



wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2014 – 05:55 PM BST

PDB ID : 4V4T
Title : Crystal structure of the whole ribosomal complex with a stop codon in the A-site.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.46 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

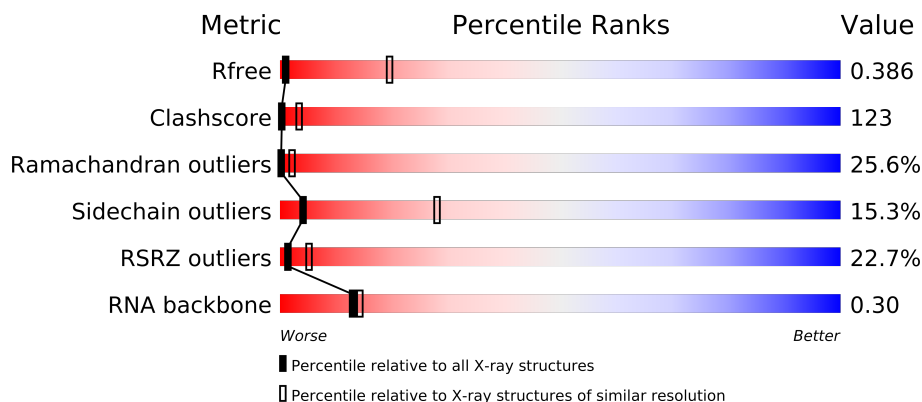
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 6.46 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}	66092	1095 (9.00-3.50)
Clashscore	79885	1033 (9.00-3.52)
Ramachandran outliers	78287	1289 (9.00-3.50)
Sidechain outliers	78261	1264 (9.00-3.50)
RSRZ outliers	66119	1094 (9.00-3.50)
RNA backbone	1838	1045 (10.00-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AV	76	
3	AW	76	
4	AX	18	
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	


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Mol	Chain	Length	Quality of chain
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	BB	123	
26	BA	2916	
27	BD	173	
28	BE	338	
29	BF	246	
30	BG	176	
31	BH	177	
32	BI	149	
33	BN	145	
34	BO	122	
35	BP	164	
36	BQ	138	
37	BS	186	
38	BT	66	
39	BW	113	
40	BX	84	
41	BY	119	
42	BZ	253	
43	BR	118	
44	BU	118	
45	BV	100	
46	B2	70	
47	B3	60	
48	B0	91	
49	B4	73	
50	B5	60	
51	B6	82	
52	B7	47	
53	B8	64	
54	B9	36	

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Mol	Chain	Length	Quality of chain
55	BK	141	 A horizontal bar chart representing the quality of chain BK. The bar is divided into segments of different colors: red, green, yellow, orange, and grey. The red segment is the largest, followed by green, yellow, orange, and a small grey segment at the end.

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 142447 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	416	G	-	INSERTION	GB 155076
AA	905	U	-	INSERTION	GB 155076
AA	1395	C	-	INSERTION	GB 155076

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*C
P*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AX	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O			
			1011	639	198	174	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S		
			794	499	156	138	1	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AK	119	Total	C	N	O	S		
			885	549	168	165	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AL	124	Total	C	N	O	S		
			970	611	195	163	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S		
			997	617	207	171	2	0	0

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S		
			734	459	147	126	2	0	0

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AR	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2814	Total	C	N	O	P	0	0	0
			60600	26974	11331	19482	2813			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BP	84	Total	C	N	O	0	0	0
			639	391	109	139			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BS	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BW	108	Total	C	N	O	0	0	0
			860	542	169	149			

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BX	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 41 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BY	110	Total	C	N	O	0	0	0
			879	531	166	182			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BZ	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BR	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

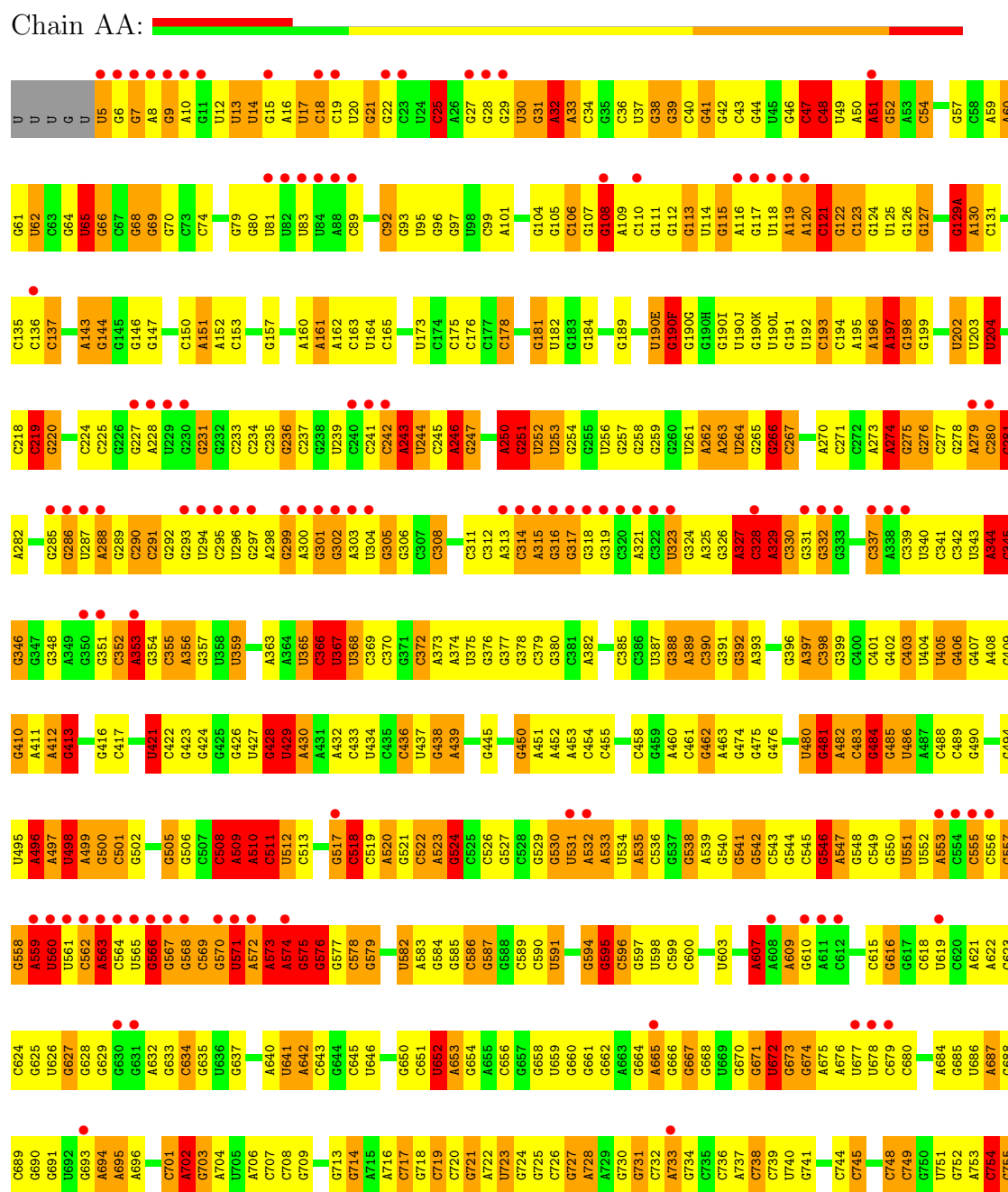
- Molecule 55 is a protein called 50S ribosomal protein L11.

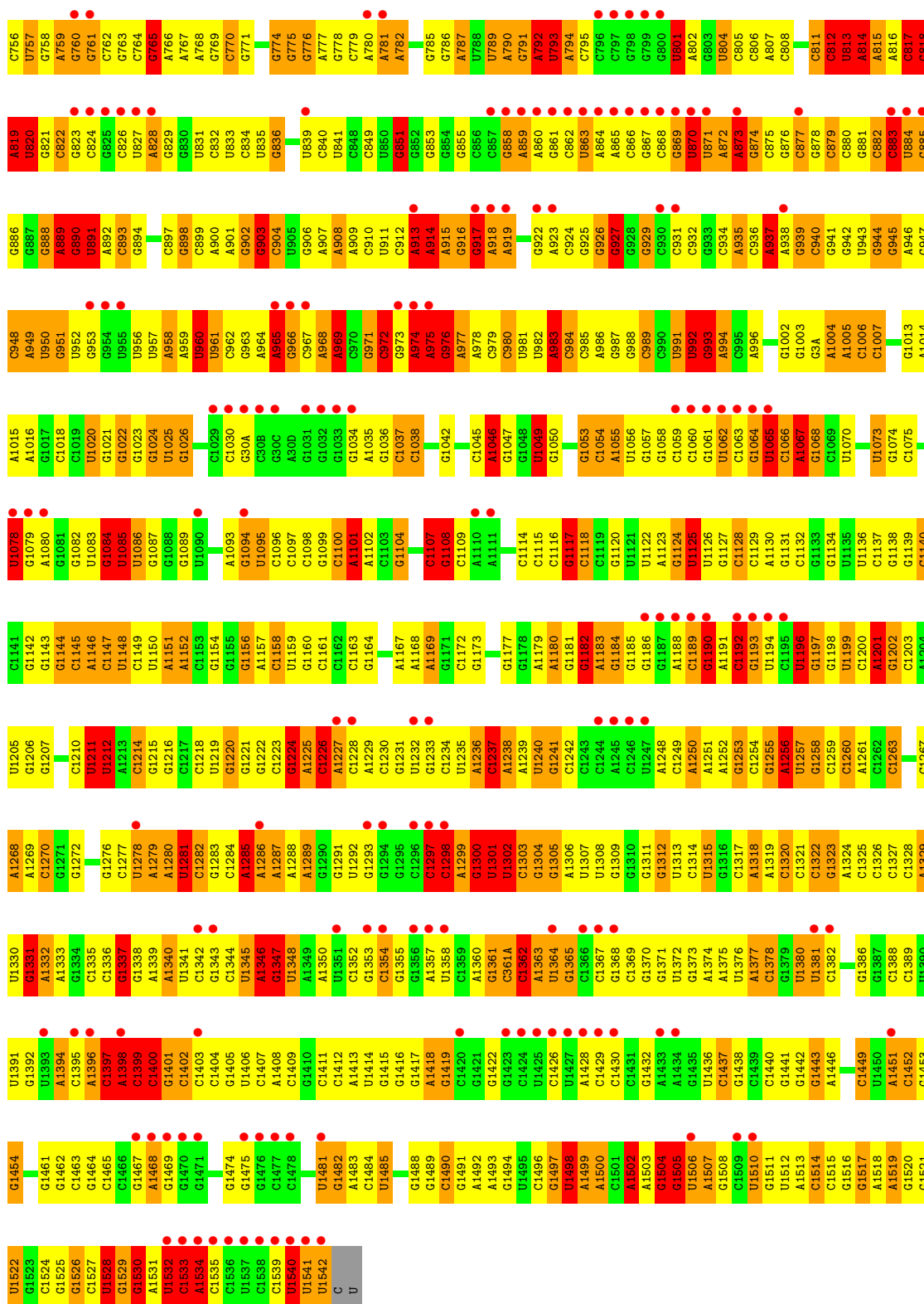
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

3 Residue-property plots

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

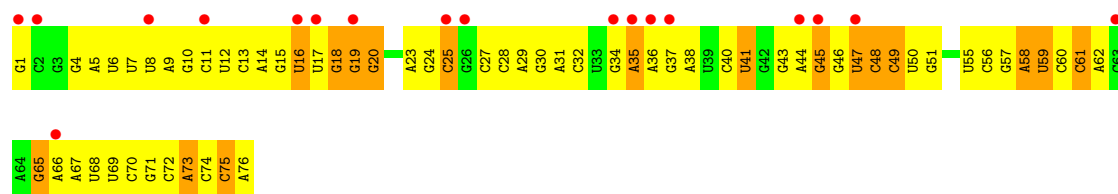
• Molecule 1: 16S ribosomal RNA





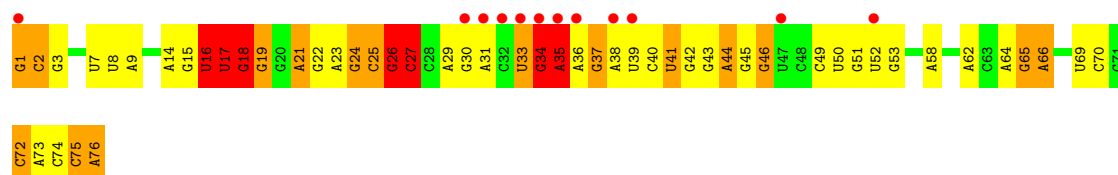
• Molecule 2: P-site tRNA (Phe)

Chain AV:



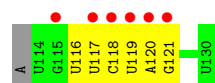
• Molecule 3: E-site tRNA (Phe)

Chain AW:



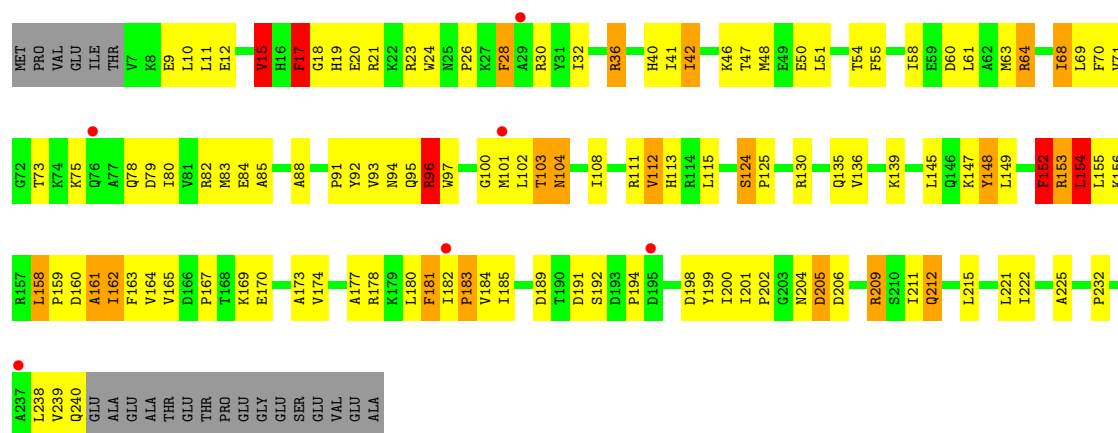
• Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

Chain AX:



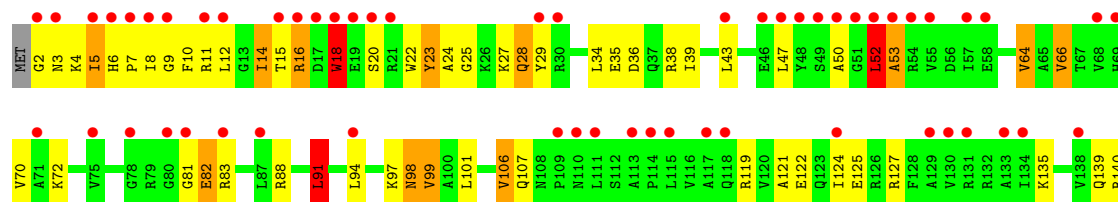
• Molecule 5: 30S ribosomal protein S2

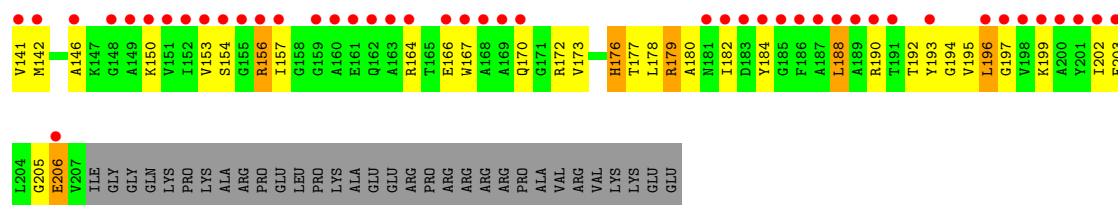
Chain AB:



• Molecule 6: 30S ribosomal protein S3

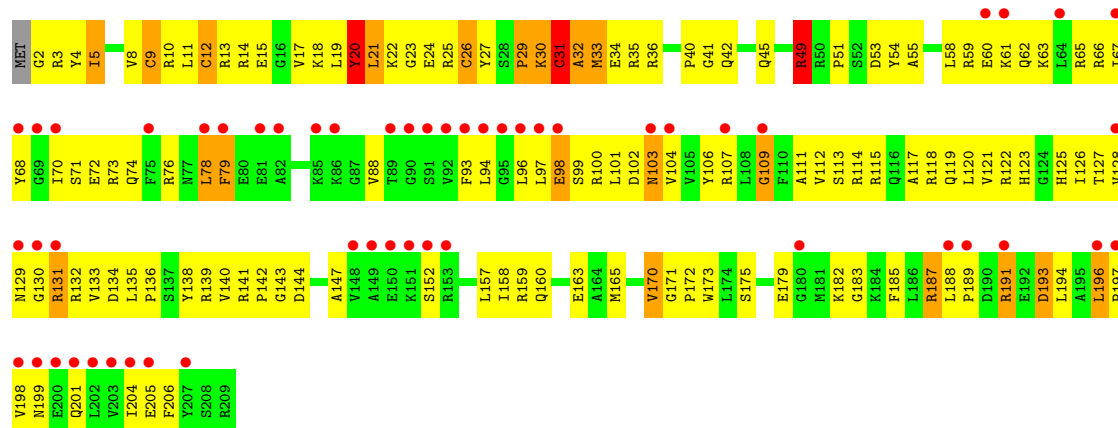
Chain AC:





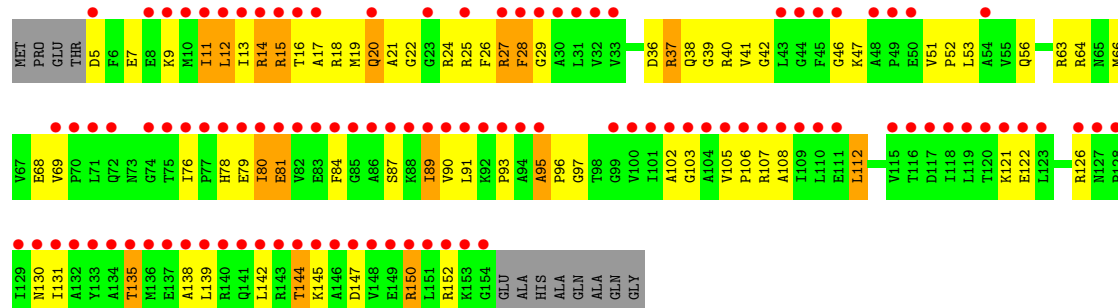
• Molecule 7: 30S ribosomal protein S4

Chain AD:



• Molecule 8: 30S ribosomal protein S5

Chain AE:



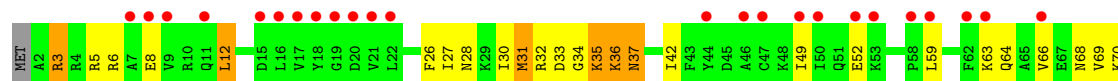
• Molecule 9: 30S ribosomal protein S6

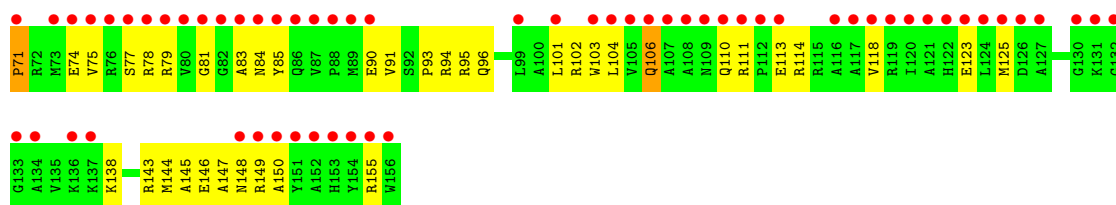
Chain AF:



• Molecule 10: 30S ribosomal protein S7

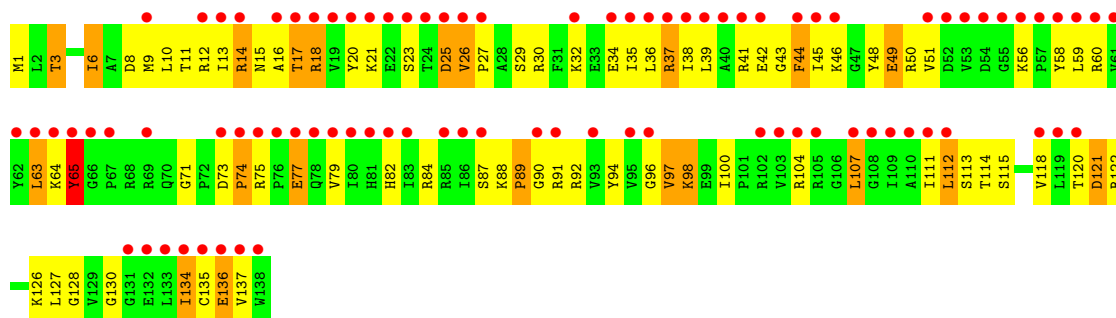
Chain AG:





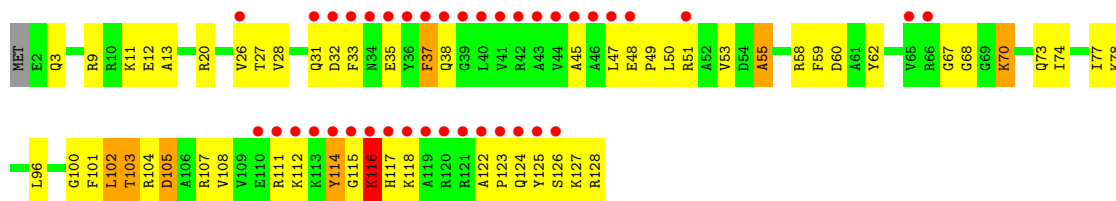
• Molecule 11: 30S ribosomal protein S8

Chain AH:



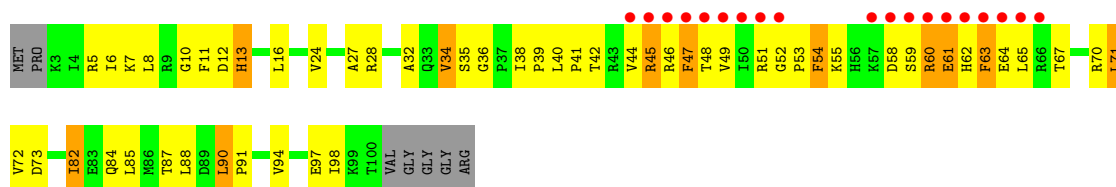
• Molecule 12: 30S ribosomal protein S9

Chain AI:



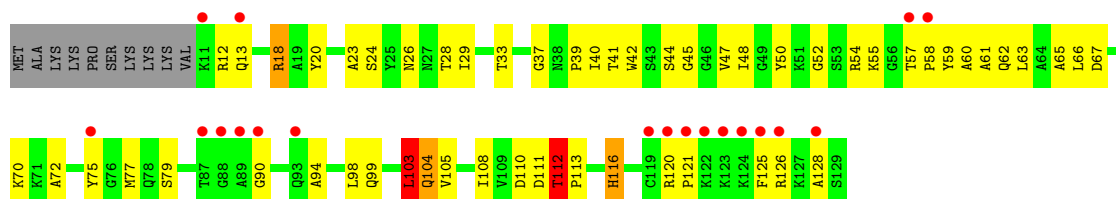
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



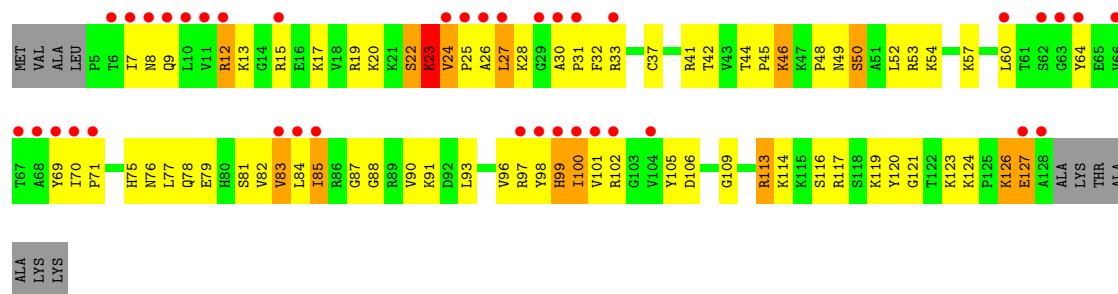
• Molecule 14: 30S ribosomal protein S11

Chain AK:



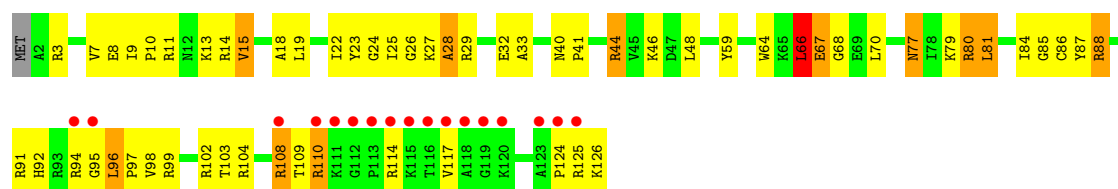
• Molecule 15: 30S ribosomal protein S12

Chain AL: 



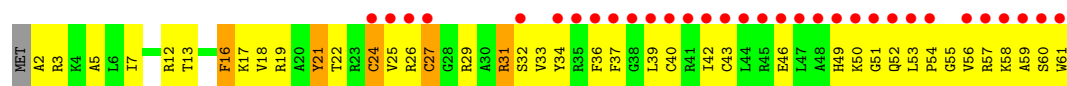
- Molecule 16: 30S ribosomal protein S13

Chain AM: 



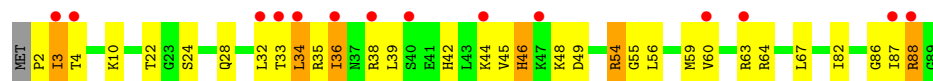
- Molecule 17: 30S ribosomal protein S14

Chain AN: 



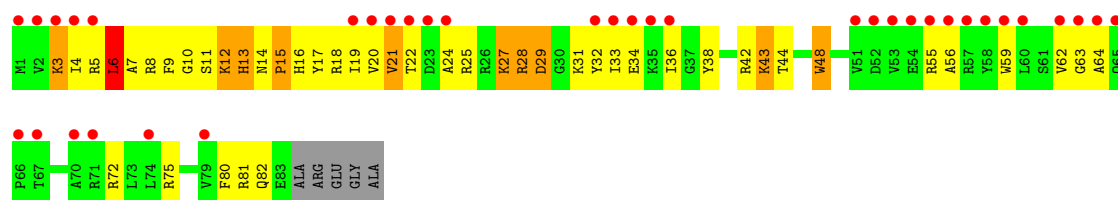
- Molecule 18: 30S ribosomal protein S15

Chain AO: 



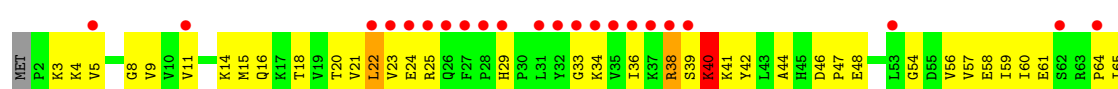
- Molecule 19: 30S ribosomal protein S16

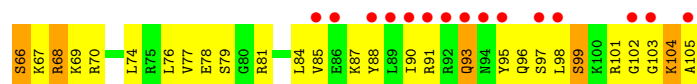
Chain AP: 



- Molecule 20: 30S ribosomal protein S17

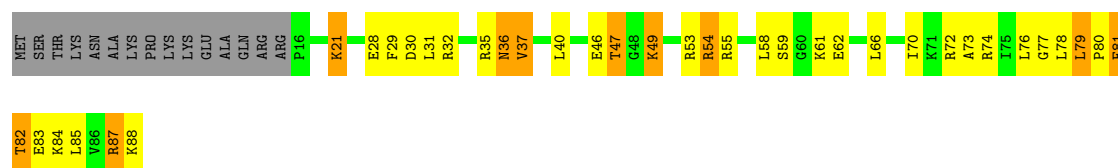
Chain AQ: 





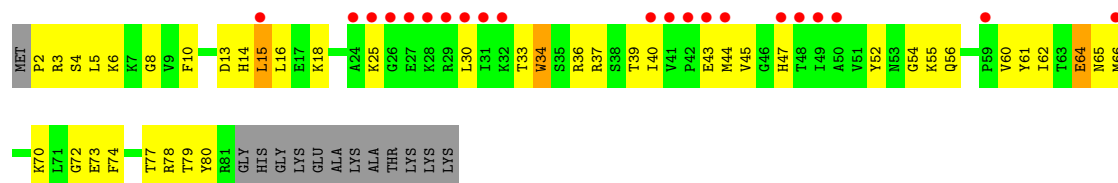
- Molecule 21: 30S ribosomal protein S18

Chain AR:



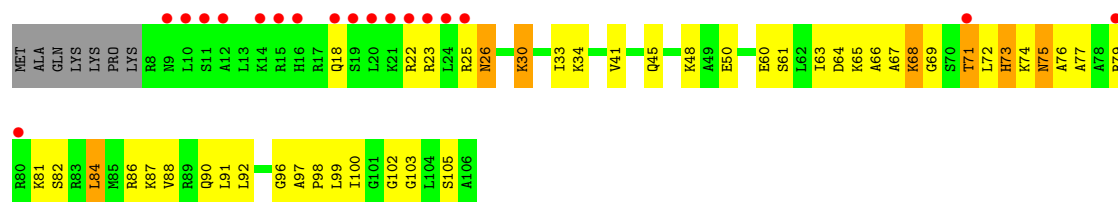
- Molecule 22: 30S ribosomal protein S19

Chain AS:



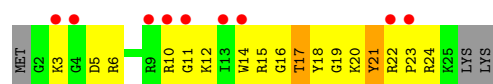
- Molecule 23: 30S ribosomal protein S20

Chain AT:



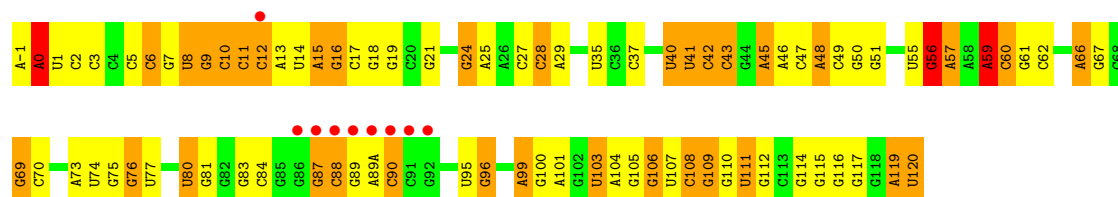
- Molecule 24: 30S ribosomal protein Thx

Chain AU:



- Molecule 25: 5S ribosomal RNA

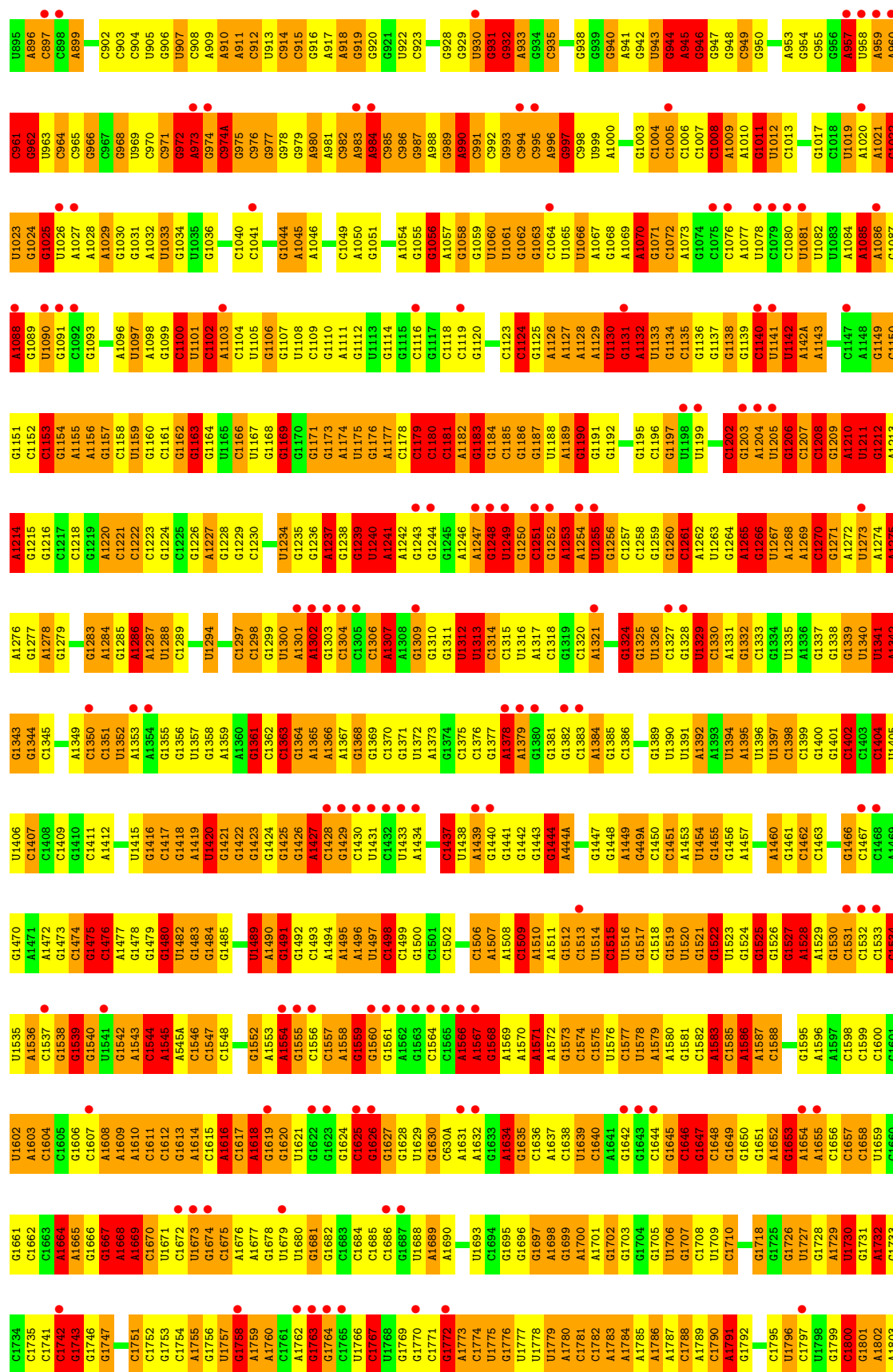
Chain BB:



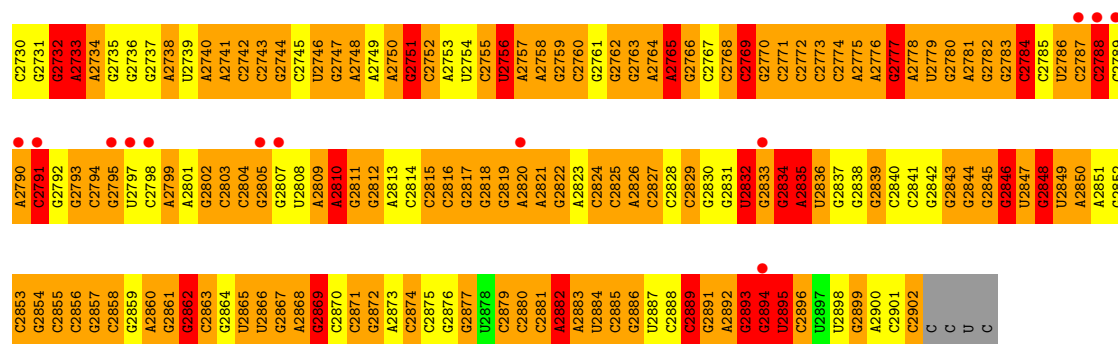
- Molecule 26: 23S ribosomal RNA

Chain BA:

A829	G830	G831	G832	G833	G834	A835	G836	G837	G838	G839	G840	G845	G846	U847	G848	A849	C850	U851	G852	G853	G854	G855	C856	C857	U858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	C885	C886	A887	C888	A889	C890	C894							
G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	A781	A782	A783	A784	G785	G786	G787	A788	A789	G790	G791	G792	A793	G794	G795	G796	G797	G798	G799	A800	G801	A802	G803	A804	G805	G806	U807	G808	G809	U810	U811	U812	U813	C814	C815	C816	C817	A818	A819	A820	A821	U822	G823	A824	C825	U826	U827	U828				
G708	U709	G710	G711	G712	G713	G714	G715	G716	A717	A718	G719	G720	G721	A722	G723	U724	G725	G726	A727	G728	G729	G730	G731	G732	G733	A734	A735	G736	G737	G738	G739	U740	G741	G742	G743	A746	U747	G748	G749	C	G	C	A	A	G	C	G	G	C	A	C	C	G										
A483	C484	C485	C486	G487	G488	G489	G490	G491	A492	G493	G494	G495	G496	A497	G498	A499	G500	A501	A502	A503	U504	A505	G506	A507	G508	C509	C510	U511	G512	C513	A514	A515	A516	C517	G518	U519	G520	G521	G522	U525	A526	G527	A528	A529	G530	C531	G532	A533	A534	C535	C536	C537	A538	A539	A540	A541	C542	G543	A544	G545	A546	A547	A548
G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	C565	G566	A567	U568	U569	G570	A571	A572	G573	C574	A575	U576	G577	A578	G579	C580	G581	G582	G583	C584	G585	A586	C587	U588	C589	A590	C591	G592	G593	U594	C595	G596	U597	G598	G599	G600	C601	G602	A603	G604	C605	U606	U607	A608	A609	G609A		
C610	C611	G612	U613	U614	G615	A616	G617	G618	A619	G620	A621	G622	G623	C624	G625	U626	G627	G628	A629	A630	A631	A632	A633	C634	C635	G636	A637	G638	U639	C640	C641	A642	A643	A644	C645	A646	G647	G648	G649	C	G	C	A	A	G	C	G	G	C	A	C	A	C	C	G								
G	C	C650	G651	G652	A653	A654	A655	A656	A657	C658	C659	G660	C661	G662	G663	G664	G665	G666	G667	G668	G669	A670	A671	A672	C673	C674	C675	C676	A677	G678	G679	G680	C681	G682	C683	G684	A685	G686	C687	U688	A689	G690	C691	C692	C693	U694	G695	G696	C697	G698	A699	G700	A701	U702	G703	G704	A705	A706	G707				
G708	U709	G710	G711	G712	G713	G714	G715	A716	A717	A718	G719	G720	G721	A722	G723	U724	G725	G726	A727	G728	G729	G730	G731	G732	G733	A734	A735	G736	G737	G738	G739	U740	G741	G742	G743	A746	U747	G748	G749	C	G	C	A	A	G	C	G	G	C	A	C	A	C	C	G								
G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	A781	A782	A783	A784	G785	G786	G787	A788	A789	G790	G791	G792	A793	G794	G795	G796	G797	G798	G799	A800	G801	A802	G803	A804	G805	G806	U807	G808	G809	U810	U811	U812	U813	C814	C815	C816	C817	A818	A819	A820	A821	U822	G823	A824	C825	U826	U827	U828				

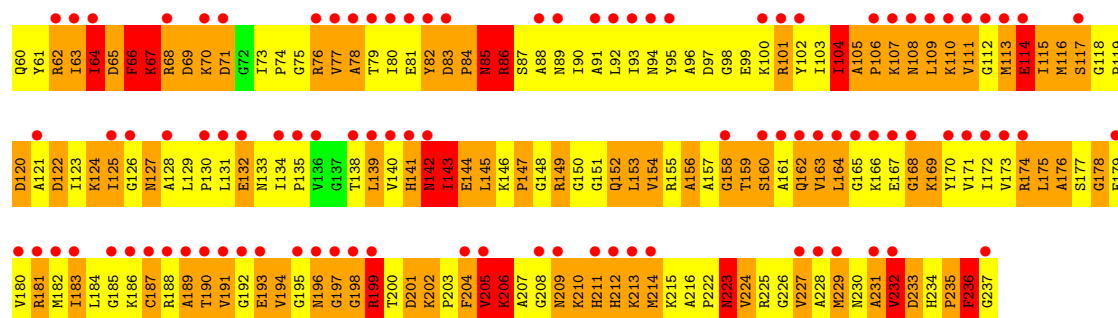


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U2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670										
C2551	U2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610										
U2491	U2492	U2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550										
U2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489											
C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430										
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G2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130
G2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060									
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A1872	G1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939		
C1804	U1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871		



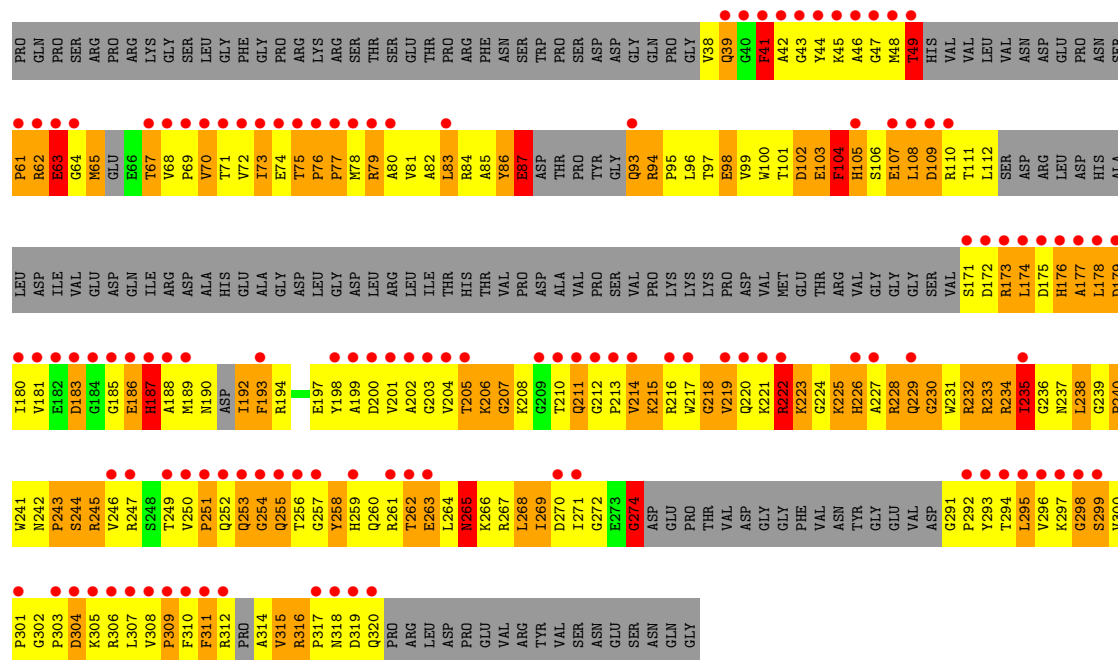
• Molecule 27: 50S ribosomal protein L2

Chain BD:



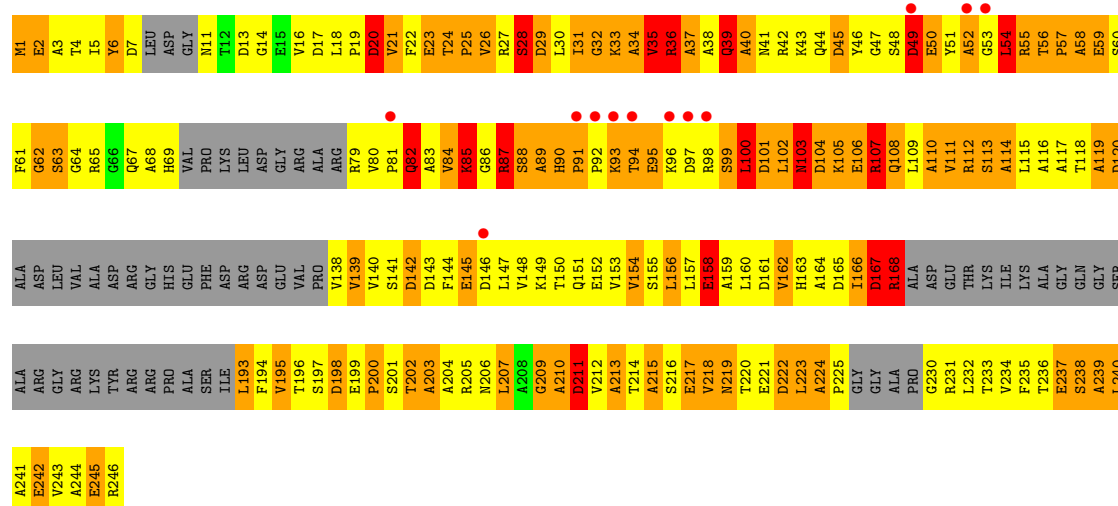
• Molecule 28: 50S ribosomal protein L3

Chain BE:



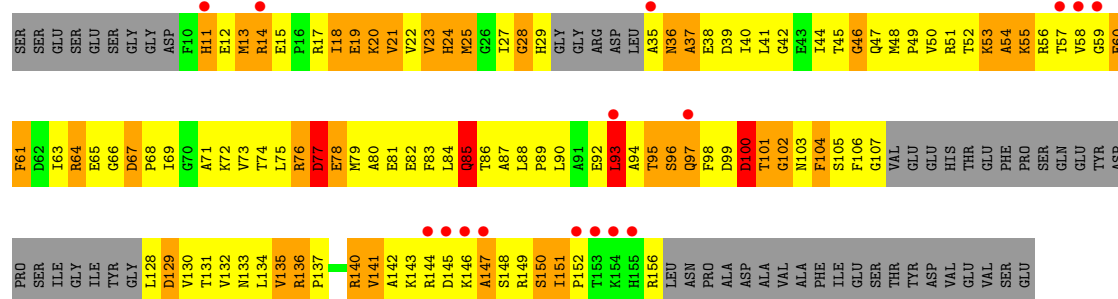
• Molecule 29: 50S ribosomal protein L4

Chain BF:



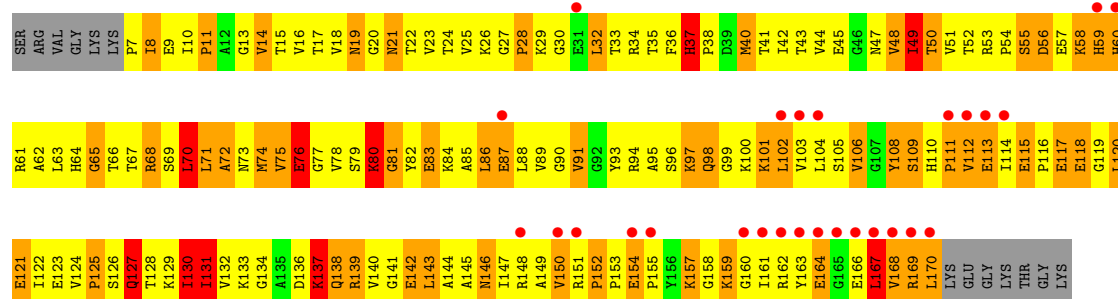
• Molecule 30: 50S ribosomal protein L5

Chain BG:



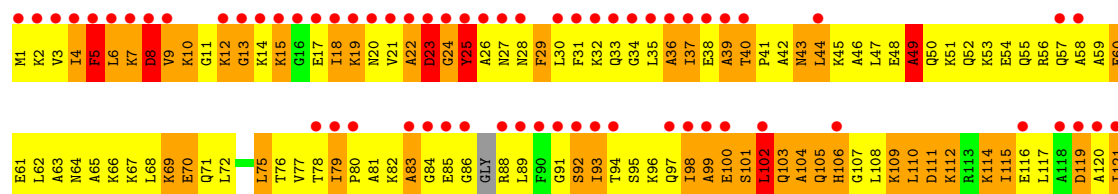
• Molecule 31: 50S ribosomal protein L6

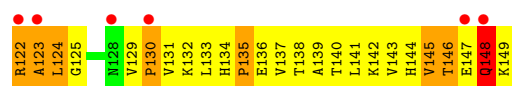
Chain BH:



• Molecule 32: 50S ribosomal protein L9

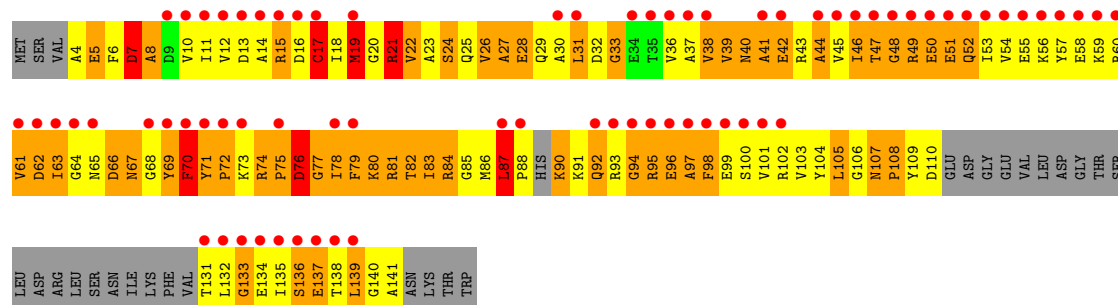
Chain BI:





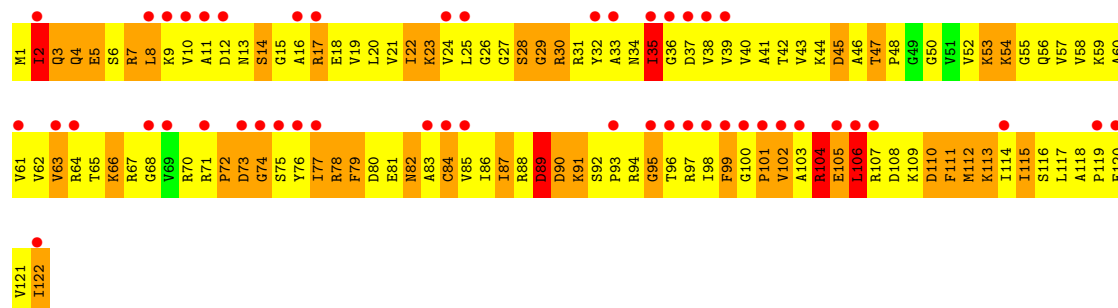
- Molecule 33: 50S ribosomal protein L13

Chain BN: 



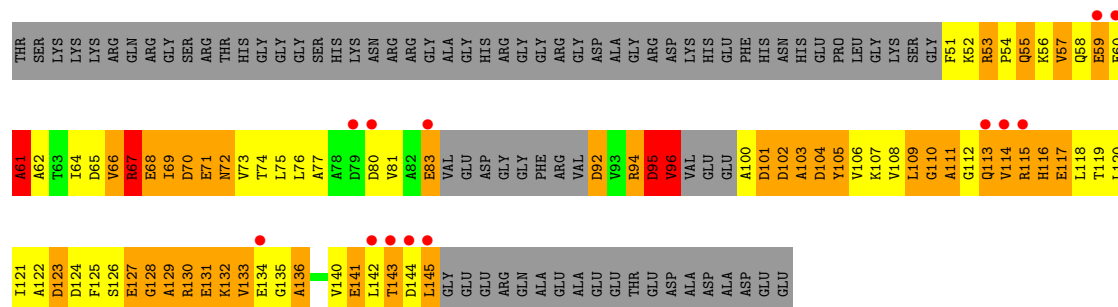
- Molecule 34: 50S ribosomal protein L14

Chain BO:



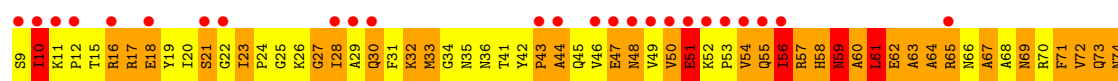
- Molecule 35: 50S ribosomal protein L15

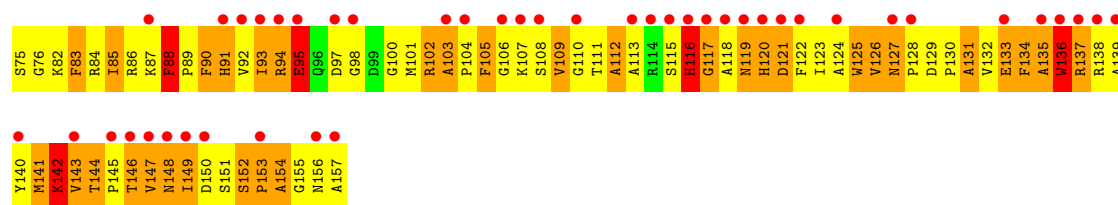
Chain BP: 



- Molecule 36: 50S ribosomal protein L16

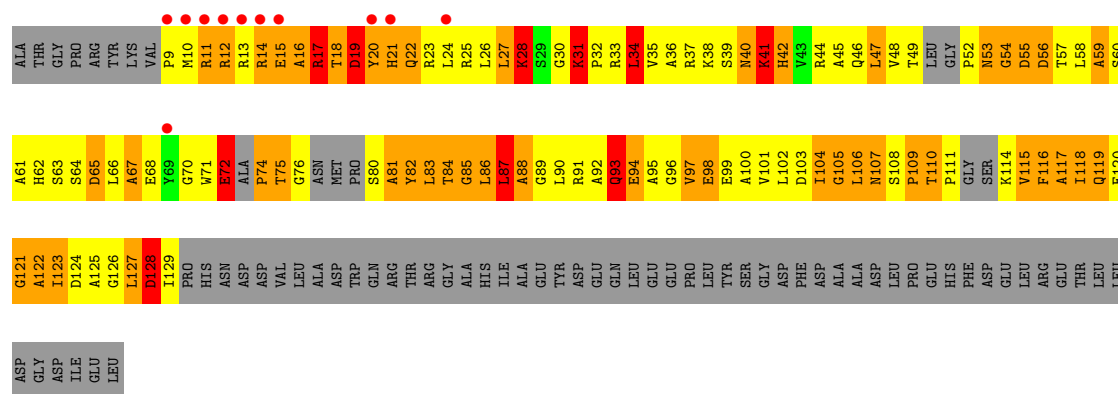
Chain BQ: 





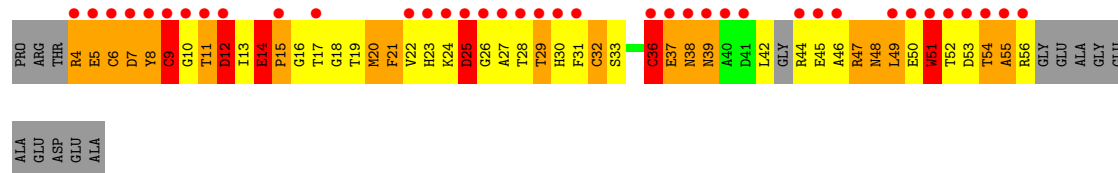
• Molecule 37: 50S ribosomal protein L18

Chain BS:



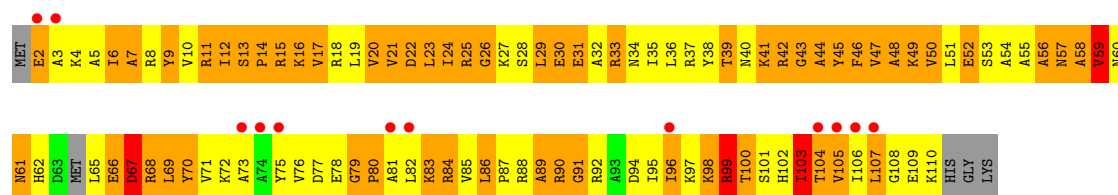
• Molecule 38: 50S ribosomal protein L19

Chain BT:



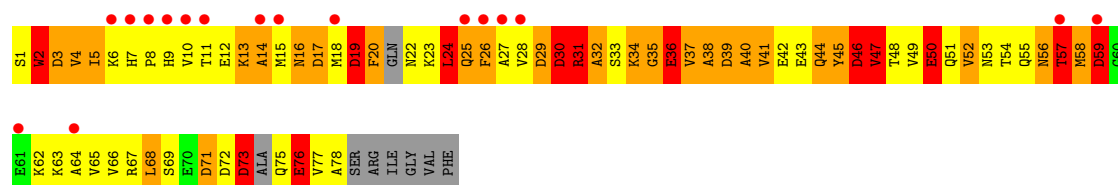
• Molecule 39: 50S ribosomal protein L22

Chain BW:



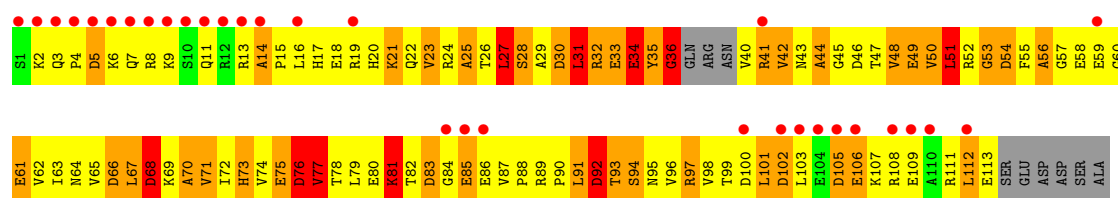
• Molecule 40: 50S ribosomal protein L23

Chain BX:



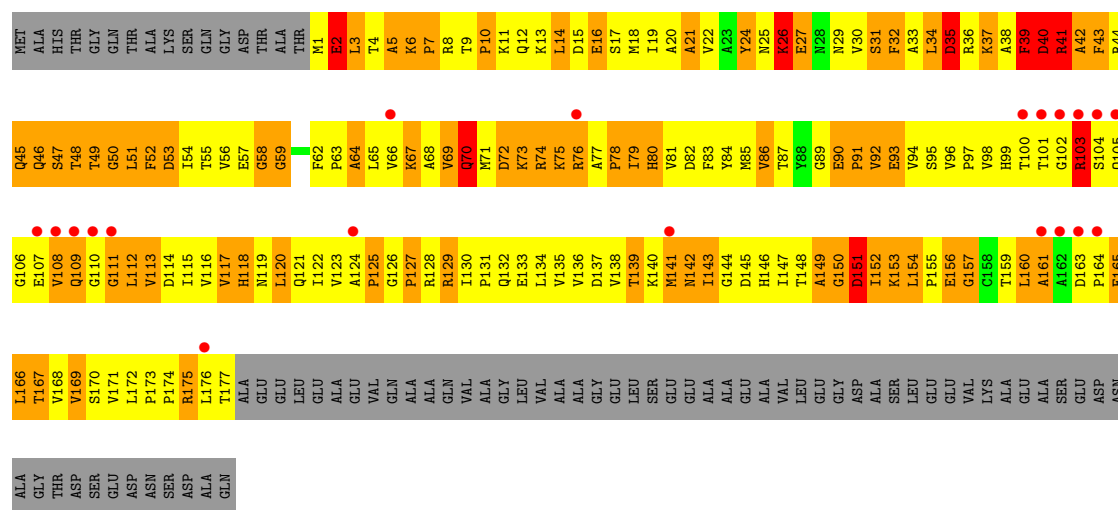
- Molecule 41: 50S ribosomal protein 24

Chain BY:



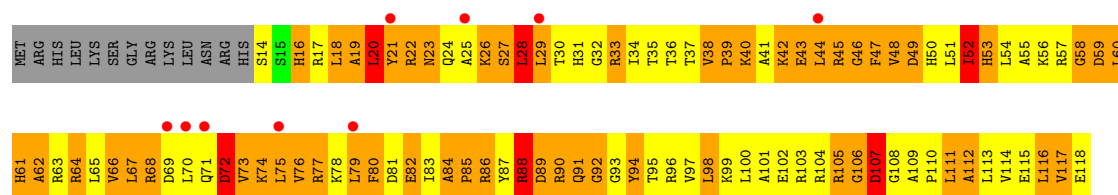
- Molecule 42: 50S ribosomal protein CTC

Chain BZ:



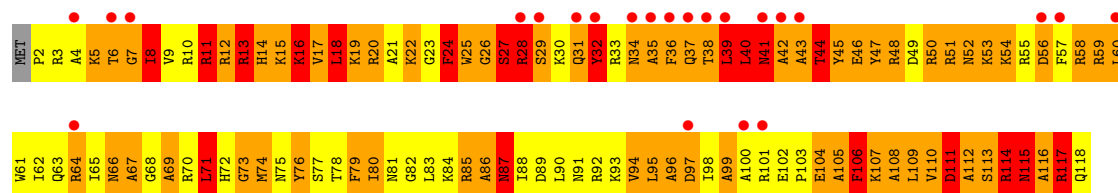
- Molecule 43: 50S ribosomal protein L17

Chain BR:



- Molecule 44: 50S ribosomal protein L20

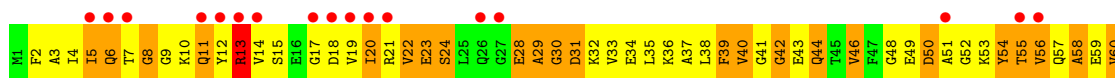
Chain BU:



- Molecule 45: 50S ribosomal protein L21

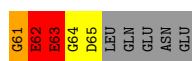
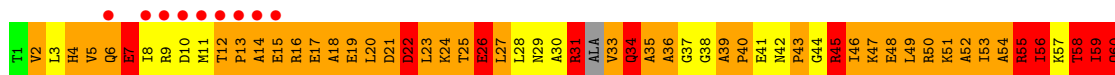
Chain BV:





• Molecule 46: 50S ribosomal protein L29

Chain B2:



• Molecule 47: 50S ribosomal protein L30

Chain B3:



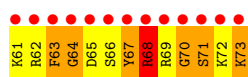
• Molecule 48: 50S ribosomal protein L27

Chain B0:



• Molecule 49: 50S ribosomal protein L31

Chain B4:



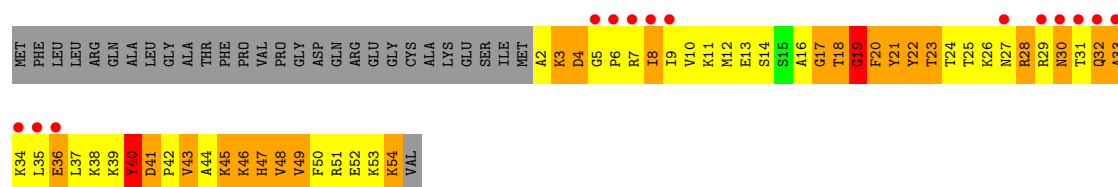
• Molecule 50: 50S ribosomal protein L32

Chain B5:



• Molecule 51: 50S ribosomal protein L33

Chain B6:



- Molecule 52: 50S ribosomal protein L34

Chain B7:



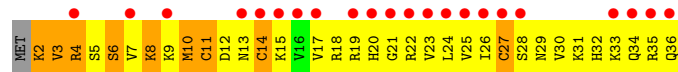
- Molecule 53: 50S ribosomal protein L35

Chain B8:



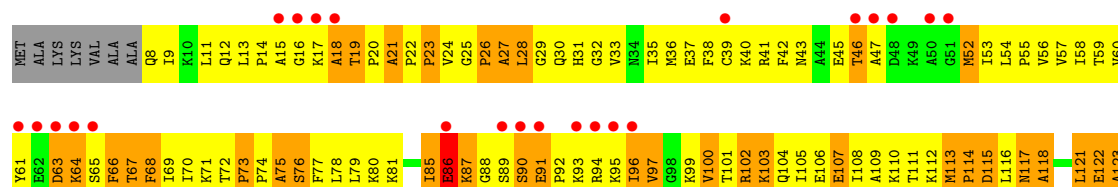
- Molecule 54: 50S ribosomal protein L36

Chain B9:



- Molecule 55: 50S ribosomal protein L11

Chain BK:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	517.41 Å 517.41 Å 365.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46 99.57 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-6.46) 99.7 (99.57-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 6.19 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.354 , 0.361 0.372 , 0.386	Depositor DCC
R_{free} test set	6075 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	240.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 76.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 123103 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	142447	wwPDB-VP
Average B, all atoms (Å ²)	314.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AA	1.32	68/36413 (0.2%)	1.49	439/56777 (0.8%)
2	AV	0.74	3/1812 (0.2%)	1.20	8/2819 (0.3%)
3	AW	1.81	19/1739 (1.1%)	2.15	47/2698 (1.7%)
4	AX	0.18	0/139	0.67	0/213
5	AB	0.60	2/1935 (0.1%)	0.61	0/2609
6	AC	0.73	2/1636 (0.1%)	0.61	4/2205 (0.2%)
7	AD	0.70	4/1733 (0.2%)	1.03	11/2318 (0.5%)
8	AE	0.83	1/1162 (0.1%)	0.63	1/1564 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.34	0/1276	0.59	3/1709 (0.2%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.59	1/900 (0.1%)	0.54	0/1213
15	AL	1.33	1/986 (0.1%)	1.11	3/1320 (0.2%)
16	AM	0.92	1/1007 (0.1%)	0.59	1/1344 (0.1%)
17	AN	0.49	1/501 (0.2%)	0.65	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.23	2/870 (0.2%)	1.38	6/1159 (0.5%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.49	0/277
25	BB	1.25	6/2950 (0.2%)	1.44	25/4602 (0.5%)
26	BA	1.17	153/67839 (0.2%)	1.46	906/105818 (0.9%)
27	BD	0.38	0/1328	0.60	0/1783
28	BE	0.65	4/1540 (0.3%)	1.07	7/2078 (0.3%)
29	BF	0.76	3/1444 (0.2%)	0.83	1/1954 (0.1%)
30	BG	0.25	0/971	0.46	0/1304
31	BH	0.54	1/1272 (0.1%)	0.80	3/1721 (0.2%)
32	BI	0.32	0/1156	0.71	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BN	0.35	0/927	0.55	0/1245
34	BO	0.32	0/946	0.57	0/1269
35	BP	1.59	3/643 (0.5%)	1.31	5/870 (0.6%)
36	BQ	0.32	0/1106	0.53	0/1490
37	BS	1.13	3/877 (0.3%)	0.69	1/1179 (0.1%)
38	BT	0.39	0/412	0.70	0/554
39	BW	0.75	3/869 (0.3%)	0.75	4/1166 (0.3%)
40	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
41	BY	0.26	0/887	0.83	3/1195 (0.3%)
42	BZ	0.32	1/1385 (0.1%)	0.62	3/1883 (0.2%)
43	BR	0.30	0/867	0.50	0/1162
44	BU	0.64	1/994 (0.1%)	0.74	3/1323 (0.2%)
45	BV	0.82	1/796 (0.1%)	0.91	3/1058 (0.3%)
46	B2	0.37	0/497	1.00	2/668 (0.3%)
47	B3	0.31	0/482	0.50	0/646
48	B0	0.38	1/649 (0.2%)	0.87	3/860 (0.3%)
49	B4	0.89	2/620 (0.3%)	0.54	0/831
50	B5	0.36	0/469	0.90	3/629 (0.5%)
51	B6	0.32	0/438	0.55	1/583 (0.2%)
52	B7	0.38	0/387	0.64	0/509
53	B8	0.91	2/503 (0.4%)	0.92	3/657 (0.5%)
54	B9	0.33	0/286	0.59	0/375
55	BK	0.27	1/1014 (0.1%)	0.44	0/1363
All	All	1.09	291/154800 (0.2%)	1.33	1508/231822 (0.7%)

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	AW	1	5
5	AB	0	1
6	AC	0	1
7	AD	0	1
14	AK	0	1
15	AL	0	1
20	AQ	0	1
27	BD	0	1
28	BE	0	3
29	BF	0	4
31	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	BI	0	1
35	BP	0	1
37	BS	0	1
40	BX	0	1
41	BY	0	1
46	B2	0	1
50	B5	0	1
55	BK	0	1
All	All	1	28

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2199	A	O3'-P	-71.04	0.75	1.61
1	AA	1278	U	O3'-P	-56.53	0.93	1.61
1	AA	1337	G	O3'-P	-53.91	0.96	1.61
26	BA	1546	C	O3'-P	-51.62	0.99	1.61
1	AA	1004	A	O3'-P	48.18	2.19	1.61

The worst 5 of 1508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	65	G	P-O3'-C3'	-50.68	58.88	119.70
26	BA	712(A)	A	P-O3'-C3'	-43.62	67.36	119.70
26	BA	2199	A	O3'-P-O5'	-43.07	22.17	104.00
2	AV	65	G	P-O3'-C3'	39.88	167.56	119.70
1	AA	1255	G	P-O3'-C3'	-38.36	73.67	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32551	0	16459	2042	3
2	AV	1622	0	821	231	0
3	AW	1638	0	836	243	0
4	AX	136	0	63	26	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	99	0
7	AD	1703	0	1761	289	0
8	AE	1146	0	1206	68	0
9	AF	843	0	857	30	0
10	AG	1257	0	1295	102	0
11	AH	1116	0	1177	100	0
12	AI	1011	0	1040	80	0
13	AJ	794	0	840	81	0
14	AK	885	0	904	53	0
15	AL	970	0	1056	72	0
16	AM	997	0	1070	149	0
17	AN	492	0	529	82	0
18	AO	734	0	771	28	0
19	AP	700	0	720	70	0
20	AQ	857	0	928	80	0
21	AR	597	0	668	40	0
22	AS	647	0	673	155	0
23	AT	762	0	859	37	0
24	AU	208	0	221	84	0
25	BB	2637	0	1339	219	1
26	BA	60600	0	30514	11060	138
27	BD	1308	0	1346	1086	0
28	BE	1507	0	1478	1144	3
29	BF	1430	0	1357	1085	0
30	BG	957	0	952	692	0
31	BH	1251	0	1291	754	0
32	BI	1145	0	1225	625	3
33	BN	917	0	896	771	2
34	BO	937	0	992	613	0
35	BP	639	0	605	482	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BQ	1081	0	1047	932	0
37	BS	866	0	866	677	0
38	BT	406	0	359	167	0
39	BW	860	0	909	557	0
40	BX	602	0	558	460	0
41	BY	879	0	860	755	0
42	BZ	1360	0	1378	902	0
43	BR	855	0	904	579	0
44	BU	978	0	996	895	0
45	BV	787	0	782	635	0
46	B2	494	0	504	393	0
47	B3	477	0	527	460	0
48	B0	641	0	661	531	0
49	B4	604	0	587	489	0
50	B5	457	0	456	279	0
51	B6	431	0	454	289	0
52	B7	383	0	409	382	0
53	B8	496	0	539	349	0
54	B9	285	0	312	195	0
55	BK	999	0	1064	573	0
All	All	142447	0	94546	28969	145

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 123.

The worst 5 of 28969 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
50:B5:33:CYS:SG	50:B5:36:CYS:HB2	1.24	1.69
26:BA:2470:G:C2	26:BA:2471:C:C5	1.81	1.68
52:B7:30:ILE:HA	52:B7:33:ARG:CD	1.21	1.67
26:BA:2712:U:C6	26:BA:712(A):A:C8	1.77	1.67
26:BA:2580:U:C6	26:BA:2581:G:C8	1.82	1.66

The worst 5 of 145 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	Distance(Å)	Clash(Å)
26:BA:6:A:O4'	26:BA:2902:C:C2'[8_554]	0.72	1.48
26:BA:2899:G:N1	26:BA:2901:C:C4[8_554]	0.79	1.41
26:BA:6:A:C4'	26:BA:2902:C:C2'[8_554]	0.97	1.23
26:BA:2900:A:N7	26:BA:2900:A:N6[8_554]	1.03	1.17
26:BA:3:U:O4	26:BA:2899:G:O2'[8_554]	1.09	1.11

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
5	AB	232/256 (91%)	183 (79%)	33 (14%)	16 (7%)	2	32
6	AC	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	2	32
7	AD	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1	28
8	AE	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	11	67
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	5	49
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	8	60
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	2	30
12	AI	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	2	35
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	23
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	37
15	AL	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0	8
16	AM	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	3	42
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	2	32
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	19	77
19	AP	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	2	30
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	2	38
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	26
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	5	50
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	36
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	24
27	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
28	BE	183/338 (54%)	89 (49%)	34 (19%)	60 (33%)	0	0
29	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
30	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
31	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	1
33	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
34	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	2
35	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
36	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
37	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
38	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
39	BW	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0	0
40	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
41	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
42	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
43	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
44	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
45	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
46	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
47	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
48	B0	84/91 (92%)	32 (38%)	17 (20%)	35 (42%)	0	0
49	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
50	B5	56/60 (93%)	16 (29%)	18 (32%)	22 (39%)	0	0
51	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
52	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
53	B8	61/64 (95%)	22 (36%)	10 (16%)	29 (48%)	0	0
54	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	1
55	BK	129/141 (92%)	73 (57%)	18 (14%)	38 (30%)	0	1
All	All	5325/6250 (85%)	2945 (55%)	1015 (19%)	1365 (26%)	0	2

5 of 1365 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
5	AB	202/220 (92%)	173 (86%)	29 (14%)	5	31
6	AC	160/188 (85%)	146 (91%)	14 (9%)	14	57
7	AD	180/181 (99%)	162 (90%)	18 (10%)	11	50
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2	17
9	AF	90/90 (100%)	83 (92%)	7 (8%)	18	63
10	AG	126/127 (99%)	116 (92%)	10 (8%)	18	62
11	AH	119/119 (100%)	92 (77%)	27 (23%)	1	10
12	AI	98/99 (99%)	90 (92%)	8 (8%)	17	60
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	7	38
14	AK	90/99 (91%)	85 (94%)	5 (6%)	30	75
15	AL	104/111 (94%)	93 (89%)	11 (11%)	10	47
16	AM	100/101 (99%)	87 (87%)	13 (13%)	6	36
17	AN	49/50 (98%)	43 (88%)	6 (12%)	7	39
18	AO	79/80 (99%)	70 (89%)	9 (11%)	8	42
19	AP	72/74 (97%)	62 (86%)	10 (14%)	5	33
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	13	53
21	AR	64/77 (83%)	57 (89%)	7 (11%)	9	46
22	AS	71/80 (89%)	64 (90%)	7 (10%)	11	50
23	AT	76/82 (93%)	68 (90%)	8 (10%)	10	47
24	AU	19/22 (86%)	19 (100%)	0	100	100
27	BD	135/135 (100%)	99 (73%)	36 (27%)	1	6
28	BE	156/284 (55%)	128 (82%)	28 (18%)	2	19
29	BF	152/193 (79%)	124 (82%)	28 (18%)	2	17
30	BG	102/147 (69%)	93 (91%)	9 (9%)	14	57
31	BH	137/147 (93%)	111 (81%)	26 (19%)	2	16
32	BI	119/119 (100%)	98 (82%)	21 (18%)	3	20
33	BN	95/121 (78%)	80 (84%)	15 (16%)	4	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BO	101/101 (100%)	81 (80%)	20 (20%)	2	14
35	BP	67/126 (53%)	56 (84%)	11 (16%)	3	24
36	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	8
37	BS	89/149 (60%)	73 (82%)	16 (18%)	2	18
38	BT	44/52 (85%)	30 (68%)	14 (32%)	0	4
39	BW	88/92 (96%)	74 (84%)	14 (16%)	4	26
40	BX	67/73 (92%)	44 (66%)	23 (34%)	0	3
41	BY	97/105 (92%)	80 (82%)	17 (18%)	3	20
42	BZ	151/203 (74%)	130 (86%)	21 (14%)	5	33
43	BR	89/101 (88%)	71 (80%)	18 (20%)	2	14
44	BU	96/97 (99%)	68 (71%)	28 (29%)	0	5
45	BV	79/79 (100%)	69 (87%)	10 (13%)	6	37
46	B2	51/56 (91%)	37 (72%)	14 (28%)	0	6
47	B3	52/52 (100%)	47 (90%)	5 (10%)	12	52
48	B0	64/67 (96%)	57 (89%)	7 (11%)	9	46
49	B4	66/66 (100%)	54 (82%)	12 (18%)	2	18
50	B5	51/53 (96%)	43 (84%)	8 (16%)	4	27
51	B6	46/69 (67%)	39 (85%)	7 (15%)	4	28
52	B7	39/40 (98%)	31 (80%)	8 (20%)	2	13
53	B8	50/51 (98%)	39 (78%)	11 (22%)	1	11
54	B9	34/35 (97%)	30 (88%)	4 (12%)	8	41
55	BK	108/113 (96%)	104 (96%)	4 (4%)	45	85
All	All	4533/5148 (88%)	3841 (85%)	692 (15%)	4	28

5 of 692 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BF	120	ASP
33	BN	87	LEU
49	B4	15	ILE
30	BG	13	MET
31	BH	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
28	BE	242	ASN
32	BI	64	ASN
48	B0	71	ASN
28	BE	260	GLN
29	BF	219	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1497/1522 (98%)	520 (34%)	164 (10%)
2	AV	73/76 (96%)	16 (21%)	1 (1%)
25	BB	122/123 (99%)	45 (36%)	3 (2%)
26	BA	2780/2916 (95%)	1487 (53%)	360 (12%)
3	AW	70/76 (92%)	16 (22%)	3 (4%)
4	AX	5/18 (27%)	0	0
All	All	4547/4731 (96%)	2084 (45%)	531 (11%)

5 of 2084 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 531 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	646	A
26	BA	1126	A
26	BA	2612	C
26	BA	704	G
26	BA	827	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
3	YYG	AW	37	10,3	40,42,43	1.09	3 (7%)	50,62,65	11.23	12 (24%)
3	PSU	AW	39	3	19,21,22	0.95	0	23,30,33	0.81	0
3	PSU	AW	55	3	19,21,22	1.10	2 (10%)	23,30,33	1.02	2 (8%)

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
3	YYG	AW	37	10,3	1/1/8/9	0/25/42/43	0/4/4/4
3	PSU	AW	39	3	-	0/8/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/8/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C6-N1	2.69	1.42	1.37
3	AW	55	PSU	C4-N3	2.68	1.40	1.36
3	AW	37	YYG	P-OP1	2.43	1.49	1.46
3	AW	37	YYG	C2-N1	-2.16	1.36	1.41
3	AW	55	PSU	P-OP1	2.16	1.49	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	37	YYG	C6-C5-N7	-76.04	130.19	134.24
3	AW	37	YYG	C11-C12-N1	18.61	111.41	104.24
3	AW	37	YYG	C24-O23-C21	6.08	123.13	115.64
3	AW	37	YYG	C13-C12-C11	-5.34	123.52	131.05
3	AW	37	YYG	C3-N3-C4	4.55	125.55	118.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	58
1	AA	45
3	AW	6
36	BQ	3
25	BB	2
2	AV	2
6	AC	2
45	BV	2
16	AM	2
44	BU	1
20	AQ	1
5	AB	1
8	AE	1
29	BF	1
27	BD	1
37	BS	1
55	BK	1
35	BP	1
7	AD	1
31	BH	1
15	AL	1

The worst 5 of 134 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	30(D):A	O3'	1031:G	P	5.01
1	BA	142(A):A	O3'	1143:A	P	4.98
1	AW	73:A	O3'	74:C	P	4.88
1	BA	1171:G	O3'	1173:G	P	4.41
1	AA	440:A	O3'	442:C	P	4.34

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	AA	1515/1522 (99%)	0.77	265 (17%) 2 7	188, 339, 400, 400	0
2	AV	76/76 (100%)	1.49	18 (23%) 1 5	242, 299, 394, 394	0
3	AW	75/76 (98%)	0.67	12 (16%) 3 8	253, 400, 400, 400	0
4	AX	17/18 (94%)	1.69	6 (35%) 1 4	400, 400, 400, 400	0
5	AB	234/256 (91%)	0.29	6 (2%) 53 46	395, 395, 400, 400	0
6	AC	206/239 (86%)	2.68	101 (49%) 1 3	393, 398, 398, 398	0
7	AD	208/209 (99%)	1.44	53 (25%) 1 5	257, 391, 400, 400	0
8	AE	150/162 (92%)	3.79	106 (70%) 0 3	371, 400, 400, 400	0
9	AF	101/101 (100%)	-0.01	1 (0%) 79 68	400, 400, 400, 400	0
10	AG	155/156 (99%)	2.98	84 (54%) 0 3	358, 400, 400, 400	0
11	AH	138/138 (100%)	2.89	87 (63%) 0 3	396, 396, 396, 396	0
12	AI	127/128 (99%)	1.56	39 (30%) 1 4	395, 395, 395, 395	0
13	AJ	98/105 (93%)	2.14	19 (19%) 2 6	400, 400, 400, 400	0
14	AK	119/129 (92%)	0.72	19 (15%) 3 8	202, 202, 400, 400	0
15	AL	124/135 (91%)	1.55	38 (30%) 1 4	399, 399, 400, 400	0
16	AM	125/126 (99%)	0.66	17 (13%) 4 10	348, 400, 400, 400	0
17	AN	60/61 (98%)	3.28	32 (53%) 0 3	400, 400, 400, 400	0
18	AO	88/89 (98%)	0.59	14 (15%) 3 8	400, 400, 400, 400	0
19	AP	83/88 (94%)	2.33	36 (43%) 1 3	400, 400, 400, 400	0
20	AQ	104/105 (99%)	1.83	37 (35%) 1 4	400, 400, 400, 400	0
21	AR	73/88 (82%)	0.08	0 100 100	400, 400, 400, 400	0
22	AS	80/93 (86%)	1.20	21 (26%) 1 5	400, 400, 400, 400	0
23	AT	99/106 (93%)	0.61	18 (18%) 2 6	400, 400, 400, 400	0
24	AU	24/27 (88%)	1.88	9 (37%) 1 4	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BB	123/123 (100%)	0.07	9 (7%) 15 21	267, 323, 388, 388	0
26	BA	2814/2916 (96%)	0.56	318 (11%) 6 13	65, 238, 393, 400	0
27	BD	173/173 (100%)	2.32	97 (56%) 0 3	392, 392, 400, 400	0
28	BE	191/338 (56%)	2.99	120 (62%) 0 3	400, 400, 400, 400	0
29	BF	189/246 (76%)	0.08	12 (6%) 19 25	393, 396, 396, 396	0
30	BG	122/176 (69%)	0.58	16 (13%) 4 11	400, 400, 400, 400	0
31	BH	164/177 (92%)	0.79	27 (16%) 2 8	400, 400, 400, 400	0
32	BI	148/149 (99%)	2.48	71 (47%) 1 3	400, 400, 400, 400	0
33	BN	117/145 (80%)	3.14	72 (61%) 0 3	400, 400, 400, 400	0
34	BO	122/122 (100%)	1.81	48 (39%) 1 3	400, 400, 400, 400	0
35	BP	84/164 (51%)	1.20	13 (15%) 3 8	395, 395, 400, 400	0
36	BQ	138/138 (100%)	2.34	69 (50%) 0 3	393, 393, 393, 393	0
37	BS	113/186 (60%)	0.47	11 (9%) 8 16	278, 400, 400, 400	0
38	BT	52/66 (78%)	3.95	38 (73%) 0 3	400, 400, 400, 400	0
39	BW	108/113 (95%)	0.67	12 (11%) 6 13	278, 395, 400, 400	0
40	BX	76/84 (90%)	0.95	17 (22%) 1 5	400, 400, 400, 400	0
41	BY	110/119 (92%)	1.55	31 (28%) 1 4	400, 400, 400, 400	0
42	BZ	177/253 (69%)	0.71	20 (11%) 6 13	396, 398, 398, 398	0
43	BR	105/118 (88%)	0.57	9 (8%) 11 18	400, 400, 400, 400	0
44	BU	117/118 (99%)	1.06	23 (19%) 2 6	391, 391, 400, 400	0
45	BV	100/100 (100%)	1.58	30 (30%) 1 4	400, 400, 400, 400	0
46	B2	64/70 (91%)	0.53	9 (14%) 3 9	400, 400, 400, 400	0
47	B3	60/60 (100%)	0.79	6 (10%) 8 15	398, 398, 398, 398	0
48	B0	86/91 (94%)	2.00	31 (36%) 1 4	396, 400, 400, 400	0
49	B4	73/73 (100%)	2.61	43 (58%) 0 3	396, 397, 397, 397	0
50	B5	58/60 (96%)	0.52	2 (3%) 43 40	400, 400, 400, 400	0
51	B6	53/82 (64%)	0.96	14 (26%) 1 5	400, 400, 400, 400	0
52	B7	46/47 (97%)	1.05	9 (19%) 2 6	396, 396, 396, 396	0
53	B8	63/64 (98%)	2.17	29 (46%) 1 3	400, 400, 400, 400	0
54	B9	35/36 (97%)	3.60	22 (62%) 0 3	400, 400, 400, 400	0
55	BK	133/141 (94%)	0.98	26 (19%) 2 6	392, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10093/10981 (91%)	1.14	2292 (22%) 1 5	65, 395, 400, 400	0

The worst 5 of 2292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AJ	62	HIS	28.3
13	AJ	61	GLU	24.3
13	AJ	60	ARG	16.3
13	AJ	48	THR	16.2
8	AE	134	ALA	14.9

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PSU	AW	39	20/21	0.39	-	399,399,399,399	0
3	YYG	AW	37	39/40	0.91	-	399,399,399,399	0
3	PSU	AW	55	20/21	0.09	-	400,400,400,400	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.