wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:43 PM BST

PDB ID	:	4V92
EMDB ID:	:	EMD-2604
Title	:	Kluyveromyces lactis 80S ribosome in complex with CrPV-IRES
Authors	:	Fernandez, I.S.; Bai, X.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-03-21
Resolution	:	3.70 Å(reported)
Based on PDB ID	:	3B31

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

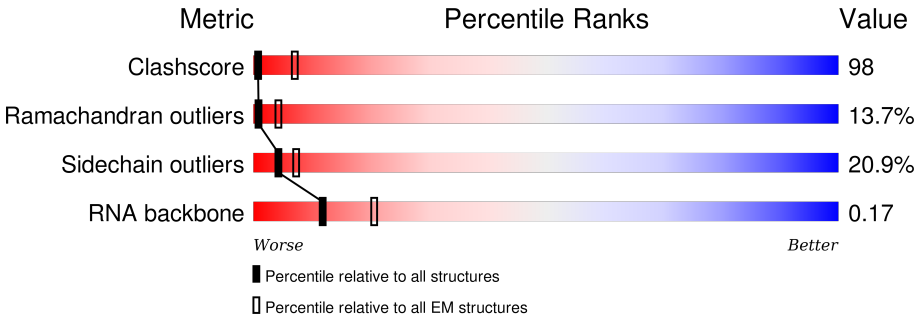
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 3.70 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A2	1767	7% 37% 38% 18%
2	AZ	190	9% 28% 48% 15%
3	BA	206	27% 47% 18% 8%
4	BB	213	32% 46% 18% •
5	BC	216	30% 58% 9% •
6	BD	222	40% 43% 13% 5%
7	BE	260	20% 59% 18% •
8	BF	206	37% 45% 15% •

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Mol	Chain	Length	Quality of chain
9	BG	226	19% 57% 18% 5%
10	BH	184	33% 52% 12%
11	BI	187	26% 45% 26%
12	BJ	179	27% 51% 18%
13	BK	93	30% 49% 19%
14	BL	142	37% 46% 11% 6%
15	BM	120	48% 39% 12%
16	BN	150	29% 48% 21%
17	BO	127	36% 46% 12% 6%
18	BP	115	30% 53% 15%
19	BQ	140	28% 47% 22%
20	BR	121	26% 53% 18%
21	BS	140	29% 46% 19% 6%
22	BT	142	26% 56% 15%
23	BU	104	28% 55% 14%
24	BV	87	40% 46% 9% 5%
25	BW	129	22% 64% 15%
26	BX	142	14% 65% 18%
27	BY	134	19% 60% 19%
28	BZ	64	34% 42% 19% 5%
29	Ba	97	72% 19% 9%
30	Bb	81	74% 23%
31	Bc	63	76% 19% 5%
32	Bd	52	63% 33%
33	Be	55	67% 27% 5%

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Mol	Chain	Length	Quality of chain
34	Bf	64	
35	Bg	315	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 79002 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
1	A2	1764	Total	C	N	O	P	0	0
			37579	16801	6644	12370	1764		

- Molecule 2 is a RNA chain called RNA OF CRICKET-PARALYSIS-VIRUS-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AZ	190	Total	C	N	O	P	0	0
			4018	1801	685	1342	190		

- Molecule 3 is a protein called US2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BA	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 4 is a protein called ES1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BB	213	Total	C	N	O	S	0	0
			1686	1070	302	310	4		

- Molecule 5 is a protein called US5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 6 is a protein called US3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 7 is a protein called ES4.

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

- Molecule 8 is a protein called US7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BF	206	Total	C	N	O	S	0	0
			1603	1004	297	299	3		

- Molecule 9 is a protein called ES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BG	226	Total	C	N	O	S	0	0
			1790	1123	343	321	3		

- Molecule 10 is a protein called ES7.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	BH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 11 is a protein called ES8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BI	187	Total	C	N	O	S	0	0
			1480	919	296	263	2		

- Molecule 12 is a protein called US4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BJ	179	Total	C	N	O	S	0	0
			1452	919	282	250	1		

- Molecule 13 is a protein called ES10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BK	93	Total	C	N	O	S	0	0
			765	496	123	144	2		

- Molecule 14 is a protein called US17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BL	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 15 is a protein called ES12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BM	120	Total	C	N	O	S	0	0
			870	548	152	168	2		

- Molecule 16 is a protein called US15.

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

- Molecule 17 is a protein called US11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BO	127	Total	C	N	O	S	0	0
			905	555	183	165	2		

- Molecule 18 is a protein called US19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BP	115	Total	C	N	O	S	0	0
			914	585	165	157	7		

- Molecule 19 is a protein called US9.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	BQ	140	Total	C	N	O	0	0
			1082	696	193	193		

- Molecule 20 is a protein called ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BR	121	Total	C	N	O	S	0	0
			934	583	179	170	2		

- Molecule 21 is a protein called US13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BS	140	Total	C	N	O	S	0	0
			1150	720	223	205	2		

- Molecule 22 is a protein called ES19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BT	142	Total	C	N	O	S	0	0
			1105	689	207	207	2		

- Molecule 23 is a protein called US10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BU	104	Total	C	N	O	S	0	0
			829	525	150	153	1		

- Molecule 24 is a protein called ES21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 25 is a protein called US8.

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

- Molecule 26 is a protein called US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BX	142	Total	C	N	O	S	0	0
			1101	698	215	186	2		

- Molecule 27 is a protein called ES24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	BY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 28 is a protein called ES25.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	64	Total	C	N	O	0	0
			518	331	95	92		

- Molecule 29 is a protein called ES26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 30 is a protein called ES27.

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

- Molecule 31 is a protein called ES28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 32 is a protein called US14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bd	52	Total	C	N	O	S	0	0
			433	269	91	69	4		

- Molecule 33 is a protein called ES30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Be	55	Total	C	N	O	S	0	0
			440	277	90	72	1		

- Molecule 34 is a protein called ES31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bf	64	Total	C	N	O	S	0	0
			458	289	83	82	4		

- Molecule 35 is a protein called RACK1.

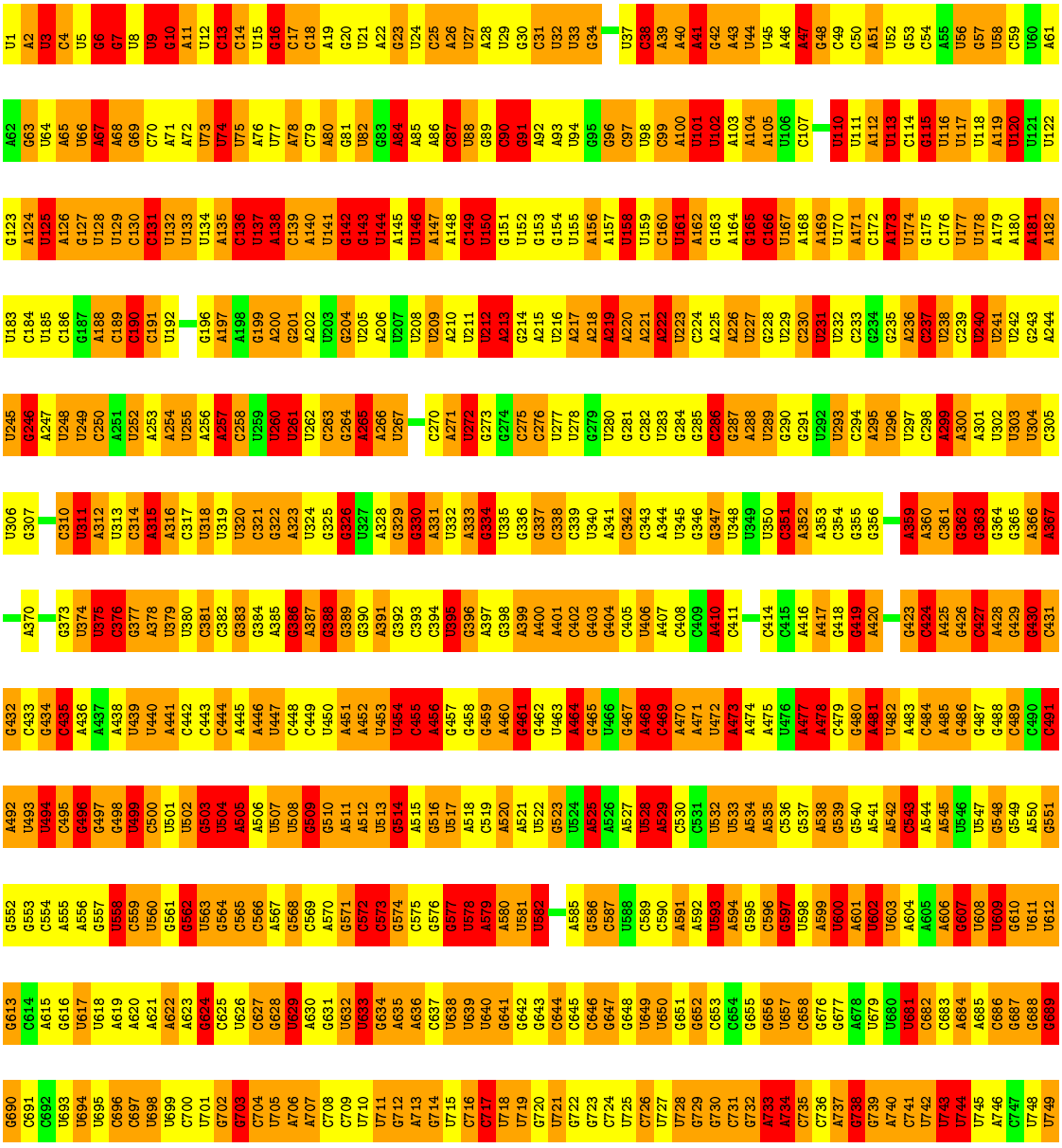
Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bg	315	Total	C	N	O	S	0	0
			2417	1531	414	464	8		

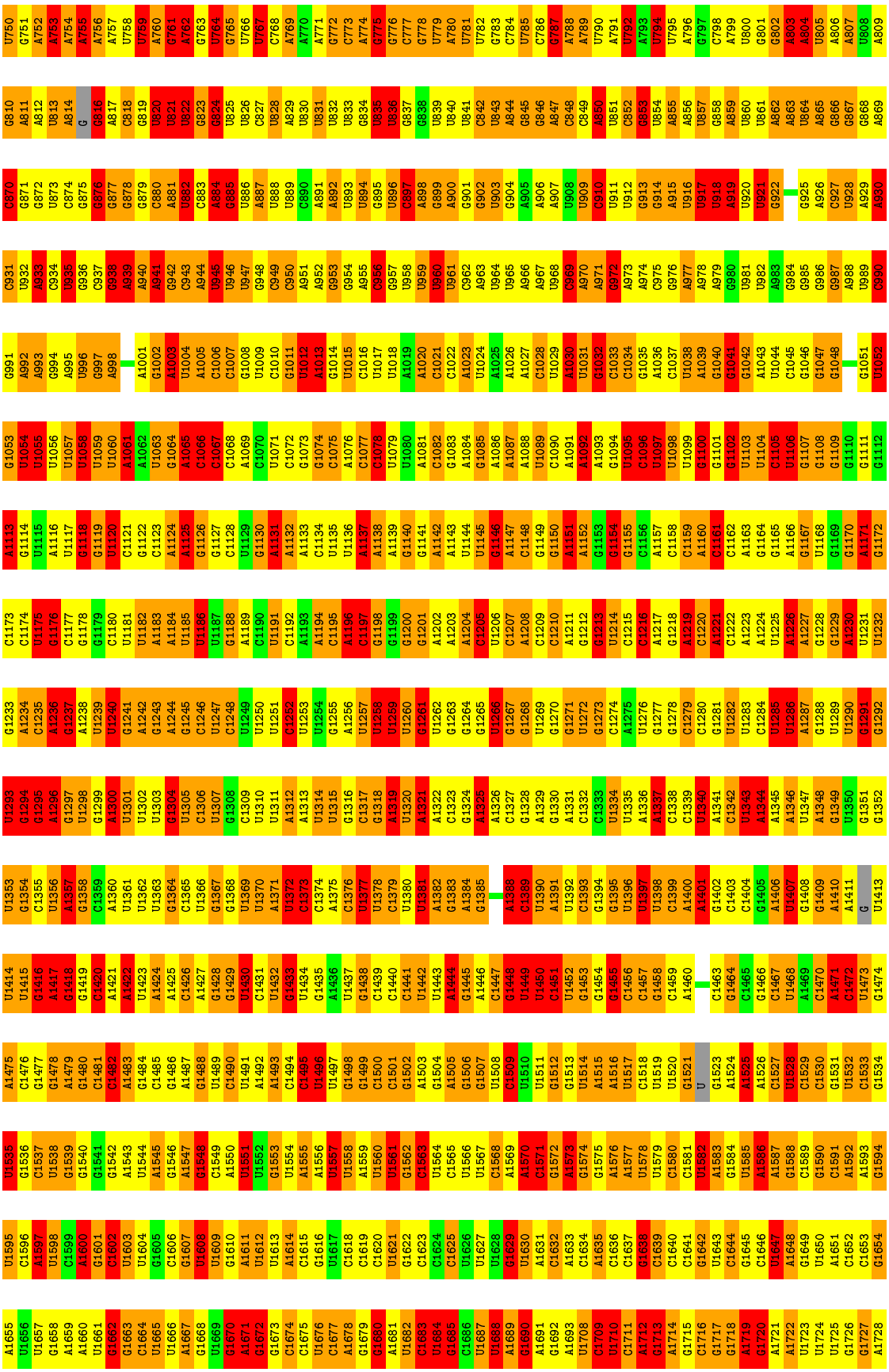
3 Residue-property plots (i)

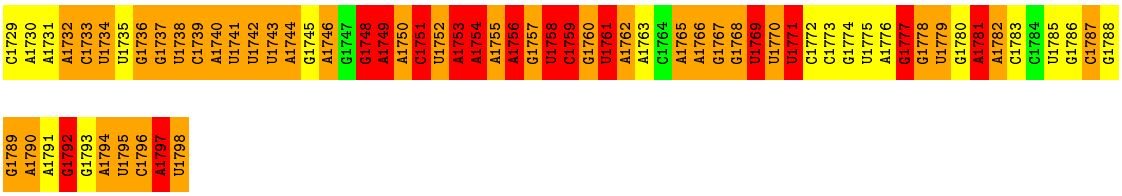
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

Chain A2: 7% 37% 38% 18%

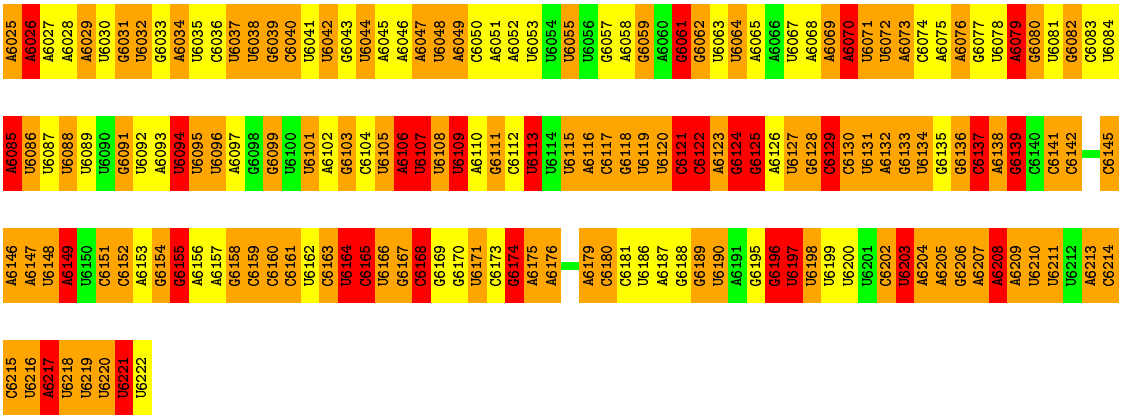






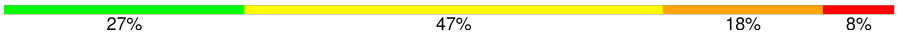
- Molecule 2: RNA OF CRICKET-PARALYSIS-VIRUS-IRES

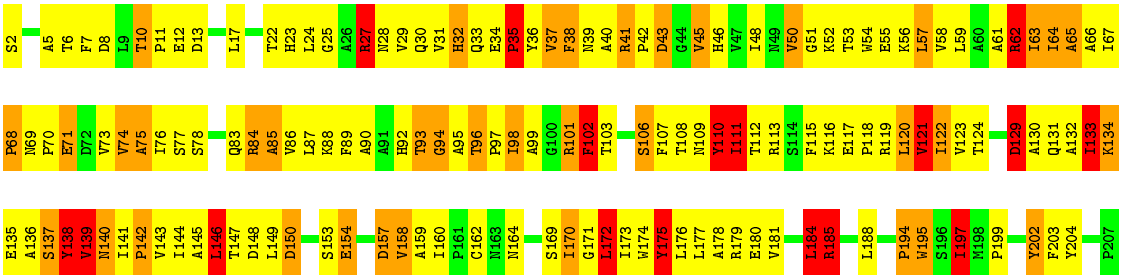
Chain AZ:



- Molecule 3: US2

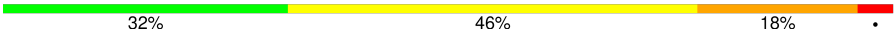
Chain BA:

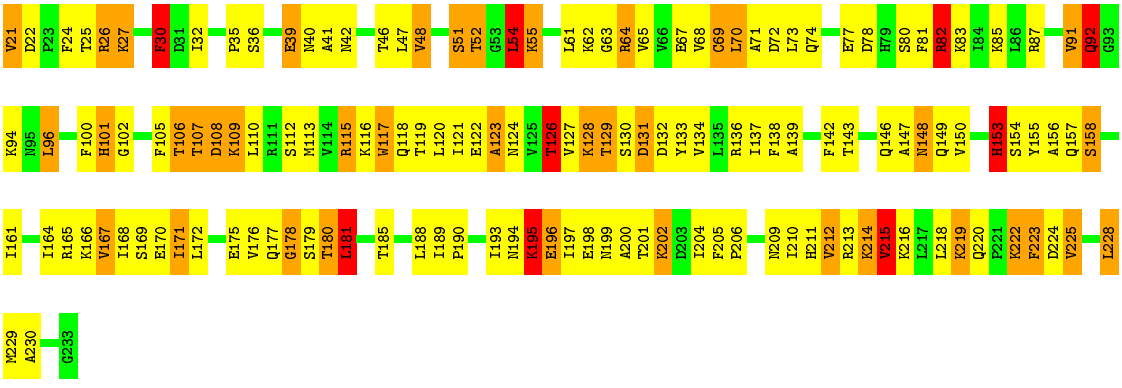




- Molecule 4: ES1

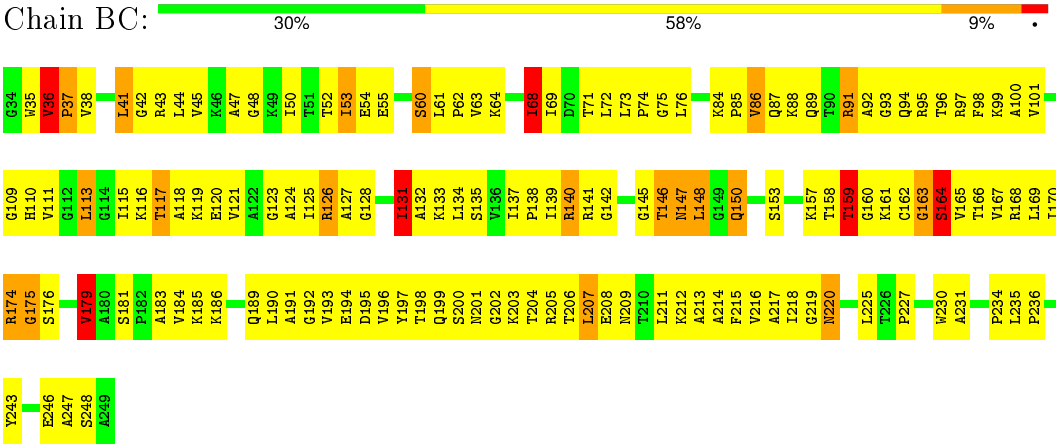
Chain BB:





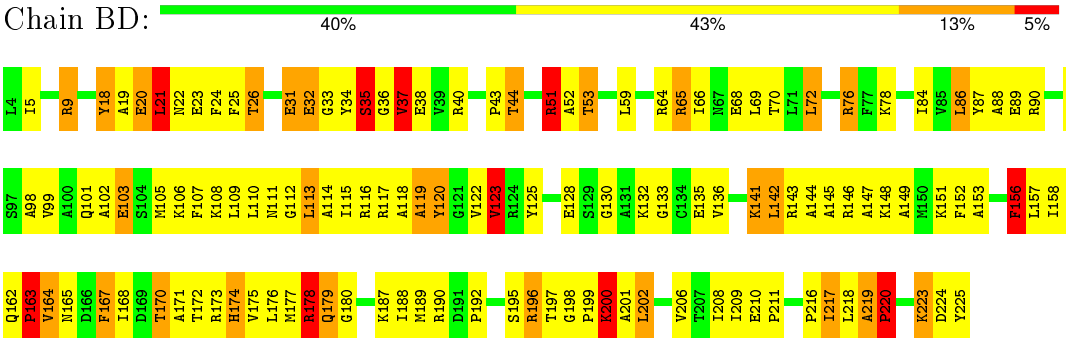
- Molecule 5: US5

Chain BC:



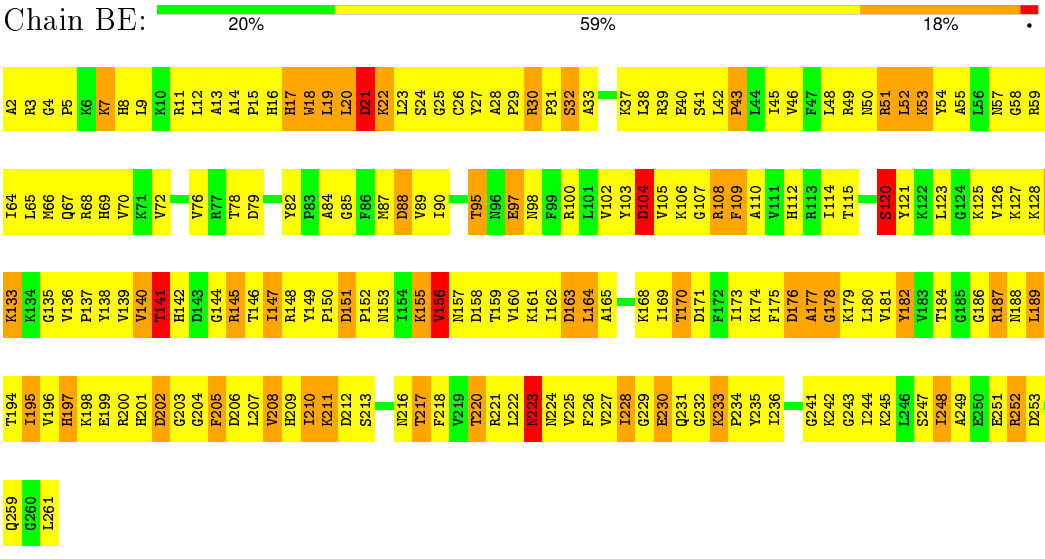
- Molecule 6: US3

Chain BD:



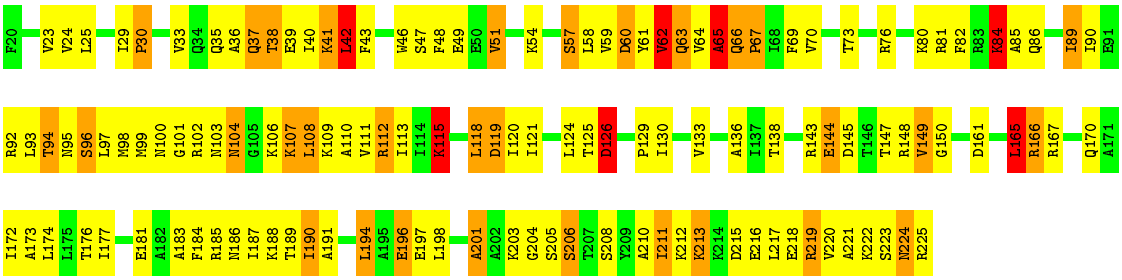
- Molecule 7: ES4

Chain BE:



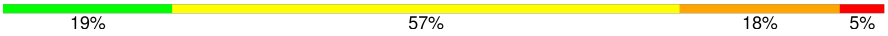
- Molecule 8: US7

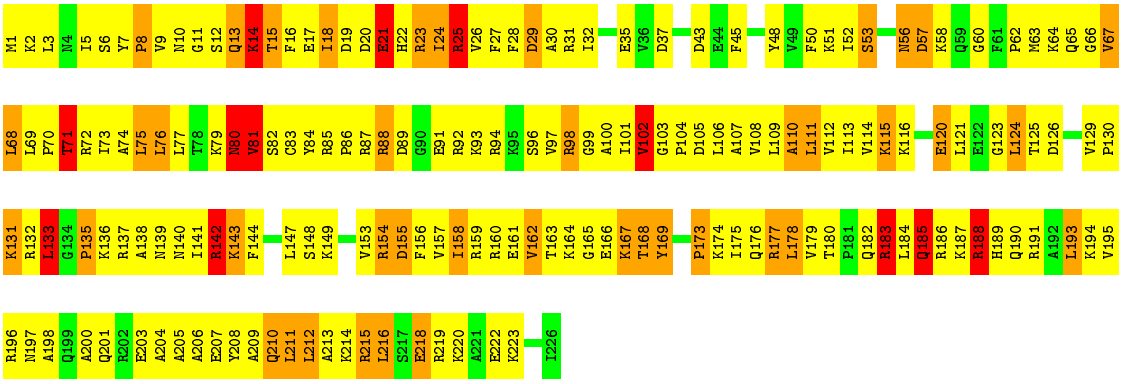
Chain BF:



- Molecule 9: ES6

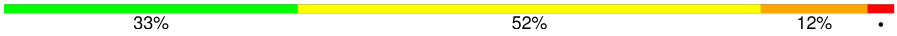
Chain BG:

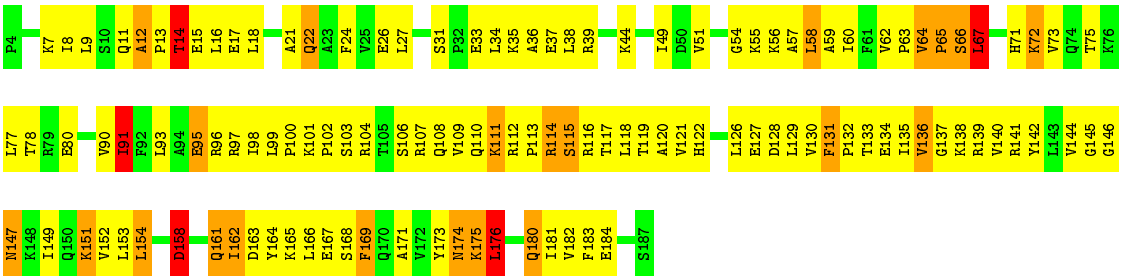




- Molecule 10: ES7

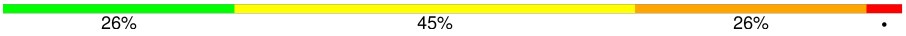
Chain BH:

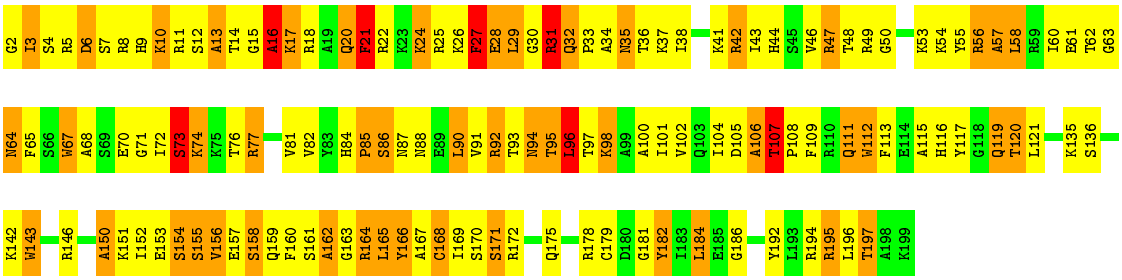




- Molecule 11: ES8

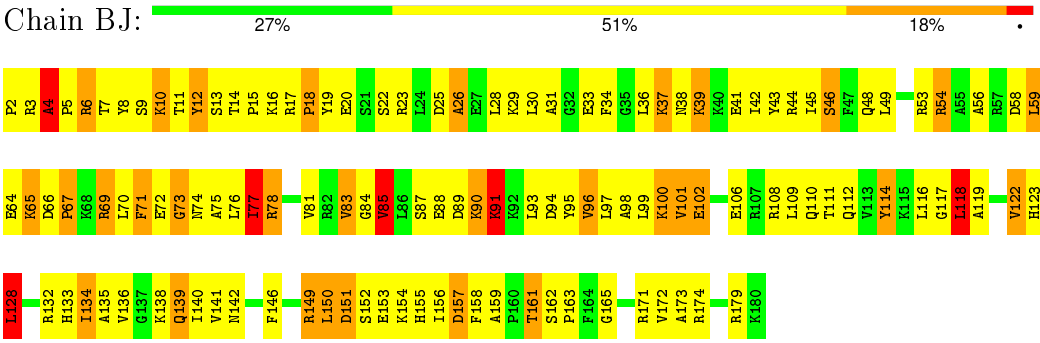
Chain BI:





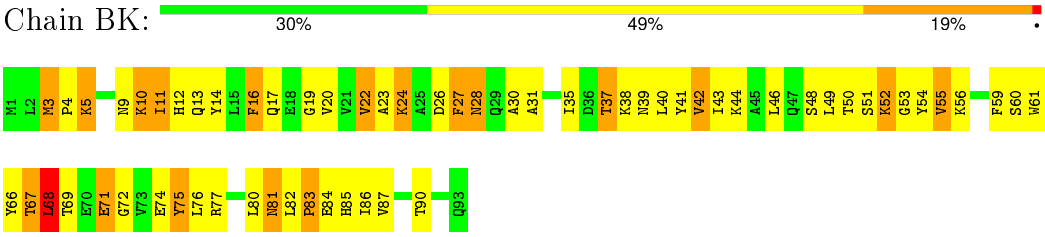
- Molecule 12: US4

Chain BJ:



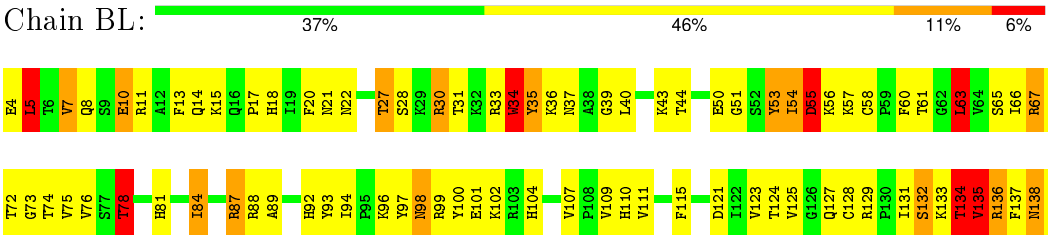
- Molecule 13: ES10

Chain BK:



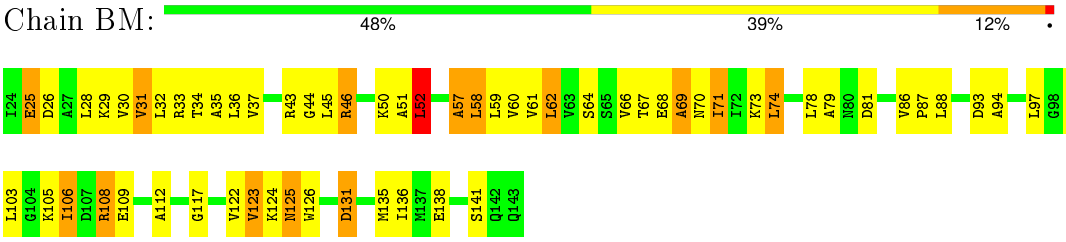
- Molecule 14: US17

Chain BL:



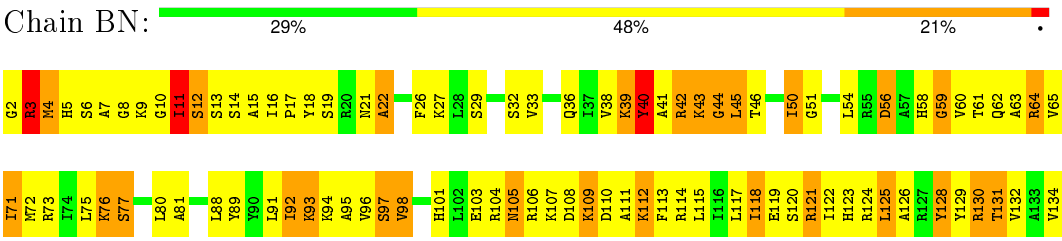
- Molecule 15: ES12

Chain BM:



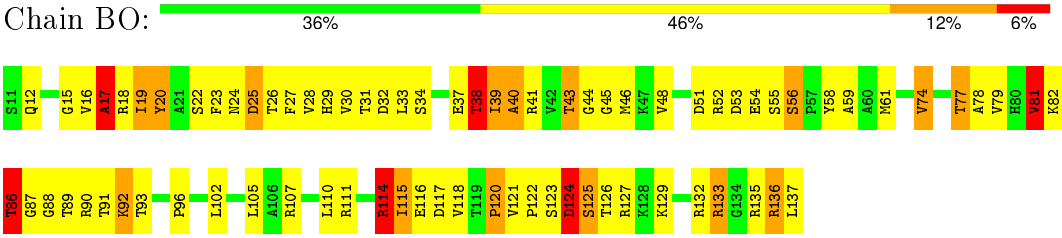
- Molecule 16: US15

Chain BN:



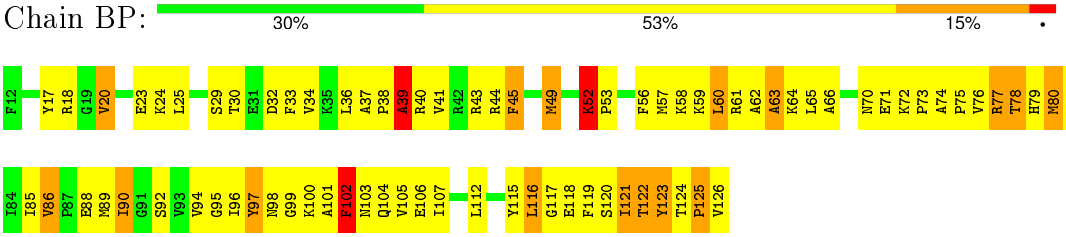
- Molecule 17: US11

Chain BO:



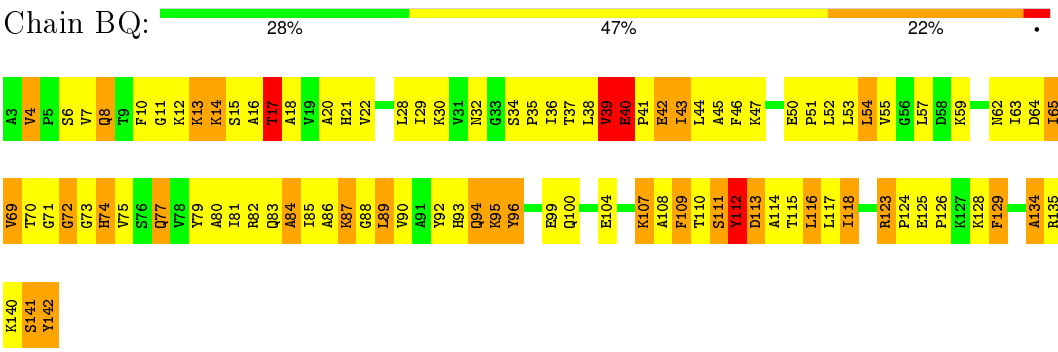
- Molecule 18: US19

Chain BP:



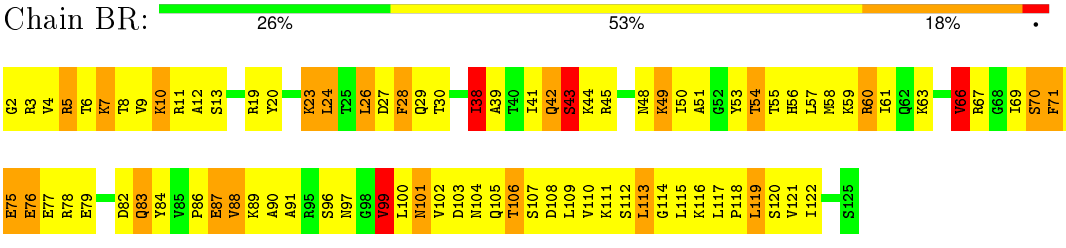
- Molecule 19: US9

Chain BQ:



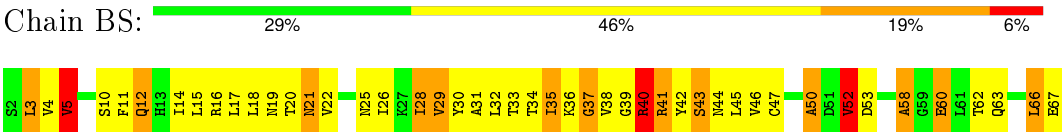
- Molecule 20: ES17

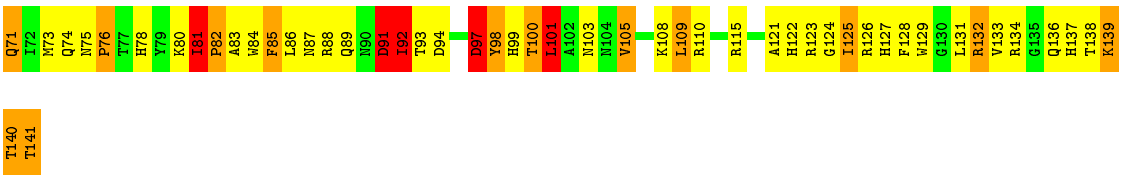
Chain BR:



- Molecule 21: US13

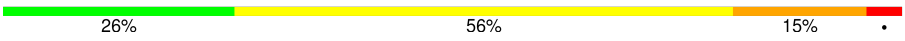
Chain BS:

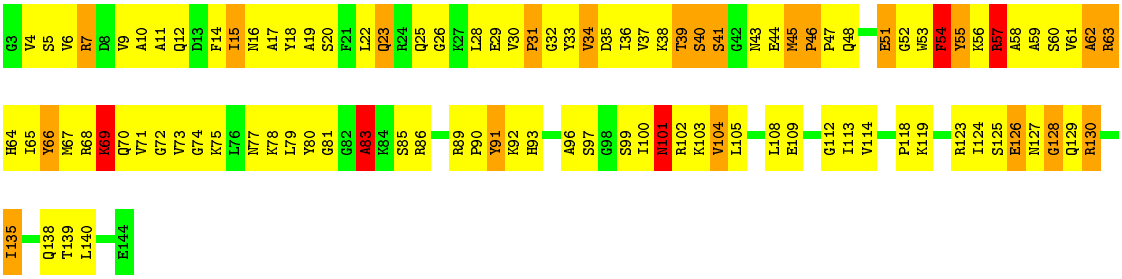




- Molecule 22: ES19

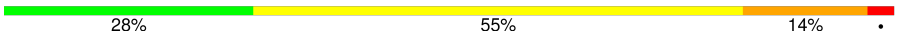
Chain BT:

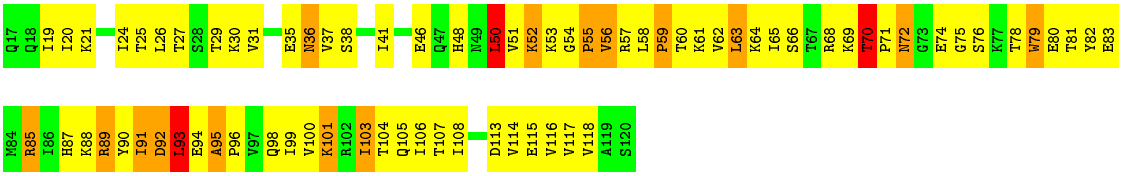




- Molecule 23: US10

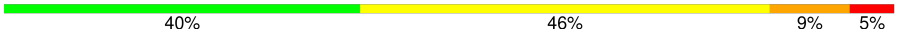
Chain BU:

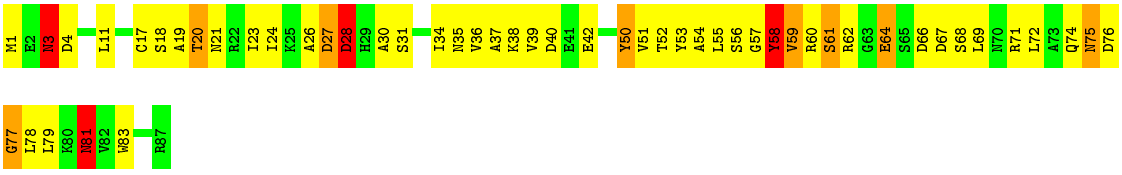




- Molecule 24: ES21

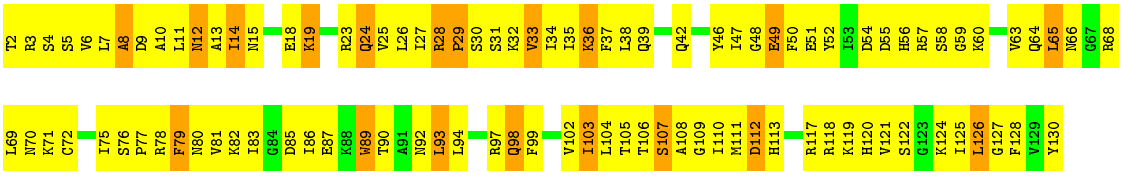
Chain BV:





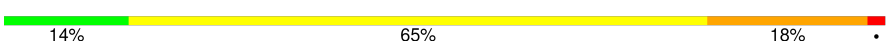
- Molecule 25: US8

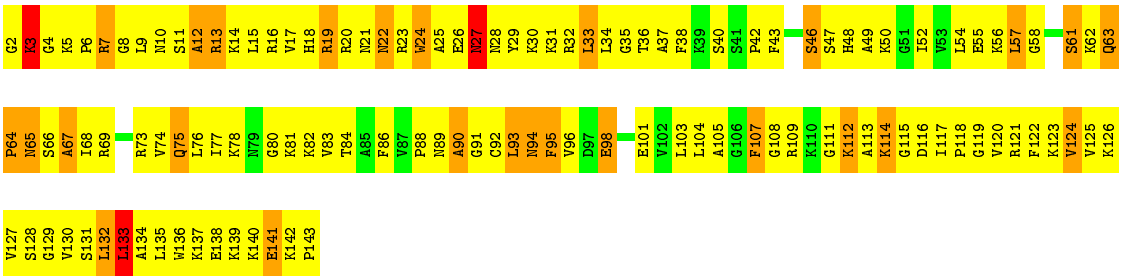
Chain BW:



- Molecule 26: US12

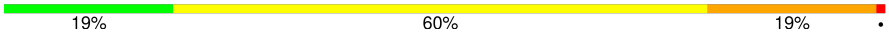
Chain BX:





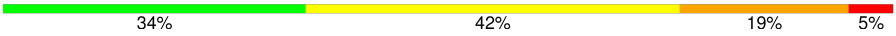
- Molecule 27: ES24

Chain BY:



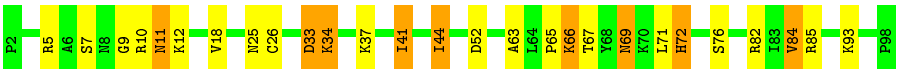
- Molecule 28: ES25

Chain BZ:



- Molecule 29: ES26

Chain Ba:

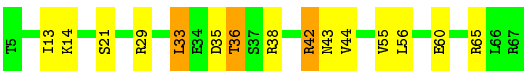


- Molecule 30: ES27

Chain Bb:

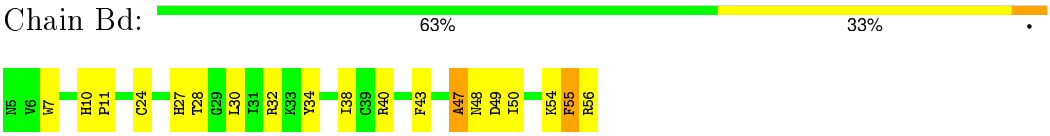
- Molecule 31: ES28

Chain Bc:



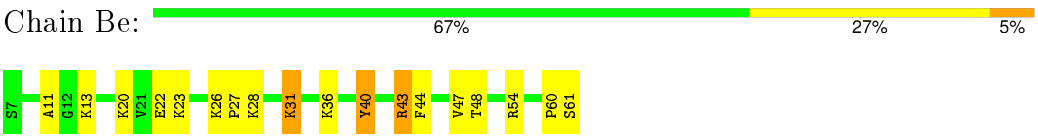
- Molecule 32: US14

Chain Bd:



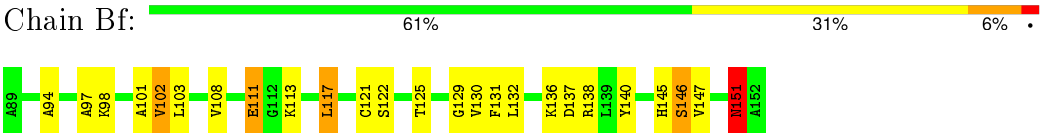
- Molecule 33: ES30

Chain Be:



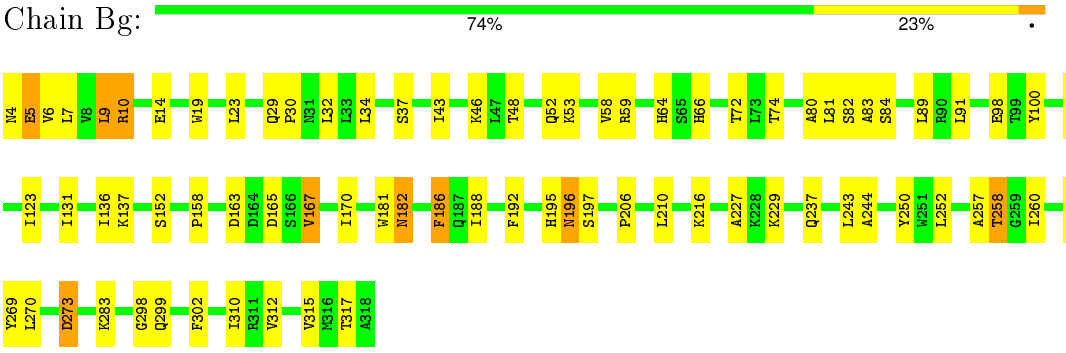
- Molecule 34: ES31

Chain Bf:



- Molecule 35: RACK1

Chain Bg:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1.8	Depositor
Maximum defocus (nm)	3	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A2	1.00	25/41655 (0.1%)	1.31	1105/63991 (1.7%)
10	BH	0.43	0/1455	1.04	17/1875 (0.9%)
11	BI	0.53	0/1448	1.18	19/1839 (1.0%)
12	BJ	0.40	0/1435	0.99	18/1854 (1.0%)
13	BK	0.56	0/759	1.07	8/988 (0.8%)
14	BL	0.52	1/1140 (0.1%)	1.12	15/1484 (1.0%)
15	BM	0.70	0/845	1.03	8/1093 (0.7%)
16	BN	0.45	0/1186	1.04	12/1551 (0.8%)
17	BO	0.39	0/893	0.96	9/1167 (0.8%)
18	BP	0.66	1/903 (0.1%)	1.09	8/1162 (0.7%)
19	BQ	0.63	1/1072 (0.1%)	1.15	13/1392 (0.9%)
2	AZ	0.91	5/4449 (0.1%)	1.28	113/6827 (1.7%)
20	BR	0.44	0/908	1.02	10/1159 (0.9%)
21	BS	0.69	0/1140	1.18	11/1487 (0.7%)
22	BT	0.92	3/1083 (0.3%)	1.16	15/1389 (1.1%)
23	BU	0.57	0/812	1.06	9/1053 (0.9%)
24	BV	0.47	0/675	0.89	4/881 (0.5%)
25	BW	0.42	0/999	0.91	4/1278 (0.3%)
26	BX	0.38	0/1079	0.97	11/1372 (0.8%)
27	BY	0.50	0/1056	1.15	14/1356 (1.0%)
28	BZ	0.73	0/511	1.11	5/663 (0.8%)
29	Ba	0.43	0/758	1.06	7/975 (0.7%)
3	BA	0.95	2/1574 (0.1%)	1.25	26/2086 (1.2%)
30	Bb	0.41	0/596	1.05	6/766 (0.8%)
31	Bc	0.42	0/485	1.03	5/628 (0.8%)
32	Bd	0.51	0/427	1.04	5/540 (0.9%)
33	Be	0.47	0/436	1.16	6/562 (1.1%)
34	Bf	0.71	0/456	1.07	5/599 (0.8%)
35	Bg	0.55	0/2390	1.01	23/3123 (0.7%)
4	BB	0.50	0/1661	1.06	16/2154 (0.7%)
5	BC	0.40	0/1610	0.99	14/2113 (0.7%)
6	BD	0.46	0/1692	1.06	19/2175 (0.9%)
7	BE	0.42	1/2045 (0.0%)	0.99	23/2647 (0.9%)
8	BF	0.53	0/1571	1.00	14/2039 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
9	BG	0.49	1/1767 (0.1%)	1.06	13/2288 (0.6%)
All	All	0.83	40/82971 (0.0%)	1.21	1610/118556 (1.4%)

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
1	A2	98	0
10	BH	7	2
11	BI	12	2
12	BJ	5	1
13	BK	2	0
14	BL	8	0
15	BM	2	0
16	BN	6	0
17	BO	4	1
18	BP	4	0
19	BQ	8	2
2	AZ	8	0
20	BR	5	0
21	BS	6	4
22	BT	6	0
23	BU	1	1
24	BV	2	1
25	BW	3	0
26	BX	5	2
27	BY	6	0
28	BZ	1	0
29	Ba	4	1
3	BA	8	3
30	Bb	5	0
31	Bc	2	0
32	Bd	3	1
33	Be	3	0
34	Bf	2	1
35	Bg	9	1
4	BB	11	2
5	BC	8	1
6	BD	6	1
7	BE	8	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	BF	6	1
9	BG	10	3
All	All	284	31

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	897	C	O3'-P	48.97	2.19	1.61
1	A2	633	U	O3'-P	48.70	2.19	1.61
1	A2	1797	A	O3'-P	47.72	2.18	1.61
1	A2	1388	A	O3'-P	46.19	2.16	1.61
1	A2	388	G	O3'-P	45.98	2.16	1.61

The worst 5 of 1610 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	104	A	P-O3'-C3'	41.97	170.06	119.70
1	A2	56	U	P-O3'-C3'	36.36	163.33	119.70
1	A2	1797	A	O3'-P-O5'	29.86	160.74	104.00
1	A2	862	A	P-O3'-C3'	26.83	151.90	119.70
1	A2	960	U	P-O3'-C3'	-25.06	89.62	119.70

5 of 284 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A2	7	G	C3'
1	A2	41	A	C3'
1	A2	67	A	C3'
1	A2	102	U	C3'
1	A2	124	A	C2'

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	BA	138	TYR	Peptide
3	BA	35	PRO	Peptide
3	BA	62	ARG	Peptide
4	BB	177	GLN	Peptide
4	BB	178	GLY	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	A2	37579	0	18988	10181	0
2	AZ	4018	0	2058	292	0
3	BA	1577	0	1518	356	0
4	BB	1686	0	1693	197	0
5	BC	1626	0	1633	602	0
6	BD	1729	0	1743	286	0
7	BE	2068	0	2055	1027	0
8	BF	1603	0	1601	319	0
9	BG	1790	0	1764	1203	0
10	BH	1481	0	1515	208	0
11	BI	1480	0	1432	502	0
12	BJ	1452	0	1479	315	0
13	BK	765	0	711	61	0
14	BL	1146	0	1175	164	0
15	BM	870	0	843	37	0
16	BN	1192	0	1210	273	0
17	BO	905	0	852	365	0
18	BP	914	0	886	535	0
19	BQ	1082	0	1104	210	0
20	BR	934	0	889	344	0
21	BS	1150	0	1130	445	0
22	BT	1105	0	1056	489	0
23	BU	829	0	853	237	0
24	BV	684	0	652	71	0
25	BW	1021	0	996	589	0
26	BX	1101	0	1103	789	0
27	BY	1073	0	1061	939	0
28	BZ	518	0	534	169	0
29	Ba	769	0	770	0	0
30	Bb	610	0	599	0	0
31	Bc	497	0	521	0	0
32	Bd	433	0	404	0	0
33	Be	440	0	473	0	0
34	Bf	458	0	452	0	0
35	Bg	2417	0	2290	0	0
All	All	79002	0	58043	12348	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 98.

The worst 5 of 12348 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:A2:782:U:P	27:BY:39:GLU:HG3	1.23	1.72
1:A2:811:A:C2	10:BH:107:ARG:HA	1.19	1.72
1:A2:1722:A:P	9:BG:73:ILE:HG13	1.23	1.72
1:A2:59:C:P	27:BY:111:LYS:HD3	1.28	1.69
1:A2:803:A:H4'	25:BW:120:HIS:CE1	1.25	1.69

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
3	BA	129/206 (63%)	60 (46%)	39 (30%)	30 (23%)	0 1
4	BB	118/213 (55%)	88 (75%)	17 (14%)	13 (11%)	0 10
5	BC	136/216 (63%)	84 (62%)	31 (23%)	21 (15%)	0 5
6	BD	116/222 (52%)	83 (72%)	17 (15%)	16 (14%)	0 6
7	BE	143/260 (55%)	100 (70%)	26 (18%)	17 (12%)	0 8
8	BF	116/206 (56%)	81 (70%)	20 (17%)	15 (13%)	0 7
9	BG	141/226 (62%)	88 (62%)	32 (23%)	21 (15%)	0 5
10	BH	100/184 (54%)	61 (61%)	22 (22%)	17 (17%)	0 4
11	BI	87/187 (46%)	51 (59%)	22 (25%)	14 (16%)	0 5
12	BJ	101/179 (56%)	58 (57%)	27 (27%)	16 (16%)	0 5
13	BK	48/93 (52%)	29 (60%)	9 (19%)	10 (21%)	0 2
14	BL	85/142 (60%)	53 (62%)	25 (29%)	7 (8%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	BM	63/120 (52%)	36 (57%)	20 (32%)	7 (11%)	0 10
16	BN	97/150 (65%)	62 (64%)	22 (23%)	13 (13%)	0 6
17	BO	84/127 (66%)	58 (69%)	16 (19%)	10 (12%)	0 8
18	BP	60/115 (52%)	40 (67%)	14 (23%)	6 (10%)	1 12
19	BQ	85/140 (61%)	56 (66%)	19 (22%)	10 (12%)	0 8
20	BR	59/121 (49%)	45 (76%)	9 (15%)	5 (8%)	1 16
21	BS	89/140 (64%)	61 (68%)	13 (15%)	15 (17%)	0 4
22	BT	72/142 (51%)	47 (65%)	14 (19%)	11 (15%)	0 5
23	BU	57/104 (55%)	38 (67%)	12 (21%)	7 (12%)	0 8
24	BV	53/87 (61%)	38 (72%)	10 (19%)	5 (9%)	1 14
25	BW	58/129 (45%)	41 (71%)	11 (19%)	6 (10%)	1 12
26	BX	70/142 (49%)	49 (70%)	12 (17%)	9 (13%)	0 7
27	BY	77/134 (58%)	55 (71%)	15 (20%)	7 (9%)	1 15
28	BZ	37/64 (58%)	22 (60%)	9 (24%)	6 (16%)	0 5
29	Ba	51/97 (53%)	29 (57%)	12 (24%)	10 (20%)	0 3
30	Bb	38/81 (47%)	24 (63%)	11 (29%)	3 (8%)	1 18
31	Bc	38/63 (60%)	29 (76%)	7 (18%)	2 (5%)	2 29
32	Bd	25/52 (48%)	15 (60%)	8 (32%)	2 (8%)	1 18
33	Be	33/55 (60%)	16 (48%)	12 (36%)	5 (15%)	0 5
34	Bf	45/64 (70%)	18 (40%)	14 (31%)	13 (29%)	0 0
35	Bg	170/315 (54%)	115 (68%)	38 (22%)	17 (10%)	1 12
All	All	2681/4776 (56%)	1730 (64%)	585 (22%)	366 (14%)	1 6

5 of 366 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	BA	27	ARG
3	BA	43	ASP
3	BA	50	VAL
3	BA	121	VAL
3	BA	122	ILE

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
3	BA	164/173 (95%)	117 (71%)	47 (29%)	0 4
4	BB	187/187 (100%)	142 (76%)	45 (24%)	1 7
5	BC	175/175 (100%)	156 (89%)	19 (11%)	8 40
6	BD	182/182 (100%)	148 (81%)	34 (19%)	2 14
7	BE	221/221 (100%)	178 (80%)	43 (20%)	2 12
8	BF	172/172 (100%)	131 (76%)	41 (24%)	1 7
9	BG	185/191 (97%)	138 (75%)	47 (25%)	1 6
10	BH	165/165 (100%)	138 (84%)	27 (16%)	3 20
11	BI	149/149 (100%)	105 (70%)	44 (30%)	0 4
12	BJ	154/154 (100%)	126 (82%)	28 (18%)	2 15
13	BK	80/84 (95%)	62 (78%)	18 (22%)	1 8
14	BL	127/127 (100%)	100 (79%)	27 (21%)	1 9
15	BM	88/97 (91%)	67 (76%)	21 (24%)	1 7
16	BN	127/127 (100%)	104 (82%)	23 (18%)	2 15
17	BO	84/96 (88%)	62 (74%)	22 (26%)	0 5
18	BP	97/97 (100%)	81 (84%)	16 (16%)	3 20
19	BQ	114/114 (100%)	80 (70%)	34 (30%)	0 3
20	BR	94/109 (86%)	71 (76%)	23 (24%)	1 7
21	BS	125/125 (100%)	96 (77%)	29 (23%)	1 8
22	BT	114/114 (100%)	94 (82%)	20 (18%)	2 17
23	BU	97/97 (100%)	77 (79%)	20 (21%)	1 10
24	BV	74/74 (100%)	62 (84%)	12 (16%)	3 21
25	BW	110/110 (100%)	97 (88%)	13 (12%)	6 36
26	BX	116/116 (100%)	101 (87%)	15 (13%)	5 32
27	BY	112/112 (100%)	94 (84%)	18 (16%)	3 22
28	BZ	57/57 (100%)	42 (74%)	15 (26%)	0 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	Ba	83/83 (100%)	65 (78%)	18 (22%)	1 9
30	Bb	70/70 (100%)	56 (80%)	14 (20%)	1 11
31	Bc	56/56 (100%)	44 (79%)	12 (21%)	1 9
32	Bd	46/46 (100%)	33 (72%)	13 (28%)	0 4
33	Be	48/48 (100%)	38 (79%)	10 (21%)	1 10
34	Bf	43/43 (100%)	31 (72%)	12 (28%)	0 4
35	Bg	257/259 (99%)	208 (81%)	49 (19%)	2 13
All	All	3973/4030 (99%)	3144 (79%)	829 (21%)	4 10

5 of 829 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	BK	5	LYS
17	BO	12	GLN
33	Be	44	PHE
13	BK	71	GLU
15	BM	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
12	BJ	131	GLN
18	BP	79	HIS
34	Bf	145	HIS
13	BK	28	ASN
14	BL	98	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1459/1767 (82%)	899 (61%)	316 (21%)
2	AZ	160/190 (84%)	128 (80%)	43 (26%)
All	All	1619/1957 (82%)	1027 (63%)	359 (22%)

5 of 1027 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	U
1	A2	4	C
1	A2	6	G
1	A2	7	G

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	930	A
1	A2	1158	C
2	AZ	6117	C
1	A2	949	C
1	A2	1065	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A2	392
35	Bg	80
7	BE	64

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Mol	Chain	Number of breaks
6	BD	62
11	BI	58
8	BF	52
4	BB	51
10	BH	51
9	BG	47
5	BC	46
3	BA	43
12	BJ	42
26	BX	40
2	AZ	40
22	BT	39
25	BW	39
20	BR	36
15	BM	33
14	BL	32
18	BP	31
27	BY	31
19	BQ	30
16	BN	29
21	BS	29
23	BU	27
13	BK	25
29	Ba	24
30	Bb	24
17	BO	23
24	BV	18
32	Bd	16
31	Bc	14
28	BZ	14
33	Be	11
34	Bf	9

The worst 5 of 1602 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	1693:A	O3'	1708:U	P	22.38
1	A2	658:C	O3'	676:G	P	18.27
1	BI	123:LYS	C	135:LYS	N	16.74
1	BA	190:ASP	C	191:ARG	N	10.15
1	BR	124:VAL	C	125:SER	N	8.71