



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:14 AM EDT

PDB ID : 6BZ8
Title : Thermus thermophilus 70S containing 16S G347U point mutation and near-cognate ASL Leucine in A site
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.74 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

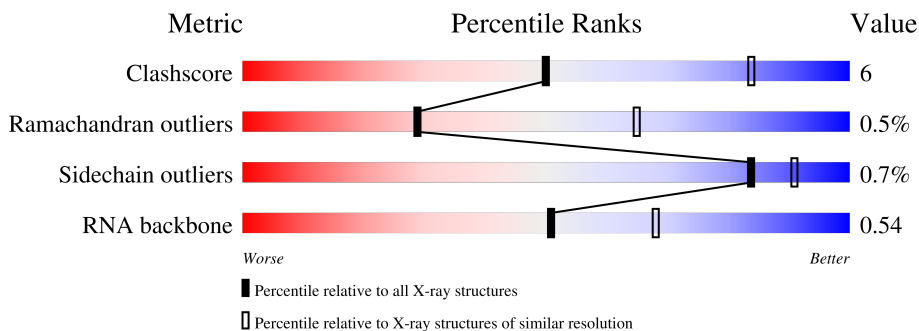
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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))
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RNA backbone	3102	1028 (4.46-3.00)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1508	
1	XA	1508	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	













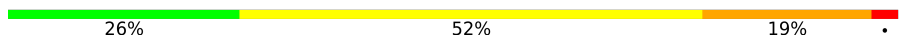












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Mol	Chain	Length	Quality of chain	
4	QD	209	80%	19%
4	XD	209	81%	18%
5	QE	162	81%	12% 7%
5	XE	162	80%	14% 7%
6	QF	101	83%	17%
6	XF	101	85%	15%
7	QG	156	88%	11% .
7	XG	156	86%	13% .
8	QH	138	82%	17% .
8	XH	138	82%	17% .
9	QI	128	77%	21% ..
9	XI	128	72%	26% ..
10	QJ	105	69%	26% 6%
10	XJ	105	69%	23% 9%
11	QK	129	73%	19% 8%
11	XK	129	73%	17% 10%
12	QL	132	78%	16% . 5%
12	XL	132	73%	18% . 8%
13	QM	126	73%	21% . 5%
13	XM	126	75%	20% 6%
14	QN	61	82%	15% ..
14	XN	61	85%	11% ..
15	QO	89	93%	6% .
15	XO	89	84%	13% .
16	QP	88	82%	13% . 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	 83% 11% 5%
17	QQ	105	 79% 16% 5%
17	XQ	105	 78% 17% 5%
18	QR	88	 67% 13% 20%
18	XR	88	 68% 11% 20%
19	QS	93	 69% 19% 11%
19	XS	93	 74% 16% 10%
20	QT	106	 80% 13% 7%
20	XT	106	 78% 15% 7%
21	QU	27	 63% 30% 7%
21	XU	27	 63% 30% 7%
22	QV	77	 60% 31% 6% .
22	QW	77	 26% 52% 19% .
22	XV	77	 61% 29% 8% .
22	XW	77	 19% 53% 25% .
23	QX	25	 28% . 68%
23	XX	25	 28% 8% 8% 56%
24	QY	17	 59% 35% 6%
24	XY	17	 59% 35% 6%
25	RA	2915	 56% 34% 8% ..
25	YA	2915	 56% 34% 8% ..
26	RB	122	 54% 37% 6% ..
26	YB	122	 54% 35% 7% ..
27	RD	276	 75% 22% ..
27	YD	276	 75% 22% ..


























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Mol	Chain	Length	Quality of chain	
28	RE	206	76%	23%
28	YE	206	75%	24%
29	RF	210	79%	17%
29	YF	210	81%	15%
30	RG	182	76%	22%
30	YG	182	73%	25%
31	RH	180	76%	19%
31	YH	180	76%	18%
32	RI	148	82%	16%
32	YI	148	82%	16%
33	RN	140	87%	11%
33	YN	140	88%	11%
34	RO	122	79%	20%
34	YO	122	80%	19%
35	RP	150	79%	21%
35	YP	150	78%	19%
36	RQ	141	73%	27%
36	YQ	141	74%	26%
37	RR	118	79%	20%
37	YR	118	85%	14%
38	RS	112	78%	21%
38	YS	112	76%	22%
39	RT	146	74%	18%
39	YT	146	71%	22%
40	RU	118	76%	20%


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Mol	Chain	Length	Quality of chain
40	YU	118	 77% 19% . .
41	RV	101	 86% 13% .
41	YV	101	 88% 10% .
42	RW	113	 84% 15% .
42	YW	113	 85% 15%
43	RX	96	 86% 9% .
43	YX	96	 85% 10% .
44	RY	110	 84% 14% .
44	YY	110	 78% 19% .
45	RZ	206	 66% 22% . 11%
45	YZ	206	 66% 21% . 11%
46	R0	85	 78% 18% 5%
46	Y0	85	 67% 21% 12%
47	R1	98	 76% 23% .
47	Y1	98	 79% 16% 5%
48	R2	72	 72% 24% .
48	Y2	72	 68% 28% .
49	R3	60	 85% 13% .
49	Y3	60	 88% 10% .
50	R4	71	 82% 13% . .
50	Y4	71	 77% 17% . .
51	R5	60	 85% 13% .
51	Y5	60	 85% 13% .
52	R6	54	 76% 22% .
52	Y6	54	 80% 19% .

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Mol	Chain	Length	Quality of chain
53	R7	49	 84% 12%
53	Y7	49	 86% 12%
54	R8	65	 78% 15% 5%
54	Y8	65	 80% 14% 5%
55	R9	37	 84% 16%
55	Y9	37	 78% 22%

2 Entry composition i

There are 58 unique types of molecules in this entry. The entry contains 295646 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	32244	14352	5978	10415	1499	0	0	0
1	XA	1500	32246	14353	5981	10413	1499	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	235	1907	1217	342	343	5	0	0	0
2	XB	236	1915	1223	343	344	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	205	1605	1011	313	280	1	0	0	0
3	XC	205	1605	1011	313	280	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	1703	1066	339	291	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
9	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	XI	126	Total	C	N	O	0	0	0
			998	633	193	172			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	QJ	99	Total 801	C 504	N 157	O 139	S 1	0	0	0
10	XJ	96	Total 777	C 487	N 153	O 136	S 1	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	QK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0
11	XK	116	Total 864	C 537	N 164	O 160	S 3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	QL	125	Total 975	C 614	N 196	O 164	S 1	0	0	0
12	XL	122	Total 956	C 603	N 193	O 159	S 1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	120	Total 955	C 591	N 197	O 165	S 2	0	0	0
13	XM	119	Total 946	C 585	N 195	O 164	S 2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	QN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
14	XN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	27	57	8			
23	XX	11	Total	C	N	O	P	0	0	0
			230	105	42	73	10			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			
24	XY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	RA	2882	Total 62071	C 27627	N 11611	O 19952	P 2881	0	0	0
25	YA	2883	Total 62091	C 27636	N 11613	O 19960	P 2882	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	RB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0
26	YB	120	Total 2573	C 1146	N 476	O 832	P 119	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	RD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0
27	YD	272	Total 2115	C 1335	N 420	O 357	S 3	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	RE	205	Total 1568	C 991	N 300	O 271	S 6	0	0	0
28	YE	205	Total 1568	C 991	N 300	O 271	S 6	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	RF	202	Total 1585	C 1011	N 297	O 275	S 2	0	0	0
29	YF	202	Total 1585	C 1011	N 297	O 275	S 2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	RG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	YG	181	1474	942	268	260	4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	RH	174	1336	848	251	236	1	0	0	0
31	YH	174	1336	848	251	236	1	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	RI	146	1136	726	201	208	1	0	0	0
32	YI	146	1136	726	201	208	1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	RN	138	1104	712	206	182	4	0	0	0
33	YN	138	1104	712	206	182	4	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	RO	122	933	588	171	170	4	0	0	0
34	YO	122	933	588	171	170	4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	RP	150	1145	712	232	198	3	0	0	0
35	YP	147	1122	698	229	192	3	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	RQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0
36	YQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
37	RR	117	Total 960	C 599	N 202	O 159	0	0	0
37	YR	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
38	RS	111	Total 882	C 556	N 176	O 150	0	0	0
38	YS	111	Total 882	C 556	N 176	O 150	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	RT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0
39	YT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	RU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
40	YU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
44	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	Y0	75	599	370	127	101	1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	R1	97	763	481	150	131	1	0	0	0
47	Y1	93	729	457	145	126	1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	R2	69	581	358	118	104	1	0	0	0
48	Y2	69	581	358	118	104	1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	R3	59	469	298	90	81	0	0	0
49	Y3	59	469	298	90	81	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	R4	69	565	356	103	101	5	0	0	0
50	Y4	69	565	356	103	101	5	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	R5	59	459	288	90	76	5	0	0	0
51	Y5	59	459	288	90	76	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
53	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	72	Total	Mg	0	0
			72	72		
56	QC	1	Total	Mg	0	0
			1	1		
56	QF	1	Total	Mg	0	0
			1	1		
56	QH	1	Total	Mg	0	0
			1	1		

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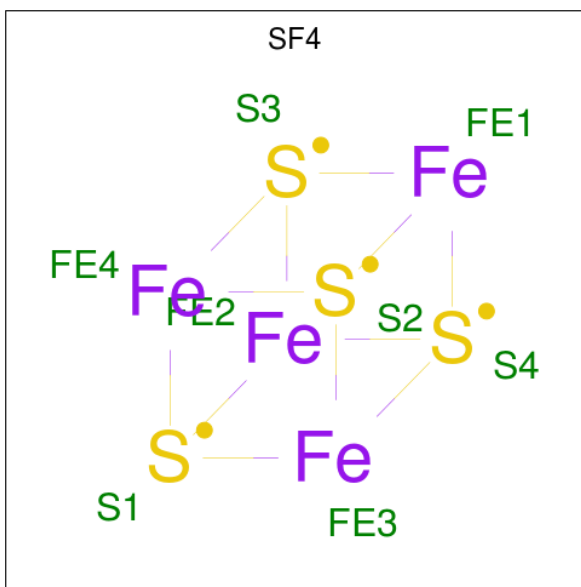
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QV	6	Total 6	Mg 6	0	0
56	QX	1	Total 1	Mg 1	0	0
56	QY	1	Total 1	Mg 1	0	0
56	RA	513	Total 513	Mg 513	0	0
56	RB	11	Total 11	Mg 11	0	0
56	RE	3	Total 3	Mg 3	0	0
56	RN	1	Total 1	Mg 1	0	0
56	RO	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	3	Total 3	Mg 3	0	0
56	R8	1	Total 1	Mg 1	0	0
56	XA	80	Total 80	Mg 80	0	0
56	XC	1	Total 1	Mg 1	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XS	1	Total 1	Mg 1	0	0
56	XV	8	Total 8	Mg 8	0	0
56	XX	1	Total 1	Mg 1	0	0
56	YA	541	Total 541	Mg 541	0	0
56	YB	12	Total 12	Mg 12	0	0
56	YD	1	Total 1	Mg 1	0	0
56	YE	3	Total 3	Mg 3	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	4	Total 4	Mg 4	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YX	2	Total 2	Mg 2	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	2	Total 2	Mg 2	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QD	1	Total	Fe S	0	0
			8	4 4		
57	XD	1	Total	Fe S	0	0
			8	4 4		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	QN	1	Total	Zn	0	0
			1	1		
58	RY	1	Total	Zn	0	0
			1	1		
58	R4	1	Total	Zn	0	0
			1	1		
58	R5	1	Total	Zn	0	0
			1	1		
58	R6	1	Total	Zn	0	0
			1	1		
58	R9	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	YY	1	Total	Zn	0	0
			1	1		
58	Y4	1	Total	Zn	0	0
			1	1		
58	Y5	1	Total	Zn	0	0
			1	1		

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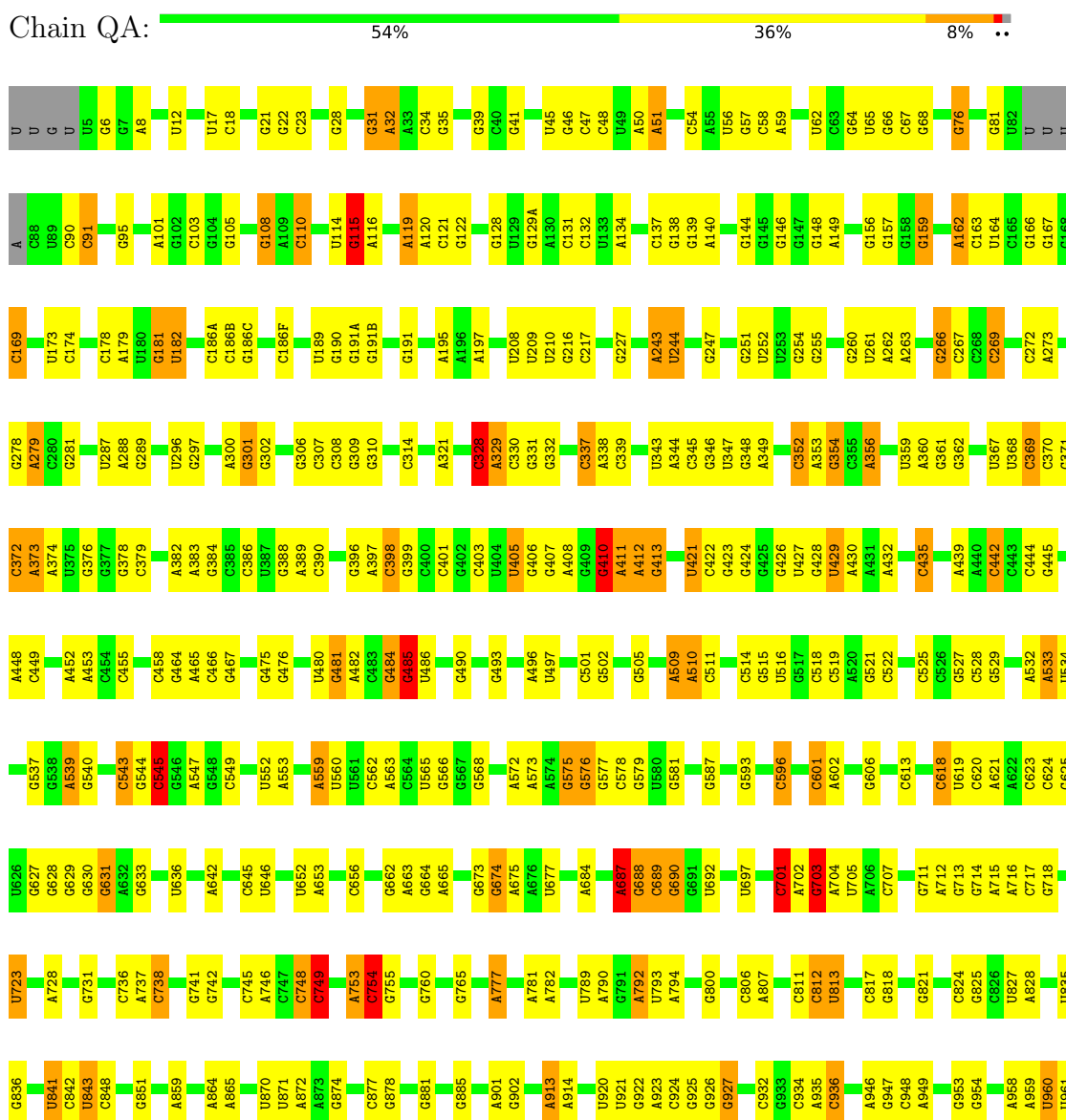
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y6	1	Total 1	Zn 1	0	0
58	Y9	1	Total 1	Zn 1	0	0

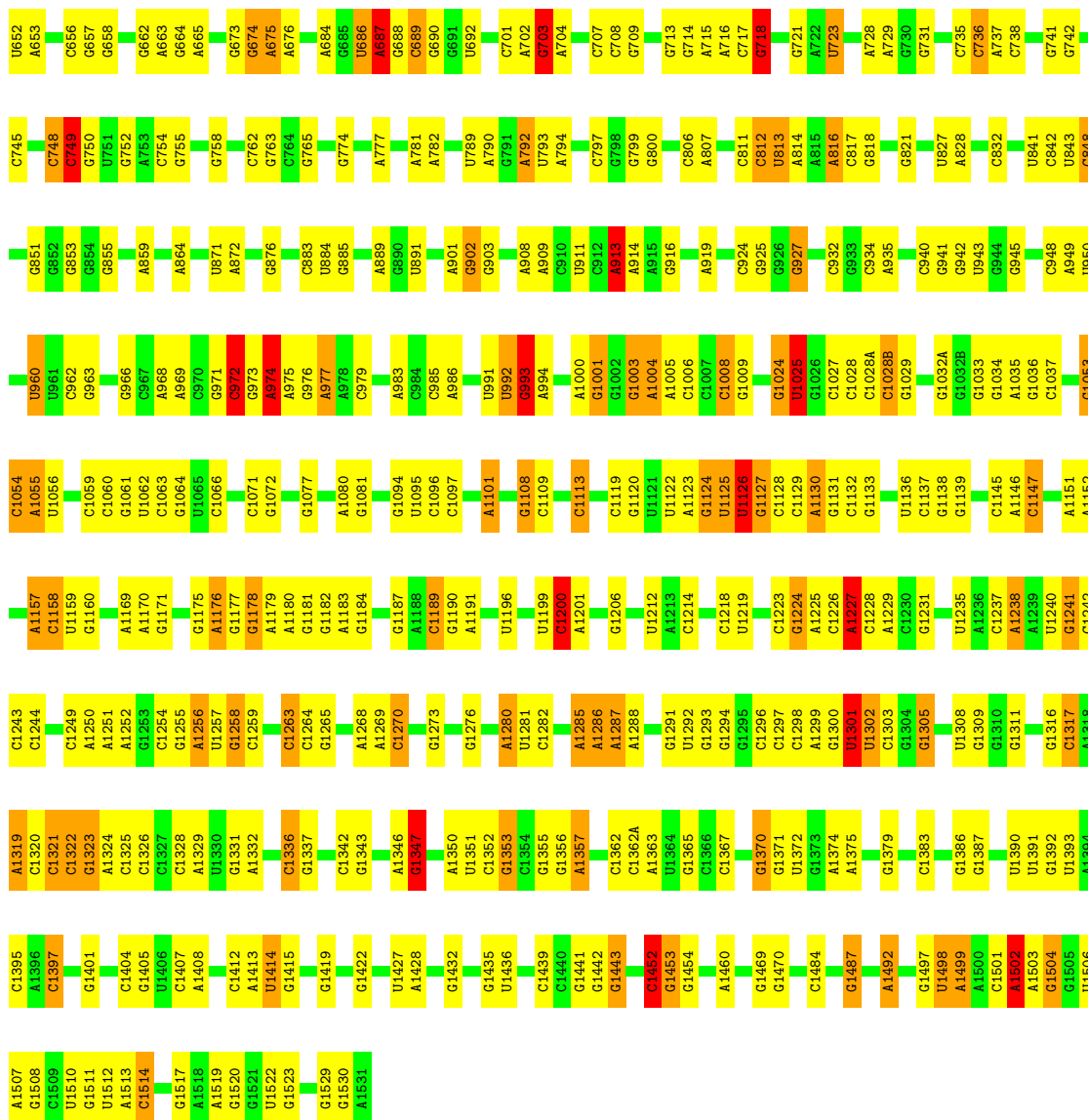
3 Residue-property plots

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.

Note EDS failed to run properly.

- Molecule 1: 16S rRNA

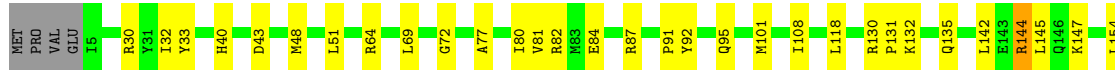
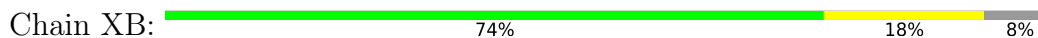




• Molecule 2: 30S ribosomal protein S2

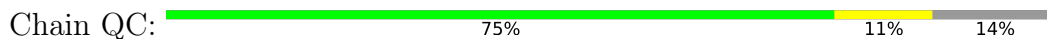


• Molecule 2: 30S ribosomal protein S2

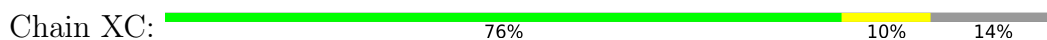




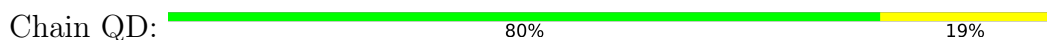
- Molecule 3: 30S ribosomal protein S3



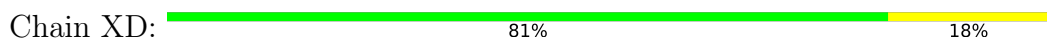
- Molecule 3: 30S ribosomal protein S3



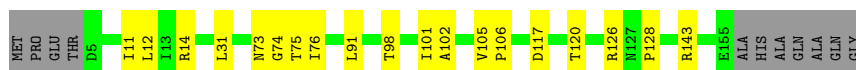
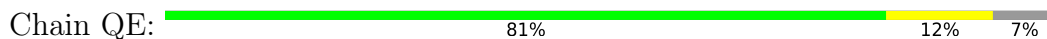
- Molecule 4: 30S ribosomal protein S4




- Molecule 4: 30S ribosomal protein S4

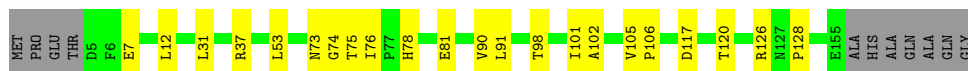


- Molecule 5: 30S ribosomal protein S5




- Molecule 5: 30S ribosomal protein S5

Chain XE:  80% 14% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  83% 17%



- Molecule 6: 30S ribosomal protein S6

Chain XF:  85% 15%




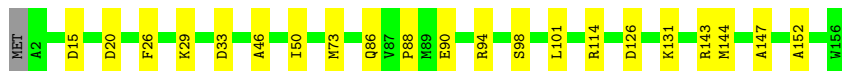
- Molecule 7: 30S ribosomal protein S7

Chain QG:  88% 11%




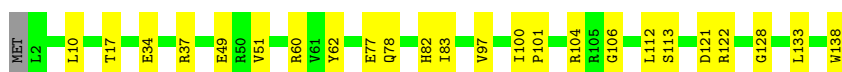
- Molecule 7: 30S ribosomal protein S7

Chain XG:  86% 13%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  82% 17%




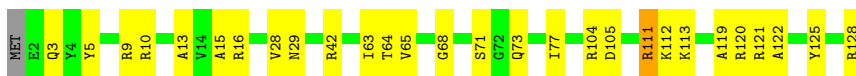
- Molecule 8: 30S ribosomal protein S8

Chain XH:  82% 17%



- Molecule 9: 30S ribosomal protein S9

Chain QI:  77% 21% ..



- Molecule 9: 30S ribosomal protein S9

Chain XI:  72% 26% ..



- Molecule 10: 30S ribosomal protein S10

Chain QJ:  69% 26% 6%



- Molecule 10: 30S ribosomal protein S10

Chain XJ:  69% 23% 9%



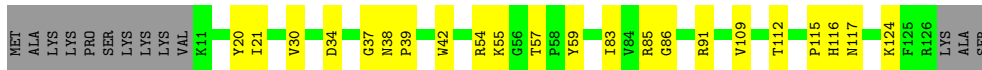
- Molecule 11: 30S ribosomal protein S11

Chain QK:  73% 19% 8%




- Molecule 11: 30S ribosomal protein S11

Chain XK:  73% 17% 10%



- Molecule 12: 30S ribosomal protein S12

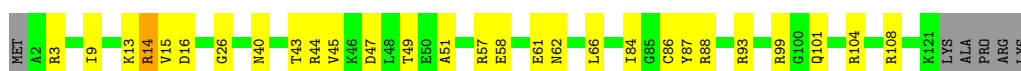
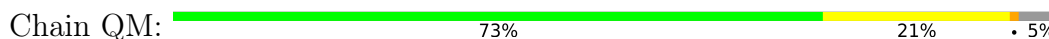
Chain QL:  78% 16% 5%



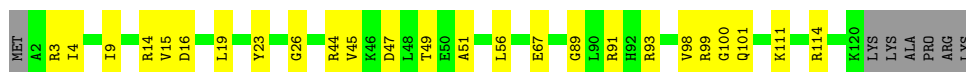
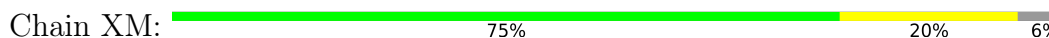
- Molecule 12: 30S ribosomal protein S12



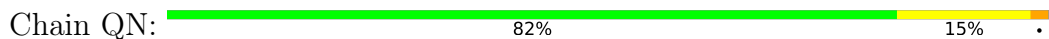
- Molecule 13: 30S ribosomal protein S13



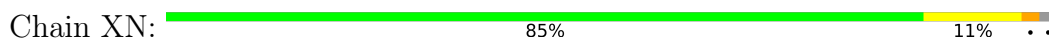
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



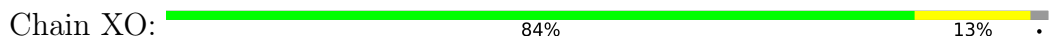
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

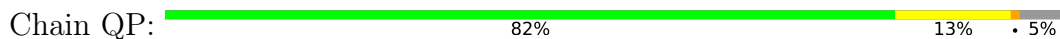


- Molecule 15: 30S ribosomal protein S15

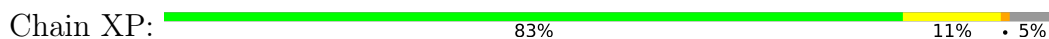




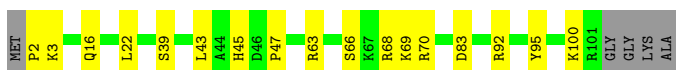
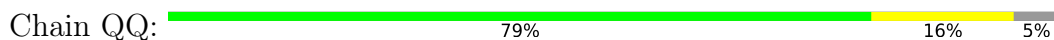
- Molecule 16: 30S ribosomal protein S16



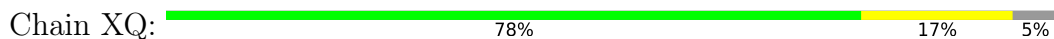
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

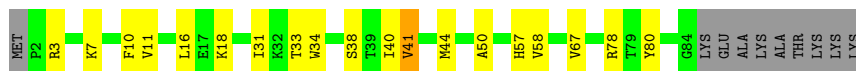


- Molecule 18: 30S ribosomal protein S18

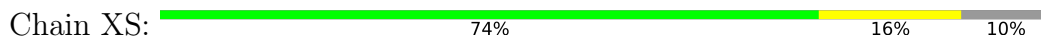


- Molecule 19: 30S ribosomal protein S19

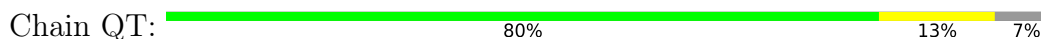




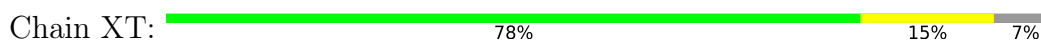
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



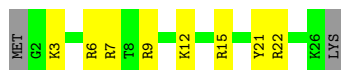
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA fMet

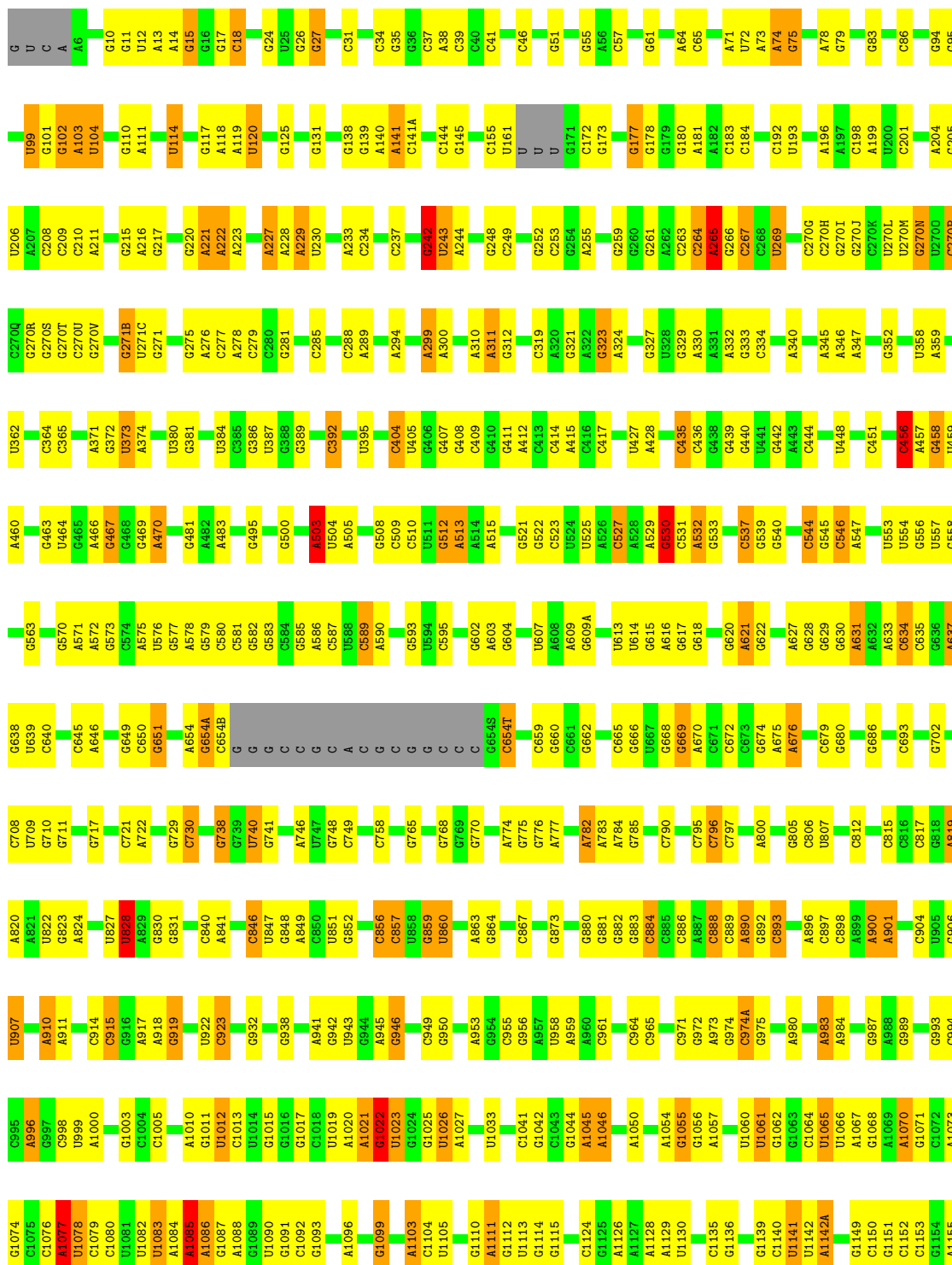


- Molecule 22: tRNA fMet

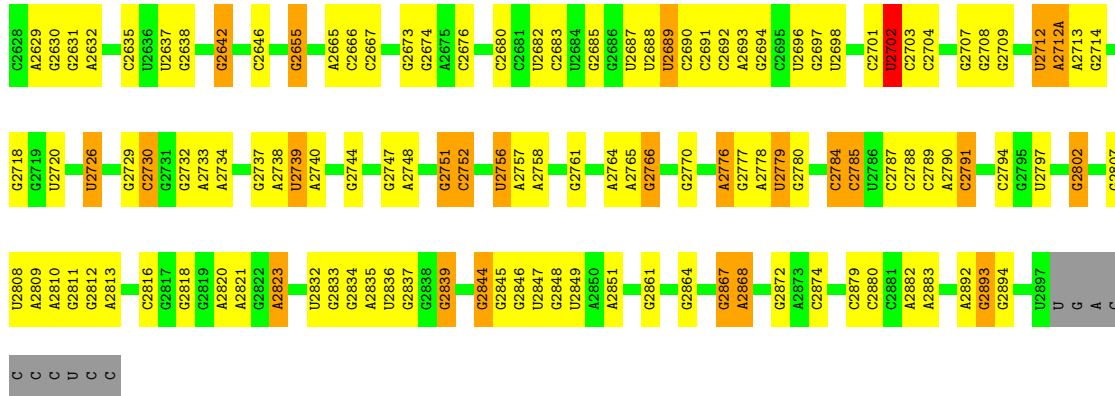




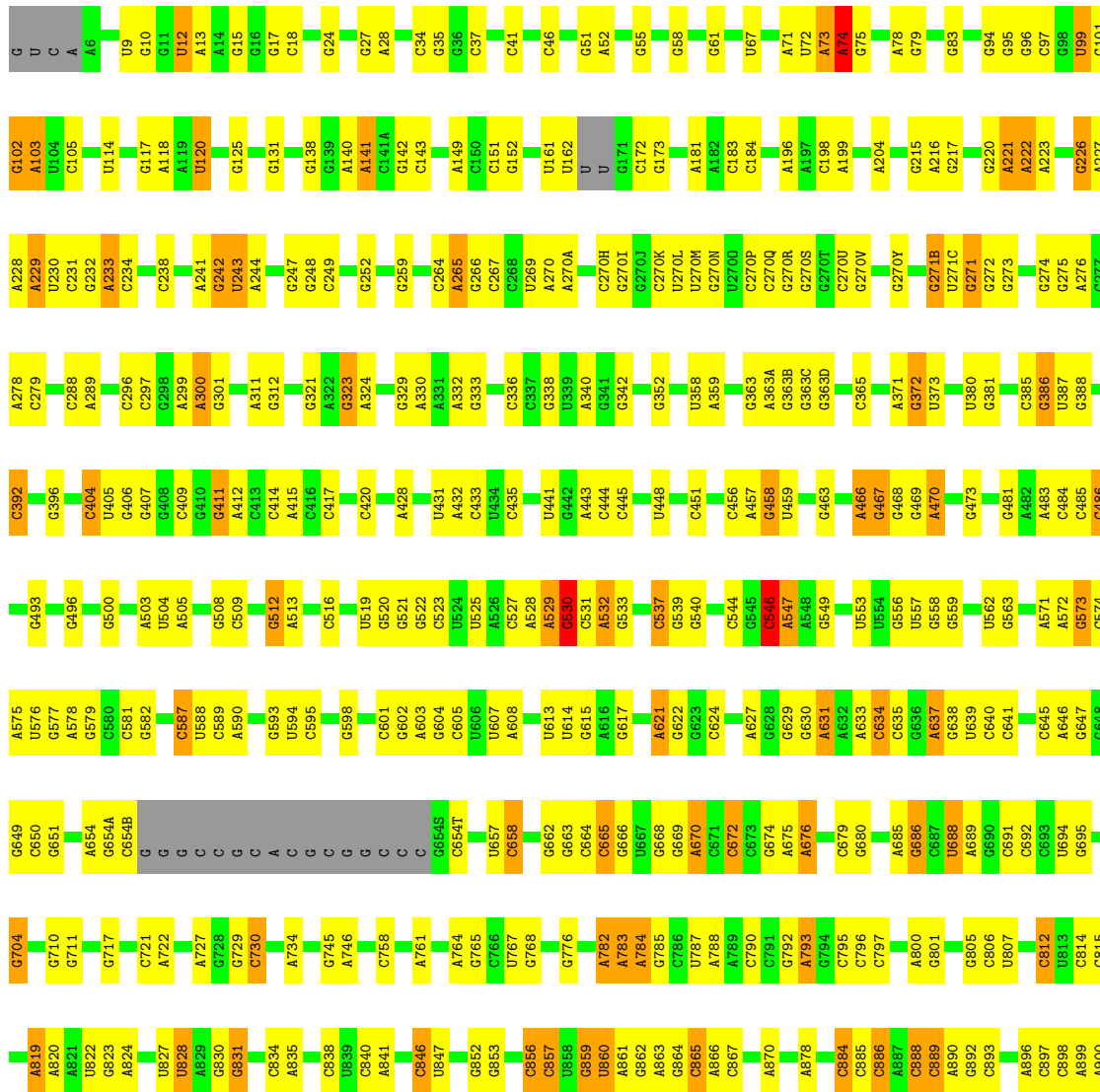
• Molecule 25: 23S rRNA



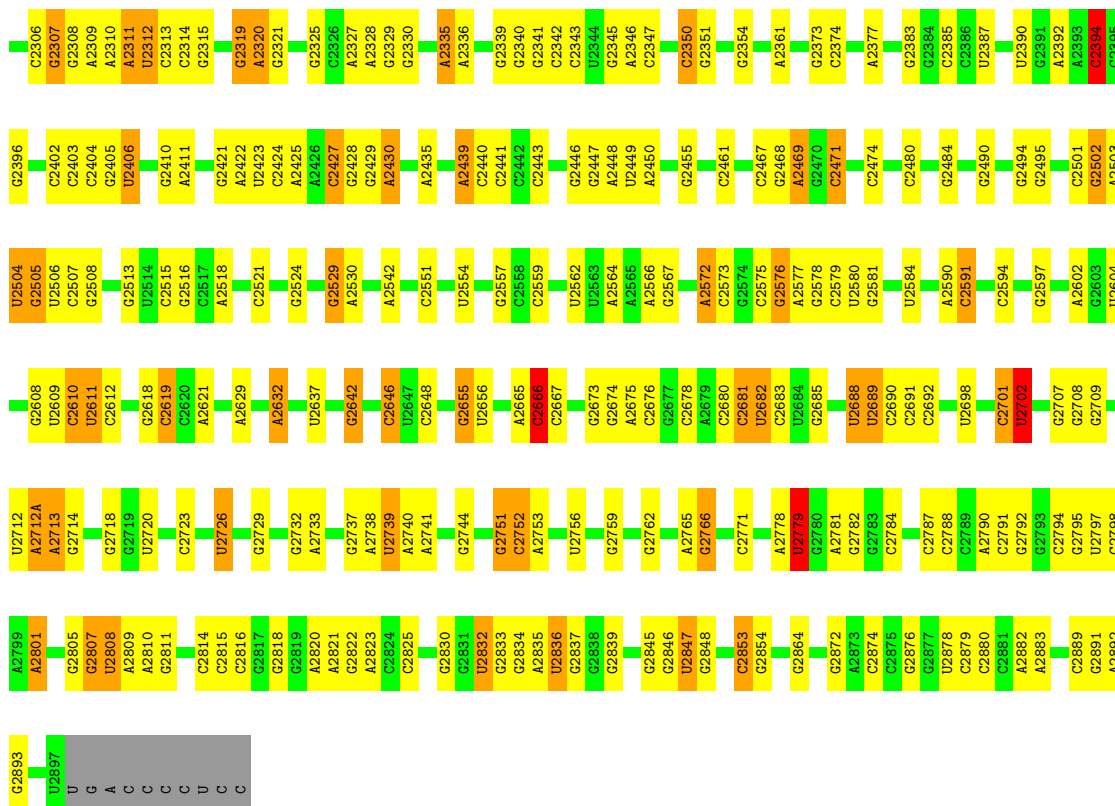
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U1267	C1270	G1271	U1272	C1273	U1274	C1275	U1276	C1277	U1278	C1279	U1280	C1281	U1282	C1283	U1284	C1285	U1286	C1287	U1288	C1289	U1290	C1291	U1292	C1293	U1294	C1295	U1296	C1297	U1298	C1299	U1300	C1301	U1302	C1303	U1304	C1305	U1306	C1307	U1308	C1309	U1310	C1311	U1312	C1313	U1314	C1315	U1316	C1317	U1318	C1319	U1320	C1321	U1322	C1323	U1324	C1325	U1326	C1327	U1328	C1329	U1330	C1331	U1332	C1333	U1334	C1335	U1336	C1337	U1338	C1339	U1340	C1341	U1342	C1343	U1344	C1345	U1346	C1347	U1348	C1349	U1350	C1351	U1352	C1353	U1354	C1355	U1356	C1357	U1358	C1359	U1360	C1361	U1362	C1363	U1364	C1365	U1366	C1367	U1368	C1369	U1370																																																																																																																																																																																																																																																																																													
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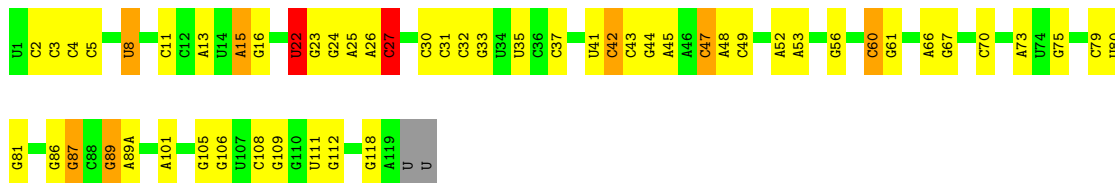
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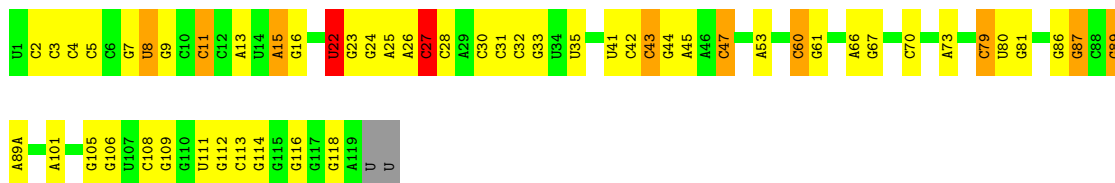
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G1244	A1247	G1248	G1252	A1253	U1254	G1255	G1256	A1262	U1263	G1264	A1265	G1266	U1267	C1270	C1271	A1272	U1273	A1287	C1290	U1294	C1295	G1296	C1297	C1298	G1299	A1300	A1301	G1306	G1309	U1310	G1311	U1312	U1313	C1314	C1315	U1329	G1332	A1331	C1333	U1341	U1342	A1349	U1352	A1353																																																																																																																																										
C1153	G1154	A1155	A1156	G1157	U1165	C1166	G1170	G1171	A1172	A1173	A1174	U1175	A1176	A1177	A1178	C1179	C1180	G1184	A1187	U1188	G1191	G1195	C1196	A1204	U1205	U1206	A1210	U1211	G1212	G1215	C1216	C1217	G1218	G1219	A1220	G1224	C1225	G1226	A1227	G1228	C1230	G1231	C1232	C1233	U1234	G1235	G1236	G1237	G1238																																																																																																																																					
C994	C995	A996	G997	C998	U999	A1000	G1003	C1004	U1002	C1005	U1008	G1011	U1012	C1013	U1014	G1015	U1019	A1020	A1021	G1022	G1023	G1024	G1025	U1026	A1027	G1031	A1032	U1033	U1035	A1045	A1046	G1047	A1050	G1051	A1054	G1055	G1059	U1060	U1061	G1062	G1063	C1064	U1065	C1066	U1067	A1068	U1069	A1070	G1071	C1072																																																																																																																																				
A1073	G1074	C1075	C1076	A1077	U1078	C1079	C1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	U1088	A1089	U1090	G1093	U1094	A1095	A1096	U1097	A1103	C1104	U1105	G1106	G1107	U1108	C1109	U1110	A1111	U1112	U1113	G1114	G1122	C1123	C1124	G1125	A1126	A1127	C1135	G1136	G1139	C1140	U1141	U1142	A1143	G1151	C1152																																																																																																																																					
A901	C902	C903	G904	U905	G906	U907	A910	A911	C912	U913	C914	C915	G916	A917	G918	U919	G920	U930	G931	G932	A941	G942	U943	U944	A945	G946	C949	G950	C955	G956	A957	U958	A959	C961	C965	C971	G972	A973	G974	C974A	A980	A983	G987	U988	G989	A990	G993																																																																																																																																							



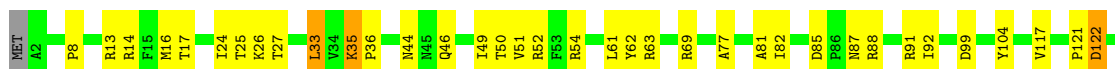
• Molecule 26: 5S rRNA



• Molecule 26: 5S rRNA



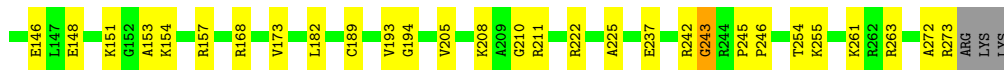
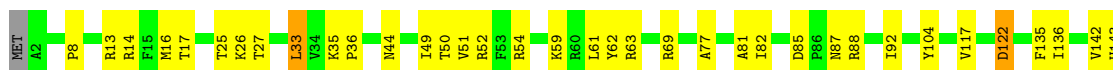
• Molecule 27: 50S ribosomal protein L2





- Molecule 27: 50S ribosomal protein L2

Chain YD: 75% 22%



- Molecule 28: 50S ribosomal protein L3

Chain RE: 76% 23%



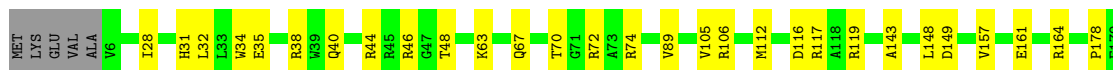
- Molecule 28: 50S ribosomal protein L3

Chain YE: 75% 24%



- Molecule 29: 50S ribosomal protein L4

Chain RF: 79% 17%



- Molecule 29: 50S ribosomal protein L4

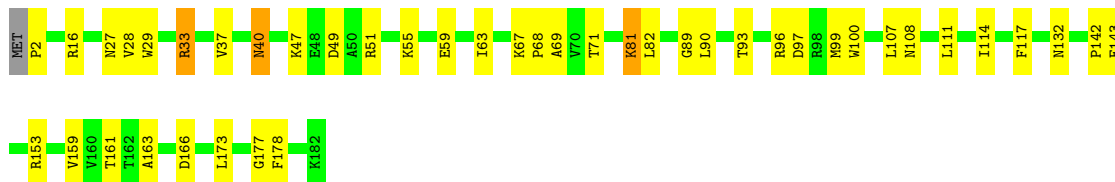
Chain YF: 81% 15%





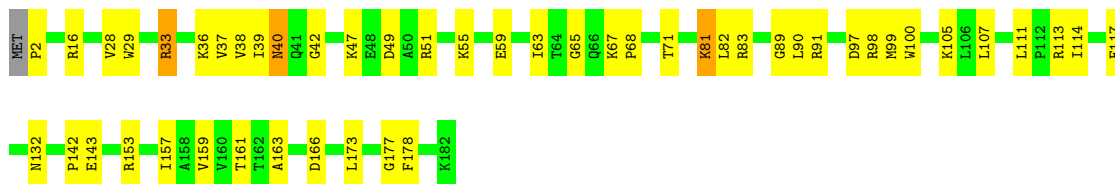
- Molecule 30: 50S ribosomal protein L5

Chain RG: 76% 22% ..



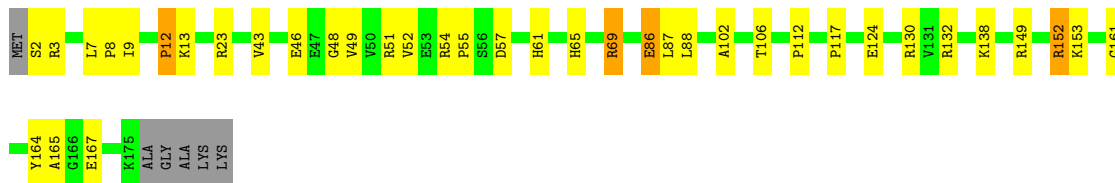
- Molecule 30: 50S ribosomal protein L5

Chain YG: 73% 25% ..



- Molecule 31: 50S ribosomal protein L6

Chain RH: 76% 19% ..



- Molecule 31: 50S ribosomal protein L6

Chain YH: 76% 18% ..




- Molecule 32: 50S ribosomal protein L9

Chain RI: 82% 16% ..



- Molecule 32: 50S ribosomal protein L9

Chain YI:  82% 16% ..




- Molecule 33: 50S ribosomal protein L13

Chain RN:  87% 11% .




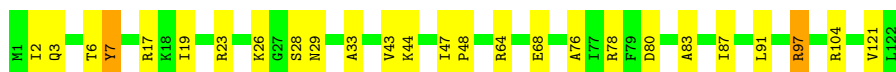
- Molecule 33: 50S ribosomal protein L13

Chain YN:  88% 11% .




- Molecule 34: 50S ribosomal protein L14

Chain RO:  79% 20% .




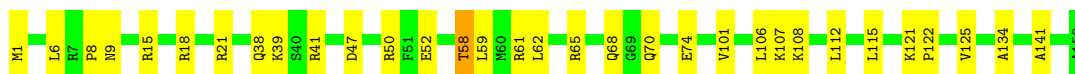
- Molecule 34: 50S ribosomal protein L14

Chain YO:  80% 19% .




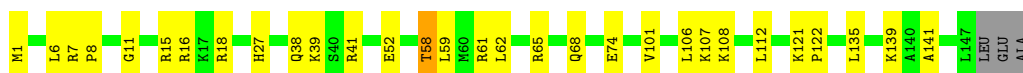
- Molecule 35: 50S ribosomal protein L15

Chain RP:  79% 21% .




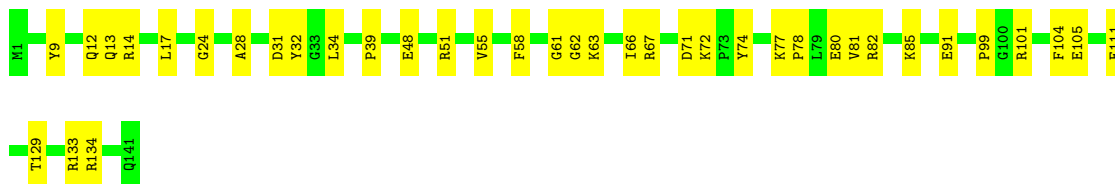
- Molecule 35: 50S ribosomal protein L15

Chain YP:  78% 19% ..




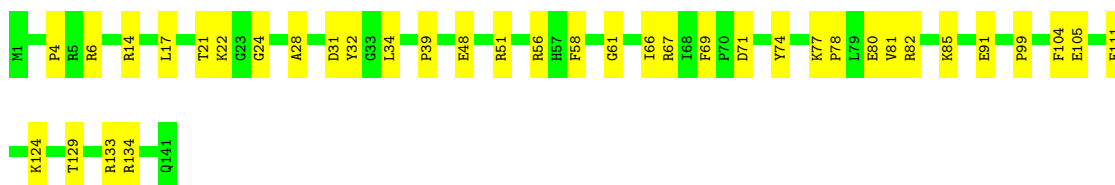
- Molecule 36: 50S ribosomal protein L16

Chain RQ:  73% 27%




- Molecule 36: 50S ribosomal protein L16

Chain YQ:  74% 26%




- Molecule 37: 50S ribosomal protein L17

Chain RR:  79% 20%




- Molecule 37: 50S ribosomal protein L17

Chain YR:  85% 14%




- Molecule 38: 50S ribosomal protein L18

Chain RS:  78% 21%




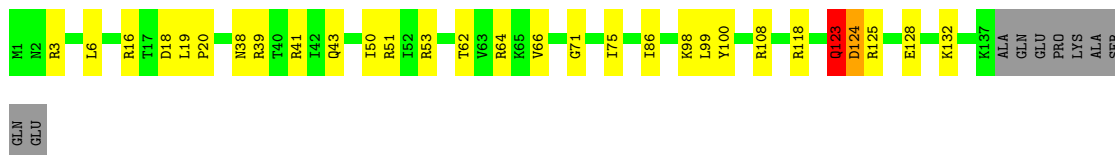
- Molecule 38: 50S ribosomal protein L18

Chain YS:  76% 22%



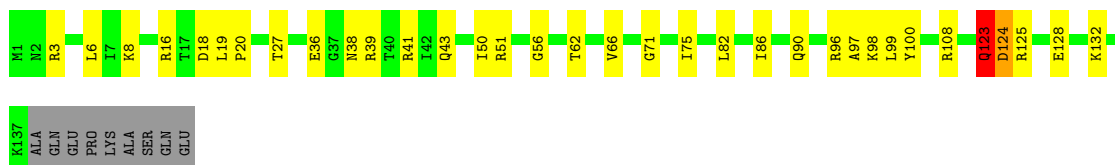
- Molecule 39: 50S ribosomal protein L19

Chain RT:  74% 18% 6%



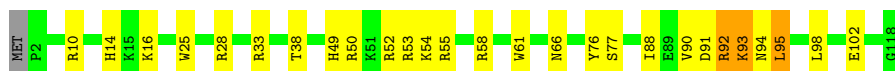
- Molecule 39: 50S ribosomal protein L19

Chain YT: 71% 22% 6%



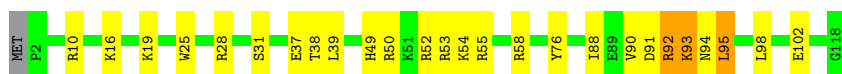
- Molecule 40: 50S ribosomal protein L20

Chain RU: 76% 20%



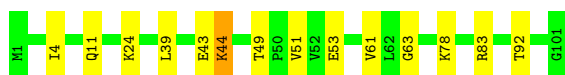
- Molecule 40: 50S ribosomal protein L20

Chain YU: 77% 19%



- Molecule 41: 50S ribosomal protein L21

Chain RV: 86% 13%



- Molecule 41: 50S ribosomal protein L21

Chain YV: 88% 10%

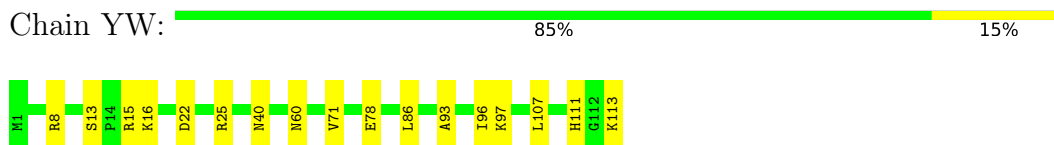


- Molecule 42: 50S ribosomal protein L22

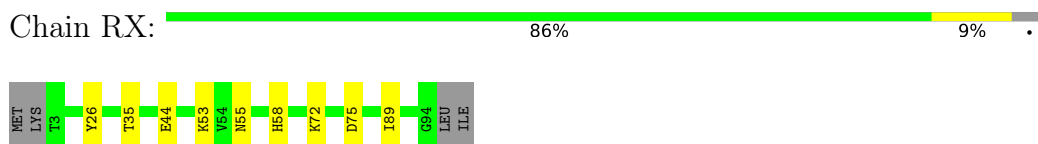
Chain RW: 84% 15%



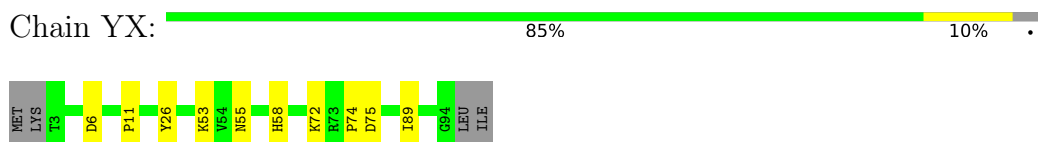
- Molecule 42: 50S ribosomal protein L22



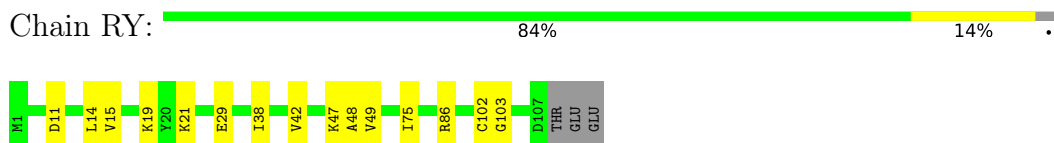
- Molecule 43: 50S ribosomal protein L23



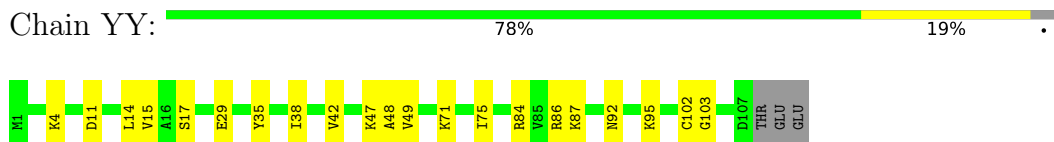
- Molecule 43: 50S ribosomal protein L23



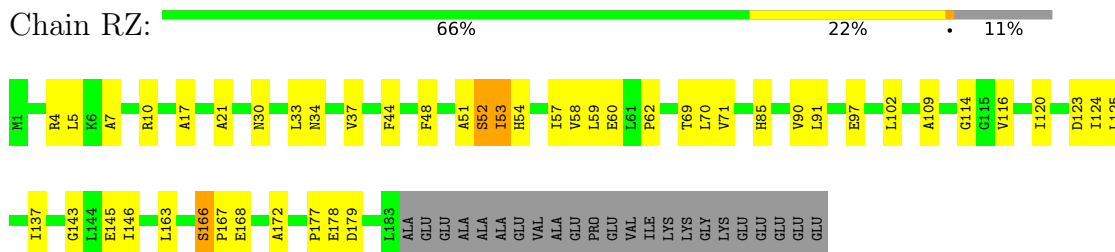
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24

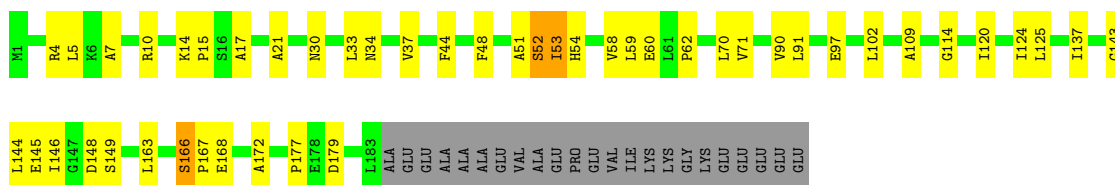


- Molecule 45: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L25





- Molecule 46: 50S ribosomal protein L27

Chain R0: 78% 18% 5%



- Molecule 46: 50S ribosomal protein L27

Chain Y0: 67% 21% 12%



- Molecule 47: 50S ribosomal protein L28

Chain R1: 76% 23% 1%



- Molecule 47: 50S ribosomal protein L28

Chain Y1: 79% 16% 5%



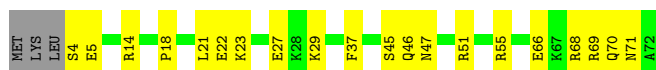
- Molecule 48: 50S ribosomal protein L29

Chain R2: 72% 24% 4%




- Molecule 48: 50S ribosomal protein L29

Chain Y2: 68% 28% 4%




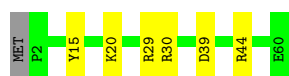
- Molecule 49: 50S ribosomal protein L30

Chain R3:  85% 13%




- Molecule 49: 50S ribosomal protein L30

Chain Y3:  88% 10%




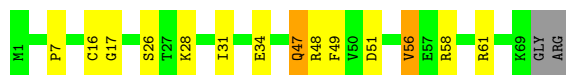
- Molecule 50: 50S ribosomal protein L31

Chain R4:  82% 13%




- Molecule 50: 50S ribosomal protein L31

Chain Y4:  77% 17%




- Molecule 51: 50S ribosomal protein L32

Chain R5:  85% 13%




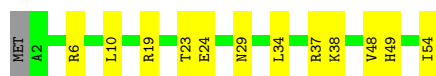
- Molecule 51: 50S ribosomal protein L32

Chain Y5:  85% 13%




- Molecule 52: 50S ribosomal protein L33

Chain R6:  76% 22%




- Molecule 52: 50S ribosomal protein L33

Chain Y6:  80% 19%




- Molecule 53: 50S ribosomal protein L34

Chain R7:  84% 12%




- Molecule 53: 50S ribosomal protein L34

Chain Y7:  86% 12%




- Molecule 54: 50S ribosomal protein L35

Chain R8:  78% 15% 5%




- Molecule 54: 50S ribosomal protein L35

Chain Y8:  80% 14% 5%




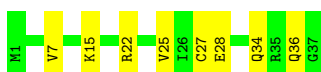
- Molecule 55: 50S ribosomal protein L36

Chain R9:  84% 16%



- Molecule 55: 50S ribosomal protein L36

Chain Y9:  78% 22%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.81Å 448.83Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.68 – 3.74	Depositor
% Data completeness (in resolution range)	100.0 (134.68-3.74)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.225	Depositor
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.103	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295646	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN, SF4, MG

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	QA	0.96	0/36094	1.18	226/56334 (0.4%)
1	XA	0.96	0/36097	1.18	214/56339 (0.4%)
2	QB	0.40	0/1942	0.62	0/2619
2	XB	0.40	0/1950	0.59	0/2630
3	QC	0.39	0/1629	0.56	0/2195
3	XC	0.39	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.57	0/2318
4	XD	0.45	0/1733	0.57	0/2318
5	QE	0.42	0/1171	0.58	0/1576
5	XE	0.42	0/1171	0.58	0/1576
6	QF	0.44	0/856	0.58	0/1154
6	XF	0.44	0/856	0.58	0/1154
7	QG	0.36	0/1276	0.51	0/1709
7	XG	0.36	0/1276	0.51	0/1709
8	QH	0.44	0/1128	0.57	0/1517
8	XH	0.44	0/1128	0.56	0/1517
9	QI	0.44	0/1029	0.64	0/1379
9	XI	0.43	1/1017 (0.1%)	0.61	0/1365
10	QJ	0.42	0/814	0.62	1/1095 (0.1%)
10	XJ	0.40	0/790	0.61	1/1063 (0.1%)
11	QK	0.45	0/900	0.55	0/1213
11	XK	0.42	0/879	0.54	0/1187
12	QL	0.50	0/991	0.66	0/1327
12	XL	0.57	1/972 (0.1%)	0.68	0/1301
13	QM	0.41	0/965	0.62	0/1292
13	XM	0.39	0/956	0.61	0/1281
14	QN	0.51	0/501	0.60	0/664
14	XN	0.51	0/501	0.60	0/664
15	QO	0.40	0/745	0.55	0/992
15	XO	0.39	0/740	0.53	0/987
16	QP	0.49	0/721	0.58	0/970
16	XP	0.49	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.45	0/847	0.58	0/1131
17	XQ	0.45	0/847	0.58	0/1131
18	QR	0.39	0/579	0.62	0/768
18	XR	0.39	0/579	0.63	0/768
19	QS	0.38	0/680	0.71	1/915 (0.1%)
19	XS	0.40	0/689	0.66	0/926
20	QT	0.35	0/765	0.61	0/1007
20	XT	0.35	0/765	0.61	0/1007
21	QU	0.46	0/221	0.74	0/288
21	XU	0.46	0/221	0.74	0/288
22	QV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	QW	0.31	0/1832	0.96	2/2855 (0.1%)
22	XV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	XW	0.29	0/1832	0.94	2/2855 (0.1%)
23	QX	0.99	0/185	0.85	0/285
23	XX	1.03	1/257 (0.4%)	0.85	0/398
24	QY	0.78	0/404	1.11	0/627
24	XY	0.78	0/404	1.11	0/627
25	RA	1.12	5/69521 (0.0%)	1.24	583/108529 (0.5%)
25	YA	1.16	13/69543 (0.0%)	1.25	546/108563 (0.5%)
26	RB	0.81	0/2878	1.23	25/4490 (0.6%)
26	YB	0.81	0/2878	1.22	25/4490 (0.6%)
27	RD	0.60	0/2165	0.71	1/2919 (0.0%)
27	YD	0.60	0/2165	0.71	1/2919 (0.0%)
28	RE	0.52	0/1601	0.71	2/2160 (0.1%)
28	YE	0.52	0/1601	0.71	2/2160 (0.1%)
29	RF	0.58	0/1620	0.62	0/2194
29	YF	0.58	0/1620	0.62	0/2194
30	RG	0.40	0/1499	0.66	1/2016 (0.0%)
30	YG	0.40	0/1499	0.66	1/2016 (0.0%)
31	RH	0.41	0/1362	0.64	0/1841
31	YH	0.41	0/1362	0.64	0/1841
32	RI	0.37	0/1151	0.65	0/1558
32	YI	0.37	0/1151	0.65	0/1558
33	RN	0.50	0/1131	0.64	0/1525
33	YN	0.50	0/1131	0.64	0/1525
34	RO	0.55	0/943	0.61	0/1269
34	YO	0.55	0/943	0.61	0/1269
35	RP	0.47	0/1162	0.76	1/1544 (0.1%)
35	YP	0.49	0/1139	0.76	1/1514 (0.1%)
36	RQ	0.48	0/1143	0.66	0/1527
36	YQ	0.48	0/1143	0.66	0/1527
37	RR	0.49	0/974	0.69	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.50	0/974	0.66	1/1302 (0.1%)
38	RS	0.38	0/892	0.70	0/1187
38	YS	0.38	0/892	0.70	0/1187
39	RT	0.46	0/1155	0.66	0/1542
39	YT	0.46	0/1155	0.66	0/1542
40	RU	0.52	0/982	0.61	0/1306
40	YU	0.52	0/982	0.61	0/1306
41	RV	0.47	0/790	0.67	0/1057
41	YV	0.46	0/790	0.67	0/1057
42	RW	0.54	0/911	0.61	0/1220
42	YW	0.55	0/911	0.61	0/1220
43	RX	0.56	0/739	0.58	0/993
43	YX	0.56	0/739	0.58	0/993
44	RY	0.53	0/831	0.56	0/1108
44	YY	0.53	0/831	0.56	0/1108
45	RZ	0.39	0/1493	0.71	0/2026
45	YZ	0.39	0/1493	0.71	0/2026
46	R0	0.51	0/652	0.57	0/867
46	Y0	0.47	0/607	0.56	0/809
47	R1	0.58	1/770 (0.1%)	0.64	0/1022
47	Y1	0.56	0/736	0.65	0/978
48	R2	0.40	0/583	0.52	0/771
48	Y2	0.40	0/583	0.52	0/771
49	R3	0.44	0/474	0.60	0/635
49	Y3	0.44	0/474	0.60	0/635
50	R4	0.37	0/578	0.64	0/776
50	Y4	0.37	0/578	0.64	0/776
51	R5	0.50	0/473	0.58	0/639
51	Y5	0.50	0/473	0.58	0/639
52	R6	0.34	0/460	0.51	0/613
52	Y6	0.34	0/460	0.51	0/613
53	R7	0.52	0/417	0.59	0/550
53	Y7	0.60	0/426	0.62	0/561
54	R8	0.55	0/525	0.76	0/691
54	Y8	0.55	0/525	0.76	0/691
55	R9	0.44	0/310	0.50	0/407
55	Y9	0.43	0/310	0.50	0/407
All	All	0.93	24/319989 (0.0%)	1.10	1680/478685 (0.4%)

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
2	QB	0	1
4	QD	0	1
4	XD	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
27	RD	0	4
27	YD	0	4
28	RE	0	3
28	YE	0	3
30	RG	0	1
30	YG	0	1
31	RH	0	1
31	YH	0	1
32	RI	0	3
32	YI	0	3
35	RP	0	1
35	YP	0	1
37	RR	0	1
39	RT	0	1
39	YT	0	1
40	RU	0	2
40	YU	0	2
41	RV	0	2
41	YV	0	2
45	RZ	0	4
45	YZ	0	4
50	R4	0	1
50	Y4	0	1
54	R8	0	4
54	Y8	0	4
All	All	0	63

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.70	1.48	1.61
22	QV	1	C	OP3-P	-10.69	1.48	1.61
25	YA	74	A	N9-C4	-6.89	1.33	1.37
25	RA	74	A	N9-C4	-6.79	1.33	1.37
23	XX	21	C	O3'-P	-6.62	1.53	1.61

The worst 5 of 1680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1158	C	C2-N1-C1'	13.01	133.12	118.80
1	QA	1301	U	N1-C2-O2	12.90	131.83	122.80
1	XA	1158	C	N1-C2-O2	12.82	126.59	118.90
1	QA	328	C	N1-C2-O2	12.57	126.44	118.90
1	QA	1301	U	N3-C2-O2	-12.21	113.65	122.20

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
4	QD	19	LEU	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
13	QM	66	LEU	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	QA	32244	0	16274	320	0
1	XA	32246	0	16277	343	1
2	QB	1907	0	1958	36	0
2	XB	1915	0	1969	25	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	15	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	29	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	12	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	QJ	801	0	849	17	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	23	0
11	XK	864	0	881	23	0
12	QL	975	0	1062	16	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	19	0
13	XM	946	0	1007	20	0
14	QN	492	0	529	8	0
14	XN	492	0	529	7	0
15	QO	734	0	771	4	0
15	XO	729	0	768	8	0
16	QP	705	0	725	11	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	8	0
18	XR	574	0	644	6	0
19	QS	665	0	686	13	0
19	XS	674	0	699	9	0
20	QT	763	0	860	9	0
20	XT	763	0	861	11	0
21	QU	217	0	234	8	0
21	XU	217	0	234	8	0
22	QV	1644	0	836	10	0
22	QW	1640	0	837	57	0
22	XV	1644	0	836	9	0
22	XW	1640	0	837	71	0
23	QX	167	0	86	3	0
23	XX	230	0	120	17	0
24	QY	362	0	183	3	0
24	XY	362	0	184	3	0
25	RA	62071	0	31285	461	0
25	YA	62091	0	31290	472	1
26	RB	2573	0	1306	26	0
26	YB	2573	0	1306	28	1
27	RD	2115	0	2195	49	0
27	YD	2115	0	2195	48	0
28	RE	1568	0	1634	29	0
28	YE	1568	0	1634	33	0
29	RF	1585	0	1632	24	0
29	YF	1585	0	1632	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	RG	1474	0	1535	26	0
30	YG	1474	0	1535	32	0
31	RH	1336	0	1418	19	0
31	YH	1336	0	1418	20	0
32	RI	1136	0	1223	12	1
32	YI	1136	0	1223	14	0
33	RN	1104	0	1180	9	0
33	YN	1104	0	1180	8	0
34	RO	933	0	996	20	0
34	YO	933	0	996	19	0
35	RP	1145	0	1227	25	0
35	YP	1122	0	1204	25	0
36	RQ	1122	0	1179	31	0
36	YQ	1122	0	1179	24	0
37	RR	960	0	1021	14	0
37	YR	960	0	1021	9	0
38	RS	882	0	943	18	0
38	YS	882	0	943	20	0
39	RT	1141	0	1202	23	0
39	YT	1141	0	1202	25	0
40	RU	964	0	1022	33	0
40	YU	964	0	1022	24	0
41	RV	779	0	852	9	0
41	YV	779	0	852	7	4
42	RW	900	0	964	13	1
42	YW	900	0	964	12	0
43	RX	725	0	778	6	0
43	YX	725	0	778	7	0
44	RY	818	0	909	8	4
44	YY	818	0	909	15	1
45	RZ	1461	0	1493	28	0
45	YZ	1461	0	1493	26	0
46	R0	643	0	667	10	0
46	Y0	599	0	617	13	0
47	R1	763	0	848	14	0
47	Y1	729	0	802	10	0
48	R2	581	0	629	9	0
48	Y2	581	0	629	11	4
49	R3	469	0	518	6	0
49	Y3	469	0	518	3	0
50	R4	565	0	557	8	0
50	Y4	565	0	557	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	R5	459	0	476	6	0
51	Y5	459	0	479	4	4
52	R6	453	0	473	8	0
52	Y6	453	0	473	6	0
53	R7	409	0	454	4	0
53	Y7	418	0	467	5	0
54	R8	517	0	582	14	0
54	Y8	517	0	582	10	0
55	R9	307	0	335	4	0
55	Y9	307	0	335	6	0
56	QA	72	0	0	0	0
56	QC	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QV	6	0	0	0	0
56	QX	1	0	0	0	0
56	QY	1	0	0	0	0
56	R0	3	0	0	0	0
56	R8	1	0	0	0	0
56	RA	513	0	0	0	0
56	RB	11	0	0	0	0
56	RE	3	0	0	0	0
56	RN	1	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	2	0	0	0	0
56	RT	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	80	0	0	0	0
56	XC	1	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	8	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	541	0	0	0	0
56	YB	12	0	0	0	0
56	YD	1	0	0	0	0
56	YE	3	0	0	0	0
56	YO	1	0	0	0	0
56	YP	4	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	0	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295646	0	199660	2768	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2768 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)
7:XG:143:ARG:CD	22:XW:42:C:O3'	1.75	1.33
7:QG:143:ARG:HD3	22:QW:42:C:O3'	1.09	1.24
7:QG:143:ARG:CD	22:QW:42:C:O3'	1.88	1.20
23:XX:22:C:H6	23:XX:22:C:H5''	1.06	1.13
11:XK:54:ARG:HH22	22:XW:40:C:H4'	1.12	1.09

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1411:C:O2'	26:YB:53:A:O2'[1_655]	1.11	1.09
41:YV:49:THR:O	51:Y5:59:GLU:OE2[4_445]	1.56	0.64
44:RY:21:LYS:NZ	48:Y2:71:ASN:CB[3_555]	1.64	0.56
44:RY:19:LYS:O	48:Y2:71:ASN:ND2[3_555]	1.71	0.49
41:YV:49:THR:OG1	51:Y5:60:VAL:O[4_445]	1.86	0.34

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	
2	QB	233/256 (91%)	207 (89%)	25 (11%)	1 (0%)	34	69
2	XB	234/256 (91%)	208 (89%)	26 (11%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
4	QD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	22	59
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	22	59
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
12	XL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	56
13	QM	118/126 (94%)	99 (84%)	18 (15%)	1 (1%)	19	56
13	XM	117/126 (93%)	98 (84%)	19 (16%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	43
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	43
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	QQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
19	XS	82/93 (88%)	67 (82%)	15 (18%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
27	RD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	34	69
27	YD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	34	69
28	RE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	15	51
28	YE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	15	51
29	RF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
29	YF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
30	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	25	61
30	YG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	25	61
31	RH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	38
32	RI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11	46
32	YI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11	46
33	RN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	59
33	YN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	59
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
35	RP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	22	59
35	YP	145/150 (97%)	113 (78%)	31 (21%)	1 (1%)	22	59
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
36	YQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
37	RR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
37	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
38	RS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
38	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
39	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	45
39	YT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	45
40	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
40	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
41	RV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
41	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
42	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	YW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	14	50
45	YZ	181/206 (88%)	149 (82%)	30 (17%)	2 (1%)	14	50
46	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
46	Y0	73/85 (86%)	67 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100
47	Y1	91/98 (93%)	77 (85%)	14 (15%)	0	100	100
48	R2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	10	45
48	Y2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	10	45
49	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	45
50	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	45
51	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	R7	45/49 (92%)	45 (100%)	0	0	100	100
53	Y7	46/49 (94%)	46 (100%)	0	0	100	100
54	R8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	32
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	32
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10311 (90%)	1088 (10%)	53 (0%)	29	65

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	RT	124	ASP
45	RZ	53	ILE
39	YT	124	ASP
45	YZ	53	ILE
14	QN	17	LYS

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	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	88	94
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	81
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	92
3	XC	159/188 (85%)	158 (99%)	1 (1%)	86	92
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	92
4	XD	180/181 (99%)	179 (99%)	1 (1%)	86	92
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	88
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	88
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	85
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	85
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	75
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	75
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	75
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	82
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	82
17	QQ	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	82
19	XS	73/80 (91%)	72 (99%)	1 (1%)	67	82
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	212 (99%)	2 (1%)	78	88
27	YD	214/218 (98%)	212 (99%)	2 (1%)	78	88
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	159 (99%)	2 (1%)	71	84
29	YF	161/166 (97%)	159 (99%)	2 (1%)	71	84
30	RG	155/156 (99%)	153 (99%)	2 (1%)	69	82
30	YG	155/156 (99%)	153 (99%)	2 (1%)	69	82
31	RH	145/148 (98%)	141 (97%)	4 (3%)	43	67
31	YH	145/148 (98%)	141 (97%)	4 (3%)	43	67
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88
33	YN	117/119 (98%)	116 (99%)	1 (1%)	78	88
34	RO	100/100 (100%)	98 (98%)	2 (2%)	55	75
34	YO	100/100 (100%)	98 (98%)	2 (2%)	55	75
35	RP	116/116 (100%)	114 (98%)	2 (2%)	60	79
35	YP	114/116 (98%)	113 (99%)	1 (1%)	78	88
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	85
38	YS	87/88 (99%)	86 (99%)	1 (1%)	73	85
39	RT	120/127 (94%)	119 (99%)	1 (1%)	81	89
39	YT	120/127 (94%)	119 (99%)	1 (1%)	81	89
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	93 (100%)	0	100	100
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	52	72
42	YW	92/92 (100%)	90 (98%)	2 (2%)	52	72
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	92
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	92
46	R0	65/67 (97%)	64 (98%)	1 (2%)	65	81
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	79
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100
49	R3	51/52 (98%)	50 (98%)	1 (2%)	55	75
49	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	75
50	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	62	79
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9622 (99%)	65 (1%)	84	91

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	YS	3	ARG
42	YW	15	ARG
35	RP	125	VAL
35	RP	58	THR
42	YW	40	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
7	XG	28	ASN
35	YP	27	HIS
7	XG	68	ASN
14	XN	49	HIS
40	YU	94	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	297 (19%)	32 (2%)
1	XA	1498/1508 (99%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	2 (2%)
22	QW	76/77 (98%)	33 (43%)	2 (2%)
22	XV	76/77 (98%)	15 (19%)	2 (2%)
22	XW	76/77 (98%)	34 (44%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	10/25 (40%)	2 (20%)	0
24	QY	16/17 (94%)	4 (25%)	0
24	XY	16/17 (94%)	4 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	RA	2879/2915 (98%)	613 (21%)	41 (1%)
25	YA	2880/2915 (98%)	609 (21%)	41 (1%)
26	RB	119/122 (97%)	24 (20%)	0
26	YB	119/122 (97%)	24 (20%)	0
All	All	9346/9482 (98%)	1956 (20%)	149 (1%)

5 of 1956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	32	A
1	QA	39	G
1	QA	41	G
1	QA	47	C

5 of 149 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	YA	404	C
25	YA	2439	A
25	YA	856	C
25	YA	1379	A
25	RA	637	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 1306 ligands modelled in this entry, 1304 are monoatomic - leaving 2 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	$\# Z > 2$
57	SF4	QD	301	4	0,12,12	-	-	-		
57	SF4	XD	301	4	0,12,12	-	-	-		

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
57	SF4	QD	301	4	-	-	0/6/5/5
57	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.