:O2	1:2:293:C:C2'	2.65	0.45
1:2:986:G:C8	16:P:137:SER:HA	2.52	0.45
1:2:1588:A:H2'	1:2:1589:A:C8	2.51	0.45
1:2:1123:C:OP1	3:C:151:ARG:NH2	2.50	0.45
9:I:142:LYS:HB2	24:X:54:ASP:HB3	1.99	0.45
11:K:94:LEU:HD23	11:K:94:LEU:H	1.82	0.45
1:2:1461:G:O2'	1:2:1464:C:N4	2.50	0.45
7:G:119:SER:OG	7:G:189:ALA:HB1	2.17	0.45
23:W:1:MET:O	23:W:1:MET:HG3	2.16	0.45
1:2:581:U:H4'	26:Z:66:GLY:HA3	1.99	0.45
1:2:373:G:H4'	13:M:85:THR:HG21	1.98	0.44
3:C:125:VAL:HG12	3:C:127:VAL:HB	2.00	0.44
2:B:156:TYR:CE1	23:W:61:ARG:HG2	2.52	0.44
1:2:110:U:H6	1:2:110:U:C5'	2.30	0.44
1:2:1315:U:O2	1:2:1315:U:O4'	2.35	0.44
1:2:551:U:H2'	1:2:552:G:C8	2.52	0.44
9:I:23:ILE:CD1	9:I:60:ILE:HD11	2.48	0.44
20:T:86:ARG:NH2	20:T:110:ASP:OD2	2.50	0.44
1:2:1035:A:H2'	1:2:1036:A:O4'	2.18	0.44
2:B:80:ARG:NH2	2:B:165:ASN:O	2.51	0.44
7:G:81:ARG:HG3	7:G:82:ASN:OD1	2.18	0.44
11:K:94:LEU:HB2	11:K:97:ILE:HD12	1.99	0.44
1:2:886:A:C8	1:2:886:A:H5''	2.53	0.44
1:2:1542:C:OP1	21:U:62:ARG:NH2	2.50	0.44
3:C:207:LEU:HD13	3:C:210:VAL:HG21	1.98	0.44
23:W:17:CYS:SG	23:W:59:ILE:HD12	2.58	0.44
1:2:1486:A:O2'	4:D:118:ALA:HB3	2.18	0.44
1:2:1619:A:OP1	17:Q:50:ARG:NH2	2.50	0.44
2:B:57:LYS:HE3	2:B:159:ILE:HG13	1.99	0.44
1:2:886:A:N3	1:2:886:A:H2'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:965:U:O2	1:2:1066:U:H1'	2.17	0.43
9:I:177:TYR:CD2	9:I:185:VAL:HG21	2.53	0.43
20:T:31:THR:HG22	20:T:37:GLY:O	2.17	0.43
4:D:139:LEU:CD1	4:D:141:LEU:HD21	2.49	0.43
23:W:1:MET:HE3	23:W:13:VAL:HG22	2.00	0.43
1:2:1139:C:O2	1:2:1139:C:O4'	2.36	0.43
10:J:202:ILE:O	10:J:206:LYS:CG	2.66	0.43
19:S:98:VAL:HG13	19:S:119:VAL:HA	2.00	0.43
20:T:35:GLY:O	20:T:97:GLN:NE2	2.48	0.43
1:2:1207:G:O2'	1:2:1837:G:N2	2.48	0.43
1:2:1295:A:H3'	1:2:1296:U:C6	2.53	0.43
23:W:37:ALA:HB1	23:W:46:PHE:CD1	2.53	0.43
24:X:75:ILE:HD11	24:X:93:LEU:HD11	1.99	0.43
5:E:25:LEU:HD12	5:E:29:LEU:HD12	1.99	0.43
18:R:112:LEU:HD12	18:R:120:LEU:HD11	2.00	0.43
1:2:575:A:OP2	26:Z:93:ARG:NH2	2.51	0.43
16:P:104:ARG:O	16:P:106:LYS:HE2	2.19	0.43
1:2:356:C:O2	1:2:356:C:C2'	2.66	0.43
1:2:1149:A:H2'	1:2:1149:A:N3	2.34	0.43
4:D:166:ARG:HB3	4:D:247:THR:HB	2.01	0.43
18:R:44:PRO:HD3	18:R:77:HIS:HB3	2.01	0.43
36:1:6518:G:N2	36:1:6531:C:N3	2.67	0.43
1:2:1491:G:H2'	1:2:1492:U:C6	2.54	0.43
3:C:35:ALA:HB2	3:C:44:ILE:HD11	2.01	0.43
6:F:61:VAL:HG12	6:F:80:ILE:HG22	2.01	0.43
1:2:446:G:H5''	10:J:49:ARG:HH22	1.84	0.42
1:2:1354:G:H5''	1:2:1354:G:H8	1.84	0.42
1:2:1395:C:H1'	1:2:1474:A:C5	2.53	0.42
1:2:1674:G:N7	18:R:17:LYS:NZ	2.48	0.42
8:H:67:VAL:CG1	8:H:99:GLY:HA2	2.49	0.42
24:X:95:PRO:HD3	24:X:130:PHE:CD1	2.54	0.42
1:2:63:U:O2'	1:2:170:A:N3	2.52	0.42
1:2:1453:C:OP1	19:S:48:ASN:ND2	2.44	0.42
1:2:126:G:OP2	8:H:198:ARG:NH1	2.52	0.42
1:2:1122:A:N3	3:C:146:ARG:NH1	2.67	0.42
2:B:8:LEU:HD11	23:W:39:VAL:HG21	2.01	0.42
15:O:128:TYR:O	15:O:131:THR:OG1	2.30	0.42
19:S:25:GLY:H	19:S:31:ASN:HD21	1.66	0.42
18:R:116:ASP:HB3	18:R:119:LEU:HD23	2.02	0.42
1:2:33:G:O2'	1:2:564:A:O2'	2.37	0.42
4:D:204:ILE:HD13	4:D:215:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:ILE:O	6:F:49:ARG:HG3	2.19	0.42
1:2:1228:A:H2'	1:2:1229:G:C8	2.55	0.42
1:2:1553:C:O2'	1:2:1554:C:O5'	2.31	0.42
4:D:135:GLY:HA2	4:D:165:VAL:HG22	2.01	0.42
15:O:60:VAL:HG23	15:O:66:VAL:HG21	2.01	0.42
23:W:1:MET:HE2	23:W:8:PHE:HD1	1.84	0.42
1:2:110:U:C6	1:2:110:U:H5''	2.55	0.42
1:2:695:C:N4	1:2:731:G:O6	2.53	0.42
7:G:25:THR:HG21	7:G:43:GLU:H	1.83	0.42
16:P:56:VAL:CG1	16:P:81:VAL:HG23	2.50	0.42
25:Y:51:VAL:HG13	25:Y:70:VAL:HG13	2.01	0.42
3:C:69:VAL:HG11	3:C:74:LEU:HD13	2.02	0.41
9:I:69:LEU:HG	9:I:96:ALA:HB2	2.02	0.41
9:I:157:HIS:HB3	9:I:190:PRO:HG3	2.02	0.41
10:J:49:ARG:HH21	10:J:49:ARG:HG3	1.85	0.41
2:B:151:ASP:N	2:B:151:ASP:OD1	2.53	0.41
17:Q:81:ARG:HG2	17:Q:81:ARG:NH1	2.35	0.41
3:C:134:LEU:HD22	3:C:218:LEU:HD12	2.03	0.41
10:J:202:ILE:HG22	10:J:206:LYS:CD	2.51	0.41
1:2:99:A:H2'	1:2:100:U:O4'	2.20	0.41
1:2:1132:C:H2'	1:2:1133:A:O4'	2.20	0.41
4:D:191:VAL:HG11	4:D:236:PHE:HA	2.01	0.41
7:G:121:PRO:O	7:G:141:VAL:HG21	2.20	0.41
12:L:35:LEU:HD22	12:L:35:LEU:HA	1.96	0.41
21:U:39:LEU:HD13	21:U:47:PRO:CG	2.50	0.41
1:2:958:G:H2'	1:2:959:G:O4'	2.21	0.41
1:2:1395:C:H2'	1:2:1396:A:N3	2.35	0.41
19:S:98:VAL:HG23	19:S:102:THR:CG2	2.51	0.41
1:2:531:A:H3'	1:2:532:C:C5'	2.43	0.41
1:2:1139:C:C2	1:2:1148:A:N6	2.89	0.41
1:2:1286:G:N2	1:2:1312:G:O2'	2.53	0.41
1:2:1521:C:O4'	17:Q:126:VAL:HG21	2.20	0.41
1:2:1834:A:H2	1:2:1837:G:H22	1.67	0.41
5:E:51:LEU:HG	5:E:91:VAL:HG22	2.03	0.41
13:M:111:VAL:HG11	13:M:128:VAL:CG1	2.50	0.41
1:2:532:C:H2'	1:2:533:A:C8	2.56	0.41
2:B:55:TRP:NE1	2:B:59:LEU:HD11	2.35	0.41
1:2:977:C:H2'	1:2:978:G:O4'	2.21	0.41
10:J:202:ILE:CG2	10:J:206:LYS:CD	2.96	0.41
18:R:37:ARG:HB3	21:U:7:LYS:HG2	2.03	0.41
36:1:6426:U:H4'	36:1:6427:G:OP1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:THR:HB	3:C:205:TYR:CE2	2.56	0.41
1:2:1619:A:OP2	17:Q:47:ARG:NH1	2.54	0.40
1:2:1622:U:O4	17:Q:122:THR:HG23	2.20	0.40
9:I:66:VAL:N	9:I:67:PRO:HD2	2.36	0.40
10:J:202:ILE:HG21	10:J:206:LYS:HZ2	1.79	0.40
1:2:1103:C:OP1	3:C:157:GLN:NE2	2.54	0.40
1:2:1284:A:C8	14:N:104:VAL:HG21	2.56	0.40
4:D:183:LYS:HA	4:D:195:LEU:O	2.22	0.40
8:H:58:LYS:HA	8:H:107:SER:HB2	2.02	0.40
16:P:76:LEU:HD22	16:P:76:LEU:HA	1.90	0.40
17:Q:81:ARG:NH2	17:Q:122:THR:HG22	2.36	0.40
1:2:183:G:N3	1:2:183:G:C2'	2.84	0.40
1:2:520:A:O2'	1:2:825:A:N3	2.41	0.40
1:2:564:A:H3'	1:2:565:G:H8	1.87	0.40
1:2:1259:A:N1	1:2:1519:U:C5	2.89	0.40
36:1:6444:G:H2'	36:1:6444:G:N3	2.35	0.40
5:E:31:GLU:O	5:E:54:ARG:NH2	2.54	0.40
1:2:1448:A:H2'	1:2:1449:G:O4'	2.21	0.40
1:2:1566:G:C2	1:2:1570:G:C6	3.10	0.40
2:B:41:ARG:HG2	2:B:47:TYR:CE1	2.56	0.40
6:F:15:PRO:HG2	6:F:18:TRP:CE2	2.56	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	215/295 (73%)	200 (93%)	14 (6%)	1 (0%)	29	64
3	C	211/264 (80%)	186 (88%)	22 (10%)	3 (1%)	11	40
4	D	219/255 (86%)	201 (92%)	16 (7%)	2 (1%)	17	52
5	E	226/281 (80%)	204 (90%)	22 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	260/263 (99%)	244 (94%)	15 (6%)	1 (0%)	34	69
7	G	180/204 (88%)	160 (89%)	17 (9%)	3 (2%)	9	36
8	H	235/249 (94%)	217 (92%)	18 (8%)	0	100	100
9	I	181/194 (93%)	162 (90%)	19 (10%)	0	100	100
10	J	204/208 (98%)	181 (89%)	16 (8%)	7 (3%)	3	21
11	K	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	29	64
12	L	94/149 (63%)	85 (90%)	8 (8%)	1 (1%)	14	46
13	M	139/158 (88%)	128 (92%)	10 (7%)	1 (1%)	22	57
14	N	115/132 (87%)	95 (83%)	19 (16%)	1 (1%)	17	52
15	O	147/151 (97%)	130 (88%)	17 (12%)	0	100	100
16	P	134/151 (89%)	115 (86%)	15 (11%)	4 (3%)	4	23
17	Q	117/145 (81%)	100 (86%)	15 (13%)	2 (2%)	9	36
18	R	140/172 (81%)	130 (93%)	8 (6%)	2 (1%)	11	40
19	S	130/135 (96%)	111 (85%)	18 (14%)	1 (1%)	19	54
20	T	139/152 (91%)	129 (93%)	7 (5%)	3 (2%)	6	29
21	U	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V	98/119 (82%)	88 (90%)	10 (10%)	0	100	100
23	W	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
24	X	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	54
25	Y	139/143 (97%)	127 (91%)	9 (6%)	3 (2%)	6	29
26	Z	122/134 (91%)	113 (93%)	9 (7%)	0	100	100
27	a	68/125 (54%)	63 (93%)	5 (7%)	0	100	100
28	b	96/115 (84%)	79 (82%)	14 (15%)	3 (3%)	4	23
29	c	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d	60/69 (87%)	55 (92%)	5 (8%)	0	100	100
31	e	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
32	f	55/133 (41%)	46 (84%)	8 (14%)	1 (2%)	8	34
33	g	66/156 (42%)	57 (86%)	9 (14%)	0	100	100
34	h	311/317 (98%)	270 (87%)	40 (13%)	1 (0%)	41	73
35	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4788/5586 (86%)	4320 (90%)	426 (9%)	42 (1%)	21	52

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ASP
7	G	19	LEU
10	J	123	ARG
16	P	137	SER
20	T	49	ASP
25	Y	62	PRO
25	Y	86	PRO
28	b	8	ASN
3	C	52	THR
4	D	77	SER
6	F	73	ASP
17	Q	18	ARG
20	T	100	ALA
28	b	26	CYS
2	B	141	ASN
7	G	136	ARG
10	J	56	ARG
10	J	71	CYS
10	J	140	LYS
16	P	136	PRO
17	Q	70	MET
18	R	127	CYS
20	T	48	ALA
25	Y	60	LYS
32	f	90	LEU
10	J	13	LYS
10	J	86	SER
11	K	147	PHE
16	P	22	ALA
34	h	264	LYS
4	D	261	PHE
13	M	151	THR
14	N	117	GLU
18	R	17	LYS
3	C	190	PRO
12	L	64	TRP
7	G	41	VAL
19	S	125	GLY
28	b	58	VAL
10	J	3	ILE
16	P	30	VAL
24	X	28	ARG



### 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	180/245 (74%)	175 (97%)	5 (3%)	43 73
3	C	194/231 (84%)	187 (96%)	7 (4%)	35 67
4	D	186/205 (91%)	174 (94%)	12 (6%)	17 47
5	E	190/232 (82%)	181 (95%)	9 (5%)	26 59
6	F	223/225 (99%)	213 (96%)	10 (4%)	27 60
7	G	156/170 (92%)	150 (96%)	6 (4%)	33 66
8	H	207/218 (95%)	203 (98%)	4 (2%)	57 81
9	I	165/174 (95%)	163 (99%)	2 (1%)	71 88
10	J	178/180 (99%)	170 (96%)	8 (4%)	27 60
11	K	161/168 (96%)	155 (96%)	6 (4%)	34 66
12	L	87/125 (70%)	84 (97%)	3 (3%)	37 69
13	M	130/142 (92%)	119 (92%)	11 (8%)	10 37
14	N	99/108 (92%)	98 (99%)	1 (1%)	76 90
15	O	130/131 (99%)	127 (98%)	3 (2%)	50 77
16	P	106/119 (89%)	100 (94%)	6 (6%)	20 52
17	Q	108/130 (83%)	97 (90%)	11 (10%)	7 27
18	R	117/140 (84%)	113 (97%)	4 (3%)	37 69
19	S	119/121 (98%)	117 (98%)	2 (2%)	60 83
20	T	123/132 (93%)	121 (98%)	2 (2%)	62 84
21	U	111/116 (96%)	108 (97%)	3 (3%)	44 74
22	V	92/107 (86%)	91 (99%)	1 (1%)	73 89
23	W	68/68 (100%)	58 (85%)	10 (15%)	3 13
24	X	112/113 (99%)	111 (99%)	1 (1%)	78 91
25	Y	113/114 (99%)	108 (96%)	5 (4%)	28 61
26	Z	107/115 (93%)	105 (98%)	2 (2%)	57 81
27	a	62/103 (60%)	62 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	86/99 (87%)	80 (93%)	6 (7%)	15	45
29	c	75/76 (99%)	74 (99%)	1 (1%)	69	87
30	d	55/62 (89%)	53 (96%)	2 (4%)	35	67
31	e	48/49 (98%)	47 (98%)	1 (2%)	53	79
32	f	47/106 (44%)	45 (96%)	2 (4%)	29	62
33	g	61/140 (44%)	60 (98%)	1 (2%)	62	84
34	h	272/275 (99%)	266 (98%)	6 (2%)	52	78
35	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4192/4763 (88%)	4039 (96%)	153 (4%)	38	67

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
2	B	128	GLN
2	B	157	VAL
2	B	189	ILE
2	B	200	ASP
3	C	29	ASP
3	C	40	ASN
3	C	49	VAL
3	C	62	LEU
3	C	94	LYS
3	C	207	LEU
3	C	212	VAL
4	D	78	LEU
4	D	102	LEU
4	D	137	VAL
4	D	141	LEU
4	D	165	VAL
4	D	182	CYS
4	D	238	LYS
4	D	254	ASP
4	D	255	LEU
4	D	260	VAL
4	D	274	MET
4	D	277	HIS
5	E	35	SER
5	E	39	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	57	ASN
5	E	74	GLN
5	E	76	ARG
5	E	94	ARG
5	E	169	ASP
5	E	208	VAL
5	E	227	LYS
6	F	3	ARG
6	F	22	LYS
6	F	32	SER
6	F	49	ARG
6	F	51	LYS
6	F	102	ILE
6	F	108	ARG
6	F	126	VAL
6	F	156	MET
6	F	220	THR
7	G	19	LEU
7	G	88	MET
7	G	112	LEU
7	G	169	ILE
7	G	173	LEU
7	G	193	LYS
8	H	63	MET
8	H	98	ARG
8	H	198	ARG
8	H	201	LYS
9	I	105	THR
9	I	121	THR
10	J	29	LEU
10	J	47	ARG
10	J	49	ARG
10	J	72	CYS
10	J	84	ASN
10	J	94	LYS
10	J	99	ASN
10	J	121	LEU
11	K	54	ARG
11	K	69	ARG
11	K	79	ARG
11	K	123	ILE
11	K	127	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	150	ARG
12	L	35	LEU
12	L	43	LEU
12	L	95	ARG
13	M	20	LYS
13	M	38	LYS
13	M	42	LEU
13	M	45	LYS
13	M	48	LYS
13	M	66	VAL
13	M	69	ARG
13	M	85	THR
13	M	101	ARG
13	M	126	VAL
13	M	153	LYS
14	N	64	LEU
15	O	60	VAL
15	O	104	ARG
15	O	121	ARG
16	P	52	THR
16	P	76	LEU
16	P	128	ARG
16	P	135	ILE
16	P	138	ASP
16	P	139	SER
17	Q	13	ARG
17	Q	37	TYR
17	Q	70	MET
17	Q	84	ILE
17	Q	104	GLN
17	Q	106	GLU
17	Q	120	SER
17	Q	121	ILE
17	Q	122	THR
17	Q	127	LYS
17	Q	130	ARG
18	R	15	ARG
18	R	18	THR
18	R	71	ARG
18	R	72	VAL
19	S	14	ARG
19	S	72	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	T	8	LYS
20	T	142	ARG
21	U	28	LEU
21	U	115	LYS
21	U	121	ARG
22	V	87	ARG
23	W	1	MET
23	W	4	ASN
23	W	11	LEU
23	W	32	ILE
23	W	38	GLU
23	W	41	LYS
23	W	49	GLN
23	W	50	SER
23	W	60	ARG
23	W	75	SER
24	X	52	ILE
25	Y	11	ARG
25	Y	60	LYS
25	Y	68	LYS
25	Y	105	PHE
25	Y	119	ARG
26	Z	21	LYS
26	Z	101	LYS
28	b	6	ARG
28	b	15	ARG
28	b	21	ILE
28	b	23	CYS
28	b	28	CYS
28	b	55	GLU
29	c	53	VAL
30	d	30	VAL
30	d	51	ARG
31	e	24	CYS
32	f	99	LYS
32	f	104	ARG
33	g	89	LYS
34	h	63	SER
34	h	107	ASP
34	h	168	CYS
34	h	213	ASP
34	h	289	LEU

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Mol	Chain	Res	Type
34	h	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
17	Q	98	ASN
17	Q	103	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1869 (90%)	415 (24%)	47 (2%)
36	1	202/253 (79%)	103 (50%)	8 (3%)
All	All	1887/2122 (88%)	518 (27%)	55 (2%)

All (518) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	17	C
1	2	33	G
1	2	41	G
1	2	44	U
1	2	45	A
1	2	46	A
1	2	56	G
1	2	58	C
1	2	60	A
1	2	65	C
1	2	67	C
1	2	68	A
1	2	70	G
1	2	73	C
1	2	74	G
1	2	79	A
1	2	99	A
1	2	101	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	102	A
1	2	103	A
1	2	104	A
1	2	110	U
1	2	111	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	123	G
1	2	126	G
1	2	127	C
1	2	128	U
1	2	130	G
1	2	142	C
1	2	143	U
1	2	149	A
1	2	155	G
1	2	162	C
1	2	163	U
1	2	168	C
1	2	175	A
1	2	177	G
1	2	178	C
1	2	182	C
1	2	183	G
1	2	184	G
1	2	188	C
1	2	189	U
1	2	190	G
1	2	192	C
1	2	197	U
1	2	198	U
1	2	204	G
1	2	215	G
1	2	291	G
1	2	292	A
1	2	294	U
1	2	302	A
1	2	306	C
1	2	307	G
1	2	309	G
1	2	312	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	313	A
1	2	316	G
1	2	319	C
1	2	320	G
1	2	322	C
1	2	323	C
1	2	330	G
1	2	331	C
1	2	332	G
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	388	U
1	2	391	C
1	2	400	C
1	2	407	G
1	2	409	C
1	2	418	A
1	2	435	A
1	2	438	G
1	2	441	C
1	2	447	A
1	2	448	A
1	2	449	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	483	C
1	2	485	A
1	2	487	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	492	C
1	2	496	C
1	2	502	C
1	2	508	A
1	2	517	C
1	2	525	A
1	2	528	A
1	2	531	A
1	2	532	C
1	2	533	A
1	2	534	G
1	2	536	A
1	2	537	C
1	2	538	U
1	2	541	U
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	553	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	561	A
1	2	562	U
1	2	564	A
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	590	A
1	2	591	U
1	2	597	G
1	2	604	A
1	2	606	G
1	2	607	U
1	2	608	C
1	2	614	C
1	2	617	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	627	U
1	2	628	A
1	2	629	A
1	2	634	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	678	U
1	2	679	A
1	2	681	U
1	2	687	C
1	2	689	U
1	2	691	G
1	2	732	U
1	2	752	G
1	2	753	C
1	2	754	G
1	2	755	C
1	2	756	C
1	2	796	G
1	2	797	C
1	2	798	G
1	2	799	U
1	2	811	A
1	2	812	A
1	2	818	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	834	C
1	2	847	A
1	2	852	G
1	2	853	C
1	2	867	G
1	2	868	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	875	A
1	2	877	C
1	2	878	G
1	2	879	C
1	2	883	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	890	U
1	2	894	G
1	2	898	U
1	2	901	G
1	2	903	A
1	2	905	C
1	2	908	A
1	2	909	G
1	2	913	A
1	2	914	U
1	2	920	A
1	2	921	G
1	2	930	C
1	2	933	G
1	2	943	U
1	2	954	U
1	2	970	G
1	2	971	G
1	2	976	G
1	2	978	G
1	2	985	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1002	U
1	2	1008	A
1	2	1017	U
1	2	1023	A
1	2	1045	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1053	C
1	2	1058	A
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1078	C
1	2	1083	A
1	2	1085	C
1	2	1089	G
1	2	1109	C
1	2	1115	U
1	2	1116	C
1	2	1121	G
1	2	1125	C
1	2	1133	A
1	2	1139	C
1	2	1143	A
1	2	1144	A
1	2	1148	A
1	2	1149	A
1	2	1150	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1170	A
1	2	1195	A
1	2	1203	G
1	2	1204	A
1	2	1207	G
1	2	1215	C
1	2	1224	G
1	2	1242	U
1	2	1251	A
1	2	1253	A
1	2	1254	C
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1267	C
1	2	1274	G
1	2	1275	G
1	2	1281	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1288	U
1	2	1293	A
1	2	1295	A
1	2	1296	U
1	2	1298	G
1	2	1299	A
1	2	1301	A
1	2	1302	G
1	2	1304	U
1	2	1307	U
1	2	1308	U
1	2	1314	U
1	2	1315	U
1	2	1320	G
1	2	1333	U
1	2	1342	U
1	2	1343	U
1	2	1348	G
1	2	1354	G
1	2	1371	U
1	2	1372	U
1	2	1373	C
1	2	1377	U
1	2	1378	A
1	2	1379	A
1	2	1396	A
1	2	1397	U
1	2	1401	A
1	2	1402	A
1	2	1403	C
1	2	1404	U
1	2	1424	G
1	2	1428	G
1	2	1429	G
1	2	1449	G
1	2	1453	C
1	2	1454	A
1	2	1459	G
1	2	1460	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1466	G
1	2	1475	G
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1479	G
1	2	1480	A
1	2	1489	A
1	2	1490	G
1	2	1497	G
1	2	1498	A
1	2	1507	G
1	2	1516	G
1	2	1517	G
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1533	A
1	2	1535	U
1	2	1536	G
1	2	1544	C
1	2	1548	G
1	2	1552	G
1	2	1553	C
1	2	1554	C
1	2	1555	U
1	2	1556	A
1	2	1557	C
1	2	1564	C
1	2	1567	G
1	2	1570	G
1	2	1573	G
1	2	1575	G
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1588	A
1	2	1596	U
1	2	1601	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1602	U
1	2	1604	G
1	2	1606	G
1	2	1607	A
1	2	1614	A
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1641	A
1	2	1647	A
1	2	1648	G
1	2	1654	G
1	2	1655	C
1	2	1661	A
1	2	1665	G
1	2	1671	G
1	2	1679	A
1	2	1680	G
1	2	1692	U
1	2	1693	G
1	2	1698	C
1	2	1706	G
1	2	1721	U
1	2	1722	G
1	2	1726	G
1	2	1742	C
1	2	1748	G
1	2	1750	C
1	2	1753	C
1	2	1756	C
1	2	1773	C
1	2	1774	C
1	2	1776	G
1	2	1777	G
1	2	1779	G
1	2	1781	A
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1801	A
1	2	1809	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	1819	A
1	2	1823	A
1	2	1824	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1836	G
1	2	1838	U
1	2	1849	G
1	2	1851	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1869	A
36	1	6419	C
36	1	6422	U
36	1	6425	A
36	1	6426	U
36	1	6427	G
36	1	6429	U
36	1	6430	U
36	1	6431	A
36	1	6434	C
36	1	6435	A
36	1	6436	U
36	1	6437	C
36	1	6444	G
36	1	6445	G
36	1	6446	A
36	1	6449	U
36	1	6451	U
36	1	6456	U
36	1	6457	A
36	1	6458	A
36	1	6459	A
36	1	6460	C
36	1	6465	G
36	1	6467	G
36	1	6472	G
36	1	6473	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	6474	U
36	1	6475	U
36	1	6481	G
36	1	6482	A
36	1	6484	G
36	1	6485	G
36	1	6486	U
36	1	6487	C
36	1	6488	G
36	1	6489	A
36	1	6490	G
36	1	6491	G
36	1	6492	U
36	1	6493	G
36	1	6494	C
36	1	6501	U
36	1	6507	G
36	1	6508	A
36	1	6511	A
36	1	6512	G
36	1	6514	C
36	1	6515	U
36	1	6516	C
36	1	6517	G
36	1	6518	G
36	1	6519	U
36	1	6520	G
36	1	6522	C
36	1	6523	A
36	1	6524	G
36	1	6525	C
36	1	6527	C
36	1	6528	C
36	1	6531	C
36	1	6532	A
36	1	6533	A
36	1	6534	A
36	1	6535	U
36	1	6539	C
36	1	6540	U
36	1	6541	A
36	1	6542	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	1	6543	U
36	1	6544	G
36	1	6545	G
36	1	6549	G
36	1	6550	G
36	1	6551	A
36	1	6552	A
36	1	6553	C
36	1	6557	U
36	1	6561	C
36	1	6562	U
36	1	6568	G
36	1	6570	U
36	1	6572	C
36	1	6573	A
36	1	6577	G
36	1	6581	U
36	1	6584	G
36	1	6585	G
36	1	6586	U
36	1	6587	A
36	1	6589	C
36	1	6590	A
36	1	6591	C
36	1	6598	C
36	1	6599	G
36	1	6603	C
36	1	6604	G
36	1	6605	A
36	1	6606	A
36	1	6607	A
36	1	6610	C
36	1	6611	C
36	1	6612	A
36	1	6613	U

All (55) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	43	U
1	2	98	C
1	2	110	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2	182	C
1	2	407	G
1	2	417	C
1	2	448	A
1	2	465	A
1	2	500	A
1	2	532	C
1	2	561	A
1	2	627	U
1	2	629	A
1	2	670	A
1	2	688	U
1	2	752	G
1	2	870	A
1	2	886	A
1	2	908	A
1	2	1016	U
1	2	1153	C
1	2	1165	G
1	2	1253	A
1	2	1298	G
1	2	1314	U
1	2	1342	U
1	2	1371	U
1	2	1377	U
1	2	1378	A
1	2	1395	C
1	2	1396	A
1	2	1475	G
1	2	1476	A
1	2	1489	A
1	2	1519	U
1	2	1520	G
1	2	1581	C
1	2	1606	G
1	2	1620	A
1	2	1637	A
1	2	1646	C
1	2	1647	A
1	2	1664	A
1	2	1679	A
1	2	1697	A

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Mol	Chain	Res	Type
1	2	1741	U
1	2	1808	U
36	1	6426	U
36	1	6428	G
36	1	6488	G
36	1	6538	U
36	1	6539	C
36	1	6541	A
36	1	6589	C
36	1	6605	A

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

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

#### 5.5 Carbohydrates [i](#)

There are no 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

This section contains visualisations of the EMDB entry EMD-20248. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.