



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:46 PM BST

PDB ID : 4V9H  
Title : Crystal structure of the ribosome bound to elongation factor G in the guanosine triphosphatase state  
Authors : Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2013-03-25  
Resolution : 2.86 Å(reported)

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

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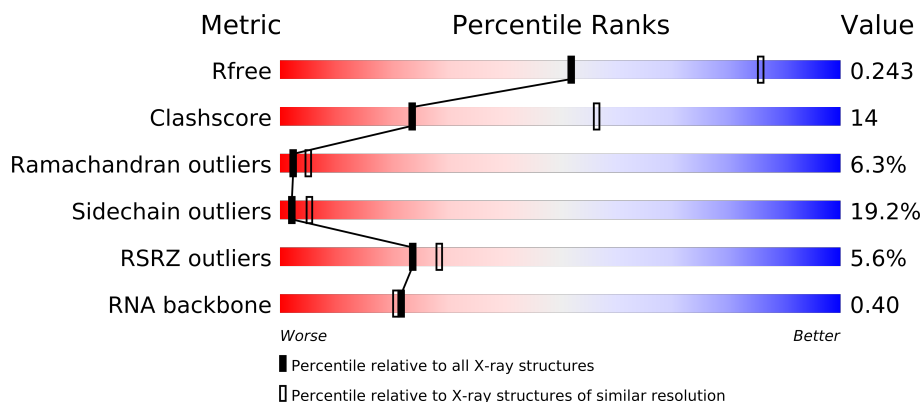
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.86 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)
RNA backbone	1838	1014 (3.32-2.40)

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  $\geq 3$ , 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	1516	
2	AV	76	
3	AX	25	
4	AJ	98	
5	AK	119	
6	AL	124	
7	AM	124	
8	AN	60	
9	AO	88	
10	AP	83	
11	AQ	99	
12	AR	70	





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Mol	Chain	Length	Quality of chain
13	AS	78	
14	AT	99	
15	AB	234	
16	AC	206	
17	AD	208	
18	AE	150	
19	AF	101	
20	AG	155	
21	AH	138	
22	AI	127	
23	AY	680	
24	AU	24	
25	BA	2915	
26	BB	122	
27	BN	140	
28	BO	122	
29	BP	150	
30	BQ	141	
31	BR	118	
32	BS	112	
33	BT	146	
34	BU	118	
35	BV	101	
36	BW	113	
37	BX	96	
38	BY	110	
39	BZ	206	
40	B0	85	
41	B1	98	
42	B2	72	
43	BD	276	
44	B3	60	
45	B4	71	
46	B5	60	
47	B6	54	
48	B7	49	
49	B8	65	
50	B9	37	
51	BC	229	
52	BE	206	
53	BF	210	
54	BG	182	

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Mol	Chain	Length	Quality of chain
55	BH	180	
56	BK	147	
57	BJ	130	
58	BL	125	

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151831 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	1514	Total	C	N	O	P	0	0	0
			32529	14480	6018	10518	1513			

- Molecule 2 is a RNA chain called PE hybrid state tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	74	Total	C	N	O	P	0	0	0
			1579	705	285	516	73			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AX	6	Total	C	N	O	P	0	0	0
			125	56	19	44	6			

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 5 is a protein called 30S ribosomal protein S11.

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

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 8 is a protein called 30S ribosomal protein S14 TYPE Z.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 14 is a protein called 30S ribosomal protein S20.

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

- Molecule 15 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 17 is a protein called 30S ribosomal protein S4.

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

- Molecule 18 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

- Molecule 19 is a protein called 30S ribosomal protein S6.

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

- Molecule 20 is a protein called 30S ribosomal protein S7.

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

- Molecule 21 is a protein called 30S ribosomal protein S8.

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

- Molecule 22 is a protein called 30S ribosomal protein S9.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	622	Total	C	N	O	S	0	0	0
			4877	3097	837	924	19			

- 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
			209	128	50	31				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2859	Total	C	N	O	P	0	0	0
			61580	27407	11519	19796	2858			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S ribosomal protein L13.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BZ	198	Total	C	N	O	S	0	0	0
			1508	960	274	272	2			

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 43 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BC	225	Total	C	N	O	S	0	0	0
			1718	1085	315	316	2			

- Molecule 52 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 53 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BH	173	Total	C	N	O	S	0	0	0
			1303	824	244	234	1			

- Molecule 56 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	127	Total	C	N	O	S	0	0	0
			936	598	161	172	5			

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

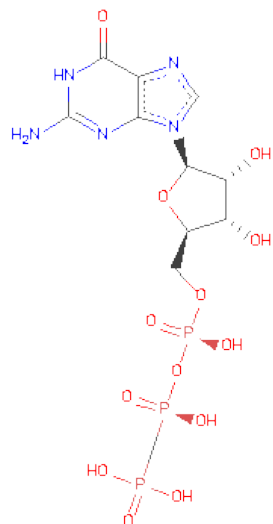
- Molecule 58 is a protein called 50S ribosomal protein L12 CTD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BL	72	Total	C	N	O		0	0	1
			356	213	72	71				

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	88	Total	Mg	0	0
			88	88		
59	BD	1	Total	Mg	0	0
			1	1		
59	BF	1	Total	Mg	0	0
			1	1		
59	B8	1	Total	Mg	0	0
			1	1		
59	BE	1	Total	Mg	0	0
			1	1		
59	AA	45	Total	Mg	0	0
			45	45		
59	AY	1	Total	Mg	0	0
			1	1		

- Molecule 60 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

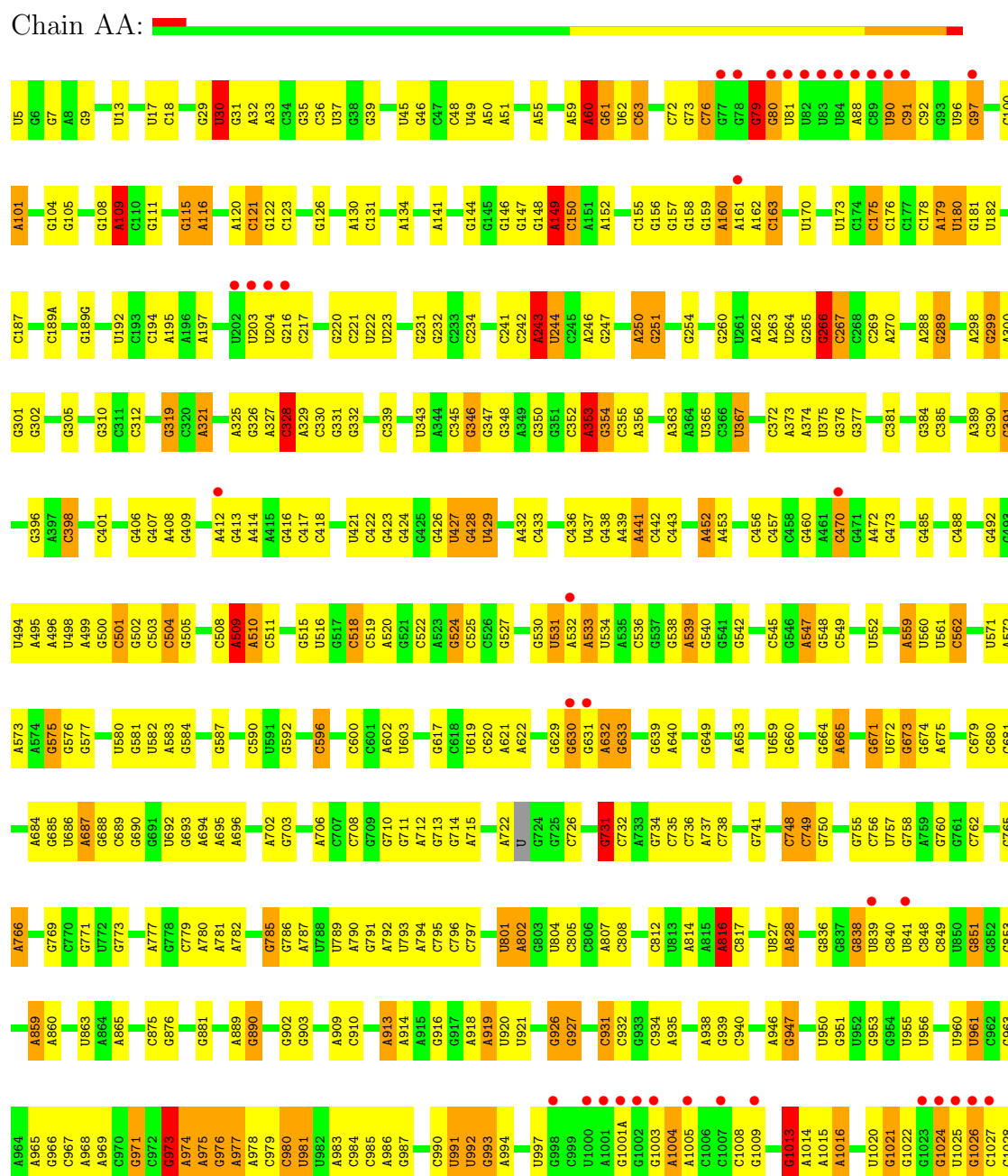
- Molecule 61 is water.

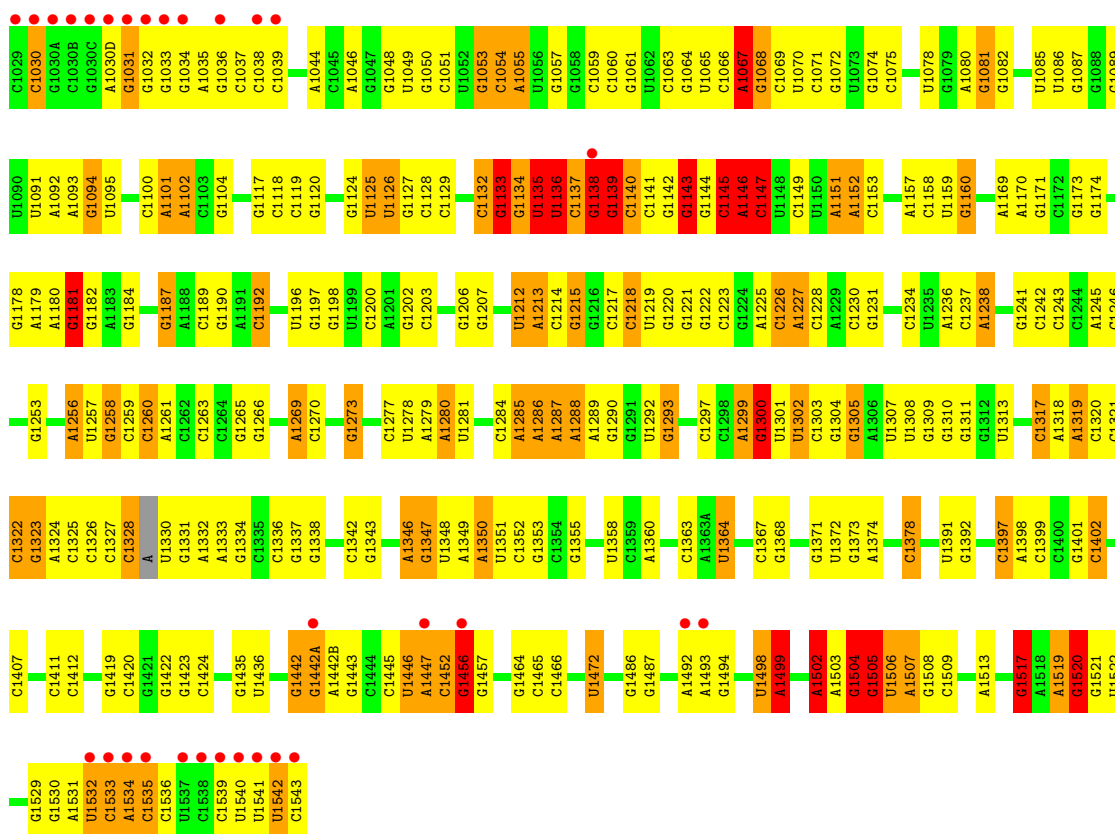
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	4	Total	O	0	0
			4	4		

### 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.

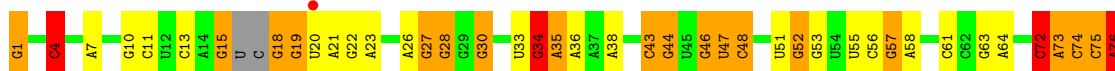
#### • Molecule 1: 16S ribosomal RNA





- Molecule 2: PE hybrid state tRNA Phe

Chain AV:



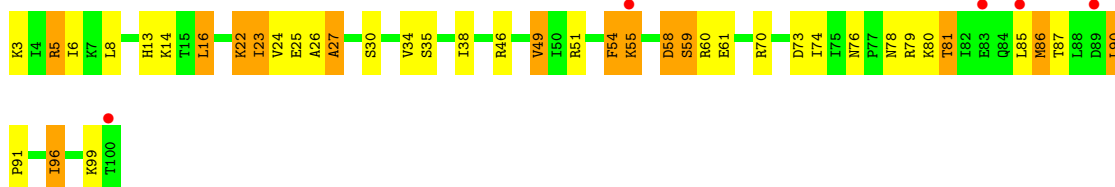
- Molecule 3: mRNA

Chain AX:



- Molecule 4: 30S ribosomal protein S10

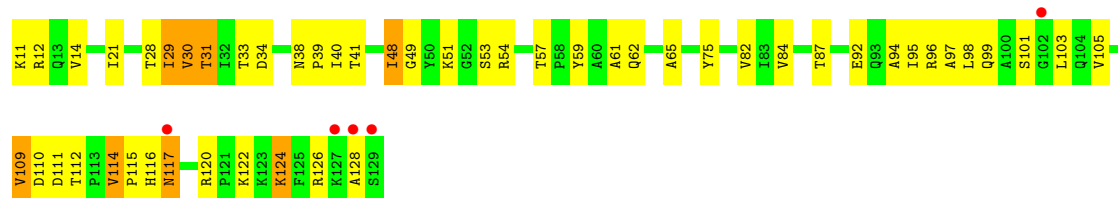
Chain AJ:



- Molecule 5: 30S ribosomal protein S11

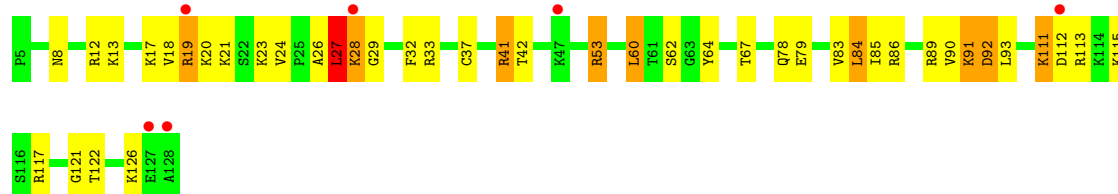
Chain AK:





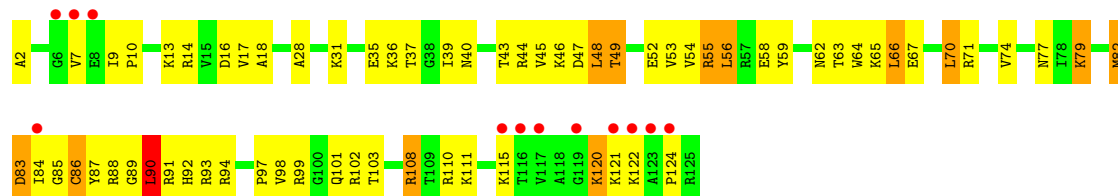
• Molecule 6: 30S ribosomal protein S12

Chain AL:



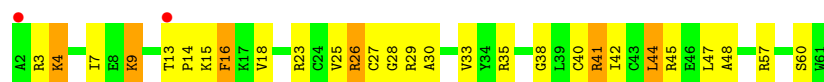
• Molecule 7: 30S ribosomal protein S13

Chain AM:



• Molecule 8: 30S ribosomal protein S14 TYPE Z

Chain AN:



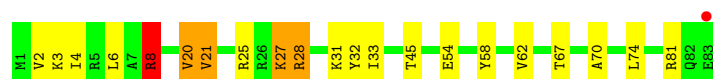
• Molecule 9: 30S ribosomal protein S15

Chain AO:



• Molecule 10: 30S ribosomal protein S16

Chain AP:



• Molecule 11: 30S ribosomal protein S17

Chain AQ:



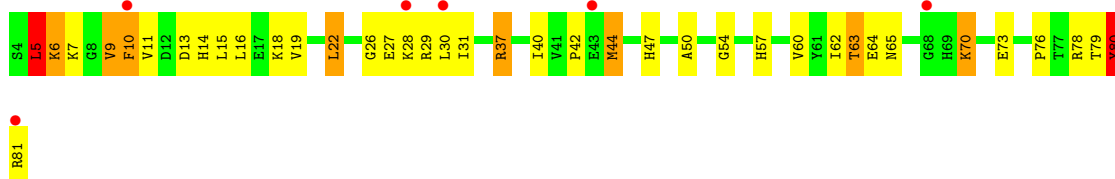
- Molecule 12: 30S ribosomal protein S18

Chain AR:



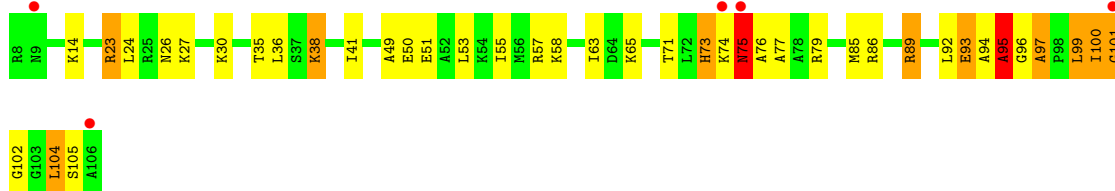
- Molecule 13: 30S ribosomal protein S19

Chain AS:



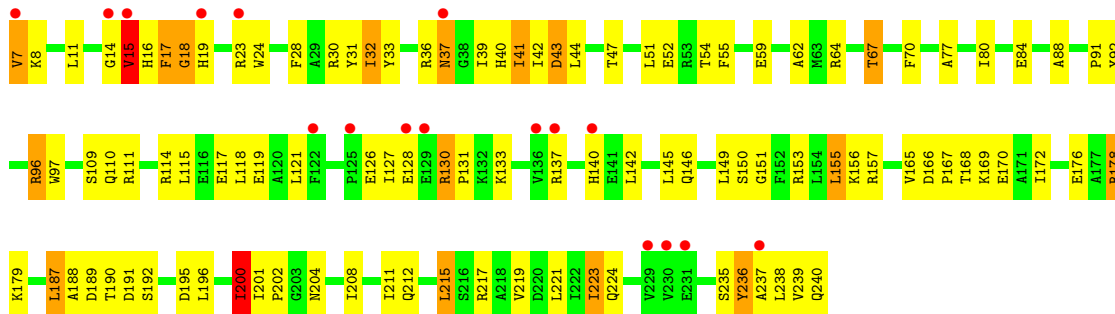
- Molecule 14: 30S ribosomal protein S20

Chain AT:



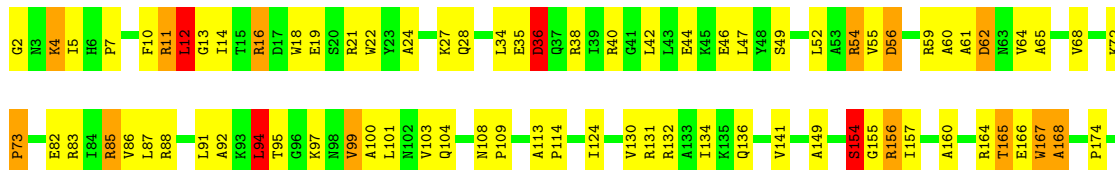
- Molecule 15: 30S ribosomal protein S2

Chain AB:



- Molecule 16: 30S ribosomal protein S3

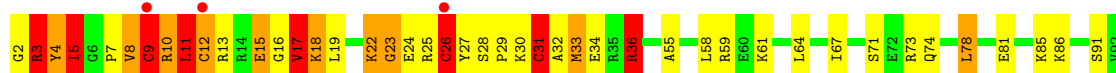
Chain AC:





- Molecule 17: 30S ribosomal protein S4

Chain AD:



- Molecule 18: 30S ribosomal protein S5

Chain AE:



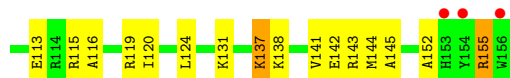
- Molecule 19: 30S ribosomal protein S6

Chain AF:



- Molecule 20: 30S ribosomal protein S7

Chain AG:



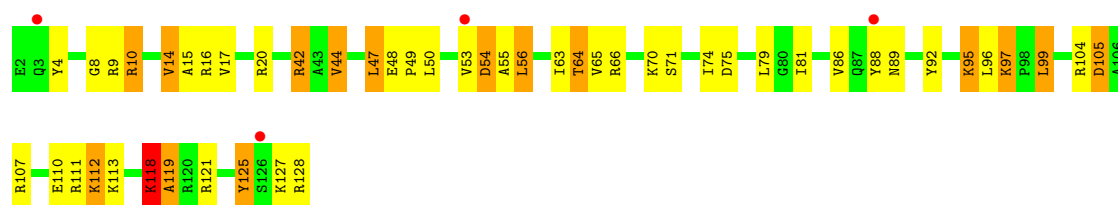
- Molecule 21: 30S ribosomal protein S8

Chain AH:



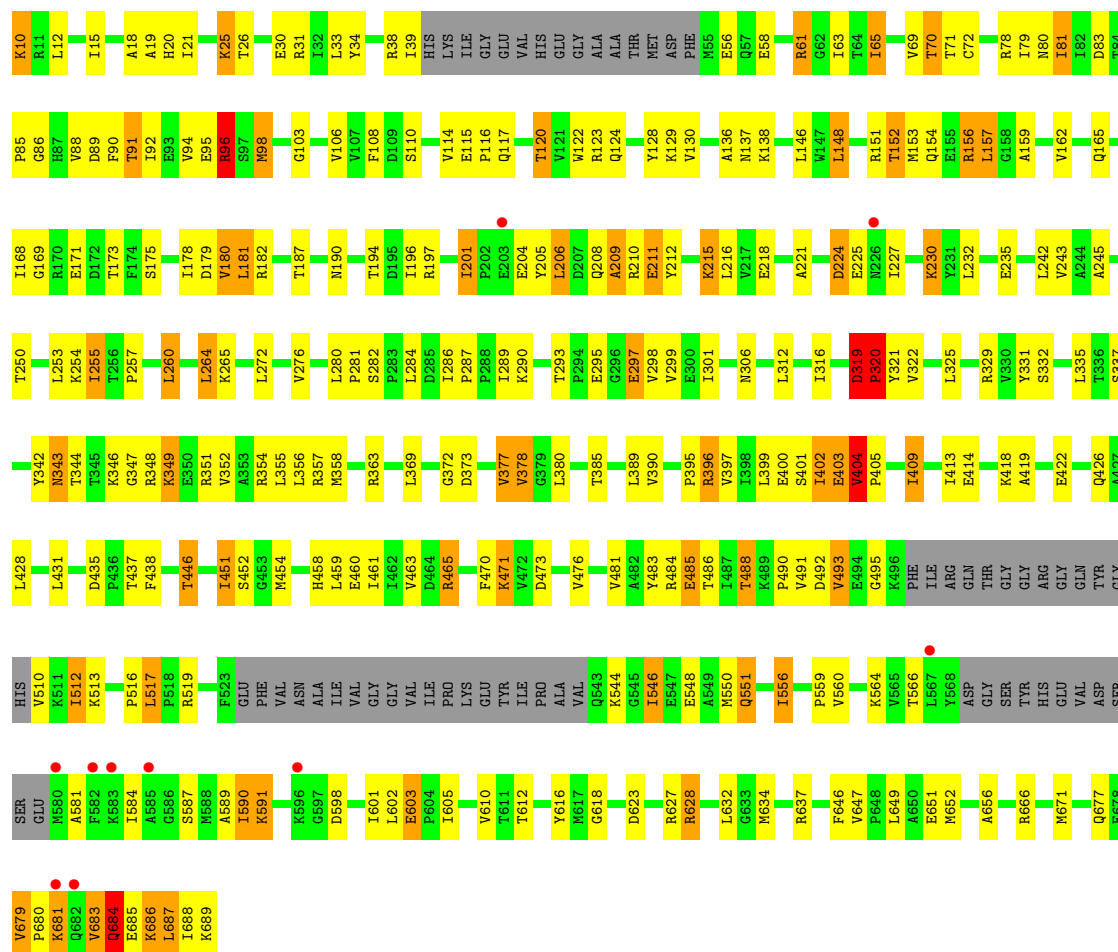
- Molecule 22: 30S ribosomal protein S9

Chain AI:



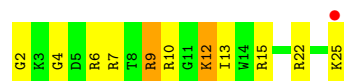
• Molecule 23: Elongation factor G

Chain AY:



• Molecule 24: 30S ribosomal protein THX

Chain AU:



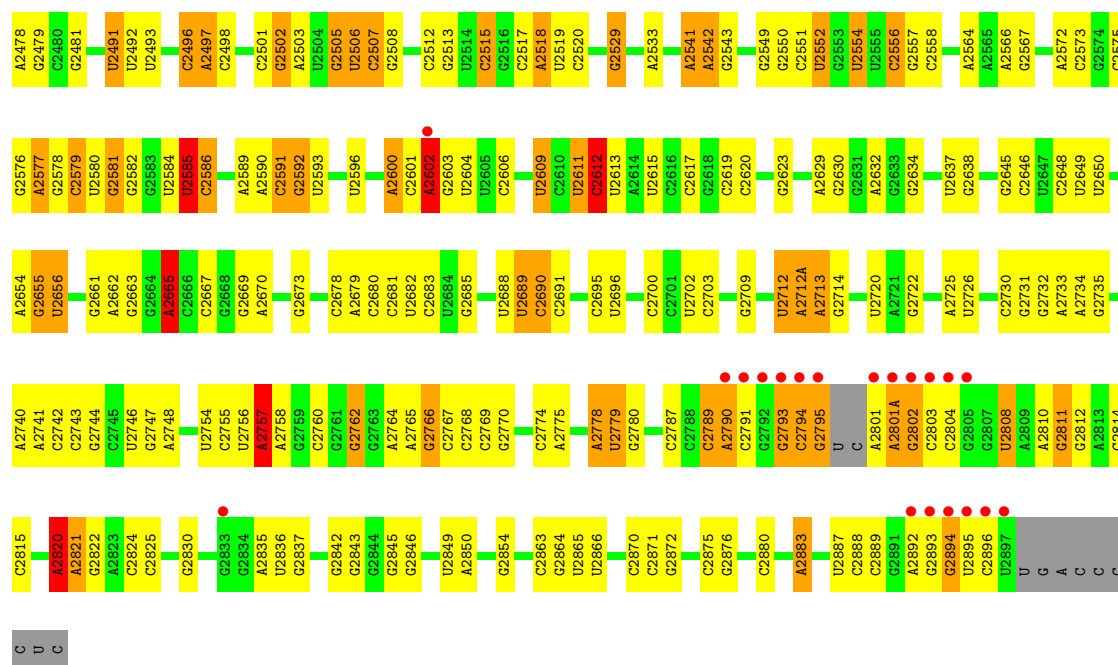
• Molecule 25: 23S ribosomal RNA

Chain BA:



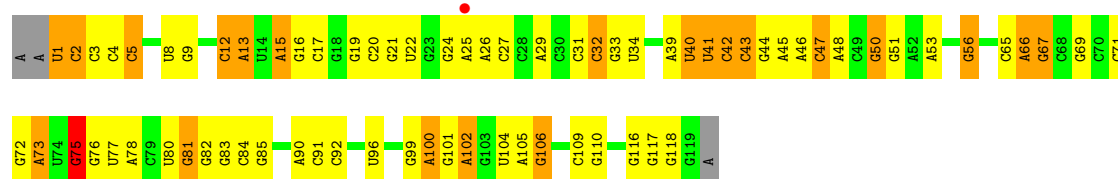
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A1182	A1098	G1025	U943	C856	G765	C661	A547	U475	G396	G317	C271F	U200	G94A
G1187	G1099	U1026	G944	C857	G766	G662	G548	A548	G396	C318	G271G	A204	G95
U1188	C1100	A1027	G945	U858	G771	G663	G549	A621	A401	C319	G271H	G205	G96
A1189	U1101	U1033	G946	C859	G772	C664	G551	A477	A402	G321	G271I	G209	C97
G1190	G1106	C1038	G947	U860	G775	G665	U555	A478	U405	G322	C271J	U99	G98
G1107	G1107	G1039	G948	G862	G776	G666	G556	A480	G406	G323	U271K	G212	G100
G1193	G1110	C1038	G954	C863	G780	C673	G558	G481	G407	A324	U271L	G217	A103
A1194	G1111	C1040	G955	C864	G781	A675	U562	A482	G407	G327	U271M	G218	A104
G1195	G1112	G1041	G956	C865	A782	A676	G563	A483	C409	U328	G271N	G214	C105
U1199	U1113	G1042	A957	C866	A783	A677	C564	C485	G410	G329	C271P	A216	C106
C1200	G1114	A1045	U958	C867	G784	G684	C565	G488	G411	A330	C271T	G217	G110
A1204	G1115	G1046	C961	U877	G785	A685	U566	A492	C414	A331	G271U	A218	A111
C1208	G1116	A1047	G962	C878	C786	A686	A567	G493	A332	A332	G271V	G219	C115
G1209	A1048	C1049	C967	U880	U787	C687	G570	G494	G333	G334	U271Y	G220	C115
A1210	G1122	A1050	C968	C881	A788	G700	G571	G495	C335	C335	G272	A221	A118
U1211	C1123	G1051	U969	C882	C790	G701	A572	G496	A422	C336	U	A223	A119
A1126	A1127	C1053	C970	C883	C842	C841	G573	G500	A423	C337	G272B	G224	G121
C1217	A1054	G1054	A973	C885	A643	A643	C574	A501	A428	U338	G272C	A228	U120
C1218	A1129	G1055	G974	C886	A644	A644	A575	A502	A429	U339	G272D	A229	G122
G1219	U1130	A1057	C979	C887	A645	A645	G579	A503	G430	G342	C272G	U230	G123
A1220	G1131	G1058	G979	C888	C708	C708	C580	U504	U431	A345	C272H	G231	A126
C1224	G1135	G1059	A980	C889	U714	G649	G581	G506	C435	A346	U272I	G232	A127
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G1239	U1142	G1069	C991	C898	C812	G729	U588	G512	C279	U358	C280	A242	A141
U1240	A1143	A1070	C992	A900	C813	C730	A359	A513	C280	A359	C281	A244	A142
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A1242	A1144	C1072	C994	C902	C815	G732	G592	G518	C445	G361	C286	G248	C164A
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G1245	C1150	C1075	C997	U907	A821	G739	G599	U525	G450	G363	A289	G251	U158
A1246	G1151	A1076	U999	A910	U827	G742	G600	C527	C451	U363E	G296	G252	G171
A1247	A1155	C1077	U999	A911	U828	G743	G602	A528	C452	A363F	G298	C263	G178
G1248	A1156	U1078	G1002	A917	A829	G744	A603	A529	C453	C364	G298	G264	A181
U1249	G1162	C1079	G1003	A918	G830	G745	G604	G530	C454	C364	A299	G266	A182
A1253	G1168	U1083	G1004	A919	G831	G746	C605	G531	C455	C365	A300	A270	U185
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G1256	G1170	G1087	C1006	C923	U833	G748	U607	G533	U457	A371	C302	G271A	A196
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G1260	G1173	G1089	C1013	G928	G836	C753	A609	C535	U464	A374	U306	G271C	C198
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U1263	U1176	C1092	U1019	A933	A849	U614A	U614B	C542	A470	U387	G309	A271A	
G1266	A1177	G1093	A1020	G934	G852	A761	G614B	C543	A471	G388	A310	G271D	
U1267	C1178	U1094	G1022	C935	G853	U762	A614C	C543	A472	G389	A311	G271D	
	C1180	A1096	U1023	A941	G854	G763	G615	G	G473	A390			

A1268	U1357	G1435	C1506	A1580	G1674	G1770	C1838	G1930	U2079	G2153	G2238	G2318	U2401
G1271	G1358	G1436	A1507	G1581	G1675	C1771	G1839	U1931	G2080	G2154	G2239	G2319	C2402
A1272	A1359	C1437	A1508	A1676	A1677	A1773	C1843	A1932	U2086	G2155	G2239	A2320	C2403
U1273	G1364	A1445	C1509	C1584	G1678	C1774	A1847	A1936	G2087	G2157	U2243	G2321	U2406
A1278	A1365	A1446	A1509A	C1586	U1679	U1775	A1848	A1937	U2092	G2159	U2244	C2324	C2407
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G1281	A1368	G1448	U1515	C1589	G1682	U1778	G1851	U1942	U2097	G2164	U2253	A2328	G2410
U1282	A1369	G1449	C1516	G1595	G1683	A1779	G1852	U1943	C2098	G2165	C2261	U2331	G2415
G1283	A1370	A1450	C1519	C1598	C1684	U1780	C1781	U1944	U2099	G2166	U2262	G2334	A2418
A1284	G1371	C1450A	U1520	C1599	G1685	C1782	A1859	U1945	U2100	U2167	C2263	G2335	U2419
G1285	U1372	A1452	G1521	C1603	G1686	A1783	U1864	U1946	G2101	G2168	A2266	A2336	C2421
A1286	C1375	U1453	U1523	A1603	U1688	A1784	G1865	C1947	U2102	C2169	A2267	U2337	A2418
A1287	C1376	U1458	U1524	A1608	A1689	A1785	C1866	A1952	C2103	A2170	A2268	A2338	U2422
U1288	A1379	C1458	G1525	A1609	U1692	A1787	A1876	U1956	U2104	U2171	U2272	G2340	A2423
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G1296	U1384	C1463	C1531	C1617	G1696	G1792	C1881	G1959	U2108	C2175	G2276	U2344	G2429
G1299	C1385	C1465	C1532	A1618	A1698	G1793	C1882	A1960	G2109	G2176	C2277	C2345	A2430
U1300	C1386	G1466	G	G1622	A1701	U1794	G1883	C1961	G2110	G2177	G2279	A2346	U2431
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U1354	U1432	U1503	U1578	U1671	G1765	U1835	C1925	G1997	G2147	C2226	C2311	U2391	G2472
G1356	A1434	C1505	U1579	U1673	G1769	U1836	U1926	U1997	G2148	G2230	C2312	A2392	G2475
							G1928	A2001	G2151	G2231	C2313	A2393	A2476
							G1929	G2002	G2152	U2232	C2314	C2394	C2477



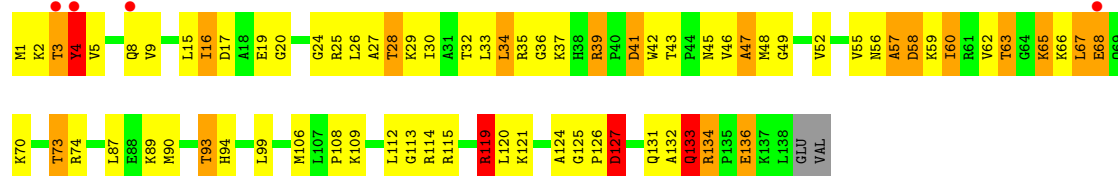
• Molecule 26: 5S ribosomal RNA

Chain BB:



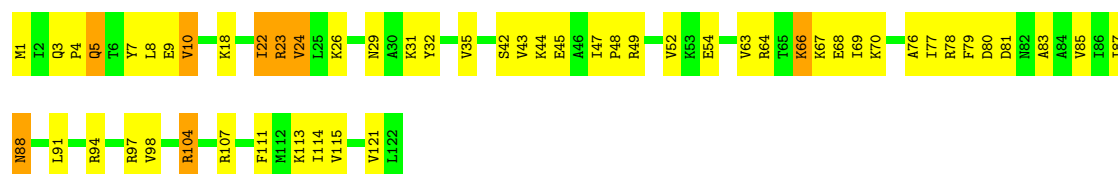
• Molecule 27: 50S ribosomal protein L13

Chain BN:



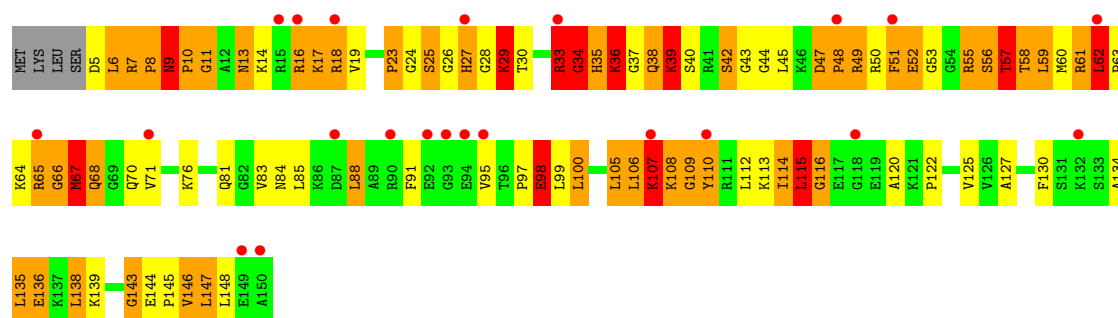
• Molecule 28: 50S ribosomal protein L14

Chain BO:



• Molecule 29: 50S ribosomal protein L15

Chain BP:



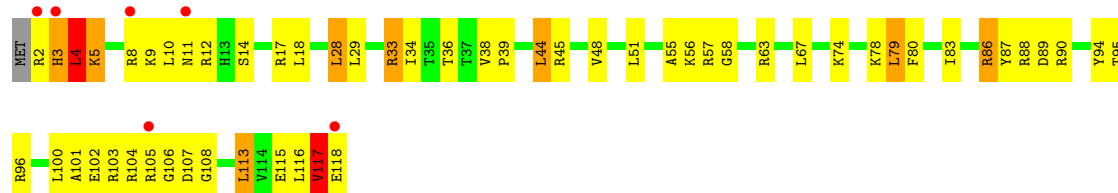
- Molecule 30: 50S ribosomal protein L16

Chain BQ:



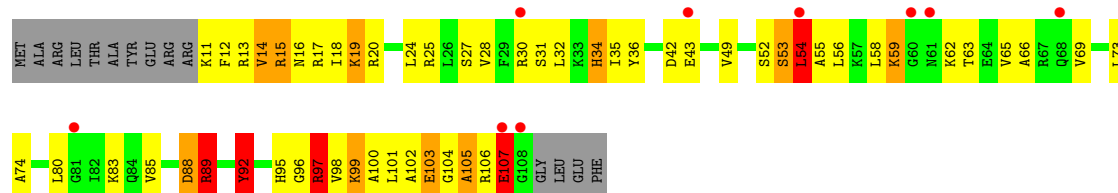
- Molecule 31: 50S ribosomal protein L17

Chain BR:



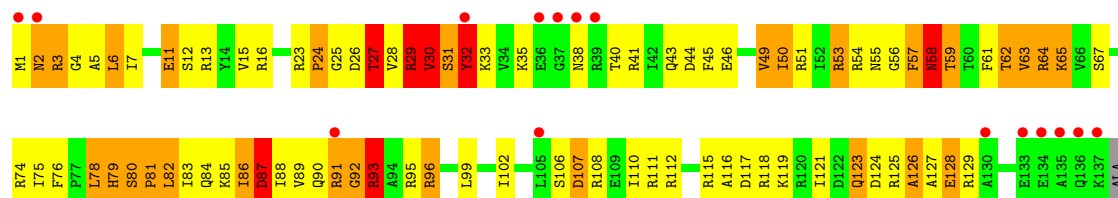
- Molecule 32: 50S ribosomal protein L18

Chain BS:



- Molecule 33: 50S ribosomal protein L19

Chain BT:

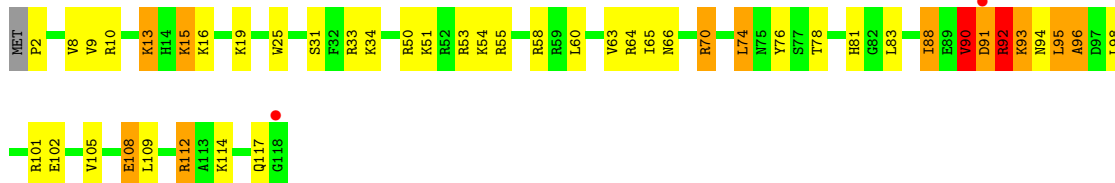




GLN  
GLU  
PRO  
LYS  
ALA  
SER  
GLN  
GLU

• Molecule 34: 50S ribosomal protein L20

Chain BU:



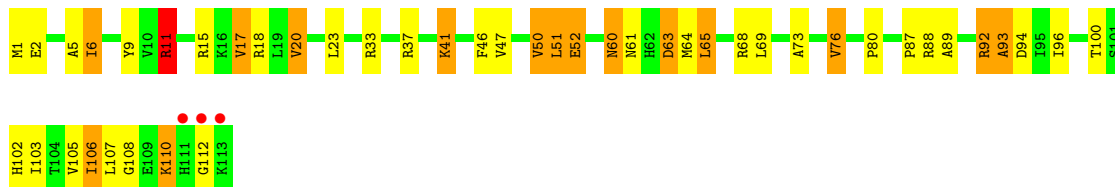
• Molecule 35: 50S ribosomal protein L21

Chain BV:



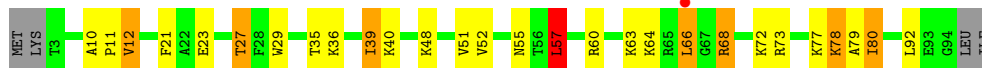
• Molecule 36: 50S ribosomal protein L22

Chain BW:



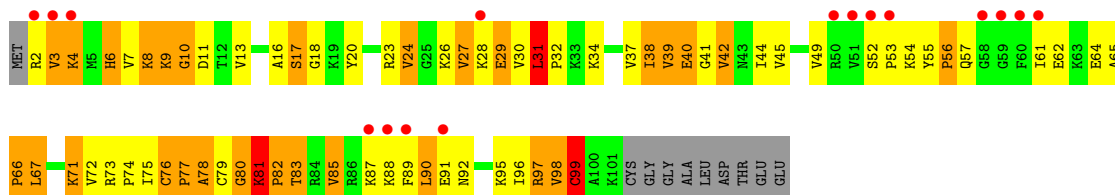
• Molecule 37: 50S ribosomal protein L23

Chain BX:



• Molecule 38: 50S ribosomal protein L24

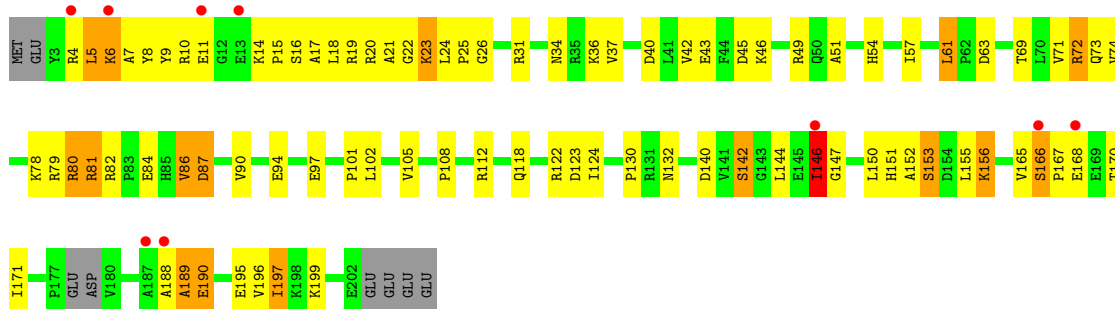
Chain BY:



• Molecule 39: 50S ribosomal protein L25

Chain BZ:





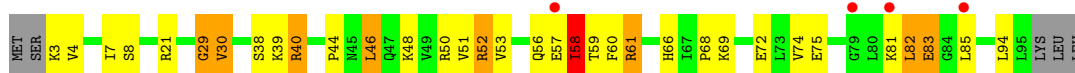
- Molecule 40: 50S ribosomal protein L27

Chain B0:



- Molecule 41: 50S ribosomal protein L28

Chain B1:



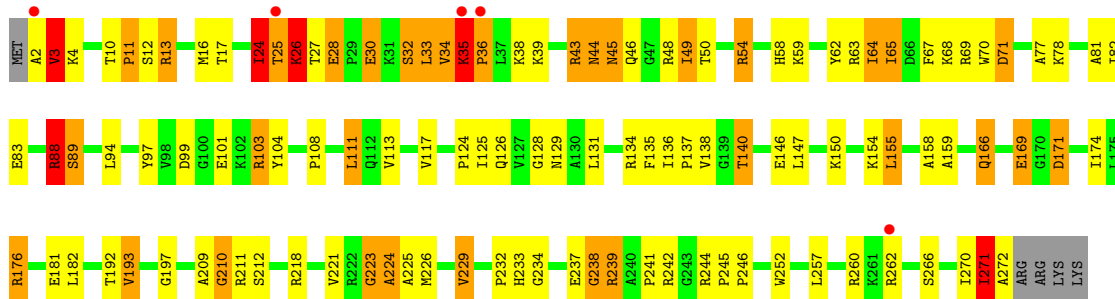
- Molecule 42: 50S ribosomal protein L29

Chain B2:



- Molecule 43: 50S ribosomal protein L2

Chain BD:



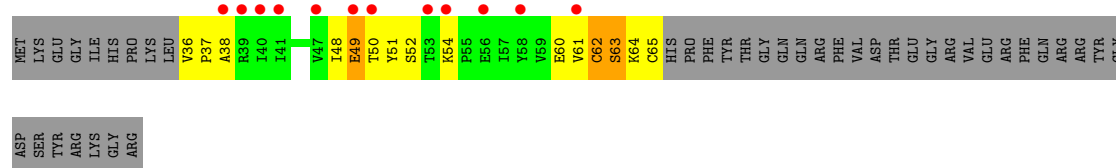
- Molecule 44: 50S ribosomal protein L30

Chain B3:



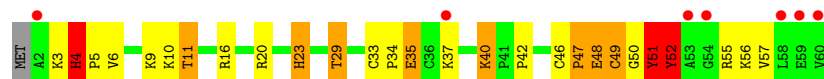
- Molecule 45: 50S ribosomal protein L31

Chain B4: 



- Molecule 46: 50S ribosomal protein L32

Chain B5: 



- Molecule 47: 50S ribosomal protein L33

Chain B6: 



- Molecule 48: 50S ribosomal protein L34

Chain B7: 



- Molecule 49: 50S ribosomal protein L35

Chain B8: 



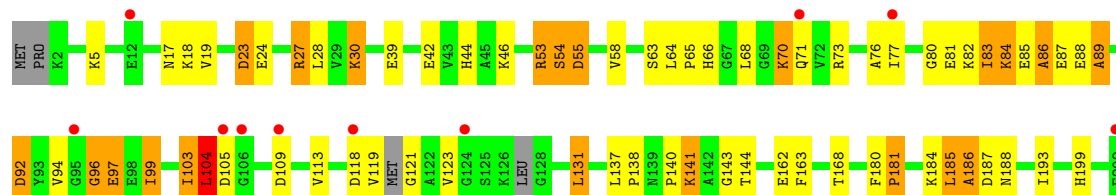
- Molecule 50: 50S ribosomal protein L36

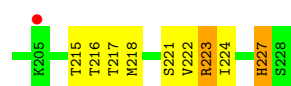
Chain B9: 



- Molecule 51: 50S ribosomal protein L1

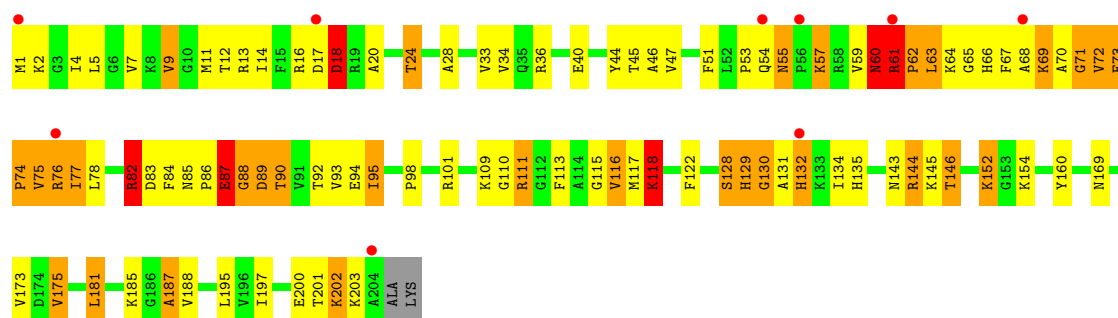
Chain BC: 





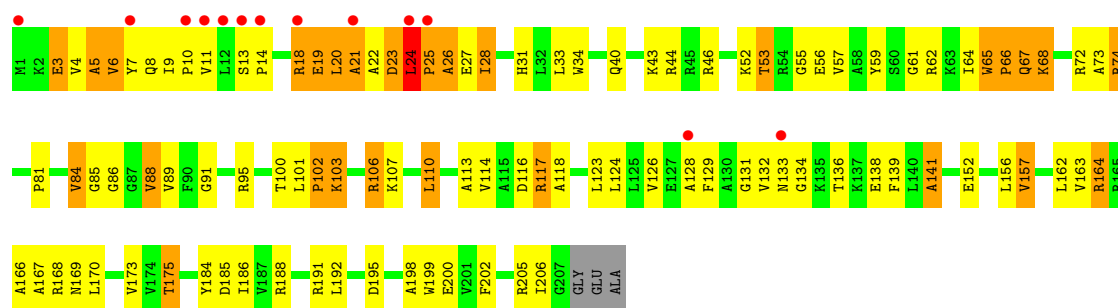
- Molecule 52: 50S ribosomal protein L3

Chain BE:



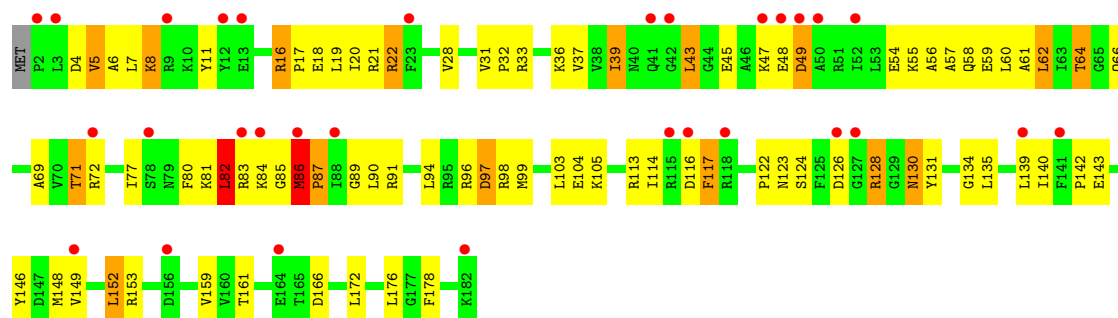
- Molecule 53: 50S ribosomal protein L4

Chain BF:



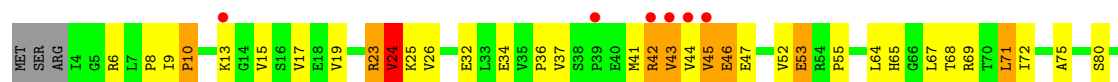
- Molecule 54: 50S ribosomal protein L5

Chain BG:



- Molecule 55: 50S ribosomal protein L6

Chain BH:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.58Å 241.65Å 305.80Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	39.60 – 2.86 39.59 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-2.86) 98.6 (39.59-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.22	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.86Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, $R_{free}$	0.200 , 0.250 0.200 , 0.243	Depositor DCC
$R_{free}$ test set	32790 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 5.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 655782 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	151831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: GCP, 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	AA	0.54	8/36408 (0.0%)	0.90	98/56818 (0.2%)
2	AV	0.49	1/1764 (0.1%)	0.96	11/2747 (0.4%)
3	AX	0.50	0/138	0.79	0/212
4	AJ	0.66	0/808	0.96	0/1085
5	AK	0.59	0/900	0.86	0/1213
6	AL	0.67	0/987	1.03	1/1320 (0.1%)
7	AM	0.54	0/999	0.89	0/1336
8	AN	0.61	0/501	1.08	2/664 (0.3%)
9	AO	0.61	0/745	0.94	1/992 (0.1%)
10	AP	0.59	0/717	0.92	2/963 (0.2%)
11	AQ	0.68	0/837	0.89	1/1117 (0.1%)
12	AR	0.60	0/579	0.84	0/768
13	AS	0.58	0/643	0.91	1/865 (0.1%)
14	AT	0.61	0/765	0.90	0/1007
15	AB	0.56	0/1936	0.83	1/2609 (0.0%)
16	AC	0.64	0/1637	0.93	3/2205 (0.1%)
17	AD	0.63	2/1733 (0.1%)	0.97	8/2318 (0.3%)
18	AE	0.71	0/1163	0.93	3/1564 (0.2%)
19	AF	0.55	0/856	0.78	0/1154
20	AG	0.54	0/1276	0.82	0/1709
21	AH	0.64	0/1136	0.95	1/1527 (0.1%)
22	AI	0.57	0/1029	0.92	0/1378
23	AY	0.53	0/4961	0.81	3/6710 (0.0%)
24	AU	0.58	0/213	0.92	0/277
25	BA	0.61	43/68964 (0.1%)	0.95	224/107644 (0.2%)
26	BB	0.40	0/2853	0.84	4/4451 (0.1%)
27	BN	0.74	1/1131 (0.1%)	1.07	5/1525 (0.3%)
28	BO	0.67	0/943	0.98	2/1269 (0.2%)
29	BP	0.86	0/1131	1.29	8/1504 (0.5%)
30	BQ	0.64	0/1143	0.92	0/1527
31	BR	0.70	0/974	1.01	1/1302 (0.1%)
32	BS	0.55	0/778	0.87	0/1036

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BT	0.70	0/1155	1.15	5/1542 (0.3%)
34	BU	0.75	0/975	1.02	1/1297 (0.1%)
35	BV	0.69	0/790	0.99	1/1057 (0.1%)
36	BW	0.67	0/907	1.02	3/1216 (0.2%)
37	BX	0.69	0/739	0.90	1/993 (0.1%)
38	BY	0.81	0/788	1.08	1/1051 (0.1%)
39	BZ	0.56	0/1539	0.87	0/2093
40	B0	0.57	0/671	0.86	0/892
41	B1	0.69	0/738	0.95	0/981
42	B2	0.57	0/600	0.86	0/793
43	BD	0.87	3/2154 (0.1%)	1.08	5/2905 (0.2%)
44	B3	0.55	0/472	0.80	0/634
45	B4	0.54	0/228	0.71	0/309
46	B5	0.85	0/473	1.22	5/639 (0.8%)
47	B6	0.94	0/387	1.36	3/518 (0.6%)
48	B7	0.74	0/426	0.85	0/561
49	B8	0.79	0/515	1.22	3/679 (0.4%)
50	B9	0.69	0/302	1.05	1/397 (0.3%)
51	BC	0.56	1/1747 (0.1%)	1.01	4/2351 (0.2%)
52	BE	0.75	0/1596	1.01	3/2153 (0.1%)
53	BF	0.69	0/1658	0.93	2/2244 (0.1%)
54	BG	0.48	0/1499	0.78	2/2016 (0.1%)
55	BH	0.59	0/1327	0.93	2/1794 (0.1%)
56	BK	0.41	0/951	0.60	0/1290
57	BJ	0.51	0/650	0.62	0/907
All	All	0.61	59/163935 (0.0%)	0.93	422/244128 (0.2%)

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
4	AJ	0	1
6	AL	0	1
8	AN	0	1
14	AT	0	2
17	AD	0	2
23	AY	0	4
27	BN	0	2
29	BP	0	15
30	BQ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BR	0	2
32	BS	0	1
33	BT	0	6
34	BU	0	3
35	BV	0	3
38	BY	0	6
41	B1	0	2
43	BD	0	4
46	B5	0	2
47	B6	0	3
51	BC	0	2
52	BE	0	5
53	BF	0	1
55	BH	0	1
58	BL	0	1
All	All	0	72

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2506	U	O3'-P	12.63	1.76	1.61
25	BA	1695	G	O3'-P	-9.03	1.50	1.61
27	BN	127	ASP	CB-CG	8.59	1.69	1.51
25	BA	1299	G	O3'-P	-7.33	1.52	1.61
25	BA	1300	U	O3'-P	-6.92	1.52	1.61

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	BC	27	ARG	NE-CZ-NH2	-24.39	108.10	120.30
25	BA	996	A	O5'-P-OP1	-17.66	89.51	110.70
1	AA	1499	A	O5'-P-OP1	-14.95	92.25	105.70
25	BA	946	G	O5'-P-OP1	-14.17	92.95	105.70
25	BA	2502	G	O5'-P-OP1	-13.94	93.15	105.70

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AJ	54	PHE	Peptide
6	AL	28	LYS	Peptide

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Mol	Chain	Res	Type	Group
8	AN	13	THR	Peptide
14	AT	73	HIS	Peptide
14	AT	95	ALA	Peptide

## 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	32529	0	16426	525	0
2	AV	1579	0	802	43	0
3	AX	125	0	64	2	0
4	AJ	795	0	840	29	0
5	AK	885	0	904	28	0
6	AL	971	0	1057	26	0
7	AM	988	0	1059	43	0
8	AN	492	0	529	21	0
9	AO	734	0	771	16	0
10	AP	701	0	720	14	0
11	AQ	824	0	891	19	0
12	AR	574	0	644	10	0
13	AS	630	0	652	25	0
14	AT	763	0	861	30	0
15	AB	1901	0	1951	86	0
16	AC	1613	0	1677	49	0
17	AD	1703	0	1763	64	0
18	AE	1147	0	1207	33	0
19	AF	843	0	857	19	0
20	AG	1257	0	1296	25	0
21	AH	1116	0	1177	27	0
22	AI	1011	0	1043	35	0
23	AY	4877	0	4964	166	0
24	AU	209	0	221	8	0
25	BA	61580	0	31049	1148	0
26	BB	2551	0	1295	55	0
27	BN	1104	0	1180	63	0
28	BO	933	0	996	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BP	1114	0	1187	142	0
30	BQ	1122	0	1179	38	0
31	BR	960	0	1021	39	0
32	BS	770	0	832	42	0
33	BT	1141	0	1202	114	0
34	BU	958	0	1015	51	0
35	BV	779	0	852	50	0
36	BW	896	0	953	27	0
37	BX	725	0	778	15	0
38	BY	775	0	870	71	0
39	BZ	1508	0	1486	56	0
40	B0	662	0	688	22	0
41	B1	731	0	808	33	0
42	B2	598	0	653	31	0
43	BD	2104	0	2182	101	0
44	B3	467	0	523	5	0
45	B4	225	0	229	10	0
46	B5	459	0	477	31	0
47	B6	380	0	390	55	0
48	B7	418	0	467	12	0
49	B8	507	0	576	58	0
50	B9	299	0	323	10	0
51	BC	1718	0	1766	54	0
52	BE	1563	0	1629	81	0
53	BF	1623	0	1677	83	0
54	BG	1474	0	1535	56	0
55	BH	1303	0	1348	55	0
56	BK	936	0	970	60	0
57	BJ	651	0	649	17	0
58	BL	356	0	75	7	0
59	AA	45	0	0	0	0
59	AY	1	0	0	0	0
59	B8	1	0	0	0	0
59	BA	88	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
60	AY	32	0	14	5	0
61	AY	4	0	0	1	0
All	All	151831	0	105250	3647	0

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 14.

The worst 5 of 3647 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:BA:2111:C:N3	25:BA:2147:G:N2	1.74	1.36
25:BA:1332:G:N2	25:BA:1609:A:O2'	1.62	1.26
47:B6:40:CYS:SG	47:B6:45:LYS:NZ	1.02	1.24
25:BA:90:U:O2'	25:BA:92:A:OP2	1.54	1.24
25:BA:1332:G:N2	25:BA:1609:A:HO2'	1.30	1.23

There are no symmetry-related clashes.

## 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	
4	AJ	96/98 (98%)	80 (83%)	10 (10%)	6 (6%)	2	5
5	AK	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	8	29
6	AL	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	4	14
7	AM	122/124 (98%)	82 (67%)	32 (26%)	8 (7%)	2	4
8	AN	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	6	21
9	AO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	19	54
10	AP	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
11	AQ	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	22	59
12	AR	68/70 (97%)	60 (88%)	5 (7%)	3 (4%)	4	13
13	AS	76/78 (97%)	60 (79%)	8 (10%)	8 (10%)	1	2
14	AT	97/99 (98%)	86 (89%)	5 (5%)	6 (6%)	2	5
15	AB	232/234 (99%)	191 (82%)	32 (14%)	9 (4%)	5	16
16	AC	204/206 (99%)	173 (85%)	22 (11%)	9 (4%)	4	13
17	AD	206/208 (99%)	171 (83%)	25 (12%)	10 (5%)	3	10
18	AE	148/150 (99%)	141 (95%)	5 (3%)	2 (1%)	16	49
19	AF	99/101 (98%)	91 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AG	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	8	29
21	AH	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	10	34
22	AI	125/127 (98%)	99 (79%)	17 (14%)	9 (7%)	2	3
23	AY	612/680 (90%)	520 (85%)	72 (12%)	20 (3%)	6	22
24	AU	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
27	BN	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	4	13
28	BO	120/122 (98%)	113 (94%)	3 (2%)	4 (3%)	6	22
29	BP	144/150 (96%)	90 (62%)	21 (15%)	33 (23%)	0	0
30	BQ	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	5	19
31	BR	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	4	13
32	BS	96/112 (86%)	61 (64%)	20 (21%)	15 (16%)	0	0
33	BT	135/146 (92%)	96 (71%)	24 (18%)	15 (11%)	1	1
34	BU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	6	20
35	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	0
36	BW	111/113 (98%)	101 (91%)	4 (4%)	6 (5%)	3	8
37	BX	90/96 (94%)	83 (92%)	7 (8%)	0	100	100
38	BY	98/110 (89%)	58 (59%)	18 (18%)	22 (22%)	0	0
39	BZ	194/206 (94%)	146 (75%)	32 (16%)	16 (8%)	1	3
40	B0	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	5	18
41	B1	91/98 (93%)	76 (84%)	12 (13%)	3 (3%)	6	22
42	B2	69/72 (96%)	58 (84%)	4 (6%)	7 (10%)	1	2
43	BD	269/276 (98%)	231 (86%)	24 (9%)	14 (5%)	3	8
44	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	13	41
45	B4	28/71 (39%)	21 (75%)	4 (14%)	3 (11%)	1	1
46	B5	57/60 (95%)	47 (82%)	4 (7%)	6 (10%)	1	2
47	B6	42/54 (78%)	20 (48%)	15 (36%)	7 (17%)	0	0
48	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	34
49	B8	61/65 (94%)	45 (74%)	11 (18%)	5 (8%)	1	3
50	B9	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
51	BC	219/229 (96%)	166 (76%)	35 (16%)	18 (8%)	1	3
52	BE	202/206 (98%)	145 (72%)	30 (15%)	27 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BF	205/210 (98%)	165 (80%)	24 (12%)	16 (8%)	1	3
54	BG	179/182 (98%)	123 (69%)	44 (25%)	12 (7%)	2	4
55	BH	171/180 (95%)	128 (75%)	26 (15%)	17 (10%)	1	2
56	BK	121/147 (82%)	84 (69%)	30 (25%)	7 (6%)	3	6
57	BJ	128/130 (98%)	84 (66%)	31 (24%)	13 (10%)	1	2
All	All	6610/6949 (95%)	5383 (81%)	812 (12%)	415 (6%)	2	5

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AJ	23	ILE
4	AJ	59	SER
4	AJ	86	MET
5	AK	117	ASN
5	AK	128	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	
4	AJ	88/88 (100%)	70 (80%)	18 (20%)	2	4
5	AK	90/90 (100%)	68 (76%)	22 (24%)	1	2
6	AL	104/104 (100%)	85 (82%)	19 (18%)	2	6
7	AM	99/99 (100%)	83 (84%)	16 (16%)	3	9
8	AN	49/49 (100%)	38 (78%)	11 (22%)	1	3
9	AO	79/79 (100%)	67 (85%)	12 (15%)	4	10
10	AP	72/72 (100%)	61 (85%)	11 (15%)	4	10
11	AQ	94/94 (100%)	79 (84%)	15 (16%)	3	9
12	AR	61/61 (100%)	52 (85%)	9 (15%)	4	11
13	AS	69/69 (100%)	52 (75%)	17 (25%)	1	2
14	AT	76/76 (100%)	61 (80%)	15 (20%)	2	5
15	AB	202/202 (100%)	172 (85%)	30 (15%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AC	160/160 (100%)	125 (78%)	35 (22%)	1	3
17	AD	180/180 (100%)	144 (80%)	36 (20%)	2	5
18	AE	115/115 (100%)	104 (90%)	11 (10%)	12	32
19	AF	90/90 (100%)	76 (84%)	14 (16%)	4	10
20	AG	126/126 (100%)	110 (87%)	16 (13%)	6	16
21	AH	119/119 (100%)	96 (81%)	23 (19%)	2	5
22	AI	98/98 (100%)	76 (78%)	22 (22%)	1	3
23	AY	528/573 (92%)	420 (80%)	108 (20%)	2	4
24	AU	19/19 (100%)	14 (74%)	5 (26%)	1	2
27	BN	117/119 (98%)	84 (72%)	33 (28%)	0	1
28	BO	100/100 (100%)	84 (84%)	16 (16%)	3	9
29	BP	112/116 (97%)	82 (73%)	30 (27%)	1	2
30	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	14
31	BR	100/101 (99%)	80 (80%)	20 (20%)	2	5
32	BS	77/88 (88%)	62 (80%)	15 (20%)	2	5
33	BT	120/127 (94%)	91 (76%)	29 (24%)	1	2
34	BU	92/94 (98%)	76 (83%)	16 (17%)	3	7
35	BV	82/82 (100%)	56 (68%)	26 (32%)	0	0
36	BW	91/92 (99%)	75 (82%)	16 (18%)	3	7
37	BX	74/78 (95%)	59 (80%)	15 (20%)	2	4
38	BY	84/91 (92%)	65 (77%)	19 (23%)	1	3
39	BZ	154/179 (86%)	127 (82%)	27 (18%)	3	7
40	B0	66/67 (98%)	56 (85%)	10 (15%)	4	10
41	B1	78/83 (94%)	63 (81%)	15 (19%)	2	5
42	B2	66/67 (98%)	51 (77%)	15 (23%)	1	3
43	BD	213/218 (98%)	170 (80%)	43 (20%)	2	4
44	B3	51/52 (98%)	41 (80%)	10 (20%)	2	5
45	B4	27/63 (43%)	23 (85%)	4 (15%)	4	11
46	B5	51/52 (98%)	42 (82%)	9 (18%)	3	7
47	B6	43/52 (83%)	31 (72%)	12 (28%)	0	1
48	B7	41/42 (98%)	35 (85%)	6 (15%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B8	53/55 (96%)	33 (62%)	20 (38%)	0	0
50	B9	33/34 (97%)	23 (70%)	10 (30%)	0	1
51	BC	177/181 (98%)	159 (90%)	18 (10%)	11	28
52	BE	165/166 (99%)	131 (79%)	34 (21%)	2	4
53	BF	165/166 (99%)	134 (81%)	31 (19%)	2	5
54	BG	155/156 (99%)	128 (83%)	27 (17%)	3	7
55	BH	136/148 (92%)	107 (79%)	29 (21%)	1	4
56	BK	96/111 (86%)	85 (88%)	11 (12%)	8	22
All	All	5448/5654 (96%)	4402 (81%)	1046 (19%)	2	5

5 of 1046 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	BN	33	LEU
32	BS	49	VAL
53	BF	102	PRO
27	BN	73	THR
29	BP	88	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
31	BR	23	ASN
36	BW	102	HIS
53	BF	31	HIS
33	BT	90	GLN
39	BZ	34	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1512/1516 (99%)	315 (20%)	65 (4%)
2	AV	73/76 (96%)	28 (38%)	9 (12%)
25	BA	2849/2915 (97%)	756 (26%)	130 (4%)
26	BB	119/122 (97%)	34 (28%)	4 (3%)
3	AX	5/25 (20%)	0	0
All	All	4558/4654 (97%)	1133 (24%)	208 (4%)



5 of 1133 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	U
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	405	U
25	BA	974	G
25	BA	2497	A
25	BA	542	C
25	BA	746	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 139 ligands modelled in this entry, 138 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	GCP	AY	702	59	34,34,34	2.23	12 (35%)	52,54,54	3.45	21 (40%)

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
60	GCP	AY	702	59	-	0/20/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AY	702	GCP	PG-O2G	-4.06	1.46	1.54
60	AY	702	GCP	C2'-C3'	-3.96	1.42	1.53
60	AY	702	GCP	C5-N7	-3.93	1.33	1.38
60	AY	702	GCP	PB-O2B	-3.87	1.46	1.56
60	AY	702	GCP	PG-O3G	-3.64	1.47	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	702	GCP	C6-C5-N7	-19.03	131.58	134.14
60	AY	702	GCP	N2-C2-N1	4.85	123.02	117.82
60	AY	702	GCP	C1'-N9-C4	-4.75	118.43	126.64
60	AY	702	GCP	O4'-C4'-C5'	-4.38	93.80	109.37
60	AY	702	GCP	C2-N3-C4	4.38	120.56	115.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1514/1516 (99%)	0.01	68 (4%) 32 38	9, 32, 113, 247	0
2	AV	74/76 (97%)	0.29	1 (1%) 72 80	23, 54, 91, 134	0
3	AX	6/25 (24%)	0.40	1 (16%) 2 3	18, 22, 53, 75	0
4	AJ	98/98 (100%)	0.27	5 (5%) 27 32	22, 49, 98, 108	0
5	AK	119/119 (100%)	-0.01	5 (4%) 35 41	18, 41, 65, 104	0
6	AL	124/124 (100%)	-0.10	6 (4%) 29 35	16, 32, 64, 107	0
7	AM	124/124 (100%)	0.81	12 (9%) 8 10	31, 69, 118, 161	0
8	AN	60/60 (100%)	-0.07	2 (3%) 44 53	21, 33, 69, 83	0
9	AO	88/88 (100%)	-0.22	0 100 100	24, 41, 67, 73	0
10	AP	83/83 (100%)	-0.23	1 (1%) 75 83	29, 40, 60, 112	0
11	AQ	99/99 (100%)	-0.38	0 100 100	20, 34, 53, 59	0
12	AR	70/70 (100%)	-0.20	1 (1%) 72 80	23, 41, 75, 92	0
13	AS	78/78 (100%)	0.55	6 (7%) 13 16	39, 69, 107, 121	0
14	AT	99/99 (100%)	-0.08	5 (5%) 27 32	24, 39, 78, 90	0
15	AB	234/234 (100%)	0.10	17 (7%) 15 17	21, 55, 117, 134	0
16	AC	206/206 (100%)	-0.33	0 100 100	22, 41, 67, 103	0
17	AD	208/208 (100%)	-0.05	5 (2%) 56 65	26, 49, 75, 90	0
18	AE	150/150 (100%)	-0.41	1 (0%) 84 90	19, 30, 54, 81	0
19	AF	101/101 (100%)	-0.10	2 (1%) 62 71	28, 52, 75, 87	0
20	AG	155/155 (100%)	0.10	10 (6%) 18 21	31, 53, 104, 148	0
21	AH	138/138 (100%)	-0.43	1 (0%) 84 90	19, 32, 55, 84	0
22	AI	127/127 (100%)	-0.02	4 (3%) 47 56	21, 51, 82, 108	0
23	AY	622/680 (91%)	-0.06	10 (1%) 68 77	30, 55, 97, 131	0
24	AU	24/24 (100%)	0.46	1 (4%) 35 41	33, 48, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BA	2859/2915 (98%)	-0.04	92 (3%) 45 54	7, 27, 90, 267	0
26	BB	119/122 (97%)	0.29	1 (0%) 83 89	26, 63, 95, 134	0
27	BN	138/140 (98%)	-0.15	4 (2%) 49 59	18, 35, 66, 80	0
28	BO	122/122 (100%)	-0.53	0 100 100	18, 31, 49, 60	0
29	BP	146/150 (97%)	0.69	22 (15%) 3 3	18, 55, 94, 127	0
30	BQ	141/141 (100%)	-0.20	2 (1%) 72 80	23, 35, 64, 112	0
31	BR	117/118 (99%)	-0.21	6 (5%) 27 32	15, 33, 58, 75	0
32	BS	98/112 (87%)	0.82	9 (9%) 9 11	50, 80, 106, 125	0
33	BT	137/146 (93%)	0.58	15 (10%) 6 8	23, 50, 135, 151	0
34	BU	117/118 (99%)	-0.24	2 (1%) 67 76	16, 29, 58, 85	0
35	BV	101/101 (100%)	0.10	5 (4%) 28 33	15, 49, 77, 97	0
36	BW	113/113 (100%)	-0.15	3 (2%) 52 61	18, 29, 67, 122	0
37	BX	92/96 (95%)	-0.31	1 (1%) 77 84	20, 34, 54, 61	0
38	BY	100/110 (90%)	1.09	16 (16%) 3 3	29, 56, 122, 168	0
39	BZ	198/206 (96%)	0.12	9 (4%) 32 38	33, 59, 92, 103	0
40	B0	84/85 (98%)	0.40	9 (10%) 6 8	26, 41, 96, 133	0
41	B1	93/98 (94%)	0.13	4 (4%) 34 40	18, 33, 72, 121	0
42	B2	71/72 (98%)	0.07	2 (2%) 50 60	30, 49, 82, 100	0
43	BD	271/276 (98%)	-0.38	5 (1%) 65 74	9, 20, 46, 89	0
44	B3	59/60 (98%)	0.20	2 (3%) 43 52	24, 40, 76, 137	0
45	B4	30/71 (42%)	1.93	12 (40%) 1 0	102, 130, 156, 174	0
46	B5	59/60 (98%)	0.49	7 (11%) 5 6	10, 35, 98, 134	0
47	B6	44/54 (81%)	1.21	9 (20%) 1 2	34, 59, 99, 109	0
48	B7	48/49 (97%)	-0.30	2 (4%) 35 41	10, 19, 59, 101	0
49	B8	63/65 (96%)	0.28	5 (7%) 13 15	22, 37, 61, 118	0
50	B9	36/37 (97%)	0.25	3 (8%) 11 13	26, 44, 69, 77	0
51	BC	225/229 (98%)	0.14	11 (4%) 28 34	36, 64, 111, 132	0
52	BE	204/206 (99%)	-0.12	9 (4%) 33 39	14, 32, 85, 109	0
53	BF	207/210 (98%)	0.06	13 (6%) 19 22	15, 37, 103, 187	0
54	BG	181/182 (99%)	1.11	30 (16%) 2 3	67, 101, 130, 147	0
55	BH	173/180 (96%)	0.45	14 (8%) 12 14	35, 60, 95, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BK	127/147 (86%)	4.89	105 (82%) 0 0	127, 181, 237, 263	0
57	BJ	130/130 (100%)	1.48	36 (27%) 1 1	74, 106, 140, 195	0
58	BL	0/125	-	-	-	-
All	All	11304/11728 (96%)	0.11	629 (5%) 24 28	7, 40, 108, 267	0

The worst 5 of 629 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	BH	44	VAL	21.9
7	AM	123	ALA	17.5
56	BK	136	VAL	15.3
56	BK	83	GLY	14.4
53	BF	11	VAL	13.6

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
59	MG	BA	3014	1/1	0.28	-	27,27,27,27	0
59	MG	AA	1639	1/1	0.18	-	20,20,20,20	0
59	MG	AA	1621	1/1	0.17	-	14,14,14,14	0
59	MG	BA	3073	1/1	0.26	-	14,14,14,14	0
59	MG	BA	3054	1/1	0.27	-	9,9,9,9	0
59	MG	BA	3070	1/1	0.28	-	24,24,24,24	0
59	MG	BA	3013	1/1	0.20	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1623	1/1	0.21	-	15,15,15,15	0
59	MG	AA	1624	1/1	0.17	-	14,14,14,14	0
59	MG	AA	1604	1/1	0.09	-	3,3,3,3	0
59	MG	BA	3027	1/1	0.35	-	30,30,30,30	0
59	MG	BA	3030	1/1	0.32	-	12,12,12,12	0
59	MG	BA	3077	1/1	0.14	-	17,17,17,17	0
59	MG	BA	3074	1/1	0.15	-	16,16,16,16	0
59	MG	BA	3017	1/1	0.20	-	16,16,16,16	0
59	MG	BA	3019	1/1	0.27	-	16,16,16,16	0
60	GCP	AY	702	32/32	0.13	-	27,42,47,49	0
59	MG	BA	3045	1/1	0.20	-	16,16,16,16	0
59	MG	AA	1603	1/1	0.22	-	23,23,23,23	0
59	MG	AA	1632	1/1	0.21	-	22,22,22,22	0
59	MG	BA	3060	1/1	0.30	-	22,22,22,22	0
59	MG	AA	1631	1/1	0.19	-	13,13,13,13	0
59	MG	BA	3004	1/1	0.14	-	46,46,46,46	0
59	MG	AA	1637	1/1	0.13	-	34,34,34,34	0
59	MG	AA	1613	1/1	0.17	-	6,6,6,6	0
59	MG	BA	3024	1/1	0.29	-	2,2,2,2	0
59	MG	BA	3064	1/1	0.17	-	22,22,22,22	0
59	MG	BA	3068	1/1	0.25	-	7,7,7,7	0
59	MG	BA	3083	1/1	0.13	-	37,37,37,37	0
59	MG	BA	3051	1/1	0.28	-	24,24,24,24	0
59	MG	AA	1611	1/1	0.22	-	7,7,7,7	0
59	MG	AA	1643	1/1	0.14	-	31,31,31,31	0
59	MG	BA	3032	1/1	0.27	-	21,21,21,21	0
59	MG	AA	1617	1/1	0.31	-	21,21,21,21	0
59	MG	AA	1635	1/1	0.21	-	24,24,24,24	0
59	MG	AA	1644	1/1	0.34	-	33,33,33,33	0
59	MG	BA	3039	1/1	0.19	-	24,24,24,24	0
59	MG	BA	3035	1/1	0.37	-	18,18,18,18	0
59	MG	AA	1609	1/1	0.24	-	16,16,16,16	0
59	MG	BA	3085	1/1	0.25	-	18,18,18,18	0
59	MG	AA	1615	1/1	0.17	-	24,24,24,24	0
59	MG	BA	3081	1/1	0.16	-	17,17,17,17	0
59	MG	BA	3075	1/1	0.20	-	12,12,12,12	0
59	MG	BA	3011	1/1	0.24	-	30,30,30,30	0
59	MG	BA	3015	1/1	0.22	-	10,10,10,10	0
59	MG	BA	3080	1/1	0.23	-	16,16,16,16	0
59	MG	BA	3087	1/1	0.23	-	26,26,26,26	0
59	MG	AA	1638	1/1	0.17	-	22,22,22,22	0
59	MG	BA	3055	1/1	0.20	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3031	1/1	0.30	-	16,16,16,16	0
59	MG	BA	3088	1/1	0.29	-	26,26,26,26	0
59	MG	BA	3021	1/1	0.19	-	25,25,25,25	0
59	MG	BA	3008	1/1	0.27	-	13,13,13,13	0
59	MG	AA	1640	1/1	0.14	-	21,21,21,21	0
59	MG	BA	3006	1/1	0.29	-	13,13,13,13	0
59	MG	BA	3065	1/1	0.31	-	24,24,24,24	0
59	MG	B8	101	1/1	0.12	-	15,15,15,15	0
59	MG	BA	3049	1/1	0.28	-	2,2,2,2	0
59	MG	BA	3026	1/1	0.19	-	19,19,19,19	0
59	MG	BA	3018	1/1	0.23	-	12,12,12,12	0
59	MG	AA	1628	1/1	0.06	-	18,18,18,18	0
59	MG	AA	1619	1/1	0.22	-	27,27,27,27	0
59	MG	AA	1620	1/1	0.36	-	18,18,18,18	0
59	MG	BA	3072	1/1	0.23	-	19,19,19,19	0
59	MG	AA	1612	1/1	0.15	-	14,14,14,14	0
59	MG	BA	3002	1/1	0.17	-	17,17,17,17	0
59	MG	AA	1601	1/1	0.25	-	13,13,13,13	0
59	MG	AA	1641	1/1	0.14	-	25,25,25,25	0
59	MG	BA	3022	1/1	0.32	-	13,13,13,13	0
59	MG	BA	3056	1/1	0.14	-	18,18,18,18	0
59	MG	BA	3025	1/1	0.21	-	16,16,16,16	0
59	MG	AA	1625	1/1	0.32	-	25,25,25,25	0
59	MG	BA	3084	1/1	0.19	-	22,22,22,22	0
59	MG	AY	701	1/1	0.13	-	41,41,41,41	0
59	MG	BA	3058	1/1	0.16	-	3,3,3,3	0
59	MG	AA	1622	1/1	0.23	-	25,25,25,25	0
59	MG	BA	3028	1/1	0.20	-	23,23,23,23	0
59	MG	BA	3037	1/1	0.20	-	7,7,7,7	0
59	MG	AA	1633	1/1	0.13	-	27,27,27,27	0
59	MG	BA	3033	1/1	0.26	-	12,12,12,12	0
59	MG	BA	3061	1/1	0.30	-	8,8,8,8	0
59	MG	AA	1616	1/1	0.17	-	5,5,5,5	0
59	MG	AA	1606	1/1	0.24	-	15,15,15,15	0
59	MG	BA	3041	1/1	0.32	-	11,11,11,11	0
59	MG	BA	3029	1/1	0.24	-	28,28,28,28	0
59	MG	BA	3009	1/1	0.32	-	31,31,31,31	0
59	MG	BA	3010	1/1	0.30	-	14,14,14,14	0
59	MG	AA	1636	1/1	0.10	-	24,24,24,24	0
59	MG	AA	1626	1/1	0.19	-	19,19,19,19	0
59	MG	BA	3003	1/1	0.35	-	2,2,2,2	0
59	MG	BA	3043	1/1	0.28	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BE	301	1/1	0.25	-	16,16,16,16	0
59	MG	BA	3063	1/1	0.19	-	22,22,22,22	0
59	MG	BA	3086	1/1	0.26	-	26,26,26,26	0
59	MG	BA	3050	1/1	0.27	-	10,10,10,10	0
59	MG	AA	1630	1/1	0.29	-	29,29,29,29	0
59	MG	AA	1602	1/1	0.31	-	16,16,16,16	0
59	MG	BA	3048	1/1	0.25	-	9,9,9,9	0
59	MG	BA	3057	1/1	0.21	-	8,8,8,8	0
59	MG	BA	3038	1/1	0.37	-	19,19,19,19	0
59	MG	BA	3020	1/1	0.31	-	6,6,6,6	0
59	MG	BA	3012	1/1	0.13	-	10,10,10,10	0
59	MG	BF	301	1/1	0.14	-	27,27,27,27	0
59	MG	BA	3023	1/1	0.25	-	9,9,9,9	0
59	MG	AA	1627	1/1	0.24	-	15,15,15,15	0
59	MG	BA	3067	1/1	0.19	-	16,16,16,16	0
59	MG	BA	3078	1/1	0.18	-	15,15,15,15	0
59	MG	AA	1614	1/1	0.24	-	11,11,11,11	0
59	MG	BA	3053	1/1	0.22	-	7,7,7,7	0
59	MG	BA	3076	1/1	0.22	-	8,8,8,8	0
59	MG	AA	1608	1/1	0.41	-	23,23,23,23	0
59	MG	BA	3047	1/1	0.32	-	27,27,27,27	0
59	MG	BA	3082	1/1	0.24	-	21,21,21,21	0
59	MG	AA	1645	1/1	0.37	-	35,35,35,35	0
59	MG	AA	1607	1/1	0.16	-	24,24,24,24	0
59	MG	BA	3071	1/1	0.32	-	29,29,29,29	0
59	MG	AA	1642	1/1	0.19	-	30,30,30,30	0
59	MG	BA	3040	1/1	0.25	-	10,10,10,10	0
59	MG	BA	3007	1/1	0.29	-	4,4,4,4	0
59	MG	AA	1605	1/1	0.11	-	25,25,25,25	0
59	MG	BA	3016	1/1	0.07	-	15,15,15,15	0
59	MG	BA	3059	1/1	0.22	-	9,9,9,9	0
59	MG	AA	1634	1/1	0.07	-	6,6,6,6	0
59	MG	BA	3046	1/1	0.19	-	14,14,14,14	0
59	MG	AA	1629	1/1	0.13	-	38,38,38,38	0
59	MG	BA	3036	1/1	0.26	-	20,20,20,20	0
59	MG	AA	1618	1/1	0.19	-	22,22,22,22	0
59	MG	BA	3044	1/1	0.16	-	15,15,15,15	0
59	MG	BA	3069	1/1	0.33	-	14,14,14,14	0
59	MG	BA	3005	1/1	0.33	-	12,12,12,12	0
59	MG	AA	1610	1/1	0.23	-	14,14,14,14	0
59	MG	BA	3062	1/1	0.22	-	18,18,18,18	0
59	MG	BA	3066	1/1	0.25	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3079	1/1	0.22	-	14,14,14,14	0
59	MG	BD	301	1/1	0.26	-	7,7,7,7	0
59	MG	BA	3034	1/1	0.26	-	5,5,5,5	0
59	MG	BA	3042	1/1	0.32	-	11,11,11,11	0
59	MG	BA	3001	1/1	0.32	-	32,32,32,32	0
59	MG	BA	3052	1/1	0.23	-	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.