wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 08:19 AM EDT

PDB ID	:	5DM7
Title	:	Crystal structure of the 50S ribosomal subunit from Deinococcus radiodurans in complex with hygromycin A
Authors	:	Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on	:	2015-09-08
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

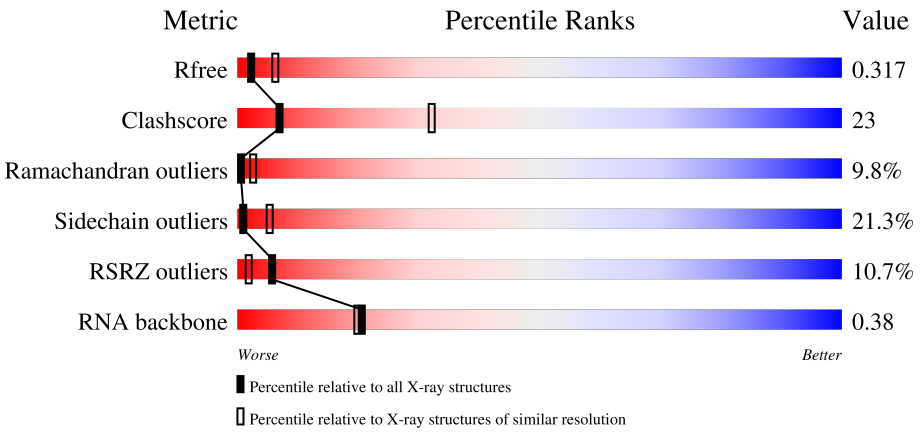
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	224	80%; 54%, 39%, 6%
2	A	274	14%; 43%, 47%, 9%, •
3	B	205	2%; 33%, 50%, 17%

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Mol	Chain	Length	Quality of chain
4	C	197	5% 30% 50% 17%
5	D	177	8% 38% 49% 13%
6	E	171	6% 46% 44% 9%
7	F	144	42% 60% 33% 6%
8	G	142	6% 47% 45% 6%
9	H	134	3% 29% 46% 23%
10	I	141	24% 43% 43% 11%
11	J	136	18% 39% 44% 15%
12	K	113	5% 29% 51% 17%
13	L	104	25% 29% 46% 24%
14	M	109	3% 32% 44% 23%
15	N	117	9% 30% 62% 8%
16	O	94	6% 38% 45% 16%
17	P	127	5% 31% 53% 15%
18	Q	93	13% 46% 39% 14%
19	R	110	7% 34% 41% 25%
20	S	175	14% 41% 43% 13%
21	T	84	20% 42% 46% 11%
22	U	72	29% 24% 51% 17% 8%
23	V	66	18% 61% 32% 8%
24	W	55	11% 38% 56% 5%
25	Z	57	5% 30% 51% 18%
26	1	54	43% 46% 39% 13%
27	2	47	4% 40% 47% 13%
28	3	65	40% 17% 60% 20%

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Mol	Chain	Length	Quality of chain
29	X	2881	3% 22% 44% 25% 5%
30	Y	122	2% 28% 51% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6006	-	-	-	X
31	MG	X	6035	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6101	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6139	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6176	-	-	-	X
31	MG	Y	205	-	-	-	X

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 89361 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	0	224	1651	1031	302	313	5	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	274	2107	1313	423	368	3	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	205	1540	965	295	272	8	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	197	1507	935	287	283	2	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	177	1401	892	247	255	7	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	171	1287	812	237	237	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	F	144	1048	663	183	197	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ARG	LYS	conflict	UNP Q9RSS7
F	3	ARG	LYS	conflict	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	142	1115	704	209	199	3	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	134	997	614	198	180	5	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	141	1068	655	216	197	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	136	1091	696	202	186	7	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	113	879	541	178	158	2	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	L	104	778	476	159	143	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	M	109	867	540	171	156	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LEU	deletion	UNP Q9RWB4
M	?	-	ARG	deletion	UNP Q9RWB4
M	?	-	GLU	deletion	UNP Q9RWB4
M	?	-	LEU	deletion	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	117	978	608	210	159	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	O	94	742	465	139	138	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	127	1014	639	199	174	2	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	93	727	458	136	131	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	R	110	826	513	160	152	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	175	1346	849	236	255	6	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	T	84	626	393	122	110	1	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	U	72	553	341	116	96	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	V	66	534	327	107	97	3	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	W	55	424	264	82	76	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Z	57	453	278	93	77	5	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	1	54	404	256	73	74	1	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	insertion	UNP Q9RSS4
1	1	ALA	-	insertion	UNP Q9RSS4
1	3	GLY	LYS	conflict	UNP Q9RSS4
1	4	ALA	ASP	conflict	UNP Q9RSS4
1	5	ALA	GLY	conflict	UNP Q9RSS4
1	45	ALA	LYS	conflict	UNP Q9RSS4
1	46	HIS	LYS	conflict	UNP Q9RSS4
1	47	VAL	HIS	conflict	UNP Q9RSS4
1	49	PHE	VAL	conflict	UNP Q9RSS4
1	50	ALA	PHE	conflict	UNP Q9RSS4
1	51	ALA	-	insertion	UNP Q9RSS4
1	52	ALA	-	insertion	UNP Q9RSS4
1	53	ALA	-	insertion	UNP Q9RSS4

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	2	47	393	235	92	64	2	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	3	65	509	320	104	80	5	0	0	0

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
29	X	2780	59673	26617	11011	19265	2780	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

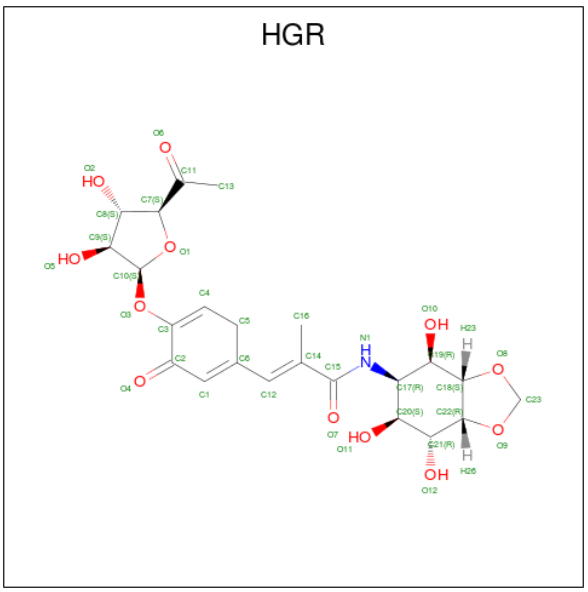
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
30	Y	122	2601	1161	476	842	122	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
31	A	1	1	1	0	0
31	H	1	1	1	0	0
31	M	1	1	1	0	0
31	N	1	1	1	0	0
31	X	177	177	177	0	0
31	Y	5	5	5	0	0

- Molecule 32 is Hygromycin A (three-letter code: HGR) (formula: $C_{23}H_{29}NO_{12}$).



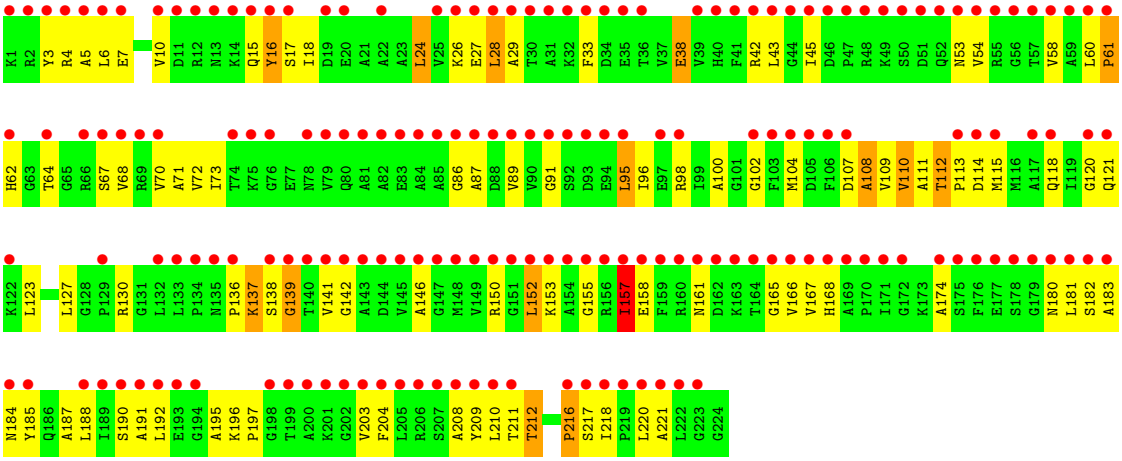
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	36	23	1	12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

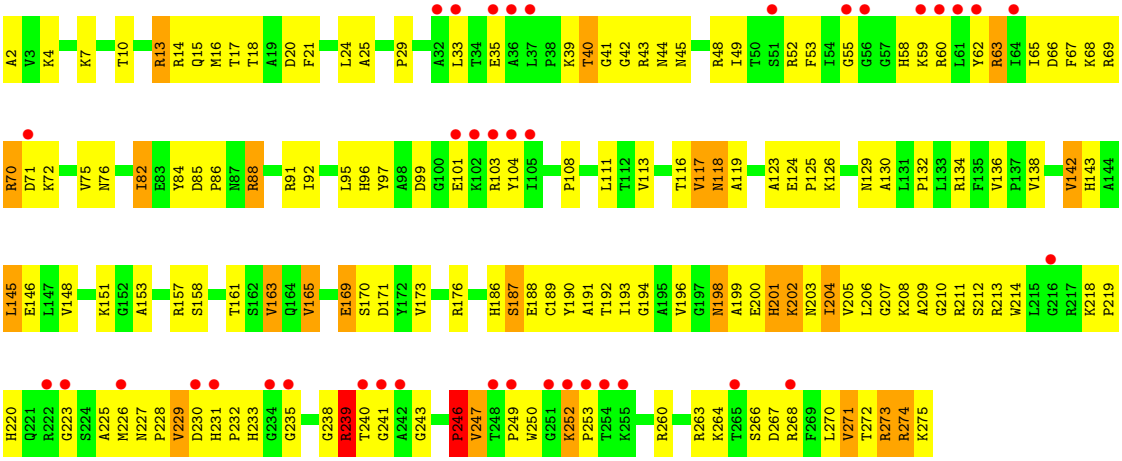
- Molecule 1: 50S ribosomal protein L1

Chain 0:



- Molecule 2: 50S ribosomal protein L2

Chain A:



- Molecule 3: 50S ribosomal protein L3

Chain B: 2% 33% 50% 17%

M1 K2 G3 I4 L5 G6 T7 K8 I9 G10 M11 T12 Q13 I14 V15 K16 N17 D18 R19 A20 I21 P22 V23 T24 V25 V26 L27 A28 G29 P30 C31 P32 I33 V34 Q35 R36 K37 T38 A39 Q40 T41 D42 G43 Y44 Q48 I49 G50 Y51 A52 A55 E56 R57 K58 V59 N60 K61 P62 M63

Q64 G65 H66 F67 G71 V72 A73 F74 T75 R76 I77 L78 R79 E80 F81 F84 A85 P86 D87 S90 V91 N92 V93 D94 I95 G99 E100 K101 I102 D103 A104 T105 G106 T107 S108 K109 G110 K111 G112 T113 Q114 G115 V116 M117 K118 R119 W120 A123 P126 A127 S128 H129 G130 S131

K132 K133 W134 H135 R136 R137 P138 G139 S140 I141 R144 K145 T146 P147 G148 R149 K152 G153 K154 R155 M156 A157 G158 H159 M160 G161 M162 E163 R164 V167 Q168 N169 L170 E171 V172 V173 E174 I175 R176 E179 N180 L181 I182 L183 A187 I188 P189 G190 A191 N192 G193 G194 L195 V196 V197

L198 R199 S200 K203 A204 S205

- Molecule 4: 50S ribosomal protein L4

Chain C: 5% 30% 50% 17%

A2 Q3 I4 N5 V6 I7 G8 Q9 N10 G11 G12 R13 T14 I15 E16 L17 P18 L19 P20 E21 V22 L27 H28 V31 T32 W33 Q34 L35 A36 S37 R38 R39 R40 G41 T42 A43 R46 T47 R48 A49 Q50 V51 S52 K53 T54 G55 R56 Y59 G60 Q61 K62 A67 R68 H69 G70

D71 R72 S73 V74 P75 T76 F77 A83 F84 G85 P86 K87 S90 Y91 D92 Y93 T94 L95 P96 R97 Q98 V99 R100 Q101 L102 G103 M106 A107 I108 A109 S110 R111 Q112 E113 G114 G115 K116 L117 V118 A119 V120 D121 G122 F123 D124 I125 A126 K129 T130 K131 N132 F133 I134 A137

N140 G141 L142 D143 G144 T145 E146 K147 V148 L149 L150 V151 T152 D153 D154 E155 R158 R159 A160 A161 R162 N163 V164 S165 W166 V167 S168 V169 L170 P171 V172 A173 G174 V175 N176 V177 Y178 D179 I180 L181 R182 H183 D184 R185 L186 V187 I188 D189 A190 L193 E194 I195 V196 E197 E198

- Molecule 5: 50S ribosomal protein L5

Chain D: 8% 38% 49% 13%

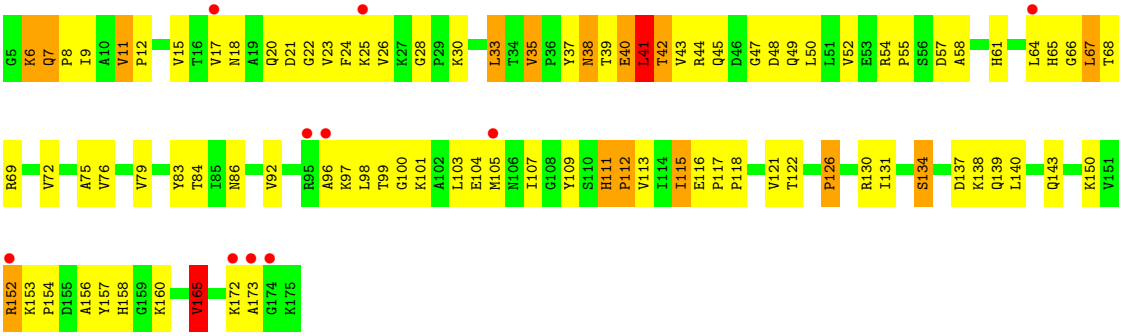
Q3 I4 K5 T6 K7 Y8 N9 D10 Q11 V12 R13 P14 M17 F20 G21 Y22 S23 S24 V25 M26 A27 V28 P29 K33 I34 V35 V36 N37 E38 G39 L40 G41 S42 S43 K44 E45 D46 A49 I50 D51 K52 A53 A54 K55 E56 L57 I60 T61 K64 P65 I66 I67 T68 K69

A70 K71 K72 S73 I74 S75 N76 F77 K78 L79 R80 Q81 G82 M83 P84 V85 G86 I87 K88 V89 T90 L91 R92 F99 L100 E101 K102 L103 I104 N105 I106 G107 L108 I111 R112 D113 F114 R115 G116 I117 N118 F122 D123 G124 R125 G126 N127 Y128 N129 L130 G131 I132 K133 E134 Q135 L136 I137

F138 P139 E140 I141 T142 Y143 D144 M145 V146 D147 K148 T149 R150 I154 T155 I156 Y157 T158 T159 A160 E164 E165 L169 M173 G174 L175 R178 K179

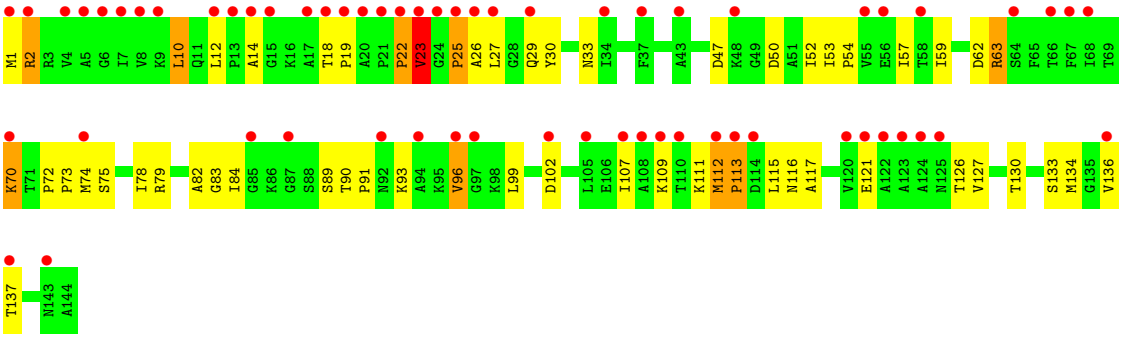
- Molecule 6: 50S ribosomal protein L6

Chain E: 6% 46% 44% 9%



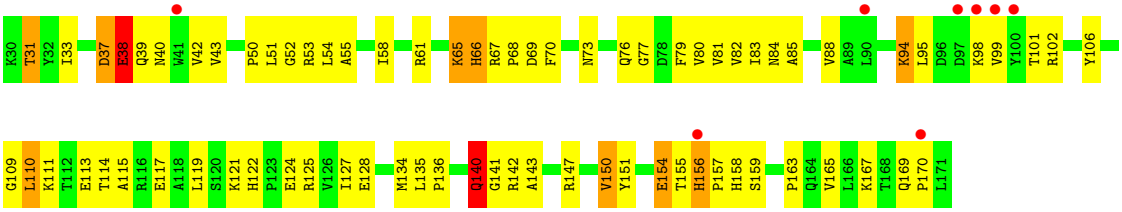
- Molecule 7: 50S ribosomal protein L11

Chain F:



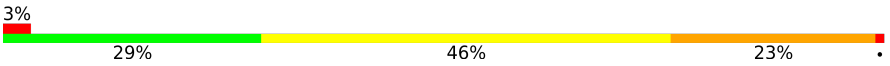
- Molecule 8: 50S ribosomal protein L13

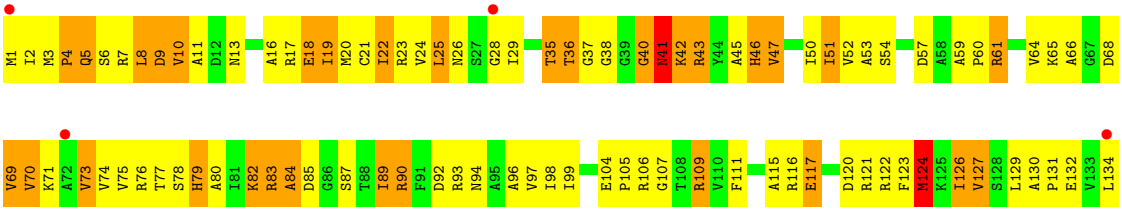
Chain G:



- Molecule 9: 50S ribosomal protein L14

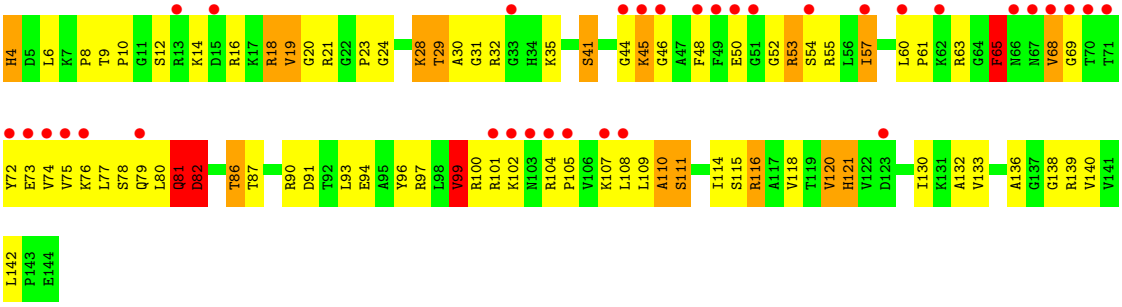
Chain H:





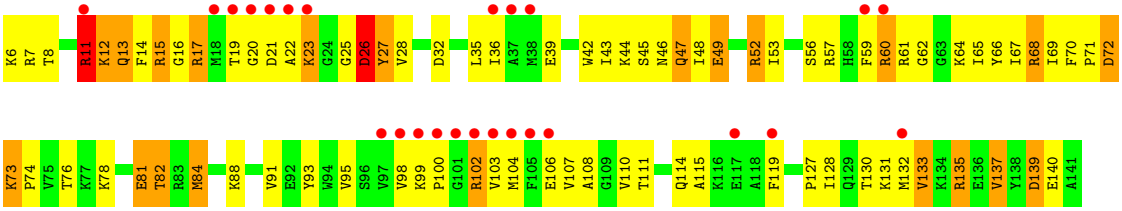
- Molecule 10: 50S ribosomal protein L15

Chain I:



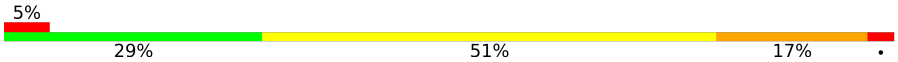
- Molecule 11: 50S ribosomal protein L16

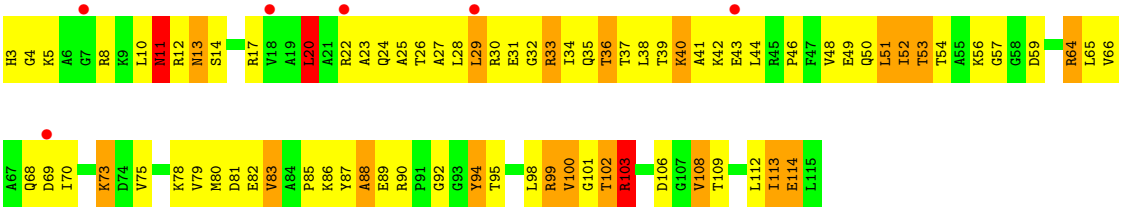
Chain J:



- Molecule 12: 50S ribosomal protein L17

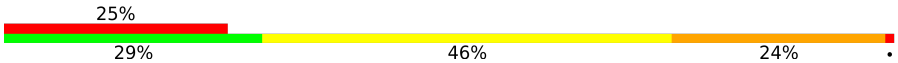
Chain K:

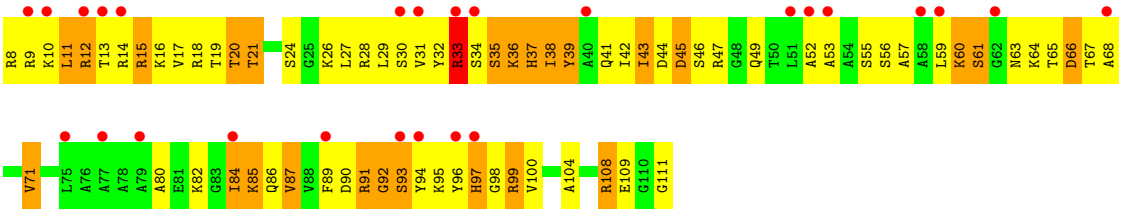




- Molecule 13: 50S ribosomal protein L18

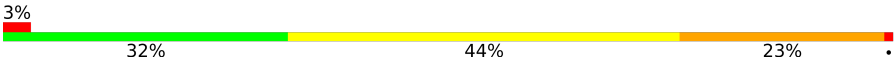
Chain L:

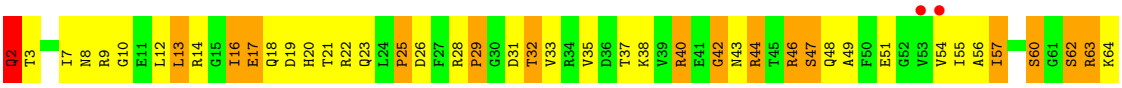


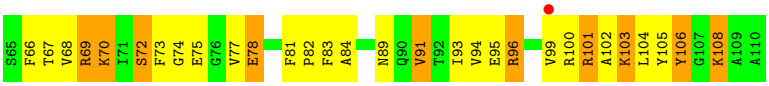


- Molecule 14: 50S ribosomal protein L19

Chain M:

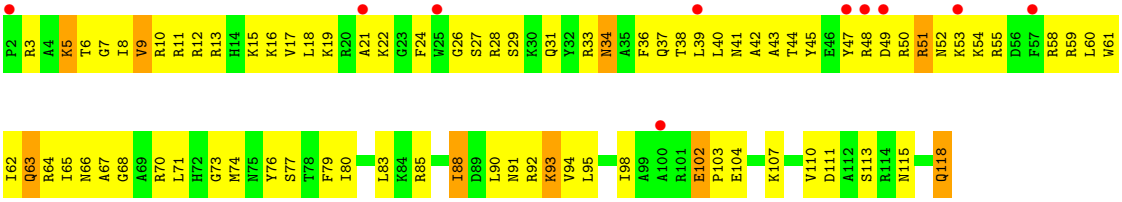






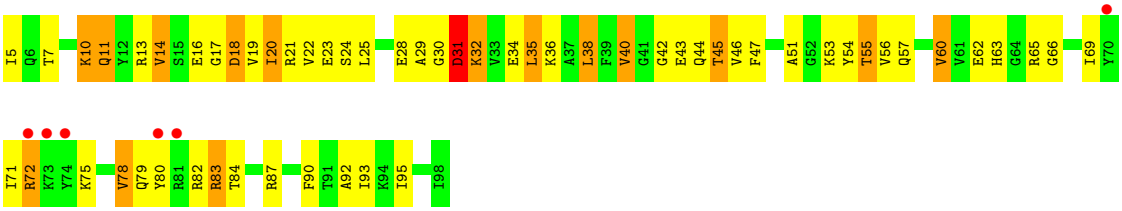
• Molecule 15: 50S ribosomal protein L20

Chain N:



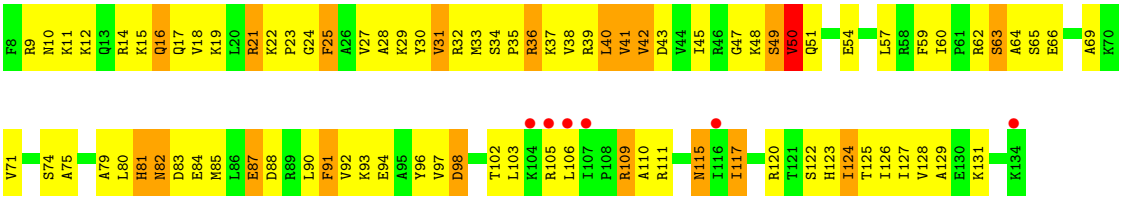
• Molecule 16: 50S ribosomal protein L21

Chain O:



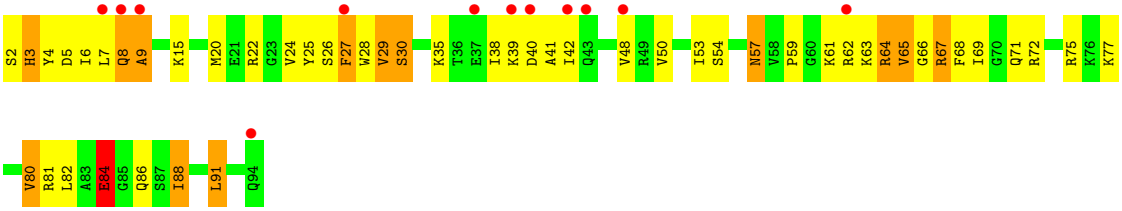
• Molecule 17: 50S ribosomal protein L22

Chain P:



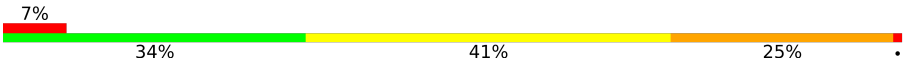
• Molecule 18: 50S ribosomal protein L23

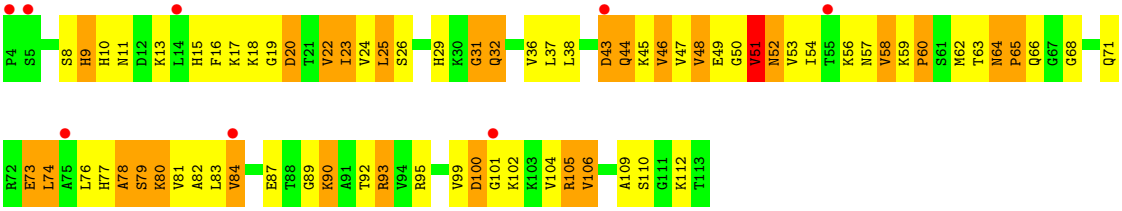
Chain Q:



• Molecule 19: 50S ribosomal protein L24

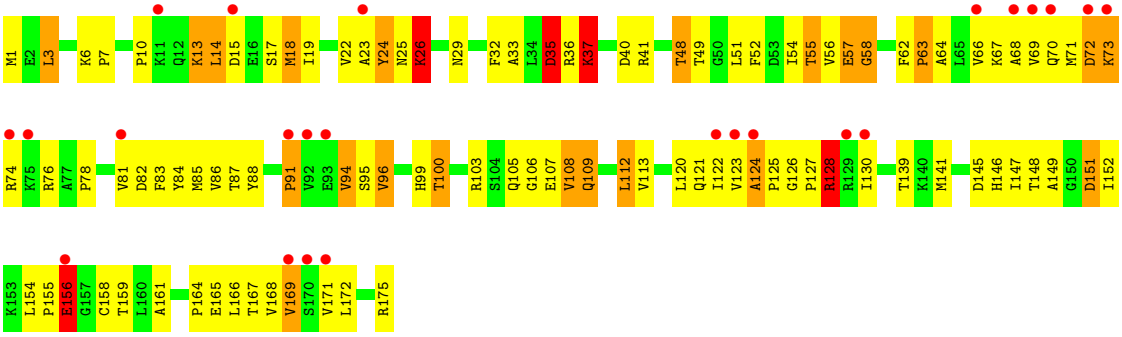
Chain R:





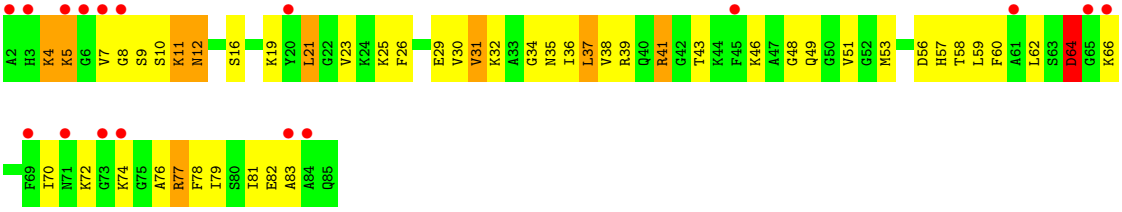
- Molecule 20: 50S ribosomal protein L25

Chain S: 14% 41% 43% 13%



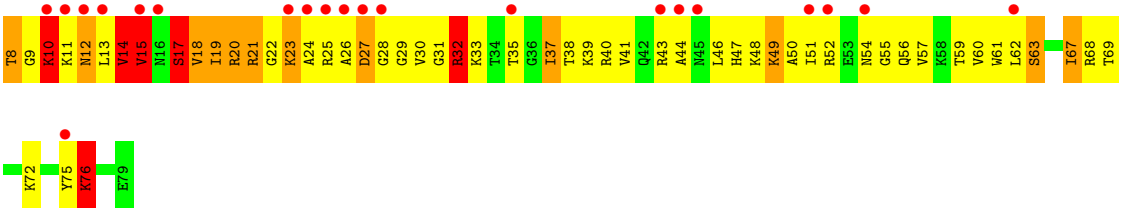
- Molecule 21: 50S ribosomal protein L27

Chain T: 20% 42% 46% 11%



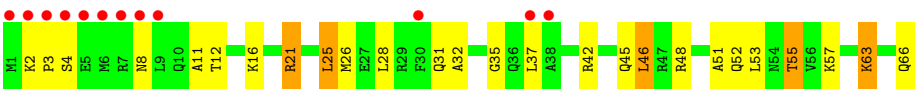
- Molecule 22: 50S ribosomal protein L28

Chain U: 29% 24% 51% 17% 8%



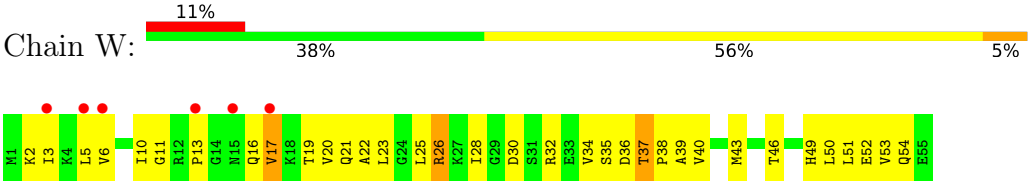
- Molecule 23: 50S ribosomal protein L29

Chain V: 18% 61% 32% 8%



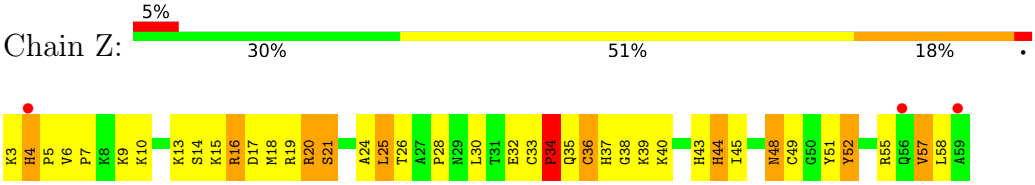
• Molecule 24: 50S ribosomal protein L30

Chain W:



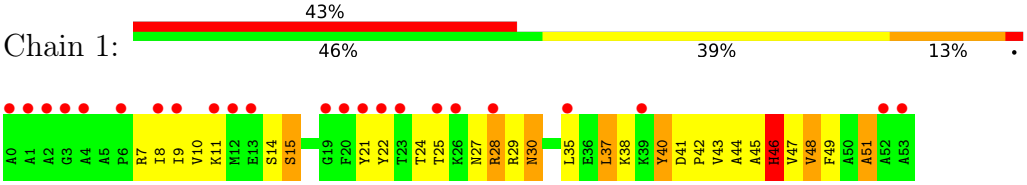
• Molecule 25: 50S ribosomal protein L32

Chain Z:



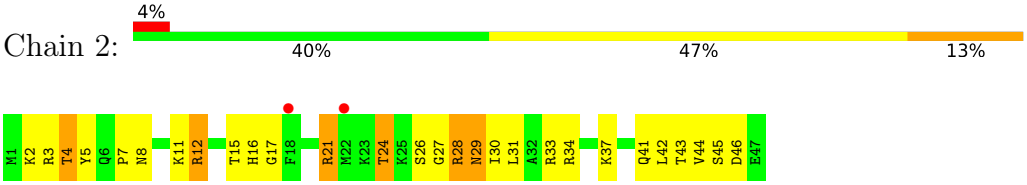
• Molecule 26: 50S ribosomal protein L33

Chain 1:



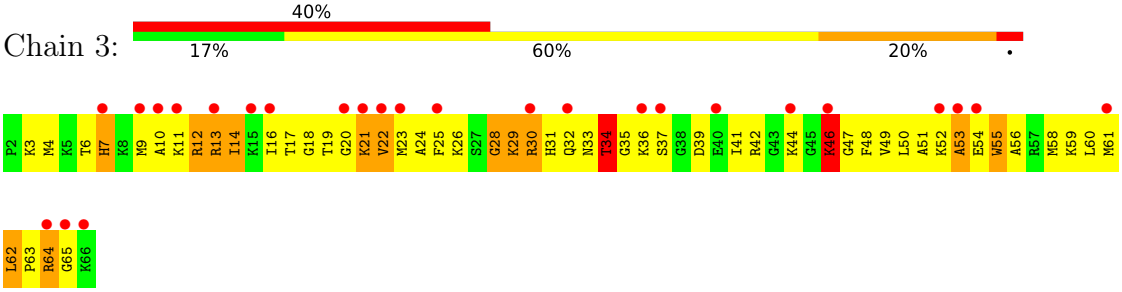
• Molecule 27: 50S ribosomal protein L34

Chain 2:



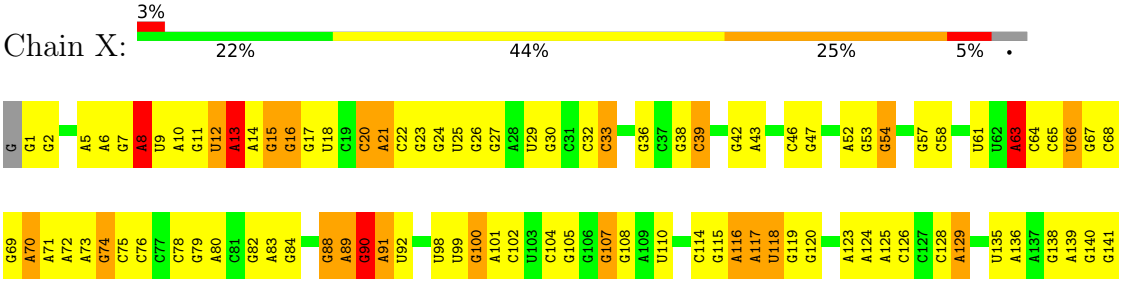
• Molecule 28: 50S ribosomal protein L35

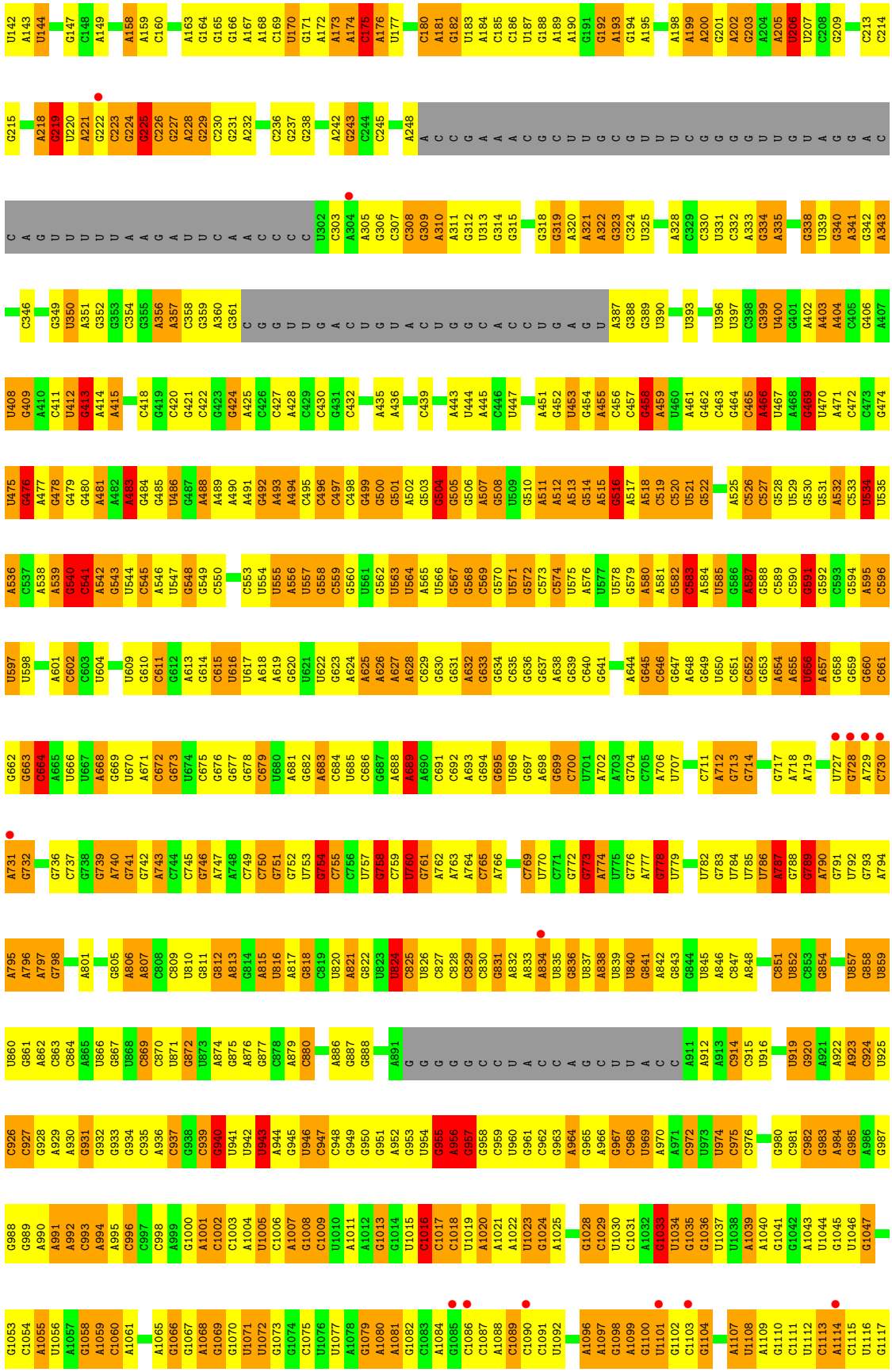
Chain 3:

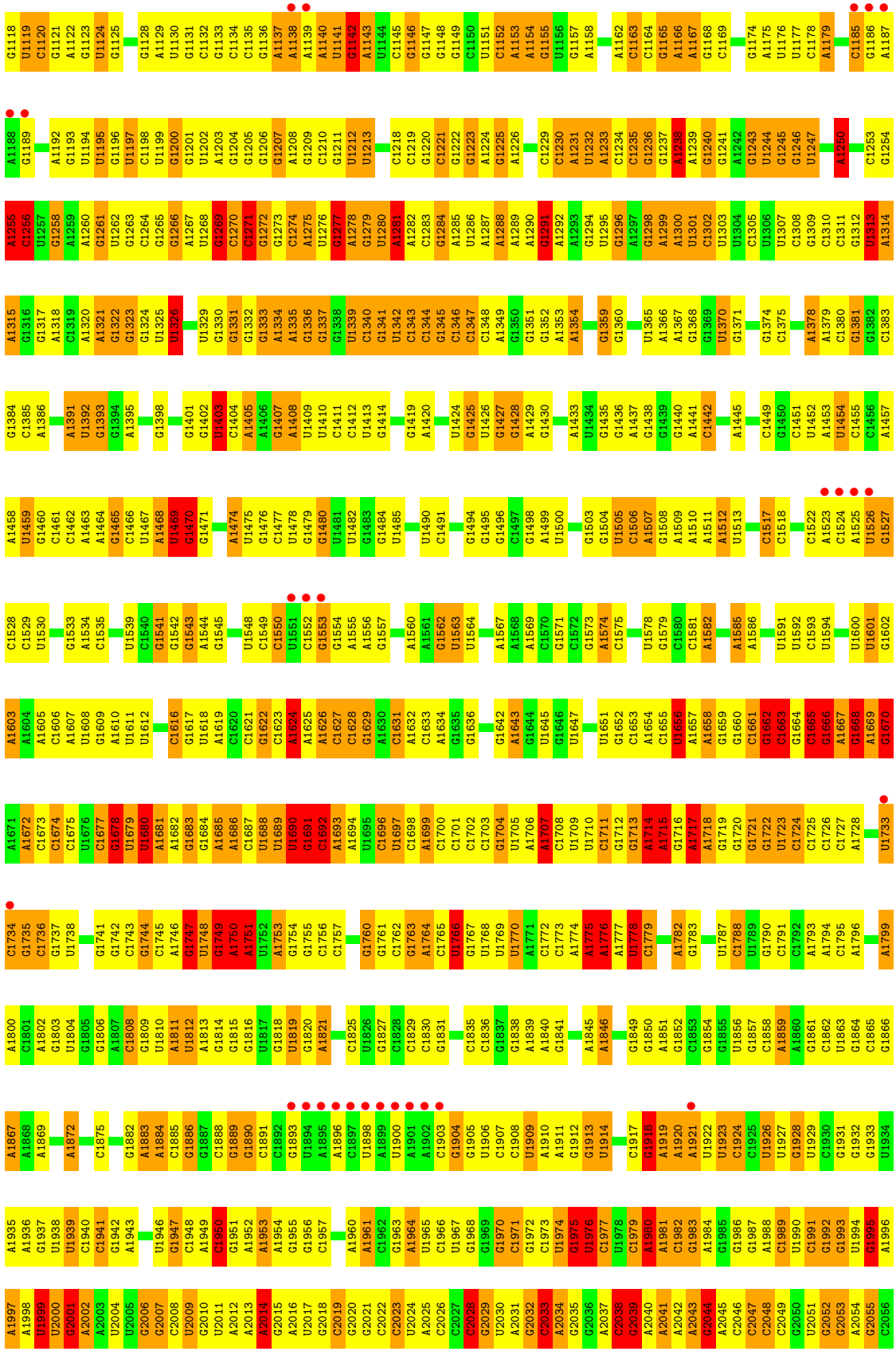


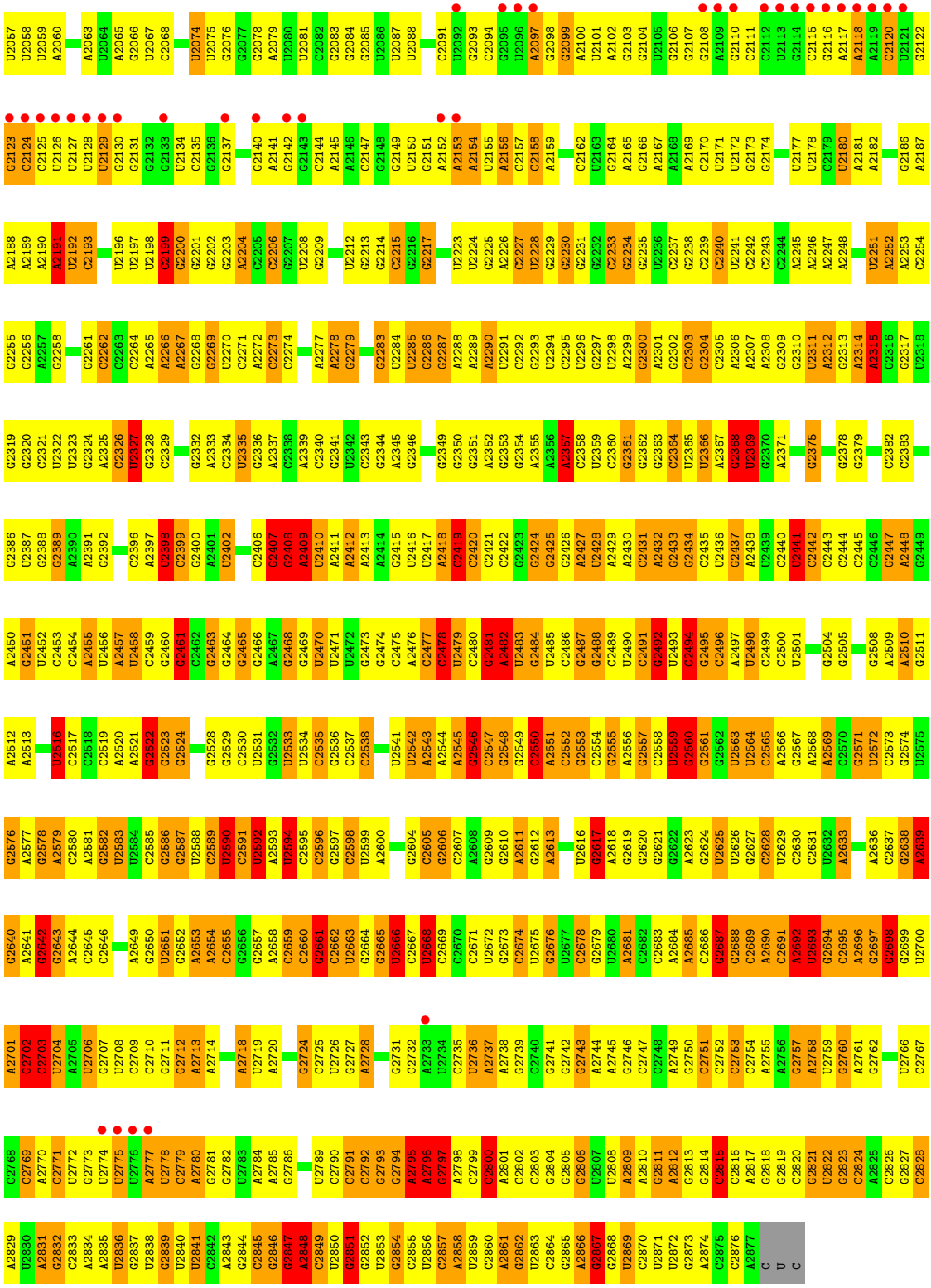
• Molecule 29: 23S ribosomal RNA

Chain X:



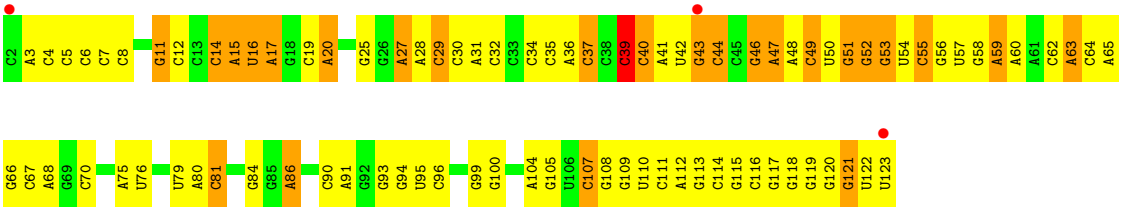






• Molecule 30: 5S ribosomal RNA

Chain Y: 2% 28% 51% 20%


C2
A3
C4
C5
C6
C7
C8
G11
C12
C13
C14
A15
U16
A17
G18
C19
A20
G25
G26
A27
A28
C29
C30
A31
C32
C33
C34
C35
A36
C37
C38
C39
C40
A41
U42
G43
C44
C45
G46
A47
A48
C49
U50
G51
G52
G53
U54
C55
G56
U57
G58
A59
A60
A61
C62
A63
C64
A65
G66
C67
A68
G69
C70
A75
U76
U79
A80
C81
G84
G85
A86
C90
A91
G92
G93
G94
U95
C96
G99
G100
A104
G105
U106
C107
G108
G109
U110
C111
A112
G113
C114
G115
C116
G117
G118
G119
G120
G121
U122
U123

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.82Å 411.54Å 695.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 3.00 59.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.02-3.00) 76.2 (59.03-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.284 , 0.326 0.272 , 0.317	Depositor DCC
R_{free} test set	22814 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	89361	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0	0.25	0/1674	0.46	0/2257
2	A	0.40	0/2149	0.62	0/2890
3	B	0.66	0/1568	0.92	2/2105 (0.1%)
4	C	0.50	0/1530	0.75	0/2070
5	D	0.36	0/1420	0.59	0/1903
6	E	0.39	0/1309	0.61	0/1771
7	F	0.30	0/1067	0.55	0/1446
8	G	0.47	0/1139	0.74	0/1539
9	H	0.72	0/1007	1.02	1/1352 (0.1%)
10	I	0.49	0/1082	0.78	0/1448
11	J	0.60	0/1114	0.83	1/1486 (0.1%)
12	K	0.81	0/887	1.11	4/1188 (0.3%)
13	L	0.54	0/784	0.79	1/1045 (0.1%)
14	M	0.76	0/880	1.02	3/1179 (0.3%)
15	N	0.65	0/994	0.77	0/1323
16	O	0.54	0/751	0.75	0/1000
17	P	0.75	0/1027	0.93	0/1373
18	Q	0.46	0/738	0.63	0/988
19	R	0.58	0/836	0.87	0/1121
20	S	0.40	0/1371	0.68	0/1862
21	T	0.52	0/634	0.70	0/838
22	U	0.52	0/557	0.88	1/741 (0.1%)
23	V	0.40	0/538	0.58	0/714
24	W	0.51	0/426	0.74	0/568
25	Z	0.67	0/465	0.99	1/622 (0.2%)
26	1	0.47	0/411	0.68	0/554
27	2	0.47	0/397	0.70	0/521
28	3	0.56	0/516	0.75	0/673
29	X	0.79	28/66826 (0.0%)	1.38	1078/104247 (1.0%)
30	Y	0.61	0/2907	1.12	10/4529 (0.2%)
All	All	0.73	28/97004 (0.0%)	1.25	1102/145353 (0.8%)

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
9	H	0	1
10	I	0	1
13	L	0	1
14	M	0	2
19	R	0	1
All	All	0	7

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	774	A	N3-C4	7.61	1.39	1.34
29	X	774	A	C5-C4	7.18	1.43	1.38
29	X	1682	A	N7-C5	-6.86	1.35	1.39
29	X	1975	G	N7-C5	6.29	1.43	1.39
29	X	2823	G	N9-C8	-6.08	1.33	1.37

The worst 5 of 1102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	1678	G	C8-N9-C4	14.96	112.38	106.40
29	X	1292	A	C8-N9-C4	14.80	111.72	105.80
29	X	774	A	N1-C6-N6	13.97	126.98	118.60
29	X	1679	U	C5-C6-N1	-13.00	116.20	122.70
29	X	1678	G	N7-C8-N9	-12.95	106.62	113.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	85	ALA	Peptide
9	H	36	THR	Peptide
10	I	52	GLY	Peptide
13	L	87	VAL	Peptide
14	M	2	GLN	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	0	1651	0	1693	51	0
2	A	2107	0	2190	133	0
3	B	1540	0	1600	117	0
4	C	1507	0	1525	115	0
5	D	1401	0	1481	81	0
6	E	1287	0	1336	53	0
7	F	1048	0	1088	35	0
8	G	1115	0	1144	50	0
9	H	997	0	1046	81	0
10	I	1068	0	1103	68	0
11	J	1091	0	1125	66	0
12	K	879	0	930	79	0
13	L	778	0	820	57	0
14	M	867	0	890	64	0
15	N	978	0	1020	95	0
16	O	742	0	756	37	0
17	P	1014	0	1096	80	0
18	Q	727	0	753	31	0
19	R	826	0	881	65	0
20	S	1346	0	1372	71	0
21	T	626	0	655	38	0
22	U	553	0	604	50	0
23	V	534	0	558	13	0
24	W	424	0	470	24	0
25	Z	453	0	455	49	0
26	1	404	0	416	25	0
27	2	393	0	420	24	0
28	3	509	0	565	56	0
29	X	59673	0	30060	1967	0
30	Y	2601	0	1327	91	0
31	A	1	0	0	0	0
31	H	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	X	177	0	0	1	0
31	Y	5	0	0	0	0
32	X	36	0	29	2	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	89361	0	59408	3326	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 23.

The worst 5 of 3326 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)
3:B:14:ILE:HB	14:M:20:HIS:HD2	1.16	1.11
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.35	1.06
29:X:1225:G:H1'	29:X:1250:A:H61	1.21	1.03
29:X:517:A:H5"	29:X:518:A:H5'	1.37	1.02
29:X:2690:A:OP1	29:X:2692:A:OP2	1.78	0.99

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 X-ray entries followed by that with respect to entries of similar resolution.

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
1	0	222/224 (99%)	139 (63%)	58 (26%)	25 (11%)	0 2
2	A	272/274 (99%)	206 (76%)	50 (18%)	16 (6%)	1 9
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1 3
4	C	195/197 (99%)	123 (63%)	50 (26%)	22 (11%)	0 2
5	D	175/177 (99%)	117 (67%)	42 (24%)	16 (9%)	1 3
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	0 2
7	F	142/144 (99%)	100 (70%)	27 (19%)	15 (11%)	0 2
8	G	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1 5
9	H	132/134 (98%)	96 (73%)	18 (14%)	18 (14%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	2
11	J	134/136 (98%)	97 (72%)	28 (21%)	9 (7%)	1	6
12	K	111/113 (98%)	81 (73%)	18 (16%)	12 (11%)	0	2
13	L	102/104 (98%)	68 (67%)	18 (18%)	16 (16%)	0	1
14	M	107/109 (98%)	83 (78%)	14 (13%)	10 (9%)	0	3
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	2	12
16	O	92/94 (98%)	69 (75%)	13 (14%)	10 (11%)	0	2
17	P	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	13
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	1	3
19	R	108/110 (98%)	63 (58%)	28 (26%)	17 (16%)	0	1
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	2
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1	5
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0	0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	9	40
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	5
25	Z	55/57 (96%)	36 (66%)	13 (24%)	6 (11%)	0	2
26	1	52/54 (96%)	31 (60%)	13 (25%)	8 (15%)	0	1
27	2	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	6	31
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0	1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	0	2

5 of 335 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	17	SER
1	0	61	PRO
1	0	157	ILE
1	0	216	PRO
2	A	25	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
1	0	167/167 (100%)	150 (90%)	17 (10%)	7	28
2	A	214/214 (100%)	177 (83%)	37 (17%)	2	10
3	B	155/155 (100%)	123 (79%)	32 (21%)	1	6
4	C	157/157 (100%)	117 (74%)	40 (26%)	0	3
5	D	153/153 (100%)	126 (82%)	27 (18%)	2	10
6	E	136/136 (100%)	111 (82%)	25 (18%)	1	9
7	F	107/107 (100%)	94 (88%)	13 (12%)	5	21
8	G	118/118 (100%)	97 (82%)	21 (18%)	2	9
9	H	103/103 (100%)	73 (71%)	30 (29%)	0	2
10	I	108/108 (100%)	88 (82%)	20 (18%)	1	8
11	J	110/110 (100%)	82 (74%)	28 (26%)	0	3
12	K	90/90 (100%)	68 (76%)	22 (24%)	0	3
13	L	74/74 (100%)	46 (62%)	28 (38%)	0	0
14	M	92/92 (100%)	58 (63%)	34 (37%)	0	0
15	N	96/96 (100%)	82 (85%)	14 (15%)	3	15
16	O	75/75 (100%)	59 (79%)	16 (21%)	1	5
17	P	109/109 (100%)	85 (78%)	24 (22%)	1	4
18	Q	75/75 (100%)	57 (76%)	18 (24%)	0	3
19	R	91/91 (100%)	71 (78%)	20 (22%)	1	4
20	S	149/149 (100%)	119 (80%)	30 (20%)	1	6
21	T	62/62 (100%)	42 (68%)	20 (32%)	0	1
22	U	57/57 (100%)	38 (67%)	19 (33%)	0	1
23	V	54/54 (100%)	45 (83%)	9 (17%)	2	11
24	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	13
26	1	38/38 (100%)	33 (87%)	5 (13%)	4	18
27	2	40/40 (100%)	32 (80%)	8 (20%)	1	7
28	3	51/51 (100%)	34 (67%)	17 (33%)	0	1
All	All	2780/2780 (100%)	2188 (79%)	592 (21%)	1	5

5 of 592 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	90	LYS
27	2	29	ASN
20	S	55	THR
19	R	84	VAL
22	U	15	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
26	1	30	ASN
28	3	7	HIS
7	F	11	GLN
13	L	37	HIS
14	M	48	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	839 (30%)	30 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	874 (30%)	31 (1%)

5 of 874 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	8	A
29	X	13	A
29	X	15	G
29	X	54	G
29	X	63	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1506	C
29	X	2758	A
29	X	1602	G
29	X	2854	G
29	X	2551	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)

Of 187 ligands modelled in this entry, 186 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	HGR	X	6178	-	39,39,39	1.81	7 (17%)	50,58,58	1.72	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HGR	X	6178	-	-	4/20/79/79	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	6178	HGR	C5-C6	-4.19	1.42	1.50
32	X	6178	HGR	C1-C6	4.15	1.41	1.35
32	X	6178	HGR	C12-C14	4.14	1.43	1.33
32	X	6178	HGR	C12-C6	3.87	1.55	1.44
32	X	6178	HGR	C3-C2	-3.78	1.41	1.48

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	6178	HGR	C10-O3-C3	4.73	126.09	115.36
32	X	6178	HGR	C4-C5-C6	4.24	121.49	112.36
32	X	6178	HGR	C23-O8-C18	-4.00	100.22	106.31
32	X	6178	HGR	C4-C3-C2	-3.98	118.17	121.83
32	X	6178	HGR	O3-C3-C2	3.09	118.43	112.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

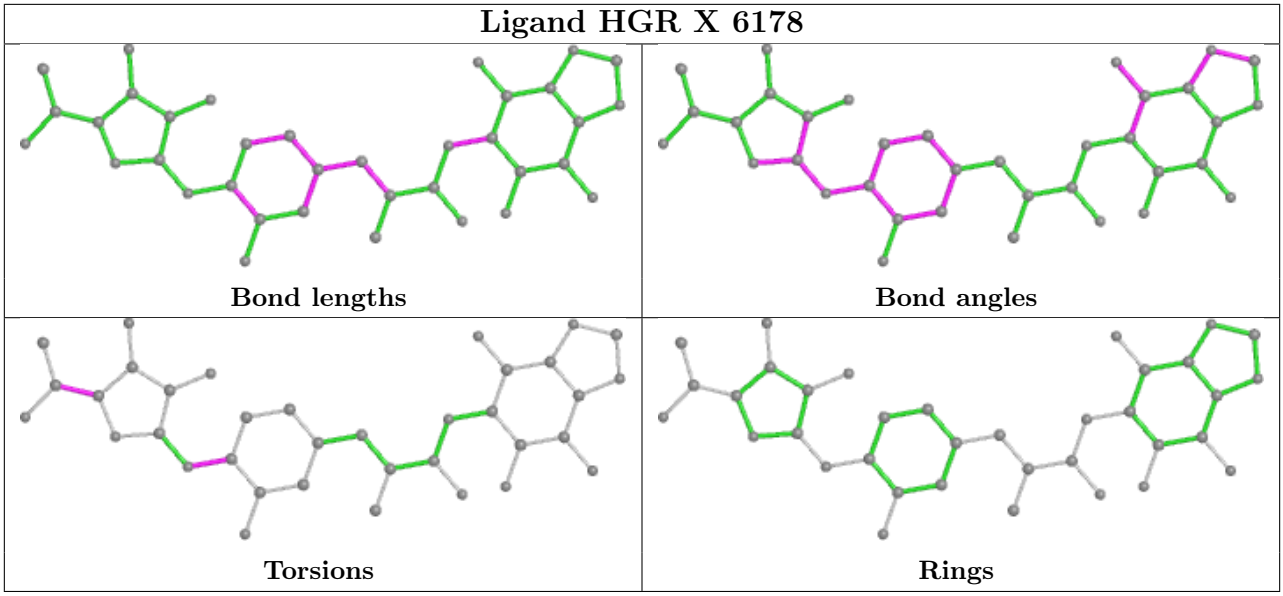
Mol	Chain	Res	Type	Atoms
32	X	6178	HGR	C2-C3-O3-C10
32	X	6178	HGR	C13-C11-C7-O1
32	X	6178	HGR	C13-C11-C7-C8
32	X	6178	HGR	O6-C11-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	6178	HGR	2	0

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	0	224/224 (100%)	4.90	179 (79%)	0	0	291, 311, 319, 322	0
2	A	274/274 (100%)	0.62	39 (14%)	2	1	108, 151, 172, 185	0
3	B	205/205 (100%)	0.04	5 (2%)	59	30	67, 102, 129, 146	0
4	C	197/197 (100%)	0.12	10 (5%)	28	10	93, 133, 158, 177	0
5	D	177/177 (100%)	0.30	14 (7%)	12	4	165, 183, 200, 214	0
6	E	171/171 (100%)	0.09	10 (5%)	23	7	116, 167, 191, 198	0
7	F	144/144 (100%)	2.34	61 (42%)	0	0	233, 259, 275, 281	0
8	G	142/142 (100%)	0.28	8 (5%)	24	8	87, 125, 139, 169	0
9	H	134/134 (100%)	-0.10	4 (2%)	50	22	70, 92, 108, 118	0
10	I	141/141 (100%)	1.05	34 (24%)	0	0	98, 150, 173, 182	0
11	J	136/136 (100%)	0.94	25 (18%)	1	0	107, 126, 156, 159	0
12	K	113/113 (100%)	0.22	6 (5%)	26	10	63, 82, 95, 99	0
13	L	104/104 (100%)	1.12	26 (25%)	0	0	126, 147, 162, 173	0
14	M	109/109 (100%)	-0.06	3 (2%)	53	25	72, 89, 117, 147	0
15	N	117/117 (100%)	0.36	10 (8%)	10	3	90, 118, 144, 153	0
16	O	94/94 (100%)	-0.28	6 (6%)	19	6	103, 129, 156, 173	0
17	P	127/127 (100%)	0.16	6 (4%)	31	11	81, 96, 120, 180	0
18	Q	93/93 (100%)	0.59	12 (12%)	3	1	108, 137, 160, 176	0
19	R	110/110 (100%)	0.37	8 (7%)	15	4	111, 131, 166, 180	0
20	S	175/175 (100%)	0.48	24 (13%)	3	1	134, 167, 185, 193	0
21	T	84/84 (100%)	1.16	17 (20%)	1	0	111, 130, 148, 171	0
22	U	72/72 (100%)	1.51	21 (29%)	0	0	134, 163, 177, 182	0
23	V	66/66 (100%)	0.82	12 (18%)	1	0	147, 163, 190, 201	0
24	W	55/55 (100%)	0.66	6 (10%)	5	2	112, 124, 142, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	57/57 (100%)	0.05	3 (5%) 26 10	82, 97, 120, 130	0
26	1	54/54 (100%)	1.72	23 (42%) 0 0	140, 153, 179, 189	0
27	2	47/47 (100%)	0.17	2 (4%) 35 13	108, 121, 132, 134	0
28	3	65/65 (100%)	1.63	26 (40%) 0 0	115, 132, 143, 153	0
29	X	2780/2881 (96%)	-0.16	79 (2%) 53 25	59, 127, 241, 397	0
30	Y	122/122 (100%)	-0.36	3 (2%) 57 29	110, 157, 182, 203	0
All	All	6389/6490 (98%)	0.37	682 (10%) 6 2	59, 134, 276, 397	0

The worst 5 of 682 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	0	204	PHE	18.3
1	0	200	ALA	18.1
1	0	205	LEU	17.5
1	0	85	ALA	15.5
1	0	47	PRO	15.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	6101	1/1	0.05	1.26	138,138,138,138	0
31	MG	X	6135	1/1	0.44	1.17	129,129,129,129	0
31	MG	X	6140	1/1	0.45	0.42	97,97,97,97	0
31	MG	X	6103	1/1	0.49	0.23	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	6168	1/1	0.55	0.67	100,100,100,100	0
31	MG	X	6152	1/1	0.57	0.30	158,158,158,158	0
31	MG	X	6099	1/1	0.58	0.86	120,120,120,120	0
31	MG	X	6114	1/1	0.62	0.70	93,93,93,93	0
31	MG	X	6118	1/1	0.62	0.41	82,82,82,82	0
31	MG	X	6093	1/1	0.66	0.34	96,96,96,96	0
31	MG	X	6124	1/1	0.68	0.58	100,100,100,100	0
31	MG	X	6161	1/1	0.69	0.23	113,113,113,113	0
31	MG	X	6176	1/1	0.69	0.55	73,73,73,73	0
31	MG	X	6139	1/1	0.71	0.42	113,113,113,113	0
31	MG	X	6111	1/1	0.71	0.41	98,98,98,98	0
31	MG	X	6125	1/1	0.72	0.49	109,109,109,109	0
31	MG	X	6112	1/1	0.72	0.33	80,80,80,80	0
31	MG	X	6051	1/1	0.73	0.54	83,83,83,83	0
31	MG	A	301	1/1	0.73	0.35	108,108,108,108	0
31	MG	X	6163	1/1	0.74	0.34	82,82,82,82	0
31	MG	X	6160	1/1	0.74	0.72	108,108,108,108	0
31	MG	X	6174	1/1	0.74	0.30	117,117,117,117	0
31	MG	X	6076	1/1	0.74	0.55	73,73,73,73	0
31	MG	X	6149	1/1	0.75	0.40	99,99,99,99	0
31	MG	Y	205	1/1	0.75	0.64	123,123,123,123	0
31	MG	X	6162	1/1	0.76	0.76	104,104,104,104	0
31	MG	X	6035	1/1	0.76	0.46	80,80,80,80	0
31	MG	N	201	1/1	0.77	0.38	74,74,74,74	0
31	MG	X	6169	1/1	0.78	0.48	91,91,91,91	0
31	MG	X	6172	1/1	0.78	0.34	88,88,88,88	0
31	MG	X	6006	1/1	0.78	0.56	70,70,70,70	0
31	MG	X	6116	1/1	0.78	0.67	99,99,99,99	0
31	MG	X	6049	1/1	0.78	0.40	91,91,91,91	0
31	MG	X	6141	1/1	0.79	0.38	87,87,87,87	0
31	MG	X	6159	1/1	0.79	1.13	109,109,109,109	0
31	MG	X	6131	1/1	0.80	0.39	80,80,80,80	0
31	MG	X	6090	1/1	0.80	0.46	72,72,72,72	0
31	MG	X	6150	1/1	0.80	0.46	97,97,97,97	0
31	MG	X	6075	1/1	0.80	0.26	85,85,85,85	0
31	MG	Y	203	1/1	0.80	0.76	96,96,96,96	0
31	MG	X	6127	1/1	0.80	0.62	81,81,81,81	0
31	MG	X	6070	1/1	0.81	0.47	69,69,69,69	0
31	MG	X	6014	1/1	0.81	0.47	99,99,99,99	0
31	MG	X	6144	1/1	0.81	0.26	132,132,132,132	0
31	MG	X	6133	1/1	0.81	0.48	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	Y	201	1/1	0.81	0.41	96,96,96,96	0
31	MG	X	6052	1/1	0.81	0.43	86,86,86,86	0
31	MG	X	6078	1/1	0.81	0.36	89,89,89,89	0
31	MG	X	6173	1/1	0.82	0.14	87,87,87,87	0
31	MG	X	6155	1/1	0.82	0.79	108,108,108,108	0
31	MG	X	6156	1/1	0.82	0.25	91,91,91,91	0
31	MG	X	6085	1/1	0.82	0.41	66,66,66,66	0
31	MG	X	6003	1/1	0.82	0.31	72,72,72,72	0
31	MG	X	6030	1/1	0.82	0.33	101,101,101,101	0
31	MG	X	6033	1/1	0.83	0.69	76,76,76,76	0
31	MG	X	6020	1/1	0.83	0.44	76,76,76,76	0
31	MG	X	6061	1/1	0.83	0.23	100,100,100,100	0
31	MG	X	6087	1/1	0.83	0.62	85,85,85,85	0
31	MG	X	6047	1/1	0.83	0.25	79,79,79,79	0
31	MG	X	6015	1/1	0.83	0.27	74,74,74,74	0
31	MG	X	6170	1/1	0.83	0.37	97,97,97,97	0
31	MG	X	6074	1/1	0.84	0.39	89,89,89,89	0
31	MG	X	6022	1/1	0.84	0.58	92,92,92,92	0
31	MG	X	6137	1/1	0.84	0.47	136,136,136,136	0
31	MG	X	6148	1/1	0.85	0.31	104,104,104,104	0
31	MG	X	6002	1/1	0.85	0.32	91,91,91,91	0
31	MG	X	6171	1/1	0.85	0.32	118,118,118,118	0
31	MG	X	6064	1/1	0.85	0.48	77,77,77,77	0
31	MG	X	6046	1/1	0.85	0.58	76,76,76,76	0
31	MG	X	6017	1/1	0.86	0.45	54,54,54,54	0
31	MG	X	6079	1/1	0.86	0.33	99,99,99,99	0
31	MG	X	6012	1/1	0.86	0.24	78,78,78,78	0
31	MG	X	6058	1/1	0.86	0.34	70,70,70,70	0
31	MG	X	6175	1/1	0.86	0.54	121,121,121,121	0
31	MG	X	6164	1/1	0.86	0.23	86,86,86,86	0
31	MG	X	6042	1/1	0.86	1.02	96,96,96,96	0
31	MG	X	6130	1/1	0.86	0.41	132,132,132,132	0
31	MG	X	6062	1/1	0.86	0.72	87,87,87,87	0
31	MG	X	6045	1/1	0.87	0.72	94,94,94,94	0
31	MG	X	6065	1/1	0.87	0.28	93,93,93,93	0
31	MG	X	6158	1/1	0.87	0.20	76,76,76,76	0
31	MG	X	6098	1/1	0.88	0.20	71,71,71,71	0
31	MG	X	6091	1/1	0.88	0.27	72,72,72,72	0
31	MG	X	6153	1/1	0.88	0.30	114,114,114,114	0
31	MG	X	6126	1/1	0.88	0.41	114,114,114,114	0
31	MG	X	6083	1/1	0.88	0.28	83,83,83,83	0
31	MG	Y	204	1/1	0.88	0.59	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	6120	1/1	0.88	0.27	78,78,78,78	0
31	MG	H	201	1/1	0.89	0.14	104,104,104,104	0
31	MG	X	6071	1/1	0.89	0.34	99,99,99,99	0
31	MG	X	6001	1/1	0.89	0.72	67,67,67,67	0
31	MG	X	6037	1/1	0.89	0.40	65,65,65,65	0
31	MG	X	6165	1/1	0.89	0.44	88,88,88,88	0
31	MG	X	6146	1/1	0.89	0.15	125,125,125,125	0
31	MG	X	6039	1/1	0.90	0.39	79,79,79,79	0
31	MG	X	6157	1/1	0.90	0.56	96,96,96,96	0
31	MG	X	6129	1/1	0.90	0.45	89,89,89,89	0
31	MG	X	6117	1/1	0.90	0.42	130,130,130,130	0
31	MG	X	6097	1/1	0.90	0.52	122,122,122,122	0
31	MG	X	6105	1/1	0.90	0.40	86,86,86,86	0
31	MG	X	6122	1/1	0.90	0.36	84,84,84,84	0
31	MG	X	6059	1/1	0.90	0.24	88,88,88,88	0
31	MG	X	6177	1/1	0.90	0.49	125,125,125,125	0
31	MG	X	6011	1/1	0.90	0.39	104,104,104,104	0
31	MG	X	6154	1/1	0.90	0.66	96,96,96,96	0
31	MG	X	6167	1/1	0.90	1.06	97,97,97,97	0
31	MG	X	6100	1/1	0.90	0.42	111,111,111,111	0
32	HGR	X	6178	36/36	0.90	0.24	79,99,109,111	0
31	MG	X	6142	1/1	0.91	0.56	106,106,106,106	0
31	MG	X	6119	1/1	0.91	0.41	89,89,89,89	0
31	MG	X	6010	1/1	0.91	0.49	64,64,64,64	0
31	MG	X	6025	1/1	0.91	0.65	76,76,76,76	0
31	MG	X	6041	1/1	0.91	0.41	64,64,64,64	0
31	MG	X	6115	1/1	0.91	0.30	133,133,133,133	0
31	MG	X	6029	1/1	0.91	0.40	82,82,82,82	0
31	MG	X	6069	1/1	0.91	0.34	65,65,65,65	0
31	MG	X	6110	1/1	0.91	0.21	84,84,84,84	0
31	MG	X	6077	1/1	0.92	0.56	80,80,80,80	0
31	MG	X	6028	1/1	0.92	0.30	75,75,75,75	0
31	MG	X	6132	1/1	0.92	0.56	84,84,84,84	0
31	MG	X	6060	1/1	0.92	0.65	80,80,80,80	0
31	MG	X	6092	1/1	0.92	0.72	97,97,97,97	0
31	MG	Y	202	1/1	0.92	0.17	130,130,130,130	0
31	MG	X	6056	1/1	0.92	0.32	81,81,81,81	0
31	MG	X	6013	1/1	0.92	0.49	76,76,76,76	0
31	MG	X	6107	1/1	0.92	0.22	76,76,76,76	0
31	MG	X	6108	1/1	0.92	0.52	108,108,108,108	0
31	MG	X	6044	1/1	0.93	0.42	66,66,66,66	0
31	MG	X	6138	1/1	0.93	0.15	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	6123	1/1	0.93	0.55	89,89,89,89	0
31	MG	X	6019	1/1	0.93	0.48	75,75,75,75	0
31	MG	X	6043	1/1	0.93	0.39	106,106,106,106	0
31	MG	X	6073	1/1	0.93	0.30	105,105,105,105	0
31	MG	X	6066	1/1	0.93	0.39	105,105,105,105	0
31	MG	X	6104	1/1	0.93	0.54	89,89,89,89	0
31	MG	X	6147	1/1	0.93	1.06	93,93,93,93	0
31	MG	X	6095	1/1	0.93	0.58	78,78,78,78	0
31	MG	X	6106	1/1	0.93	0.50	100,100,100,100	0
31	MG	X	6096	1/1	0.93	0.33	99,99,99,99	0
31	MG	X	6166	1/1	0.93	0.12	76,76,76,76	0
31	MG	X	6068	1/1	0.93	0.38	111,111,111,111	0
31	MG	X	6121	1/1	0.93	0.60	85,85,85,85	0
31	MG	X	6113	1/1	0.94	0.59	143,143,143,143	0
31	MG	M	201	1/1	0.94	0.67	71,71,71,71	0
31	MG	X	6084	1/1	0.94	0.29	124,124,124,124	0
31	MG	X	6151	1/1	0.94	0.16	88,88,88,88	0
31	MG	X	6040	1/1	0.94	0.54	63,63,63,63	0
31	MG	X	6031	1/1	0.94	0.61	85,85,85,85	0
31	MG	X	6134	1/1	0.94	0.12	100,100,100,100	0
31	MG	X	6089	1/1	0.94	0.27	89,89,89,89	0
31	MG	X	6027	1/1	0.94	0.72	65,65,65,65	0
31	MG	X	6034	1/1	0.94	0.27	69,69,69,69	0
31	MG	X	6021	1/1	0.94	0.26	91,91,91,91	0
31	MG	X	6036	1/1	0.94	0.35	70,70,70,70	0
31	MG	X	6094	1/1	0.94	0.37	95,95,95,95	0
31	MG	X	6109	1/1	0.94	0.36	92,92,92,92	0
31	MG	X	6009	1/1	0.94	0.31	50,50,50,50	0
31	MG	X	6145	1/1	0.94	0.39	84,84,84,84	0
31	MG	X	6080	1/1	0.94	0.69	82,82,82,82	0
31	MG	X	6082	1/1	0.94	0.68	105,105,105,105	0
31	MG	X	6008	1/1	0.95	0.26	58,58,58,58	0
31	MG	X	6048	1/1	0.95	0.57	66,66,66,66	0
31	MG	X	6038	1/1	0.95	0.08	82,82,82,82	0
31	MG	X	6136	1/1	0.95	0.68	84,84,84,84	0
31	MG	X	6018	1/1	0.95	0.78	86,86,86,86	0
31	MG	X	6024	1/1	0.95	0.37	100,100,100,100	0
31	MG	X	6053	1/1	0.95	0.36	85,85,85,85	0
31	MG	X	6102	1/1	0.95	0.30	98,98,98,98	0
31	MG	X	6032	1/1	0.95	0.36	86,86,86,86	0
31	MG	X	6057	1/1	0.95	0.68	92,92,92,92	0
31	MG	X	6004	1/1	0.96	0.28	93,93,93,93	0

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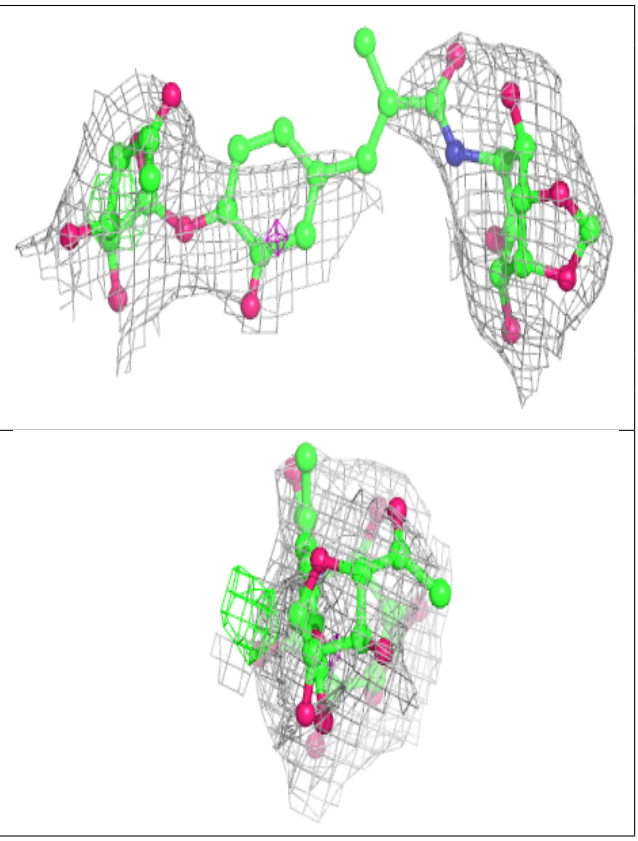
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	6128	1/1	0.96	0.21	131,131,131,131	0
31	MG	X	6054	1/1	0.96	0.39	79,79,79,79	0
31	MG	X	6086	1/1	0.96	0.17	104,104,104,104	0
31	MG	X	6007	1/1	0.96	0.39	78,78,78,78	0
31	MG	X	6081	1/1	0.96	0.34	90,90,90,90	0
31	MG	X	6016	1/1	0.96	0.35	74,74,74,74	0
31	MG	X	6072	1/1	0.96	0.51	101,101,101,101	0
31	MG	X	6055	1/1	0.97	0.45	85,85,85,85	0
31	MG	X	6026	1/1	0.97	0.34	79,79,79,79	0
31	MG	X	6063	1/1	0.97	0.31	87,87,87,87	0
31	MG	X	6023	1/1	0.97	0.37	83,83,83,83	0
31	MG	X	6143	1/1	0.97	0.63	99,99,99,99	0
31	MG	X	6050	1/1	0.98	0.44	91,91,91,91	0
31	MG	X	6067	1/1	0.98	0.18	72,72,72,72	0
31	MG	X	6005	1/1	0.98	0.55	58,58,58,58	0
31	MG	X	6088	1/1	0.99	0.29	88,88,88,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HGR X 6178:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.