



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:17 PM BST

PDB ID : 4V6A
Title : Structure of EF-P bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-06-15
Resolution : 3.10 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>

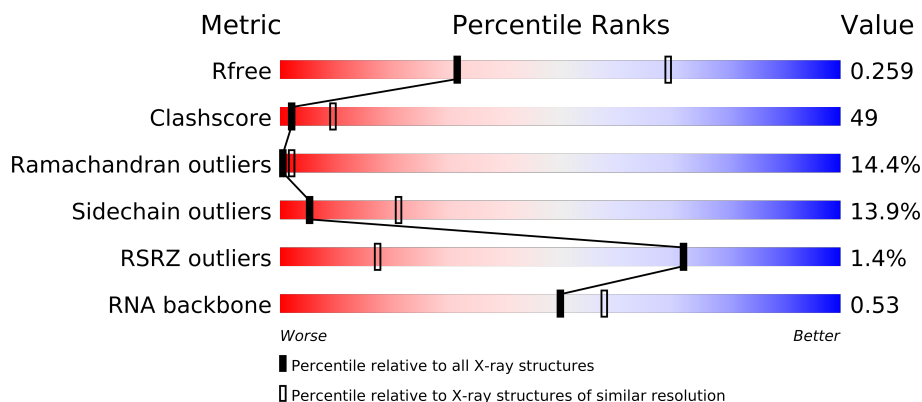
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	1509	
1	CA	1509	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	184	
22	CV	184	
23	AW	77	
23	CW	77	
24	AX	5	
24	CX	5	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BC	229	
27	DC	229	

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Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	

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Mol	Chain	Length	Quality of chain
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290405 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	1495	Total	C	N	O	P	0	0	0
			32144	14306	5964	10379	1495			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14390	5992	10446	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1004	635	195	174			
9	CI	127	Total	C	N	O	0	0	0
			1004	635	195	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			
13	CM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	80	Total	C	N	O	S	0	0	1
			613	392	110	109	2			
19	CS	78	Total	C	N	O	S	0	0	1
			619	397	111	109	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			
22	CV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			

- Molecule 23 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			
24	CX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2767	Total	C	N	O	P	0	0	0
			59596	26524	11148	19158	2766			
25	DA	2777	Total	C	N	O	P	0	0	0
			59809	26619	11186	19228	2776			

- 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			

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

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	224	Total	C	N	O	S	2	0	0
			1702	1075	309	315	3			
27	DC	220	Total	C	N	O	S	1	0	0
			1640	1033	297	307	3			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	274	Total	C	N	O	S	0	0	1
			2127	1341	425	358	3			
28	DD	274	Total	C	N	O	S	0	0	1
			2115	1335	419	358	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
29	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
30	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	168	Total	C	N	O	S	0	0	1
			1231	780	228	222	1			
32	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	1
			1043	661	185	196	1			
33	DI	146	Total	C	N	O	S	0	0	1
			871	543	162	165	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1079	672	216	189	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	139	Total	C	N	O	S	0	0	1
			1099	702	209	181	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	116	Total	C	N	O		0	0	0
			923	575	191	157				
38	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	101	Total	C	N	O		0	0	1
			777	489	156	132				
39	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	94	Total	C	N	O	S	0	0	1
			735	477	134	124				
44	DX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			757	486	144	123	4			
45	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	182	Total	C	N	O	S	0	0	1
			1438	917	258	261	2			
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	96	Total	C	N	O	S	0	0	0
			757	478	149	129	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	S	0	0	1
			460	293	90	77				
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	57	Total	C	N	O	S	0	0	1
			435	272	88	70	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	1
			401	247	82	68	4			
53	D6	48	Total	C	N	O	S	0	0	0
			322	199	62	57	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	63	Total	C	N	O	S	0	0	1
			496	317	101	76	2			
55	D8	62	Total	C	N	O	S	0	0	1
			467	299	95	71	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			294	179	66	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	459	Total	Mg	0	0
			459	459		
57	CA	109	Total	Mg	0	0
			109	109		
57	DF	1	Total	Mg	0	0
			1	1		
57	BE	1	Total	Mg	0	0
			1	1		
57	AW	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B1	1	Total 1	Mg 1	0	0
57	BP	3	Total 3	Mg 3	0	0
57	DR	1	Total 1	Mg 1	0	0
57	B5	4	Total 4	Mg 4	0	0
57	BB	9	Total 9	Mg 9	0	0
57	BT	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0
57	AA	117	Total 117	Mg 117	0	0
57	BQ	3	Total 3	Mg 3	0	0
57	D6	2	Total 2	Mg 2	0	0
57	CX	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	DD	1	Total 1	Mg 1	0	0
57	BR	1	Total 1	Mg 1	0	0
57	DA	305	Total 305	Mg 305	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	1	Total 1	Mg 1	0	0
57	DP	1	Total 1	Mg 1	0	0
57	CW	5	Total 5	Mg 5	0	0
57	D5	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BD	1	Total 1	Mg 1	0	0
57	AT	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	CE	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	0	0
57	BH	1	Total 1	Mg 1	0	0

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

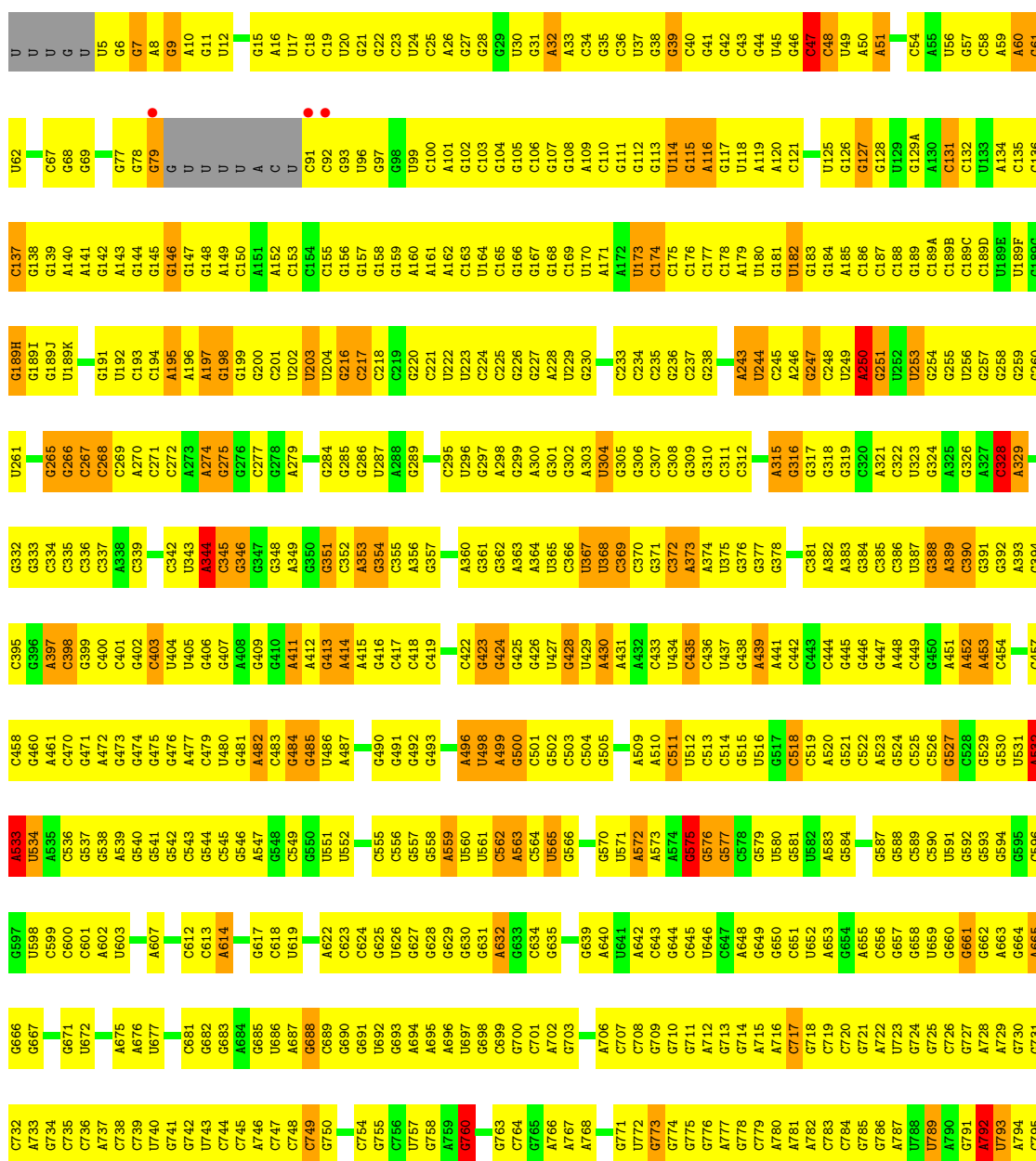
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B5	1	Total 1	Zn 1	0	0
58	AD	1	Total 1	Zn 1	0	0
58	B9	1	Total 1	Zn 1	0	0
58	D9	1	Total 1	Zn 1	0	0
58	D5	1	Total 1	Zn 1	0	0
58	CD	1	Total 1	Zn 1	0	0

3 Residue-property plots

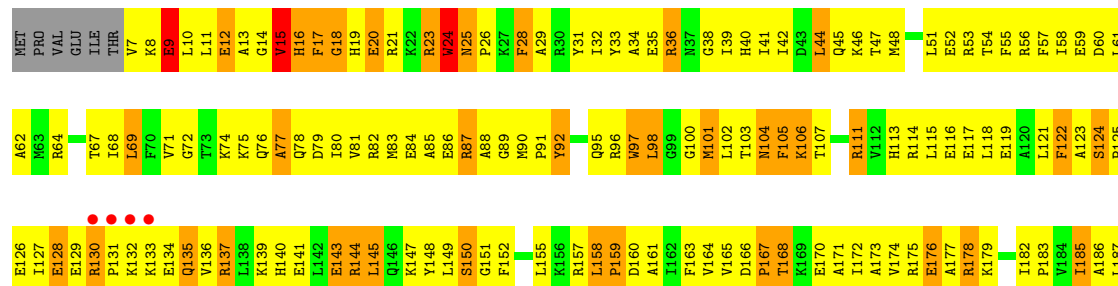
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain AA: 



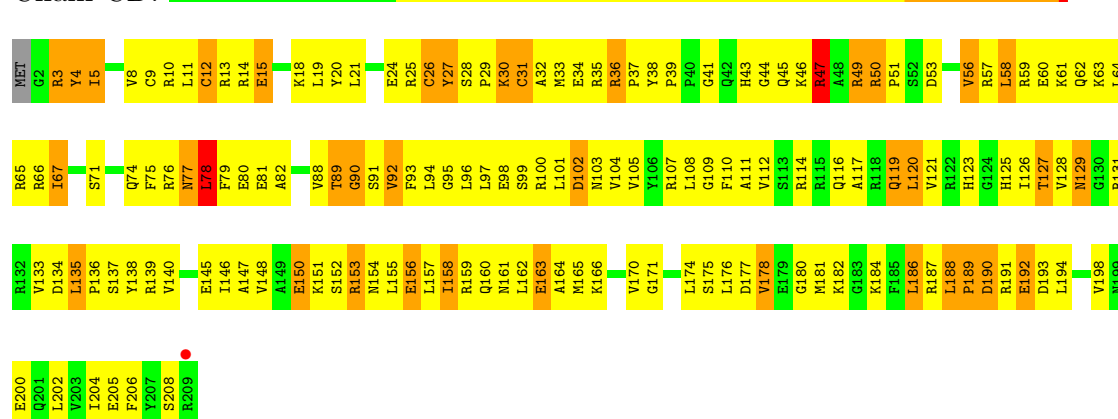






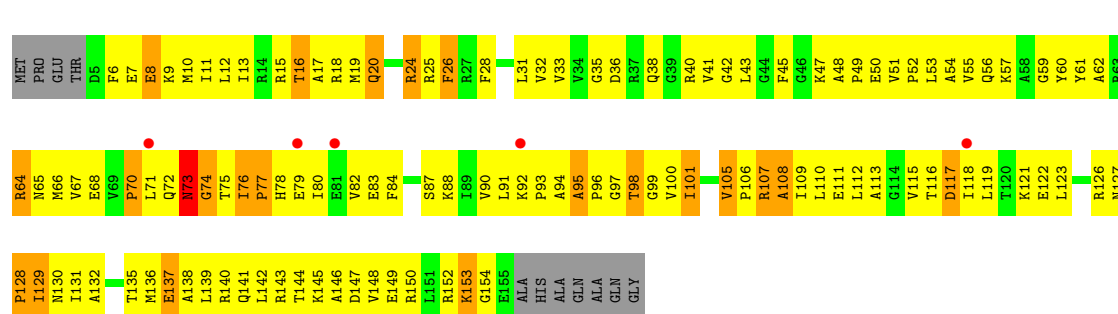
- Molecule 4: 30S ribosomal protein S4

Chain CD:



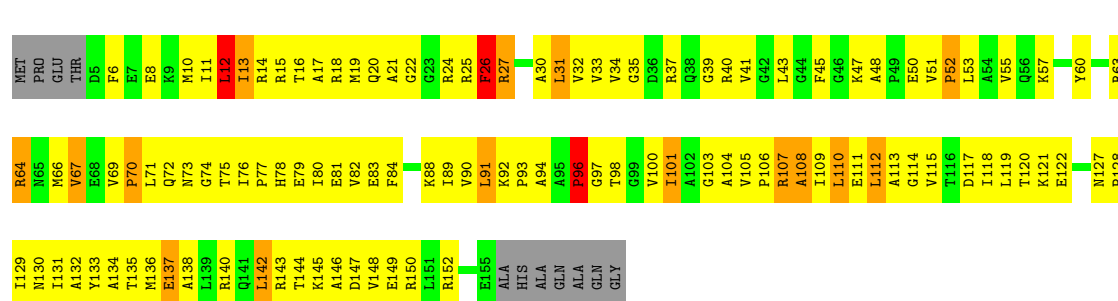
- Molecule 5: 30S ribosomal protein S5

Chain AE:



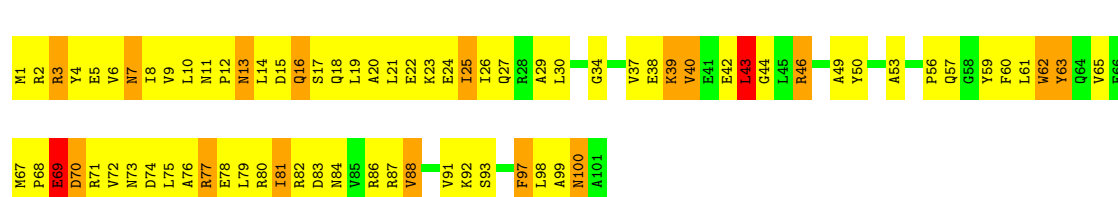
- Molecule 5: 30S ribosomal protein S5

Chain CE:



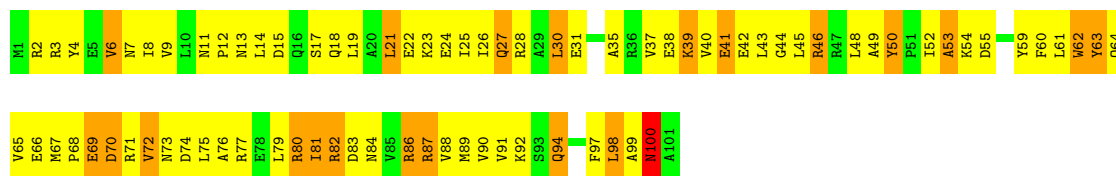
- Molecule 6: 30S ribosomal protein S6

Chain AF:



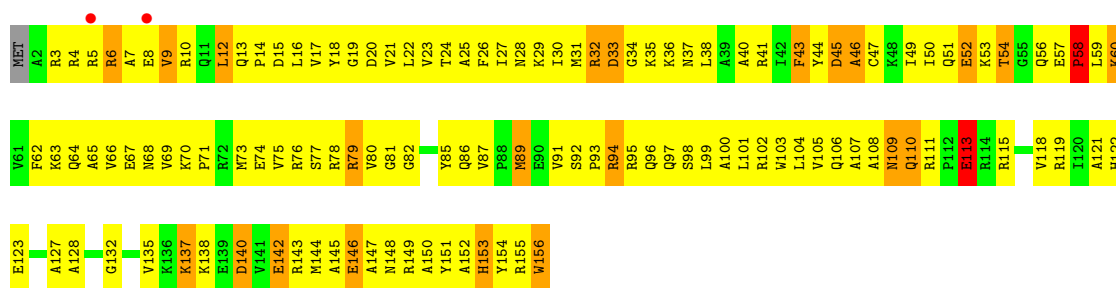
- Molecule 6: 30S ribosomal protein S6

Chain CF:



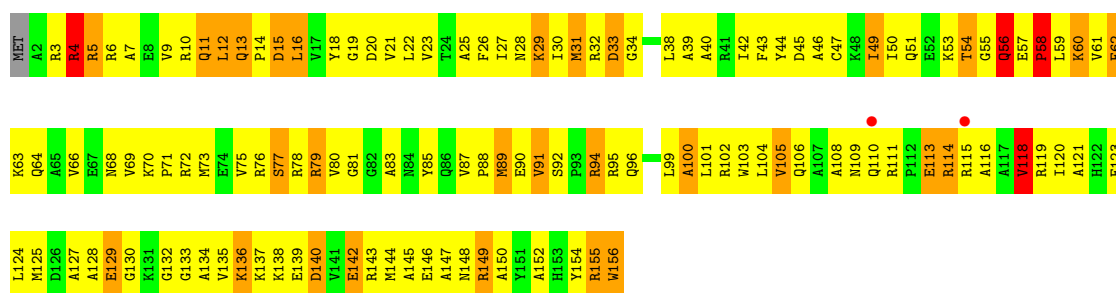
- Molecule 7: 30S ribosomal protein S7

Chain AG:



- Molecule 7: 30S ribosomal protein S7

Chain CG:



- Molecule 8: 30S ribosomal protein S8

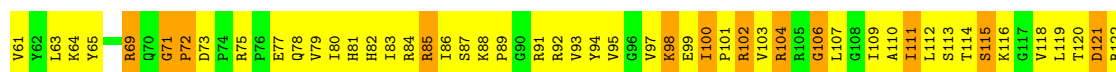
Chain AH:



- Molecule 8: 30S ribosomal protein S8

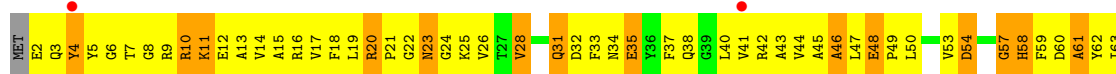
Chain CH:





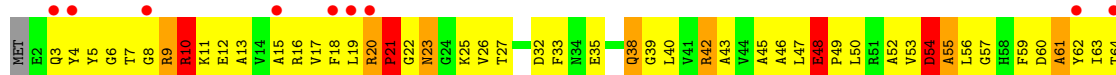
• Molecule 9: 30S ribosomal protein S9

Chain AI:



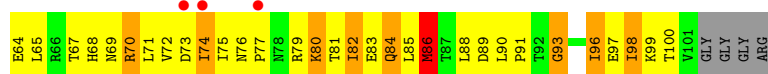
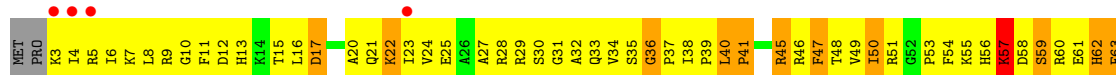
• Molecule 9: 30S ribosomal protein S9

Chain CI:



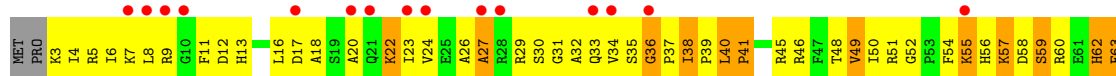
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



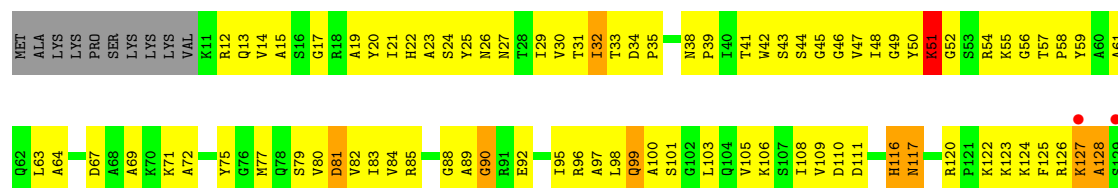
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



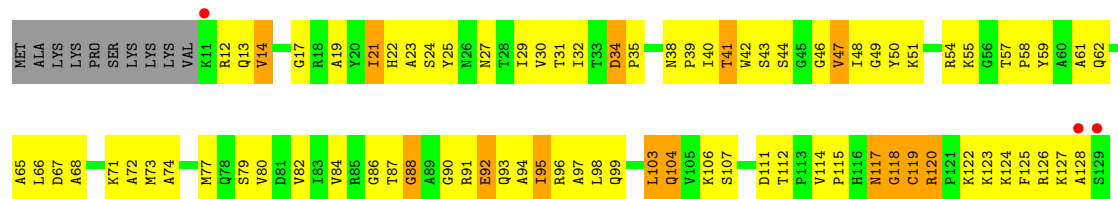
- Molecule 11: 30S ribosomal protein S11

Chain AK:



- Molecule 11: 30S ribosomal protein S11

Chain CK:



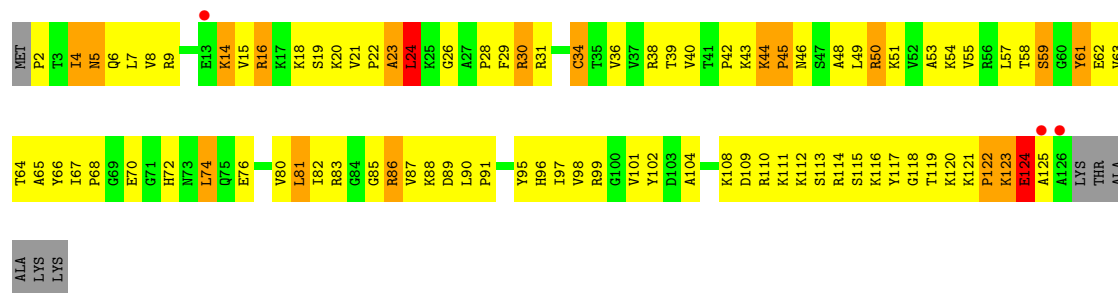
- Molecule 12: 30S ribosomal protein S12

Chain AL:



- Molecule 12: 30S ribosomal protein S12

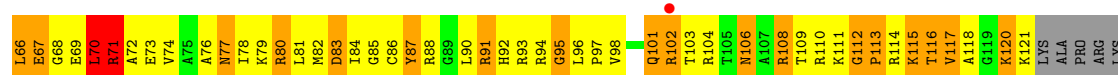
Chain CL:



- Molecule 13: 30S ribosomal protein S13

Chain AM:





- Molecule 13: 30S ribosomal protein S13

Chain CM:



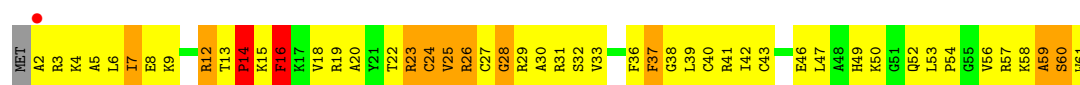
- Molecule 14: 30S ribosomal protein S14

Chain AN:



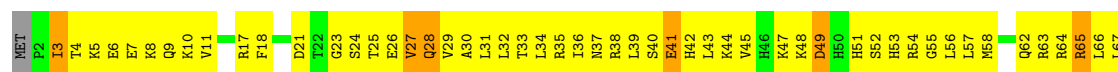
- Molecule 14: 30S ribosomal protein S14

Chain CN:



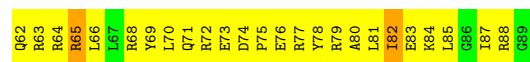
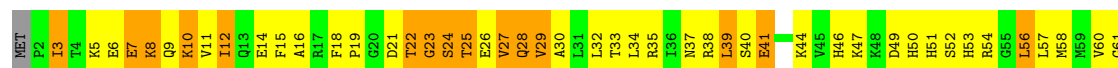
- Molecule 15: 30S ribosomal protein S15

Chain AO:



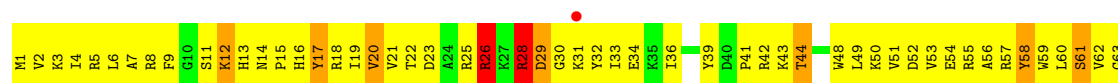
- Molecule 15: 30S ribosomal protein S15

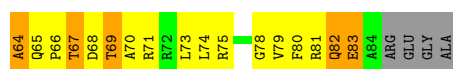
Chain CO:



- Molecule 16: 30S ribosomal protein S16

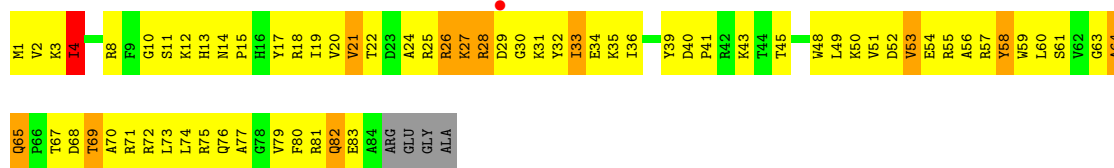
Chain AP:





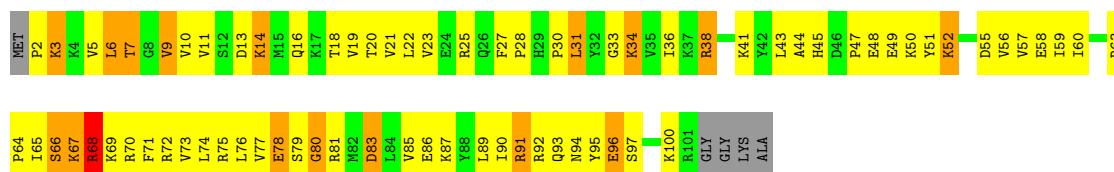
- Molecule 16: 30S ribosomal protein S16

Chain CP:



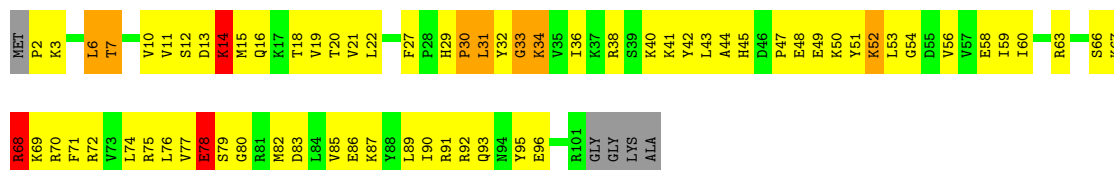
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



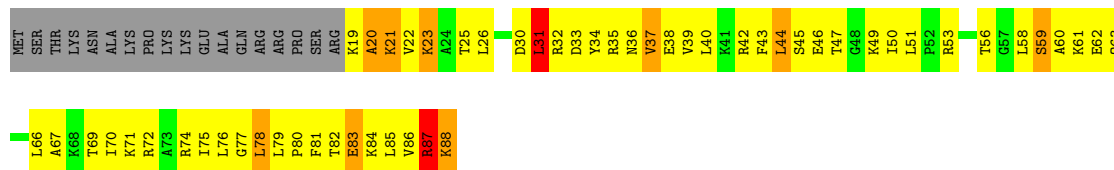
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



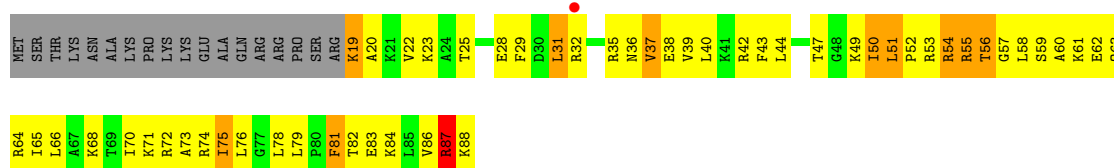
- Molecule 18: 30S ribosomal protein S18

Chain AR:



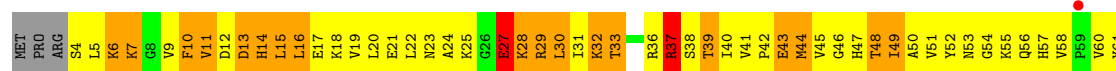
- Molecule 18: 30S ribosomal protein S18

Chain CR:



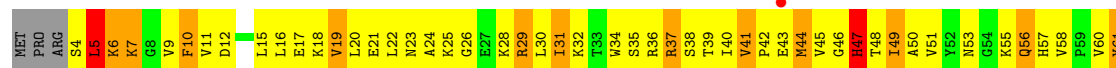
- Molecule 19: 30S ribosomal protein S19

Chain AS: 



- Molecule 19: 30S ribosomal protein S19

Chain CS: 



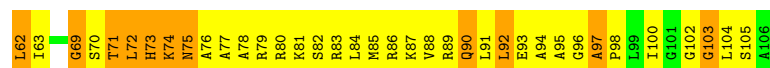
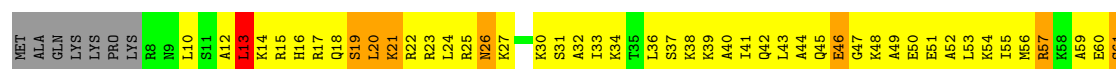
- Molecule 20: 30S ribosomal protein S20

Chain AT: 



- Molecule 20: 30S ribosomal protein S20

Chain CT: 



- Molecule 21: 30S ribosomal protein Thx

Chain AU: 



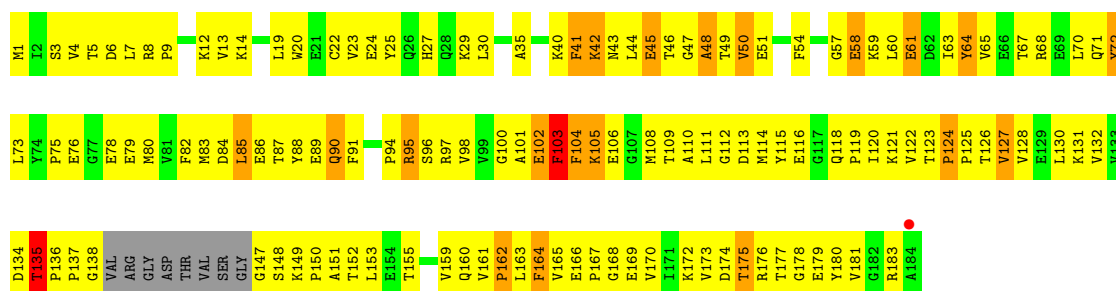
- Molecule 21: 30S ribosomal protein Thx

Chain CU: 



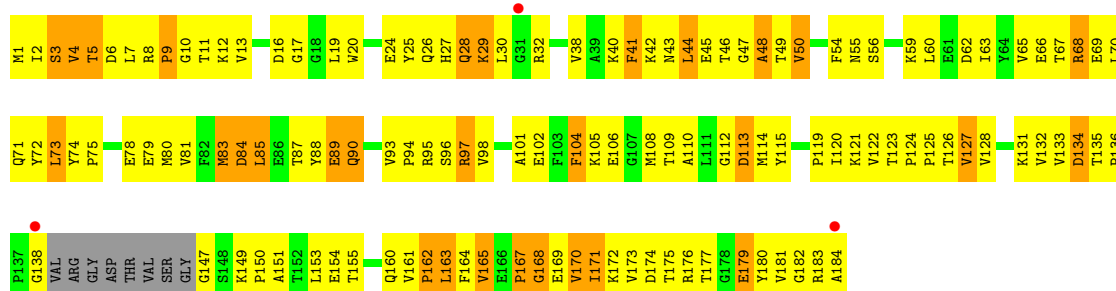
- Molecule 22: Elongation factor P

Chain AV: 



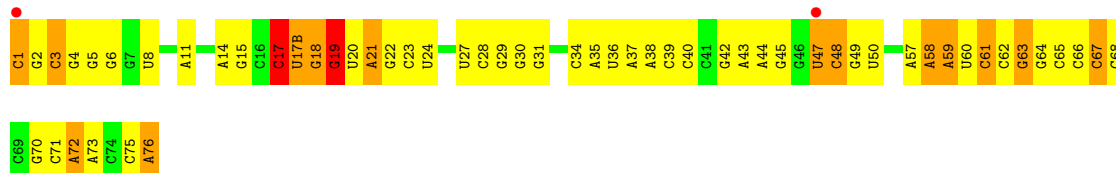
- Molecule 22: Elongation factor P

Chain CV:



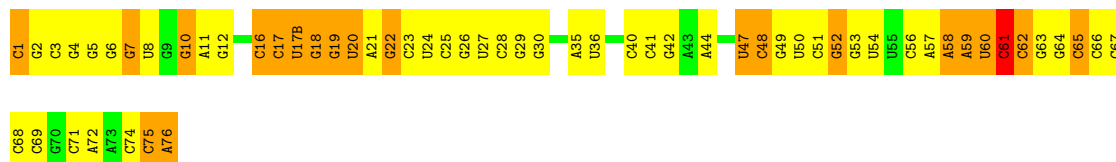
- Molecule 23: tRNA-Met

Chain AW:



- Molecule 23: tRNA-Met

Chain CW:



- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

Chain AX:



- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

Chain CX:



A1900	G1823	G1750	G1604	U	C1408	A1342	A1269	G1187	C1119	G	C995	C923
A1901	G1824	C1751	C1605	A	C1409	A1342	C1270	U1188	G1120	U	A996	C924
G1902	A1825	G1676	C1606	C	G1470	G1344	G1271	A1189	C1121	G	C997	C925
G1903	G1826	G1753	C1607	G	C1471	G1344	A1272	G1190	G122	G	C998	A926
G1906	C1827	C1754	A1608	G	G1476	C1345	U1273	G1191	C1123	C	U999	G927
G1907	G1828	A1755	A1609	G	G1476	G1346		G1195	G1124	C	A1000	G928
C1908	A1829	G1756	A1610	U	A1477	G1347	A1276		G1125	U	A1001	U930
C1909	C1830	U1757	C1611	G	G1478	G1348	G1277			U	G1002	U931
G1910	G1831	G1758	G1681	A	G1479	A1349	A1278	G1203	U1130	A	C1003	G932
U1911	U1832		G1682	C	A1418	C1350	G1279	A1204	G1131	G	A1004	G933
A1912	A1833	A1762	G1683	A1544	A1419	C1351	G1280	U1205		A	C1005	G934
A1913	G1837	G1763	C1684	A1545	U1420	G1352	G1281	G1206	G1135	A	C1006	
C1914	C1838	G1764	A1616	C1546	G1421	A1353	U1282	C1207	G1136	G		A941
U1915	G1839	C1765	C1617	C1547		A1354	G1283	C1208	G1137	C	A1009	G942
A1916	U1766	U1767	A1618	C1548	G1424	G1355	U1288	G1209	G1138	A	A1010	U943
U1917	G1768	G1772	G1688		G1425	G1356	A1210	A1210	G1139	G	G1011	U944
A1918	C1843	C1773	A1689	A1553	G1426	U1357	C1289	G1215	C1140	A	U1012	A945
G1921	G1844	G1770	A1690	A1558	A1427	G1358	C1290	G1212	U1141	C	C1013	G946
G1922	G1845	C1771	C1692	G1559	G1428	A1359	U1291	A1213	U1142	U	U1014	
U1923	G1846	A1772	U1693	G1560	G1429	A1360	U1292	A1214	A1143	C	G1017	C951
C1924	A1847	C1774	G1694	G1561	C1430	G1361	U1293	G1215	A1143	C	C1018	G952
C1925	G1850	U1775	G1695	A1562	U1431	C1362	U1294	G1216	G1144	U	U1019	A953
U1926	G1851	G1776	G1696	G1563	C1432	C1363	C1295		C1145	U	G954	
G1929	C1852	U1777	A1688	G1564	U1433	G1364	G1296	C1221	C1146	U	A1020	C955
G1930	A1853	U1778	G1699	A1667	A1434	A1365	G1297	C1221A	C1147	U	G956	
U1931	A1854	A1779	C1636	G1568	G1435	A1366	U1300	C1222	A1148	A	G1022	A957
U1932	G1855	A1780	A1637	G1569	G1436	A1367	A1301	G1223	G1149	A	U1023	U958
A1933	G1856	C1781	C1638	A1570	A1439	G1368	A1302	C1224	C1150	A	G1024	A959
C1934	G1857	C1782	U1639	C1571		C1375	G1303		G1151	G	G1025	A960
G1935	G1858	A1783	C1640	A1572	G1442	G1376	A1307	G1232	C1152	U	U1026	C961
U1936	A1859	A1784	A1641	A1573	G1443	A1377	A1308	G1233	C1153	G	A1027	G962
A1937	G1860	A1785	G1642	C1574	G1444	A1378	A1309	U1234	G1154	U	A1028	U963
A1938	G1861	A1786	C1643	C1575	A1445A	A1379	G1310	G1235	A1155	G		C964
U1939	C1862	U1787	C1644	U1576	G1446	G1380	G1311	G1236	A1156	C	U1032	G966
U1940	G1863	C1788	U1709	C1577	G1447	G1381	U1312	G1238	C1161	U	U1035	U969
C1941	U1864	A1789	C1711	C1578	G1448	G1382	U1313	U1240	G1162	A	G1036	C970
G1948	G1865	C1790	C1712	U1578	A1449	A1383	C1314	A1241	G1163	U	G1037	C971
G1949	C1866	A1791	U1713	A1579	G1450	G1385	C1315	A1242	G1164	A	C1038	G972
U1950	A1876	G1792	G1714	G1580	C1450A	C1386	U1316	G1243	U1165	G	G1039	A973
U1951	C1877		G1717	G1581	C1451	C1387	A1317	G1244	U1167	C	C1040	G974
A1952	G1878	U1796	G1718	C1582	U1452	G1388	G1245	G1245	G1168	U	C975	
G1953	C1882	U1797	G1719	C1583	U1453	G1389	C1320	A1246	G1169	C	G1042	G975A
A1954	G1883	U1798	U1720	A1586	G1455		A1321	A1247	G1170	A	C1043	C976
G1955	A1884	G1799	G1721	A1587	G1456	A1393	A1322		G1171	C	G1044	G977
U1956	C1885	C1800	A1722	C1588	A1457	U1394	U1323	C1251	G1173	U	A1045	G978
U1957	A1886	G1801	U1739	C1589	C1458	A1395	G1324	G1252	A1174	G	A	G979
C1957	C1887	A1802	G1740	U1590	G1459	U1396	G1325	A1253	U1175	A	A	A980
G1958	G1888	A1803	A1741	G1591	A1460	U1397	U1326	G1256	G1176	C	C	A981
U1959	U1805	C1804	G1742	C1592	G1461	C1398	C1327	G1256	A1177	C	C	C982
G1963	A1815	G1745	C1744	G1593	C1462	C1399	G1328	G1260	C1178	A	A	A983
C1964	G1816	A1745A	G1663	G1594	C1463	G1400	A1331	C1261	C1179	G	C	G987
C1965	G1746	G1746A	A1665	G1595	A1528	G1401	G1332	C1261	C1180	C	C	A990
A1966	G1747	G1747	G1666	A1596	G1455	C1402	C1332	U1263	G1181	C	A	C991
C1967	A1819	U1820	G1667	G1597	C1467	C1403	C1334	G1264	A1182	G	G	C992
G1968	U1821	G1747A	A1668	C1598	C1468	U1405	G1338	A1265	G1183	A	A	
A1969	G1822	A1749	C1670	C1532	A1469	U1406	G1338	G1268	C1185	G	G	C993
				G	G1470	C1407	G1339		G1186	C	G	C994

U2847	C2784	A2721	C2652	G2581	C2442	G2370	A2309	C2240	A2170	U2109	G2037	A1970
G2848	C2785	G2722	U2653	G2582	C2443	G2371	A2310	A2241	A2171	G2110	G2038	A1971
U2849	C2786	C2723	A2654	G2583	G2444	G2372	A2311	G2242	A2172	G2111	C2039	A1972
A2850	C2787	C2724	U2584	U2584	G2445	U2373	U2312	U2243	A2173	C2112	C2040	G1973
A2851	C2788	A2725	C2655	U2585	A2446	G2374	C2314	U2245	C2174	U2113	A2042	C1974
G2852	C2789	U2726	U2586	C2520	A2448	G2375	C2315	U2246	C2175	A2114	C2043	
C2853	G2727	G2727	C2662	C2521	C2452	A2376	G2316	G2247	A2176	G2115	C2044	A1981
G2854	C2791	G2728	G2663	U2522	U2455	A2377	C2317	A2248	C2177	G2116	C2049	C1982
G2855	C2792	G2729	G2664	G2523	G2456	C2380	G2318	C2249	C2178	A2117	C2050	C1983
C2856	C2793	G2730	A2665	G2524	U2457	G2381	G2319	U2249	C2179	G2120	G1984	G1985
G2857	C2794	A2732	C2666	G2525	U2458	G2382	A2320	C2254	U2180	U2121	G2051	G1986
C2863	U2795	A2733	U2667	G2526	U2459	G2383	G2321	C2261	G2181	U2122	G2052	A1987
G2864	U2796	A2734	G2668	C2527	G2458	G2384	A2322	U2262	G2182	G2123	A2053	G1988
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U2866	A2801	G2736	A2670	G2529	U2460	G2387	C2324	C2264	G2184	G2125	C2055	G1990
U2867	A2801A	G2737	A2671	A2530	C2461	G2388	U2324	C2265	G2186	A2126	G2056	U1991
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G2877	G2812	G2747	U2682	C2610	G2472	G2405	G2340	G2280	G2201	C	G2068	G2002
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C2879	G2814	A2749	U2684	C2612	C2474	C2342	A2336	G2282	U2203	C	G2070	G2004
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A2881	G2816	A2751	C2686	U2614	A2476	C2403	G2338	A2284	G2206	C	G2072	C2006
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	A2823	A2758	C2695	G2621	G2485	U2417	C2347	U2291	G2222	U	G2087	A2015
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G2833	G2833	C2768	G2706	A2632	C2498	U2431	A2358	A2299	G2232	C	U2099	G2027
A2834	G2834	G2707	U2707	U2633	G2502	U2431	A2359	G2300	G2233	C	G2100	U2028
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G2837	G2837	C2773	C2710	G2636	U2505	U2431	A2362	G2303	U2236	C	G2103	A2031
C2838	G2838	C2774	A2711	G2637	U2506	U2431	A2363	G2304	G2237	C	G2104	G2032
G2839	G2839	A2775	U2712	G2642	U2507	U2431	A2364	A2305	G2238	C	G2105	A2033
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G2841	G2841	G2777	A2714	G2644	G2509	U2431	A2366	G2307	G2240	C	G2107	G2035
C2842	G2842	A2778	G2715	G2645	U2511	U2431	A2367	G2308	G2241	C	G2108	C2036
G2843	G2843	U2779	C2716	U2647	C2512	U2431	A2368					
G2844	G2844	A2780	G2717	G2648	C2513	U2431	A2369					
G2845	G2845	G2781		U2649	U2514	U2431	A2369					
G2846	G2846			U2580								

● Molecule 25: 23S ribosomal RNA

Chain DA:

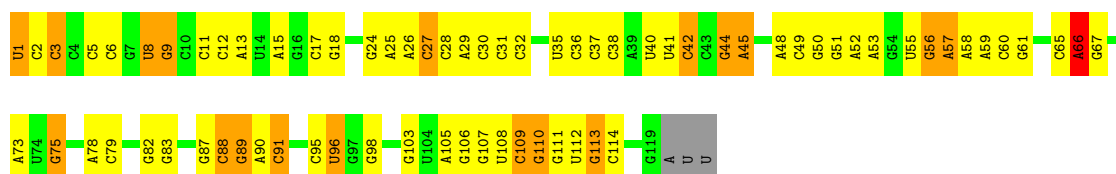
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WORLDWIDE
PDB
PROTEIN DATA BANK

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C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625
C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689
C2731	C2732	C2733	C2734	C2735	C2736	C2737	C2738	C2739	C2740	C2741	C2742	C2743	C2744	C2745	C2746	C2747	C2748	C2749	C2750	C2751	C2752	C2753
C2791	C2792	C2793	C2794	C2795	C2796	C2797	C2798	C2799	C2800	C2801	C2802	C2803	C2804	C2805	C2806	C2807	C2808	C2809	C2810	C2811	C2812	C2813
C2856	C2857	C2858	C2859	C2860	C2861	C2862	C2863	C2864	C2865	C2866	C2867	C2868	C2869	C2870	C2871	C2872	C2873	C2874	C2875	C2876	C2877	C2878
C2983	C2984	C2985	C2986	C2987	C2988	C2989	C2990	C2991	C2992	C2993	C2994	C2995	C2996	C2997	C2998	C2999	C3000	C3001	C3002	C3003	C3004	C3005
C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077
C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112
C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184
C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283
C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357
C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423
C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493
C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554
C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625
C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689
C2731	C2732	C2733	C2734	C2735	C2736	C2737	C2738	C2739	C2740	C2741	C2742	C2743	C2744	C2745	C2746	C2747	C2748	C2749	C2750	C2751	C2752	C2753
C2791	C2792	C2793	C2794	C2795	C2796	C2797	C2798	C2799	C2800	C2801	C2802	C2803	C2804	C2805	C2806	C2807	C2808	C2809	C2810	C2811	C2812	C2813
C2856	C2857	C2858	C2859	C2860	C2861	C2862	C2863	C2864	C2865	C2866	C2867	C2868	C2869	C2870	C2871	C2872	C2873	C2874	C2875	C2876	C2877	C2878
C2983	C2984	C2985	C2986	C2987	C2988	C2989	C2990	C2991	C2992	C2993	C2994	C2995	C2996	C2997	C2998	C2999	C3000	C3001	C3002	C3003	C3004	C3005

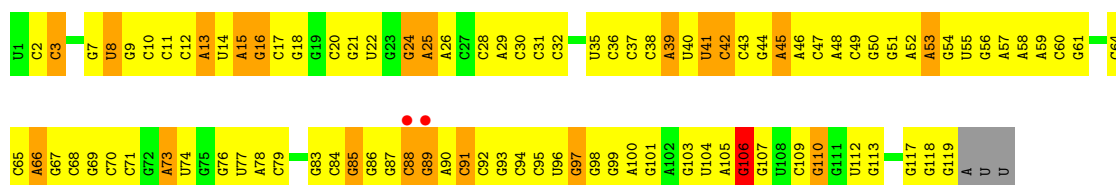
• Molecule 26: 5S ribosomal RNA

Chain BB:



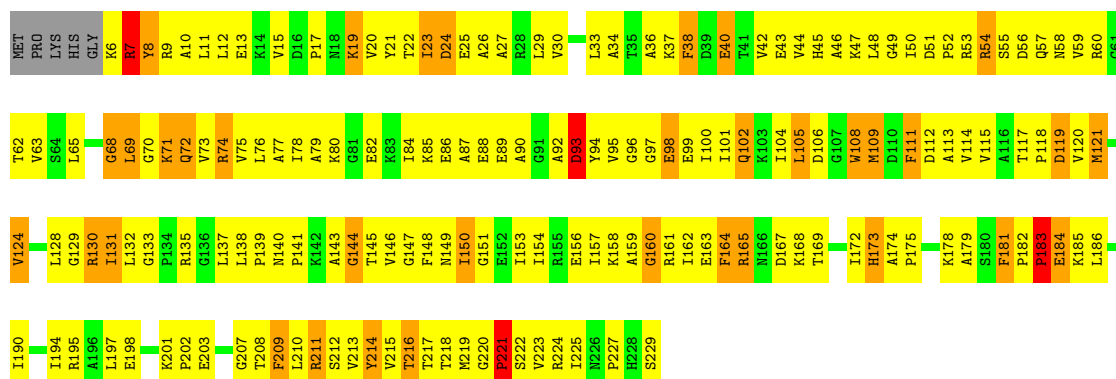
• Molecule 26: 5S ribosomal RNA

Chain DB:



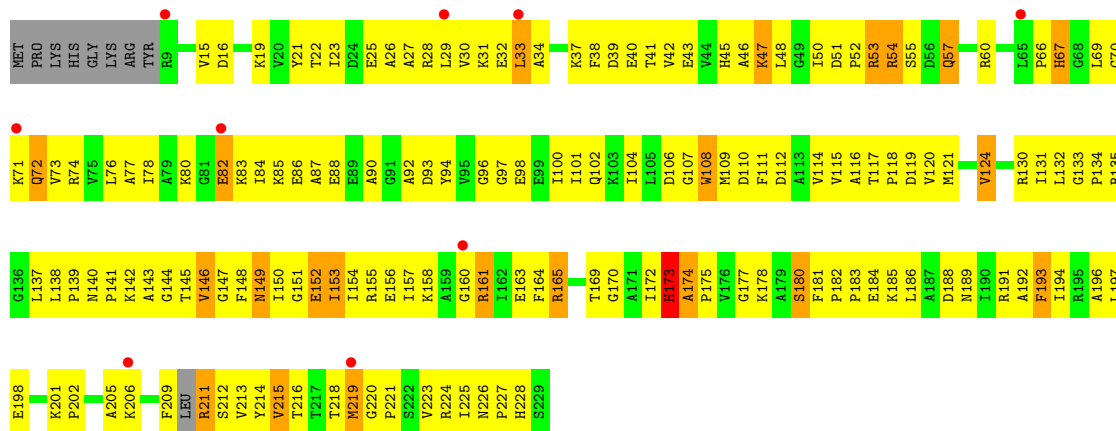
• Molecule 27: 50S ribosomal protein L1

Chain BC:



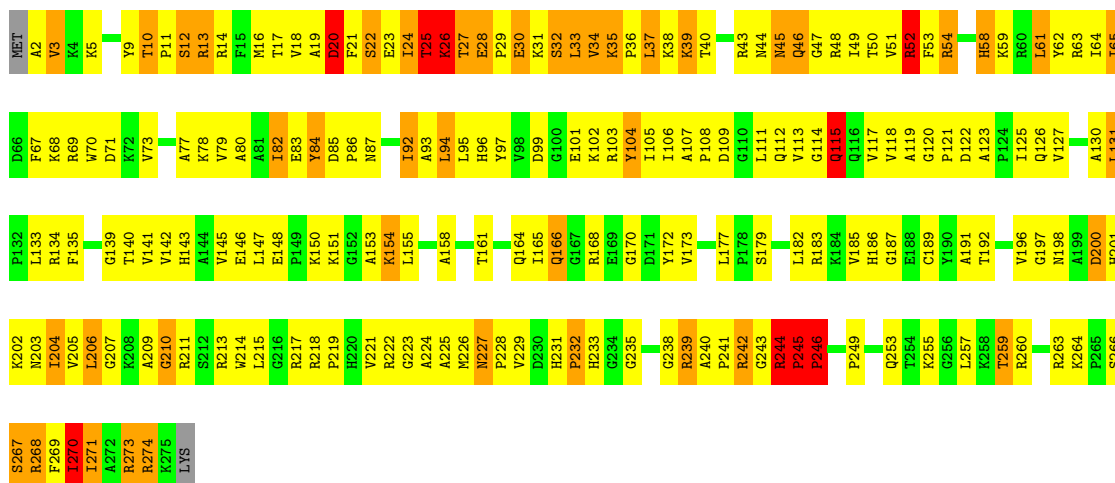
• Molecule 27: 50S ribosomal protein L1

Chain DC:



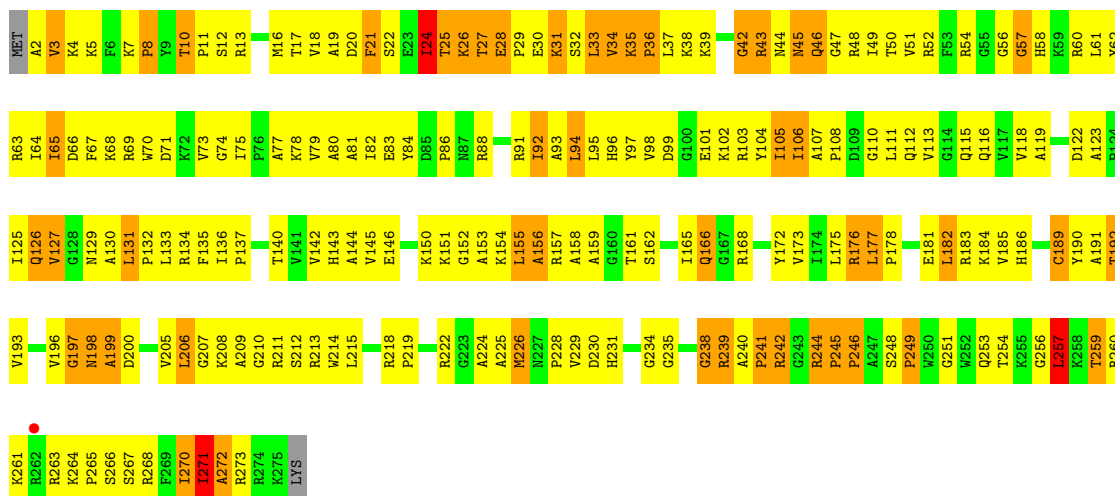
• Molecule 28: 50S ribosomal protein L2

Chain BD:



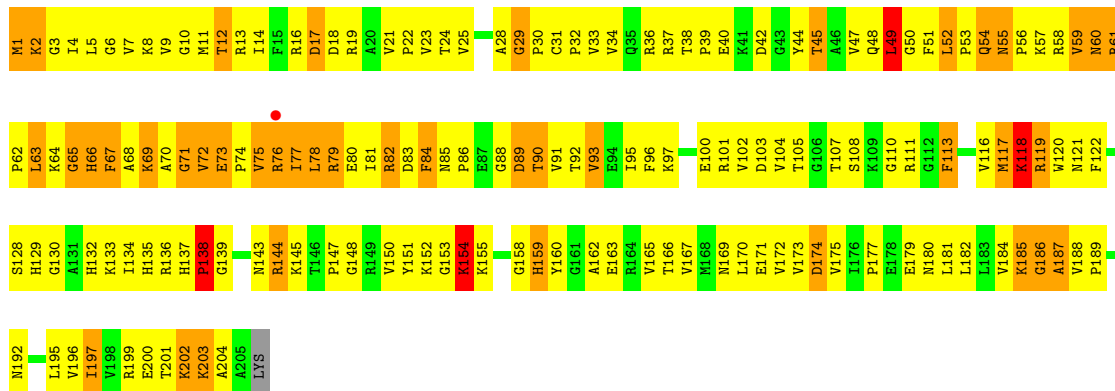
• Molecule 28: 50S ribosomal protein L2

Chain DD:



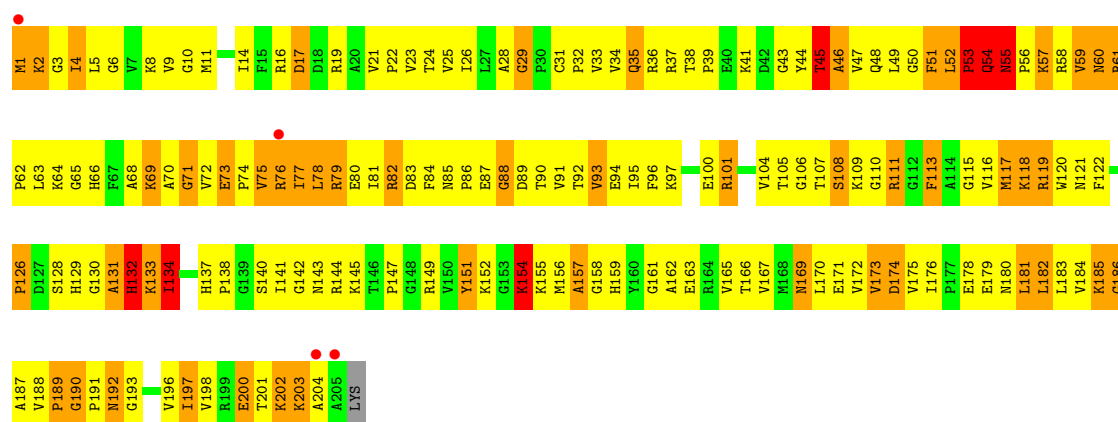
• Molecule 29: 50S ribosomal protein L3

Chain BE:



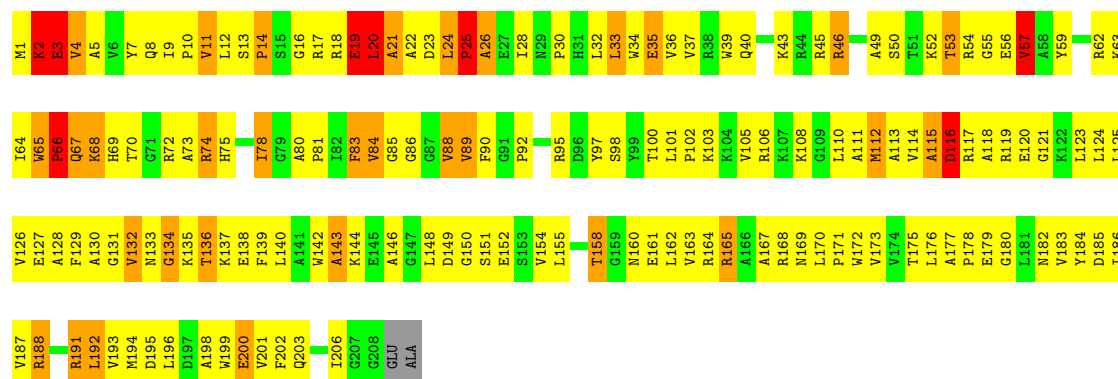
• Molecule 29: 50S ribosomal protein L3

Chain DE:



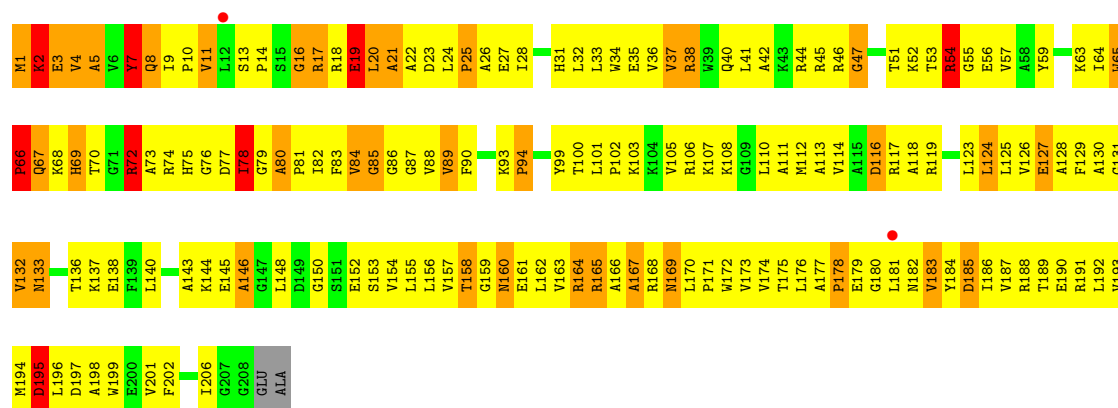
• Molecule 30: 50S ribosomal protein L4

Chain BF:



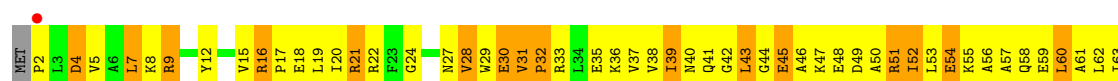
• Molecule 30: 50S ribosomal protein L4

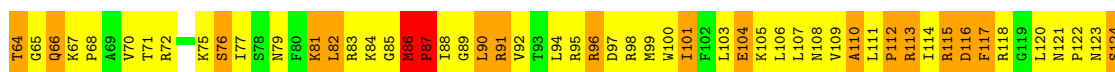
Chain DF:



• Molecule 31: 50S ribosomal protein L5

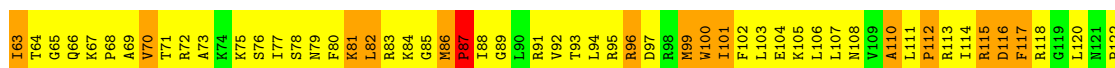
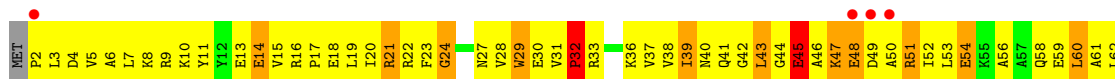
Chain BG:





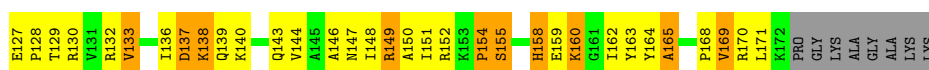
• Molecule 31: 50S ribosomal protein L5

Chain DG:



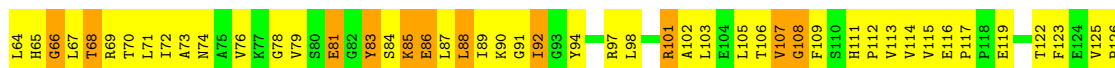
• Molecule 32: 50S ribosomal protein L6

Chain BH:



• Molecule 32: 50S ribosomal protein L6

Chain DH:



• Molecule 33: 50S ribosomal protein L9

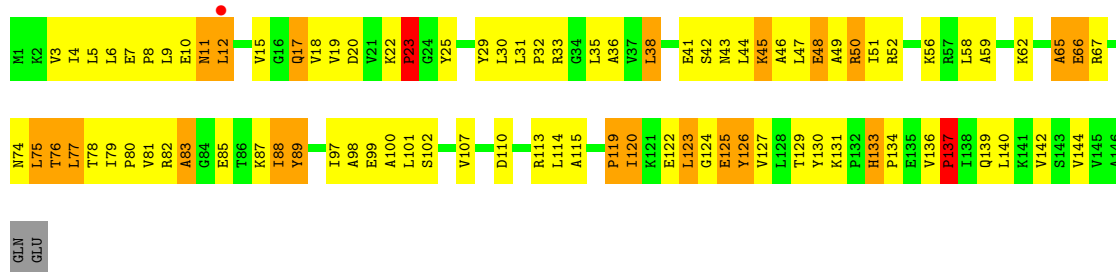
Chain BI:





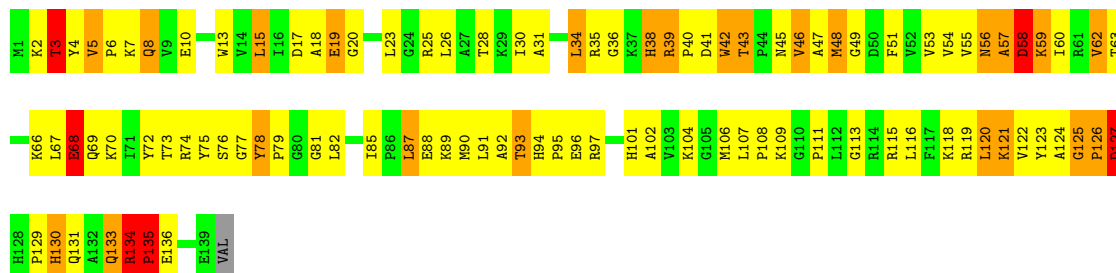
- Molecule 33: 50S ribosomal protein L9

Chain DI:



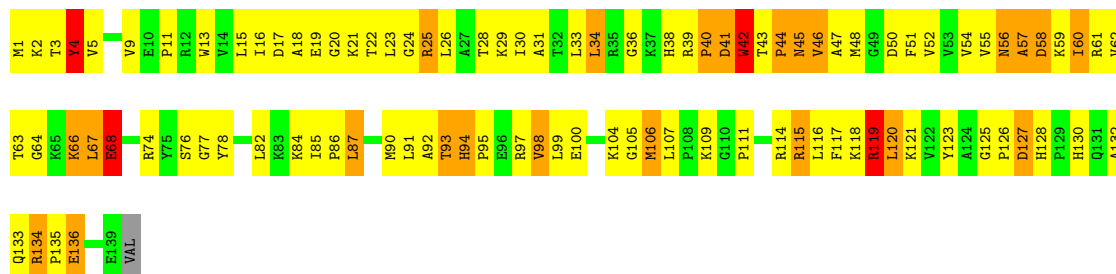
- Molecule 34: 50S ribosomal protein L13

Chain BN:



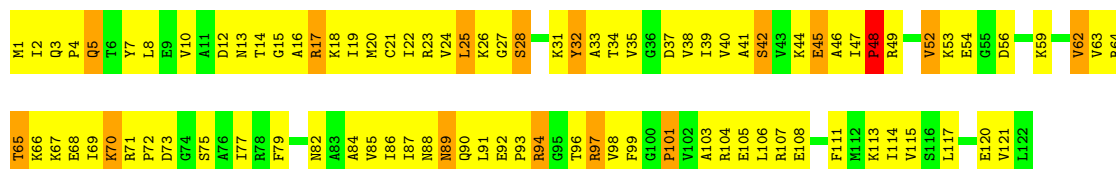
- Molecule 34: 50S ribosomal protein L13

Chain DN:



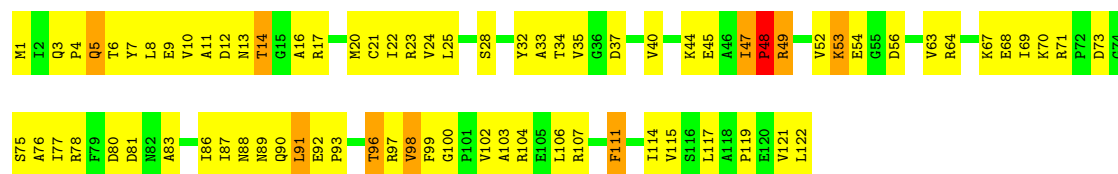
- Molecule 35: 50S ribosomal protein L14

Chain BO:



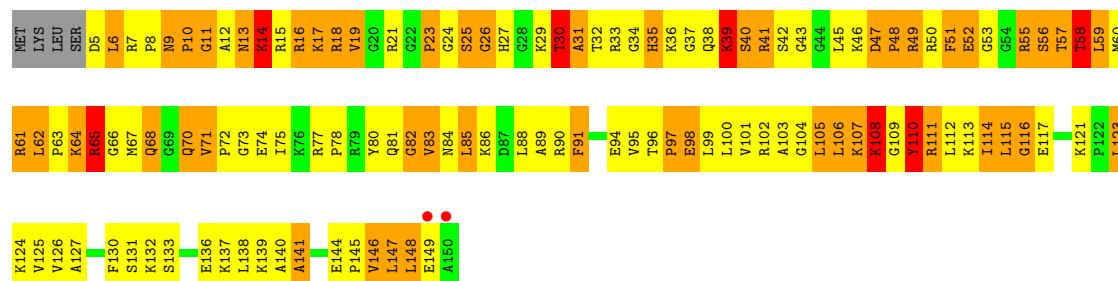
- Molecule 35: 50S ribosomal protein L14

Chain DO:



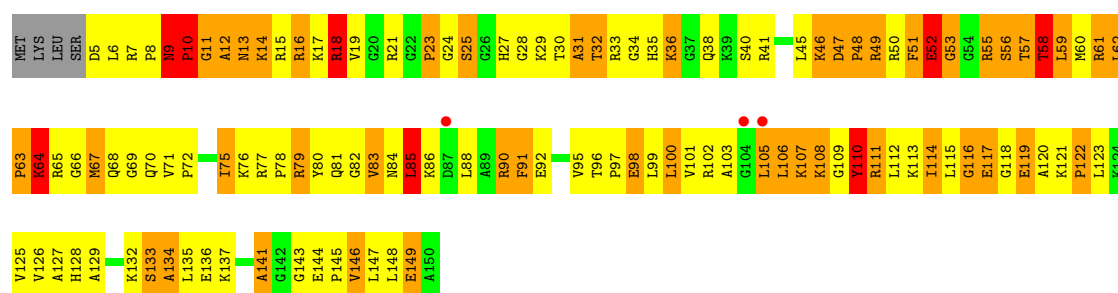
- Molecule 36: 50S ribosomal protein L15

Chain BP:



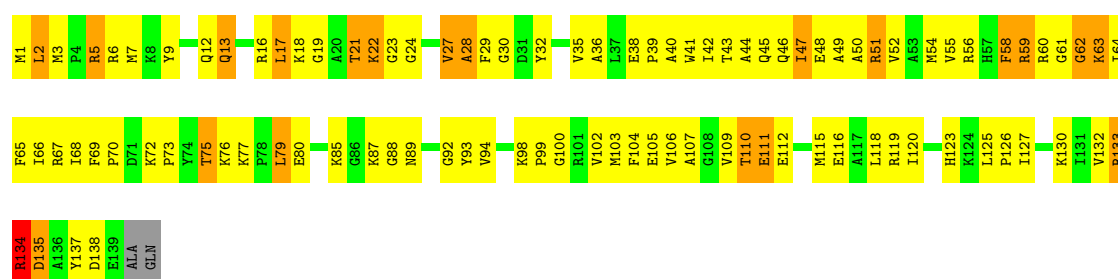
- Molecule 36: 50S ribosomal protein L15

Chain DP:



- Molecule 37: 50S ribosomal protein L16

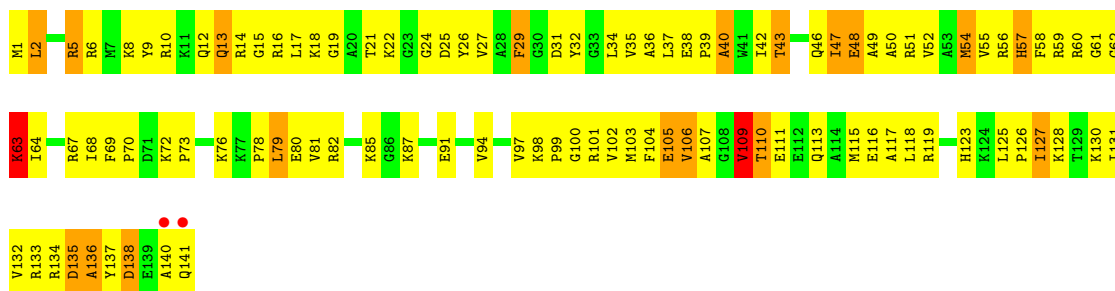
Chain BQ:



- Molecule 37: 50S ribosomal protein L16

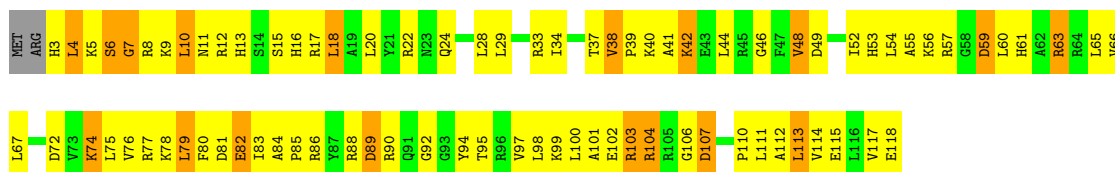
Chain DQ:





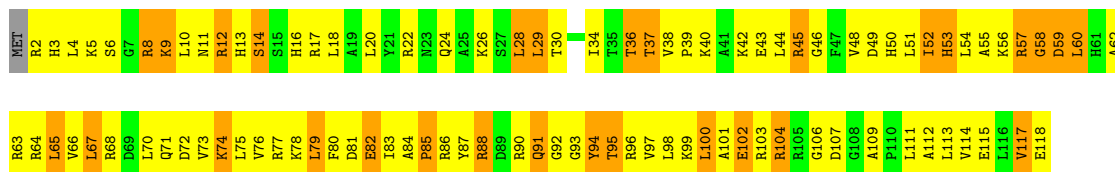
- Molecule 38: 50S ribosomal protein L17

Chain BR:



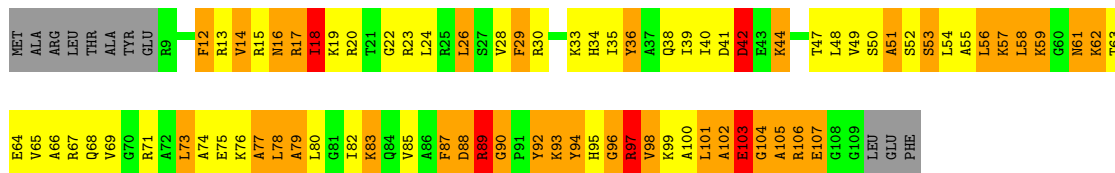
- Molecule 38: 50S ribosomal protein L17

Chain DR:



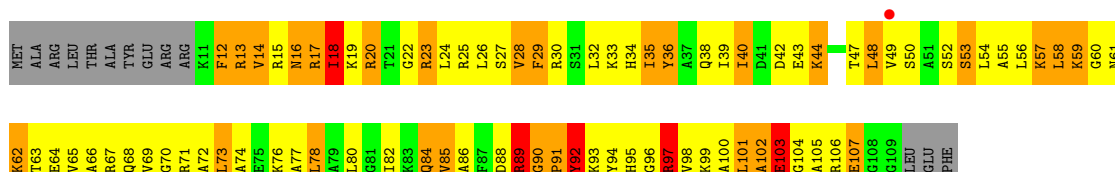
- Molecule 39: 50S ribosomal protein L18

Chain BS:



- Molecule 39: 50S ribosomal protein L18

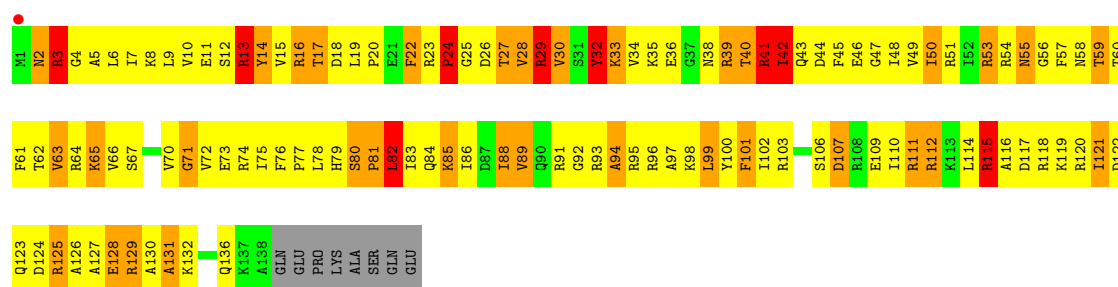
Chain DS:



- Molecule 40: 50S ribosomal protein L19

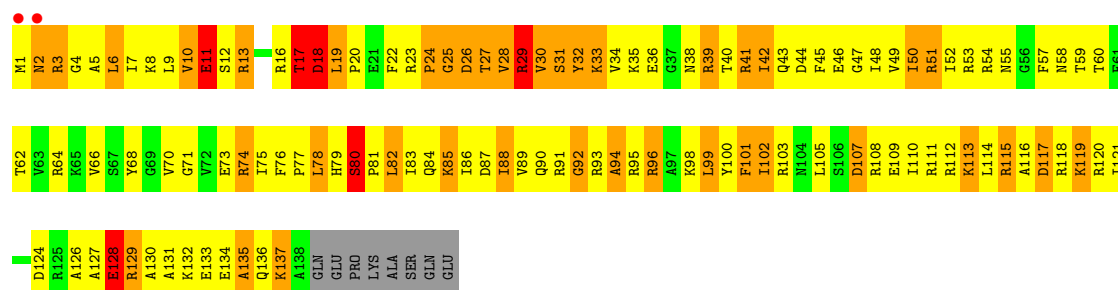
Chain BT:





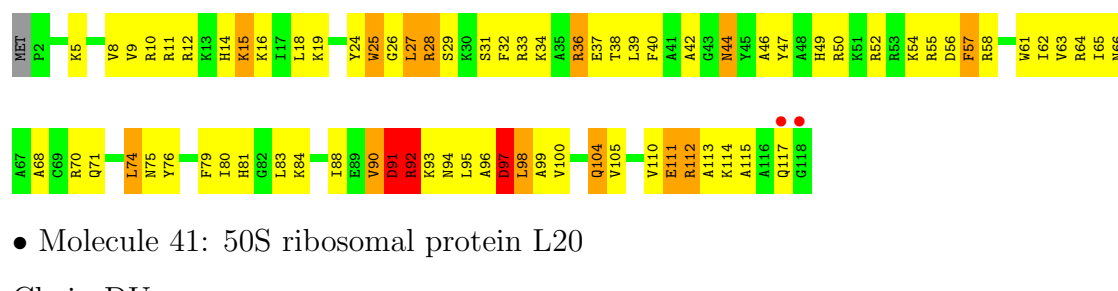
- Molecule 40: 50S ribosomal protein L19

Chain DT:



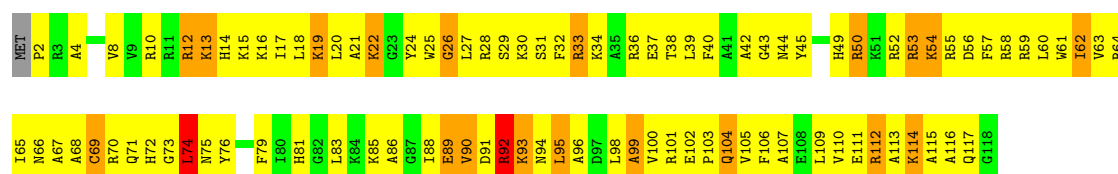
- Molecule 41: 50S ribosomal protein L20

Chain BU:



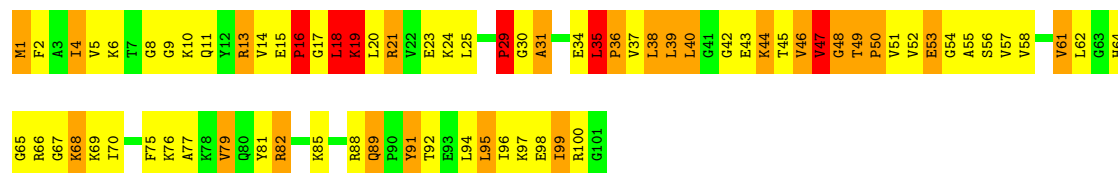
- Molecule 41: 50S ribosomal protein L20

Chain DU:



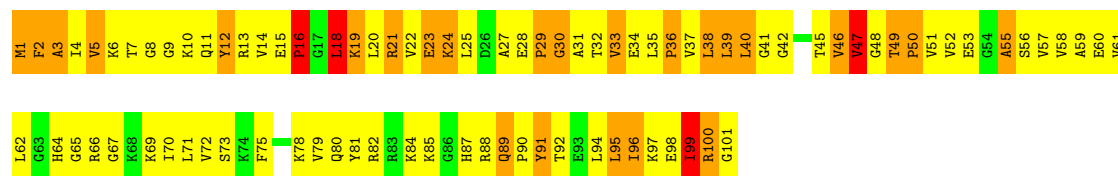
- Molecule 42: 50S ribosomal protein L21

Chain BV:



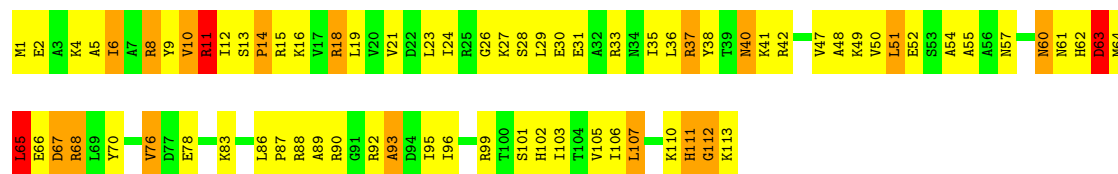
- Molecule 42: 50S ribosomal protein L21

Chain DV:



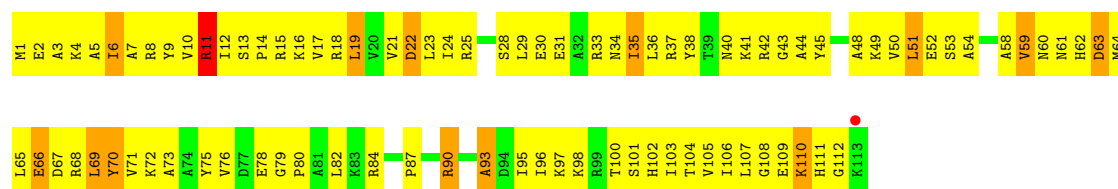
- Molecule 43: 50S ribosomal protein L22

Chain BW:



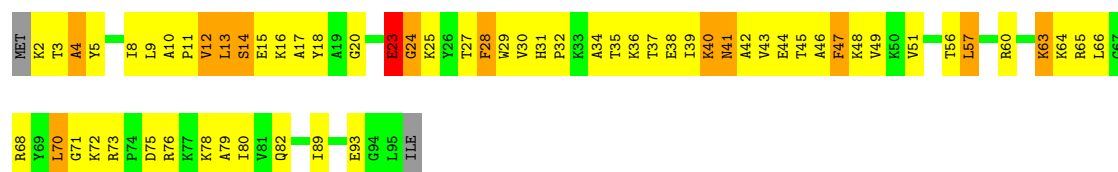
- Molecule 43: 50S ribosomal protein L22

Chain DW:



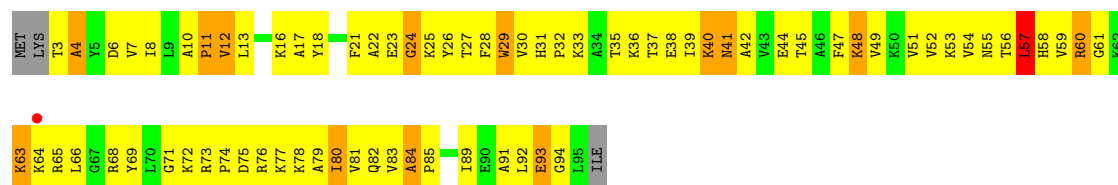
- Molecule 44: 50S ribosomal protein L23

Chain BX:



- Molecule 44: 50S ribosomal protein L23

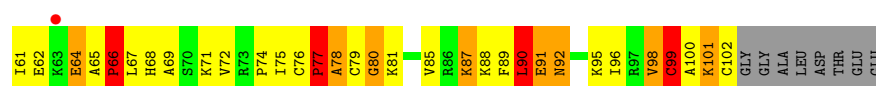
Chain DX:



- Molecule 45: 50S ribosomal protein L24

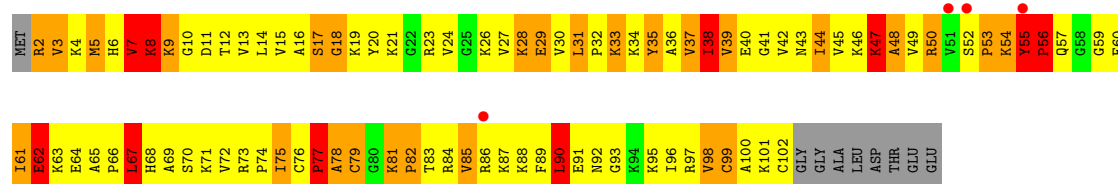
Chain BY:





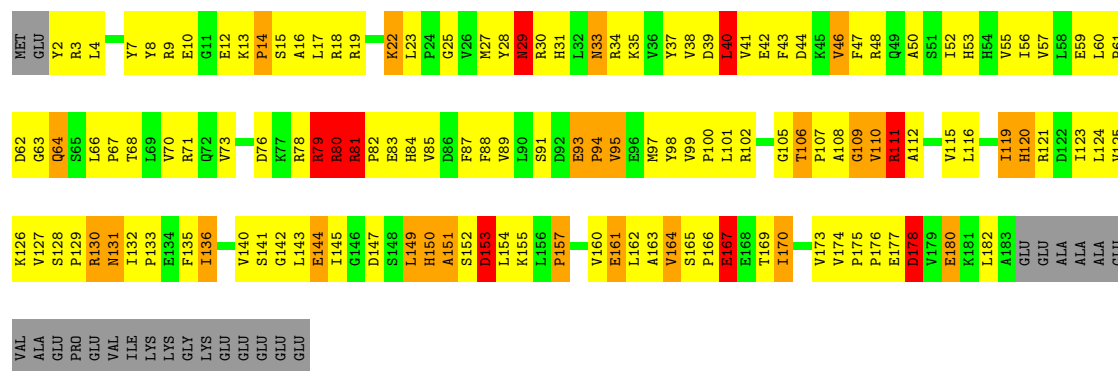
- Molecule 45: 50S ribosomal protein L24

Chain DY:



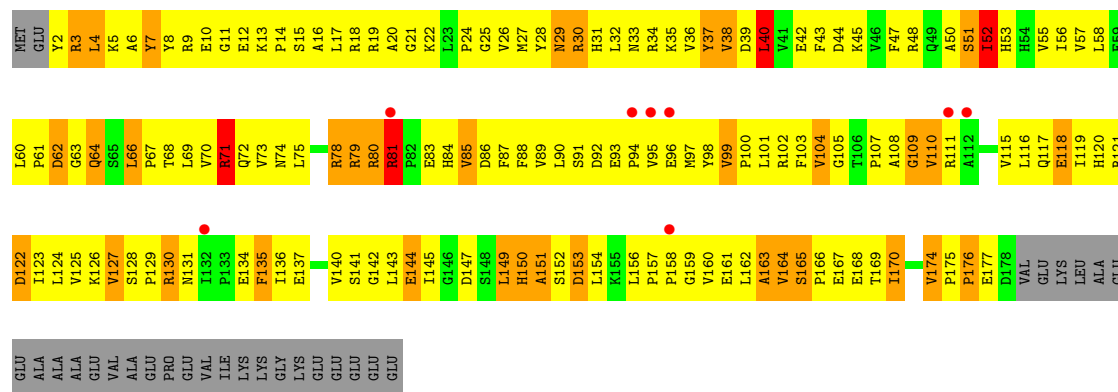
- Molecule 46: 50S ribosomal protein L25

Chain BZ:



- Molecule 46: 50S ribosomal protein L25

Chain DZ:



- Molecule 47: 50S ribosomal protein L27

Chain B0:





- Molecule 47: 50S ribosomal protein L27

Chain D0:



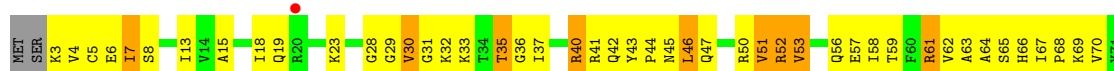
- Molecule 48: 50S ribosomal protein L28

Chain B1:



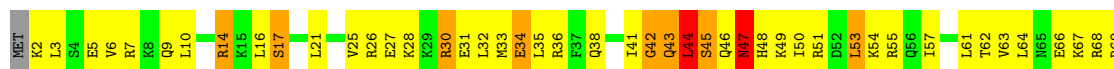
- Molecule 48: 50S ribosomal protein L28

Chain D1:



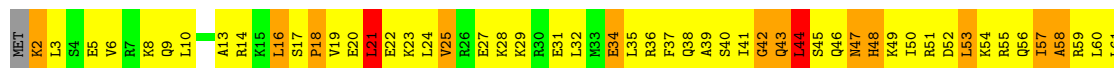
- Molecule 49: 50S ribosomal protein L29

Chain B2:



- Molecule 49: 50S ribosomal protein L29

Chain D2:



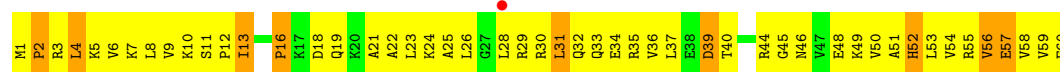
- Molecule 50: 50S ribosomal protein L30

Chain B3: 



- Molecule 50: 50S ribosomal protein L30

Chain D3: 



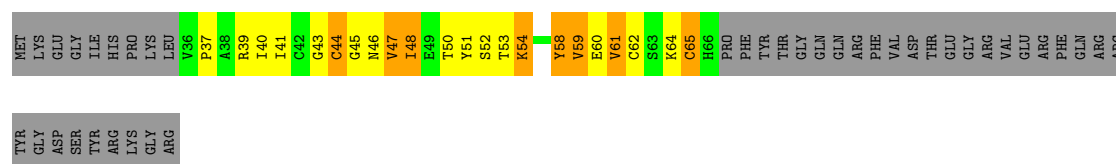
- Molecule 51: 50S ribosomal protein L31

Chain B4: 



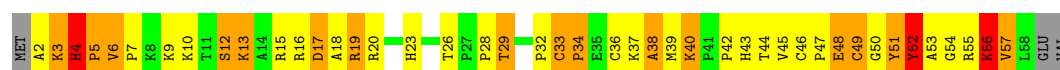
- Molecule 51: 50S ribosomal protein L31

Chain D4: 



- Molecule 52: 50S ribosomal protein L32

Chain B5: 



- Molecule 52: 50S ribosomal protein L32

Chain D5: 



- Molecule 53: 50S ribosomal protein L33

Chain B6: 



- Molecule 53: 50S ribosomal protein L33

Chain D6: 



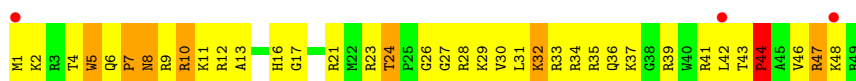
- Molecule 54: 50S ribosomal protein L34

Chain B7:



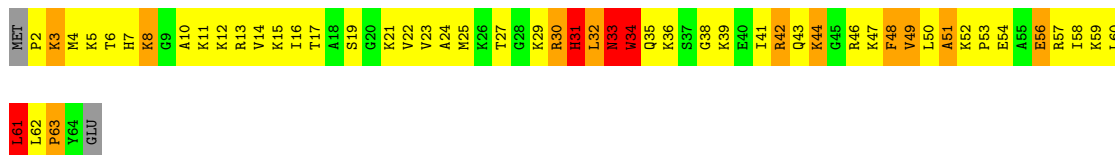
- Molecule 54: 50S ribosomal protein L34

Chain D7:



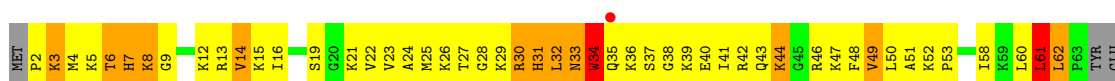
- Molecule 55: 50S ribosomal protein L35

Chain B8:



- Molecule 55: 50S ribosomal protein L35

Chain D8:



- Molecule 56: 50S ribosomal protein L36

Chain B9:



- Molecule 56: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.53Å 447.03Å 622.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10 49.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 94.7 (49.65-3.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.302 0.262 , 0.259	Depositor DCC
R_{free} test set	49631 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 23.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 989777 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290405	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: ZN, 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	0.82	6/35982 (0.0%)	0.78	24/56156 (0.0%)
1	CA	0.47	0/36193	0.72	9/56490 (0.0%)
2	AB	0.41	0/1936	0.69	0/2611
2	CB	0.43	0/1936	0.73	1/2611 (0.0%)
3	AC	0.41	0/1637	0.66	0/2207
3	CC	0.40	0/1637	0.66	0/2207
4	AD	0.41	0/1733	0.69	0/2318
4	CD	0.42	0/1733	0.72	1/2318 (0.0%)
5	AE	0.42	0/1163	0.68	0/1566
5	CE	0.40	0/1163	0.69	0/1566
6	AF	0.44	0/856	0.71	0/1154
6	CF	0.40	0/856	0.70	0/1154
7	AG	0.42	0/1276	0.67	0/1709
7	CG	0.42	0/1276	0.67	0/1709
8	AH	0.41	0/1136	0.72	0/1527
8	CH	0.39	0/1136	0.67	0/1527
9	AI	0.46	0/1022	0.69	0/1369
9	CI	0.43	0/1022	0.70	0/1369
10	AJ	0.43	0/808	0.71	0/1087
10	CJ	0.45	0/808	0.72	0/1087
11	AK	0.41	0/900	0.72	1/1213 (0.1%)
11	CK	0.39	0/900	0.67	0/1213
12	AL	0.41	0/987	0.78	0/1322
12	CL	0.41	0/987	0.77	1/1322 (0.1%)
13	AM	0.41	0/957	0.78	1/1283 (0.1%)
13	CM	0.39	0/957	0.76	1/1283 (0.1%)
14	AN	0.43	0/501	0.69	0/664
14	CN	0.45	0/501	0.66	0/664
15	AO	0.42	0/745	0.66	0/992
15	CO	0.39	0/745	0.67	1/992 (0.1%)
16	AP	0.42	0/717	0.71	1/965 (0.1%)
16	CP	0.42	0/717	0.73	1/965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.70	0/1119
18	AR	0.40	0/579	0.73	0/768
18	CR	0.45	0/579	0.75	0/768
19	AS	0.42	0/625	0.74	0/844
19	CS	0.45	0/632	0.76	0/853
20	AT	0.37	0/765	0.74	0/1007
20	CT	0.38	0/765	0.73	0/1007
21	AU	0.52	0/213	0.58	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.47	0/1393	0.68	0/1883
22	CV	0.46	0/1393	0.67	0/1883
23	AW	0.61	3/1836 (0.2%)	0.90	6/2859 (0.2%)
23	CW	0.50	1/1836 (0.1%)	0.72	1/2859 (0.0%)
24	AX	0.99	1/123 (0.8%)	0.68	0/188
24	CX	0.89	1/123 (0.8%)	0.67	0/188
25	BA	0.68	8/66745 (0.0%)	0.78	54/104189 (0.1%)
25	DA	0.56	10/66983 (0.0%)	0.76	54/104560 (0.1%)
26	BB	0.50	0/2853	0.79	3/4451 (0.1%)
26	DB	0.47	0/2853	0.72	2/4451 (0.0%)
27	BC	0.41	0/1732	0.69	0/2335
27	DC	0.87	1/1668 (0.1%)	0.65	0/2251
28	BD	0.56	0/2177	0.88	4/2935 (0.1%)
28	DD	0.48	0/2165	0.83	0/2921
29	BE	0.52	0/1597	0.84	2/2155 (0.1%)
29	DE	0.49	0/1597	0.84	1/2155 (0.0%)
30	BF	0.54	0/1659	0.82	1/2246 (0.0%)
30	DF	0.44	0/1659	0.74	0/2246
31	BG	0.45	0/1499	0.75	1/2016 (0.0%)
31	DG	0.43	0/1499	0.77	2/2016 (0.1%)
32	BH	0.55	0/1254	0.83	0/1703
32	DH	0.43	0/1246	0.75	2/1684 (0.1%)
33	BI	0.41	0/1056	0.75	0/1443
33	DI	0.37	0/881	0.73	0/1219
34	BN	0.52	0/1132	0.82	2/1527 (0.1%)
34	DN	0.41	0/1132	0.75	0/1527
35	BO	0.52	0/943	0.79	0/1269
35	DO	0.47	0/943	0.72	0/1269
36	BP	0.54	0/1131	1.08	7/1504 (0.5%)
36	DP	0.45	0/1095	0.90	4/1460 (0.3%)
37	BQ	0.46	0/1120	0.70	0/1498
37	DQ	0.45	0/1143	0.71	0/1527
38	BR	0.49	0/936	0.80	1/1256 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.42	0/974	0.78	0/1302
39	BS	0.47	0/785	0.85	2/1048 (0.2%)
39	DS	0.47	0/779	0.83	1/1038 (0.1%)
40	BT	0.49	0/1156	0.87	3/1544 (0.2%)
40	DT	0.46	0/1156	0.85	1/1544 (0.1%)
41	BU	0.53	0/975	0.79	0/1297
41	DU	0.42	0/975	0.71	0/1297
42	BV	0.54	0/790	0.88	0/1057
42	DV	0.42	0/790	0.77	0/1057
43	BW	0.52	0/907	0.77	0/1216
43	DW	0.42	0/907	0.71	0/1216
44	BX	0.56	0/749	0.81	1/1006 (0.1%)
44	DX	0.47	0/740	0.72	0/995
45	BY	0.58	0/770	0.93	1/1031 (0.1%)
45	DY	0.49	0/789	0.88	1/1053 (0.1%)
46	BZ	0.44	0/1470	0.72	1/1998 (0.1%)
46	DZ	0.42	0/1436	0.70	0/1951
47	B0	0.54	0/621	0.76	0/827
47	D0	0.45	0/671	0.68	0/892
48	B1	0.51	0/764	0.78	0/1014
48	D1	0.41	0/739	0.72	0/983
49	B2	0.45	0/600	0.69	0/793
49	D2	0.42	0/600	0.69	0/793
50	B3	0.47	0/465	0.73	0/625
50	D3	0.36	0/473	0.70	0/636
51	B4	0.57	0/229	0.83	0/311
51	D4	0.46	0/229	0.73	0/311
52	B5	0.58	0/449	0.86	0/608
52	D5	0.51	0/473	0.73	0/639
53	B6	0.68	1/408 (0.2%)	0.95	2/548 (0.4%)
53	D6	0.47	0/328	0.96	1/450 (0.2%)
54	B7	0.59	0/427	0.83	1/563 (0.2%)
54	D7	0.47	0/427	0.74	0/563
55	B8	0.55	0/503	0.94	3/663 (0.5%)
55	D8	0.49	0/473	0.82	0/626
56	B9	0.49	0/297	0.74	0/391
56	D9	0.43	0/302	0.70	0/397
All	All	0.59	32/313996 (0.0%)	0.76	207/468619 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	38
1	CA	0	17
23	AW	0	2
23	CW	0	2
25	BA	3	106
25	DA	1	76
26	BB	0	2
26	DB	0	1
28	BD	0	1
52	B5	0	1
52	D5	0	1
All	All	4	247

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1223	C	C4'-C3'	85.69	2.47	1.53
1	AA	1223	C	C3'-C2'	69.16	2.29	1.52
1	AA	1223	C	C3'-O3'	-41.26	0.84	1.42
27	DC	180	SER	CB-OG	31.26	1.82	1.42
1	AA	1223	C	N3-C4	27.30	1.53	1.33

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1223	C	C4'-C3'-C2'	-42.89	59.71	102.60
1	AA	1223	C	C3'-C2'-C1'	32.11	127.19	101.50
1	AA	1223	C	P-O3'-C3'	-30.31	83.33	119.70
1	AA	1223	C	O4'-C4'-C3'	20.77	124.77	104.00
1	AA	1223	C	N3-C4-C5	-18.18	114.63	121.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	BA	454	A	C3'
25	BA	775	G	C3'
25	BA	1992	G	C3'
25	DA	1992	G	C3'

5 of 247 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	127	G	Sidechain
1	AA	250	A	Sidechain
1	AA	253	U	Sidechain
1	AA	47	C	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	32144	0	16225	1841	0
1	CA	32332	0	16317	1680	0
2	AB	1901	0	1951	360	0
2	CB	1901	0	1951	361	0
3	AC	1613	0	1677	329	0
3	CC	1613	0	1677	275	0
4	AD	1703	0	1763	325	0
4	CD	1703	0	1763	212	0
5	AE	1147	0	1207	168	0
5	CE	1147	0	1207	177	0
6	AF	843	0	857	111	0
6	CF	843	0	857	137	0
7	AG	1257	0	1296	192	0
7	CG	1257	0	1296	213	0
8	AH	1116	0	1177	183	0
8	CH	1116	0	1177	170	0
9	AI	1004	0	1031	187	0
9	CI	1004	0	1031	200	0
10	AJ	795	0	840	215	0
10	CJ	795	0	840	192	0
11	AK	885	0	904	130	0
11	CK	885	0	904	111	0
12	AL	971	0	1057	168	0
12	CL	971	0	1057	133	0
13	AM	947	0	1008	191	0
13	CM	947	0	1008	135	0
14	AN	492	0	533	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	533	95	0
15	AO	734	0	771	102	0
15	CO	734	0	771	111	0
16	AP	701	0	720	122	0
16	CP	701	0	720	98	0
17	AQ	824	0	891	108	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	108	0
18	CR	574	0	644	102	0
19	AS	613	0	621	132	0
19	CS	619	0	639	120	0
20	AT	763	0	861	142	0
20	CT	763	0	861	138	0
21	AU	209	0	221	15	0
21	CU	209	0	221	31	0
22	AV	1367	0	1364	182	0
22	CV	1367	0	1364	199	0
23	AW	1644	0	834	67	0
23	CW	1644	0	836	75	0
24	AX	110	0	55	4	0
24	CX	110	0	55	3	0
25	BA	59596	0	30049	2582	0
25	DA	59809	0	30157	2949	0
26	BB	2551	0	1295	92	0
26	DB	2551	0	1295	145	0
27	BC	1702	0	1747	274	0
27	DC	1640	0	1651	242	0
28	BD	2127	0	2208	330	0
28	DD	2115	0	2186	338	0
29	BE	1564	0	1629	252	0
29	DE	1564	0	1629	273	0
30	BF	1624	0	1677	280	0
30	DF	1624	0	1677	300	0
31	BG	1474	0	1535	285	0
31	DG	1474	0	1535	269	0
32	BH	1231	0	1260	198	0
32	DH	1223	0	1282	234	0
33	BI	1043	0	1019	181	0
33	DI	871	0	680	103	0
34	BN	1105	0	1180	132	0
34	DN	1105	0	1180	175	0
35	BO	933	0	996	158	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DO	933	0	996	112	0
36	BP	1114	0	1187	332	0
36	DP	1079	0	1117	265	0
37	BQ	1099	0	1160	144	0
37	DQ	1122	0	1179	190	0
38	BR	923	0	949	105	0
38	DR	960	0	1021	156	0
39	BS	777	0	825	180	0
39	DS	771	0	832	159	0
40	BT	1142	0	1202	274	0
40	DT	1142	0	1202	231	0
41	BU	958	0	1015	150	0
41	DU	958	0	1015	224	0
42	BV	779	0	852	167	0
42	DV	779	0	852	217	0
43	BW	896	0	953	91	0
43	DW	896	0	953	126	0
44	BX	735	0	791	85	0
44	DX	726	0	778	122	0
45	BY	757	0	821	198	0
45	DY	776	0	870	199	0
46	BZ	1438	0	1455	202	0
46	DZ	1404	0	1432	302	0
47	B0	613	0	633	88	0
47	D0	662	0	688	109	0
48	B1	757	0	843	108	0
48	D1	732	0	808	99	0
49	B2	598	0	653	56	0
49	D2	598	0	653	101	0
50	B3	460	0	512	46	0
50	D3	468	0	523	91	0
51	B4	226	0	229	46	0
51	D4	226	0	229	39	0
52	B5	435	0	452	58	0
52	D5	459	0	477	64	0
53	B6	401	0	399	118	0
53	D6	322	0	250	85	0
54	B7	419	0	467	27	0
54	D7	419	0	467	49	0
55	B8	496	0	567	113	0
55	D8	467	0	519	114	0
56	B9	294	0	311	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D9	299	0	325	31	0
57	AA	117	0	0	0	0
57	AL	1	0	0	0	0
57	AT	1	0	0	0	0
57	AW	2	0	0	0	0
57	B0	2	0	0	0	0
57	B1	1	0	0	0	0
57	B5	4	0	0	0	0
57	B7	1	0	0	0	0
57	BA	459	0	0	1	0
57	BB	9	0	0	0	0
57	BD	1	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BH	1	0	0	0	0
57	BP	3	0	0	0	0
57	BQ	3	0	0	0	0
57	BR	1	0	0	0	0
57	BT	1	0	0	0	0
57	BU	1	0	0	0	0
57	BX	1	0	0	0	0
57	CA	109	0	0	0	0
57	CE	1	0	0	0	0
57	CW	5	0	0	0	0
57	CX	1	0	0	0	0
57	D5	2	0	0	0	0
57	D6	2	0	0	0	0
57	DA	305	0	0	0	0
57	DB	10	0	0	0	0
57	DD	1	0	0	0	0
57	DF	1	0	0	0	0
57	DP	1	0	0	0	0
57	DR	1	0	0	0	0
58	AD	1	0	0	0	0
58	B5	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0
58	D5	1	0	0	1	0
58	D9	1	0	0	2	0
All	All	290405	0	198457	23826	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 49.

The worst 5 of 23826 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:D5:49:CYS:SG	58:D5:103:ZN:ZN	0.84	1.63
56:D9:14:CYS:SG	58:D9:101:ZN:ZN	1.23	1.27
27:DC:180:SER:CB	27:DC:180:SER:OG	1.82	1.25
36:BP:59:LEU:HA	36:BP:61:ARG:NH1	1.53	1.21
39:BS:97:ARG:NH2	39:BS:98:VAL:HA	1.55	1.20

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	
2	AB	233/256 (91%)	128 (55%)	72 (31%)	33 (14%)	0	2
2	CB	233/256 (91%)	138 (59%)	54 (23%)	41 (18%)	0	0
3	AC	205/239 (86%)	106 (52%)	68 (33%)	31 (15%)	0	1
3	CC	205/239 (86%)	134 (65%)	45 (22%)	26 (13%)	0	3
4	AD	206/209 (99%)	124 (60%)	52 (25%)	30 (15%)	0	2
4	CD	206/209 (99%)	132 (64%)	46 (22%)	28 (14%)	0	2
5	AE	149/162 (92%)	107 (72%)	26 (17%)	16 (11%)	1	5
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	1	7
6	AF	99/101 (98%)	63 (64%)	27 (27%)	9 (9%)	1	8
6	CF	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
7	AG	153/156 (98%)	98 (64%)	39 (26%)	16 (10%)	1	5
7	CG	153/156 (98%)	95 (62%)	34 (22%)	24 (16%)	0	1
8	AH	136/138 (99%)	96 (71%)	28 (21%)	12 (9%)	1	8
8	CH	136/138 (99%)	93 (68%)	26 (19%)	17 (12%)	1	3
9	AI	125/128 (98%)	82 (66%)	27 (22%)	16 (13%)	0	3
9	CI	125/128 (98%)	80 (64%)	32 (26%)	13 (10%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	58 (60%)	29 (30%)	10 (10%)	1	6
10	CJ	97/105 (92%)	59 (61%)	26 (27%)	12 (12%)	1	3
11	AK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	3	22
11	CK	117/129 (91%)	86 (74%)	25 (21%)	6 (5%)	3	22
12	AL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	3
12	CL	123/132 (93%)	86 (70%)	21 (17%)	16 (13%)	0	3
13	AM	118/126 (94%)	72 (61%)	24 (20%)	22 (19%)	0	0
13	CM	118/126 (94%)	72 (61%)	22 (19%)	24 (20%)	0	0
14	AN	58/61 (95%)	34 (59%)	14 (24%)	10 (17%)	0	0
14	CN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	0
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	1	7
15	CO	86/89 (97%)	55 (64%)	19 (22%)	12 (14%)	0	2
16	AP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	1	4
16	CP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	1	4
17	AQ	98/105 (93%)	73 (74%)	14 (14%)	11 (11%)	1	5
17	CQ	98/105 (93%)	71 (72%)	19 (19%)	8 (8%)	1	10
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	0
18	CR	68/88 (77%)	37 (54%)	26 (38%)	5 (7%)	2	11
19	AS	78/93 (84%)	47 (60%)	16 (20%)	15 (19%)	0	0
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	2
20	AT	97/106 (92%)	66 (68%)	18 (19%)	13 (13%)	0	2
20	CT	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	2
21	AU	23/27 (85%)	12 (52%)	7 (30%)	4 (17%)	0	0
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	3
22	AV	172/184 (94%)	124 (72%)	31 (18%)	17 (10%)	1	6
22	CV	172/184 (94%)	126 (73%)	28 (16%)	18 (10%)	1	5
27	BC	222/229 (97%)	165 (74%)	33 (15%)	24 (11%)	1	5
27	DC	216/229 (94%)	141 (65%)	62 (29%)	13 (6%)	2	17
28	BD	272/276 (99%)	194 (71%)	47 (17%)	31 (11%)	1	4
28	DD	272/276 (99%)	187 (69%)	47 (17%)	38 (14%)	0	2
29	BE	203/206 (98%)	130 (64%)	37 (18%)	36 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DE	203/206 (98%)	122 (60%)	35 (17%)	46 (23%)	0	0
30	BF	206/210 (98%)	136 (66%)	46 (22%)	24 (12%)	1	4
30	DF	206/210 (98%)	123 (60%)	48 (23%)	35 (17%)	0	0
31	BG	179/182 (98%)	118 (66%)	43 (24%)	18 (10%)	1	6
31	DG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	2
32	BH	166/180 (92%)	98 (59%)	33 (20%)	35 (21%)	0	0
32	DH	158/180 (88%)	80 (51%)	49 (31%)	29 (18%)	0	0
33	BI	144/148 (97%)	84 (58%)	32 (22%)	28 (19%)	0	0
33	DI	144/148 (97%)	74 (51%)	41 (28%)	29 (20%)	0	0
34	BN	137/140 (98%)	104 (76%)	14 (10%)	19 (14%)	0	2
34	DN	137/140 (98%)	79 (58%)	38 (28%)	20 (15%)	0	2
35	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	1	6
35	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	4	27
36	BP	144/150 (96%)	71 (49%)	34 (24%)	39 (27%)	0	0
36	DP	144/150 (96%)	69 (48%)	34 (24%)	41 (28%)	0	0
37	BQ	137/141 (97%)	102 (74%)	23 (17%)	12 (9%)	1	8
37	DQ	139/141 (99%)	91 (66%)	35 (25%)	13 (9%)	1	7
38	BR	114/118 (97%)	82 (72%)	21 (18%)	11 (10%)	1	7
38	DR	115/118 (98%)	81 (70%)	17 (15%)	17 (15%)	0	2
39	BS	99/112 (88%)	44 (44%)	25 (25%)	30 (30%)	0	0
39	DS	97/112 (87%)	48 (50%)	25 (26%)	24 (25%)	0	0
40	BT	136/146 (93%)	86 (63%)	21 (15%)	29 (21%)	0	0
40	DT	136/146 (93%)	72 (53%)	33 (24%)	31 (23%)	0	0
41	BU	115/118 (98%)	74 (64%)	31 (27%)	10 (9%)	1	9
41	DU	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	3
42	BV	99/101 (98%)	68 (69%)	13 (13%)	18 (18%)	0	0
42	DV	99/101 (98%)	57 (58%)	20 (20%)	22 (22%)	0	0
43	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	1	5
43	DW	111/113 (98%)	82 (74%)	18 (16%)	11 (10%)	1	6
44	BX	92/96 (96%)	64 (70%)	21 (23%)	7 (8%)	2	11
44	DX	91/96 (95%)	64 (70%)	16 (18%)	11 (12%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BY	99/110 (90%)	38 (38%)	23 (23%)	38 (38%)	0	0
45	DY	99/110 (90%)	39 (39%)	26 (26%)	34 (34%)	0	0
46	BZ	180/206 (87%)	114 (63%)	41 (23%)	25 (14%)	0	2
46	DZ	175/206 (85%)	103 (59%)	46 (26%)	26 (15%)	0	1
47	B0	75/85 (88%)	60 (80%)	13 (17%)	2 (3%)	8	39
47	D0	82/85 (96%)	60 (73%)	15 (18%)	7 (8%)	1	9
48	B1	94/98 (96%)	65 (69%)	15 (16%)	14 (15%)	0	1
48	D1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	1	5
49	B2	69/72 (96%)	53 (77%)	9 (13%)	7 (10%)	1	6
49	D2	69/72 (96%)	41 (59%)	17 (25%)	11 (16%)	0	1
50	B3	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	13	52
50	D3	58/60 (97%)	38 (66%)	13 (22%)	7 (12%)	1	4
51	B4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
51	D4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
52	B5	55/60 (92%)	31 (56%)	10 (18%)	14 (26%)	0	0
52	D5	57/60 (95%)	35 (61%)	11 (19%)	11 (19%)	0	0
53	B6	47/54 (87%)	19 (40%)	13 (28%)	15 (32%)	0	0
53	D6	46/54 (85%)	19 (41%)	11 (24%)	16 (35%)	0	0
54	B7	47/49 (96%)	40 (85%)	7 (15%)	0	100	100
54	D7	47/49 (96%)	37 (79%)	6 (13%)	4 (8%)	1	9
55	B8	61/65 (94%)	36 (59%)	16 (26%)	9 (15%)	0	2
55	D8	60/65 (92%)	37 (62%)	14 (23%)	9 (15%)	0	1
56	B9	34/37 (92%)	24 (71%)	9 (26%)	1 (3%)	7	38
56	D9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
All	All	12117/12954 (94%)	7729 (64%)	2646 (22%)	1742 (14%)	0	2

5 of 1742 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	23	ARG
2	AB	26	PRO
2	AB	75	LYS
2	AB	128	GLU

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	
2	AB	202/220 (92%)	173 (86%)	29 (14%)	5	19
2	CB	202/220 (92%)	179 (89%)	23 (11%)	8	31
3	AC	160/188 (85%)	142 (89%)	18 (11%)	9	32
3	CC	160/188 (85%)	146 (91%)	14 (9%)	14	49
4	AD	180/181 (99%)	157 (87%)	23 (13%)	6	24
4	CD	180/181 (99%)	158 (88%)	22 (12%)	7	26
5	AE	115/123 (94%)	102 (89%)	13 (11%)	9	32
5	CE	115/123 (94%)	104 (90%)	11 (10%)	12	42
6	AF	90/90 (100%)	77 (86%)	13 (14%)	5	19
6	CF	90/90 (100%)	81 (90%)	9 (10%)	11	38
7	AG	126/127 (99%)	112 (89%)	14 (11%)	9	33
7	CG	126/127 (99%)	110 (87%)	16 (13%)	6	24
8	AH	119/119 (100%)	109 (92%)	10 (8%)	16	52
8	CH	119/119 (100%)	108 (91%)	11 (9%)	13	45
9	AI	97/99 (98%)	80 (82%)	17 (18%)	3	11
9	CI	97/99 (98%)	78 (80%)	19 (20%)	2	8
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	17
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	11	37
11	AK	90/99 (91%)	85 (94%)	5 (6%)	30	70
11	CK	90/99 (91%)	81 (90%)	9 (10%)	11	38
12	AL	104/109 (95%)	94 (90%)	10 (10%)	12	42
12	CL	104/109 (95%)	92 (88%)	12 (12%)	8	31
13	AM	95/101 (94%)	74 (78%)	21 (22%)	1	6
13	CM	95/101 (94%)	79 (83%)	16 (17%)	3	11
14	AN	49/50 (98%)	40 (82%)	9 (18%)	2	9
14	CN	49/50 (98%)	44 (90%)	5 (10%)	11	37
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CO	79/80 (99%)	73 (92%)	6 (8%)	19	58
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	33
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	41
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
18	AR	61/77 (79%)	57 (93%)	4 (7%)	24	64
18	CR	61/77 (79%)	54 (88%)	7 (12%)	8	31
19	AS	65/80 (81%)	52 (80%)	13 (20%)	2	8
19	CS	68/80 (85%)	56 (82%)	12 (18%)	3	10
20	AT	76/82 (93%)	67 (88%)	9 (12%)	8	29
20	CT	76/82 (93%)	66 (87%)	10 (13%)	6	23
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	35
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	72
22	AV	148/154 (96%)	136 (92%)	12 (8%)	17	53
22	CV	148/154 (96%)	129 (87%)	19 (13%)	6	24
27	BC	175/181 (97%)	148 (85%)	27 (15%)	4	15
27	DC	165/181 (91%)	146 (88%)	19 (12%)	8	31
28	BD	215/218 (99%)	179 (83%)	36 (17%)	3	11
28	DD	213/218 (98%)	184 (86%)	29 (14%)	5	21
29	BE	165/166 (99%)	144 (87%)	21 (13%)	6	24
29	DE	165/166 (99%)	140 (85%)	25 (15%)	4	16
30	BF	165/166 (99%)	137 (83%)	28 (17%)	3	11
30	DF	165/166 (99%)	143 (87%)	22 (13%)	6	22
31	BG	155/156 (99%)	126 (81%)	29 (19%)	2	9
31	DG	155/156 (99%)	132 (85%)	23 (15%)	4	17
32	BH	127/148 (86%)	115 (91%)	12 (9%)	13	43
32	DH	132/148 (89%)	111 (84%)	21 (16%)	4	13
33	BI	97/124 (78%)	78 (80%)	19 (20%)	2	8
33	DI	49/124 (40%)	41 (84%)	8 (16%)	3	12
34	BN	117/119 (98%)	95 (81%)	22 (19%)	2	9
34	DN	117/119 (98%)	100 (86%)	17 (14%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BO	100/100 (100%)	90 (90%)	10 (10%)	11	38
35	DO	100/100 (100%)	91 (91%)	9 (9%)	14	47
36	BP	112/116 (97%)	88 (79%)	24 (21%)	1	7
36	DP	103/116 (89%)	81 (79%)	22 (21%)	1	7
37	BQ	109/111 (98%)	95 (87%)	14 (13%)	6	24
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	11	39
38	BR	92/101 (91%)	80 (87%)	12 (13%)	6	23
38	DR	100/101 (99%)	83 (83%)	17 (17%)	3	11
39	BS	76/88 (86%)	61 (80%)	15 (20%)	2	8
39	DS	77/88 (88%)	60 (78%)	17 (22%)	1	6
40	BT	120/127 (94%)	94 (78%)	26 (22%)	1	6
40	DT	120/127 (94%)	97 (81%)	23 (19%)	2	9
41	BU	92/94 (98%)	77 (84%)	15 (16%)	3	12
41	DU	92/94 (98%)	82 (89%)	10 (11%)	9	34
42	BV	82/82 (100%)	63 (77%)	19 (23%)	1	5
42	DV	82/82 (100%)	66 (80%)	16 (20%)	2	8
43	BW	91/92 (99%)	77 (85%)	14 (15%)	4	15
43	DW	91/92 (99%)	84 (92%)	7 (8%)	18	57
44	BX	75/78 (96%)	64 (85%)	11 (15%)	4	18
44	DX	74/78 (95%)	66 (89%)	8 (11%)	9	34
45	BY	79/91 (87%)	64 (81%)	15 (19%)	2	9
45	DY	84/91 (92%)	69 (82%)	15 (18%)	2	10
46	BZ	158/179 (88%)	136 (86%)	22 (14%)	5	21
46	DZ	155/179 (87%)	131 (84%)	24 (16%)	4	14
47	B0	62/67 (92%)	56 (90%)	6 (10%)	12	41
47	D0	66/67 (98%)	56 (85%)	10 (15%)	4	16
48	B1	81/83 (98%)	66 (82%)	15 (18%)	2	9
48	D1	78/83 (94%)	69 (88%)	9 (12%)	8	31
49	B2	66/67 (98%)	57 (86%)	9 (14%)	5	21
49	D2	66/67 (98%)	57 (86%)	9 (14%)	5	21
50	B3	50/52 (96%)	43 (86%)	7 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	D3	51/52 (98%)	48 (94%)	3 (6%)	28	68
51	B4	27/63 (43%)	23 (85%)	4 (15%)	4	17
51	D4	27/63 (43%)	25 (93%)	2 (7%)	20	59
52	B5	48/52 (92%)	36 (75%)	12 (25%)	1	3
52	D5	51/52 (98%)	44 (86%)	7 (14%)	5	21
53	B6	43/52 (83%)	32 (74%)	11 (26%)	1	2
53	D6	24/52 (46%)	14 (58%)	10 (42%)	0	0
54	B7	41/42 (98%)	38 (93%)	3 (7%)	20	59
54	D7	41/42 (98%)	32 (78%)	9 (22%)	1	6
55	B8	52/55 (94%)	44 (85%)	8 (15%)	4	15
55	D8	46/55 (84%)	36 (78%)	10 (22%)	1	6
56	B9	32/34 (94%)	26 (81%)	6 (19%)	2	9
56	D9	33/34 (97%)	28 (85%)	5 (15%)	4	16
All	All	9998/10736 (93%)	8606 (86%)	1392 (14%)	5	21

5 of 1392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	79	ARG
4	CD	127	THR
45	DY	55	TYR
47	B0	9	THR
53	B6	24	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	46	ASN
6	CF	64	GLN
46	DZ	64	GLN
54	B7	8	ASN
3	CC	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1492/1509 (98%)	236 (15%)	40 (2%)
1	CA	1503/1509 (99%)	227 (15%)	33 (2%)
23	AW	76/77 (98%)	18 (23%)	2 (2%)
23	CW	76/77 (98%)	19 (25%)	6 (7%)
24	AX	4/5 (80%)	0	0
24	CX	4/5 (80%)	0	0
25	BA	2761/2915 (94%)	508 (18%)	77 (2%)
25	DA	2771/2915 (95%)	546 (19%)	84 (3%)
26	BB	118/122 (96%)	19 (16%)	2 (1%)
26	DB	118/122 (96%)	20 (16%)	2 (1%)
All	All	8923/9256 (96%)	1593 (17%)	246 (2%)

5 of 1593 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2610	C
1	CA	484	G
25	DA	2422	A
25	BA	2750	A
1	CA	79	G

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 1056 ligands modelled in this entry, 1056 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	1495/1509 (99%)	-0.09	28 (1%)	64	13	43, 73, 89, 96	1 (0%)
1	CA	1504/1509 (99%)	-0.11	25 (1%)	67	15	47, 71, 88, 97	1 (0%)
2	AB	235/256 (91%)	0.07	7 (2%)	48	7	65, 75, 82, 88	0
2	CB	235/256 (91%)	0.01	4 (1%)	67	15	66, 76, 82, 85	0
3	AC	207/239 (86%)	0.12	3 (1%)	72	17	67, 75, 82, 86	0
3	CC	207/239 (86%)	0.07	1 (0%)	88	39	67, 75, 81, 84	0
4	AD	208/209 (99%)	-0.15	0	100	100	61, 72, 79, 85	0
4	CD	208/209 (99%)	-0.11	1 (0%)	88	39	55, 68, 75, 83	0
5	AE	151/162 (93%)	0.05	5 (3%)	44	6	60, 69, 76, 83	0
5	CE	151/162 (93%)	-0.00	0	100	100	60, 69, 77, 90	0
6	AF	101/101 (100%)	-0.27	0	100	100	56, 67, 76, 81	0
6	CF	101/101 (100%)	-0.10	0	100	100	61, 70, 78, 83	0
7	AG	155/156 (99%)	-0.02	2 (1%)	74	19	63, 74, 80, 83	0
7	CG	155/156 (99%)	0.13	2 (1%)	74	19	67, 74, 81, 84	0
8	AH	138/138 (100%)	-0.11	2 (1%)	72	17	56, 69, 74, 79	0
8	CH	138/138 (100%)	-0.16	0	100	100	57, 70, 76, 82	0
9	AI	127/128 (99%)	0.30	3 (2%)	56	9	66, 77, 83, 87	0
9	CI	127/128 (99%)	0.68	12 (9%)	9	2	70, 77, 83, 86	0
10	AJ	99/105 (94%)	0.50	7 (7%)	16	3	66, 79, 84, 88	0
10	CJ	99/105 (94%)	1.14	19 (19%)	2	0	66, 79, 84, 87	0
11	AK	119/129 (92%)	0.15	2 (1%)	67	15	58, 68, 78, 82	0
11	CK	119/129 (92%)	-0.06	3 (2%)	54	9	64, 72, 78, 84	0
12	AL	125/132 (94%)	-0.15	1 (0%)	83	28	53, 67, 76, 85	0
12	CL	125/132 (94%)	0.11	3 (2%)	56	9	56, 65, 74, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	120/126 (95%)	0.20	1 (0%) 83 28	66, 75, 81, 83	0
13	CM	120/126 (95%)	0.06	1 (0%) 83 28	65, 75, 81, 84	0
14	AN	60/61 (98%)	0.01	0 100 100	65, 74, 80, 82	0
14	CN	60/61 (98%)	-0.06	1 (1%) 67 15	62, 74, 78, 82	0
15	AO	88/89 (98%)	-0.02	0 100 100	52, 66, 74, 79	0
15	CO	88/89 (98%)	-0.13	0 100 100	59, 68, 76, 78	0
16	AP	84/88 (95%)	-0.02	1 (1%) 75 20	62, 69, 77, 80	0
16	CP	84/88 (95%)	0.20	1 (1%) 75 20	59, 66, 75, 83	0
17	AQ	100/105 (95%)	-0.06	0 100 100	59, 68, 75, 76	0
17	CQ	100/105 (95%)	-0.20	0 100 100	58, 68, 76, 78	0
18	AR	70/88 (79%)	-0.07	0 100 100	58, 69, 78, 85	0
18	CR	70/88 (79%)	0.24	1 (1%) 72 17	63, 69, 77, 82	0
19	AS	80/93 (86%)	0.20	1 (1%) 74 19	66, 76, 83, 86	0
19	CS	78/93 (83%)	0.31	1 (1%) 74 19	70, 76, 82, 84	0
20	AT	99/106 (93%)	0.14	1 (1%) 79 23	62, 71, 79, 83	0
20	CT	99/106 (93%)	0.14	0 100 100	63, 69, 77, 83	0
21	AU	25/27 (92%)	0.85	3 (12%) 5 1	67, 74, 81, 83	0
21	CU	25/27 (92%)	1.07	2 (8%) 12 2	68, 77, 83, 85	0
22	AV	176/184 (95%)	-0.11	1 (0%) 86 36	51, 71, 79, 83	0
22	CV	176/184 (95%)	0.10	3 (1%) 67 15	58, 72, 80, 84	0
23	AW	77/77 (100%)	0.06	2 (2%) 53 8	45, 69, 81, 92	0
23	CW	77/77 (100%)	-0.39	0 100 100	58, 72, 83, 87	0
24	AX	5/5 (100%)	0.56	0 100 100	65, 65, 83, 88	0
24	CX	5/5 (100%)	0.63	1 (20%) 2 0	68, 70, 82, 88	0
25	BA	2767/2915 (94%)	-0.13	35 (1%) 74 19	25, 53, 82, 97	0
25	DA	2777/2915 (95%)	-0.12	43 (1%) 70 16	38, 65, 85, 97	0
26	BB	119/122 (97%)	-0.33	0 100 100	53, 67, 77, 86	0
26	DB	119/122 (97%)	-0.03	2 (1%) 67 15	68, 77, 83, 92	0
27	BC	224/229 (97%)	0.22	0 100 100	67, 76, 81, 86	1 (0%)
27	DC	220/229 (96%)	0.27	9 (4%) 35 5	66, 76, 82, 87	1 (0%)
28	BD	274/276 (99%)	-0.11	0 100 100	38, 53, 65, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	274/276 (99%)	-0.07	1 (0%) 90 45	42, 59, 70, 77	0
29	BE	205/206 (99%)	-0.07	1 (0%) 88 39	38, 58, 73, 77	0
29	DE	205/206 (99%)	0.02	4 (1%) 62 12	46, 65, 78, 82	0
30	BF	208/210 (99%)	0.05	0 100 100	35, 58, 78, 88	0
30	DF	208/210 (99%)	-0.03	2 (0%) 79 23	52, 69, 78, 90	0
31	BG	181/182 (99%)	-0.06	1 (0%) 86 36	60, 71, 79, 86	0
31	DG	181/182 (99%)	0.19	4 (2%) 59 11	65, 73, 81, 85	0
32	BH	168/180 (93%)	-0.05	0 100 100	25, 66, 75, 82	0
32	DH	160/180 (88%)	0.24	0 100 100	66, 76, 82, 87	0
33	BI	146/148 (98%)	-0.19	1 (0%) 84 32	55, 71, 77, 84	0
33	DI	146/148 (98%)	-0.13	1 (0%) 84 32	60, 73, 80, 83	0
34	BN	139/140 (99%)	-0.18	0 100 100	46, 59, 72, 77	0
34	DN	139/140 (99%)	0.09	0 100 100	60, 70, 77, 82	0
35	BO	122/122 (100%)	-0.17	0 100 100	44, 59, 70, 73	0
35	DO	122/122 (100%)	0.01	0 100 100	50, 63, 71, 75	0
36	BP	146/150 (97%)	0.06	2 (1%) 72 17	40, 65, 76, 81	0
36	DP	146/150 (97%)	0.34	3 (2%) 60 11	52, 70, 78, 82	0
37	BQ	139/141 (98%)	-0.15	0 100 100	45, 61, 71, 80	0
37	DQ	141/141 (100%)	0.05	2 (1%) 72 17	54, 69, 77, 83	0
38	BR	116/118 (98%)	-0.07	0 100 100	39, 57, 69, 74	0
38	DR	117/118 (99%)	-0.03	0 100 100	50, 63, 73, 78	0
39	BS	101/112 (90%)	0.20	0 100 100	49, 69, 74, 80	0
39	DS	99/112 (88%)	0.22	1 (1%) 79 23	63, 72, 79, 86	0
40	BT	138/146 (94%)	-0.00	1 (0%) 84 32	52, 65, 79, 83	0
40	DT	138/146 (94%)	0.06	2 (1%) 72 17	56, 67, 81, 84	0
41	BU	117/118 (99%)	-0.06	2 (1%) 67 15	41, 54, 68, 78	0
41	DU	117/118 (99%)	-0.09	0 100 100	55, 67, 76, 81	0
42	BV	101/101 (100%)	-0.18	0 100 100	41, 60, 71, 75	0
42	DV	101/101 (100%)	0.20	0 100 100	58, 74, 79, 85	0
43	BW	113/113 (100%)	-0.10	0 100 100	44, 53, 70, 86	0
43	DW	113/113 (100%)	-0.06	1 (0%) 81 25	56, 64, 78, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	94/96 (97%)	-0.09	0 100 100	42, 57, 69, 79	0
44	DX	93/96 (96%)	-0.00	1 (1%) 77 22	53, 67, 73, 81	0
45	BY	101/110 (91%)	0.03	1 (0%) 79 23	51, 64, 77, 81	0
45	DY	101/110 (91%)	0.18	4 (3%) 36 5	63, 74, 82, 85	0
46	BZ	182/206 (88%)	-0.03	0 100 100	56, 70, 78, 83	0
46	DZ	177/206 (85%)	0.28	8 (4%) 32 5	68, 76, 83, 87	0
47	B0	77/85 (90%)	0.00	1 (1%) 74 19	49, 59, 72, 81	0
47	D0	84/85 (98%)	0.15	2 (2%) 56 9	59, 68, 78, 84	0
48	B1	96/98 (97%)	-0.12	0 100 100	42, 60, 72, 77	0
48	D1	94/98 (95%)	0.15	2 (2%) 60 11	50, 64, 75, 78	0
49	B2	71/72 (98%)	-0.18	0 100 100	50, 61, 75, 80	0
49	D2	71/72 (98%)	-0.22	1 (1%) 72 17	60, 71, 79, 87	0
50	B3	59/60 (98%)	0.01	1 (1%) 67 15	45, 59, 71, 74	0
50	D3	60/60 (100%)	0.45	1 (1%) 67 15	62, 72, 82, 85	0
51	B4	31/71 (43%)	0.02	0 100 100	69, 75, 80, 86	0
51	D4	31/71 (43%)	-0.00	0 100 100	67, 74, 81, 84	0
52	B5	57/60 (95%)	-0.24	0 100 100	40, 55, 71, 73	0
52	D5	59/60 (98%)	0.16	2 (3%) 43 6	55, 68, 78, 86	0
53	B6	49/54 (90%)	0.18	0 100 100	39, 65, 75, 75	0
53	D6	48/54 (88%)	-0.08	0 100 100	54, 66, 73, 78	0
54	B7	49/49 (100%)	0.00	0 100 100	35, 46, 69, 76	0
54	D7	49/49 (100%)	0.49	3 (6%) 21 3	47, 58, 77, 83	0
55	B8	63/65 (96%)	0.03	0 100 100	43, 56, 69, 75	0
55	D8	62/65 (95%)	0.18	1 (1%) 68 15	54, 62, 68, 76	0
56	B9	36/37 (97%)	0.40	2 (5%) 24 3	52, 59, 69, 71	0
56	D9	36/37 (97%)	0.44	1 (2%) 50 8	60, 69, 76, 82	0
All	All	21272/22210 (95%)	-0.02	300 (1%) 72 17	25, 68, 82, 97	4 (0%)

The worst 5 of 300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	82	U	9.3
1	CA	83	U	8.3

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Mol	Chain	Res	Type	RSRZ
1	CA	81	U	6.8
23	AW	1	C	6.4
1	CA	89	C	6.3

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, 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
57	MG	BA	3274	1/1	0.31	-	27,27,27,27	0
57	MG	DA	3198	1/1	0.31	-	31,31,31,31	0
57	MG	DA	3305	1/1	0.32	-	35,35,35,35	0
57	MG	BA	3363	1/1	0.21	-	23,23,23,23	0
57	MG	DA	3113	1/1	0.36	-	26,26,26,26	0
57	MG	DB	203	1/1	0.28	-	66,66,66,66	0
57	MG	BA	3234	1/1	0.06	-	38,38,38,38	0
57	MG	CA	1694	1/1	0.66	-	51,51,51,51	0
57	MG	AA	1655	1/1	0.22	-	6,6,6,6	0
57	MG	CA	1627	1/1	0.16	-	24,24,24,24	0
57	MG	BT	201	1/1	0.20	-	32,32,32,32	0
57	MG	AA	1642	1/1	0.33	-	67,67,67,67	0
57	MG	BA	3343	1/1	0.19	-	22,22,22,22	0
57	MG	BA	3215	1/1	0.22	-	35,35,35,35	0
57	MG	AA	1652	1/1	0.17	-	44,44,44,44	0
57	MG	DA	3026	1/1	0.08	-	33,33,33,33	0
57	MG	AA	1695	1/1	0.21	-	26,26,26,26	0
57	MG	DA	3209	1/1	0.30	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CW	104	1/1	0.32	-	52,52,52,52	0
57	MG	BA	3049	1/1	0.39	-	24,24,24,24	0
57	MG	AA	1669	1/1	0.29	-	70,70,70,70	0
57	MG	BB	202	1/1	0.28	-	21,21,21,21	0
57	MG	BA	3088	1/1	0.23	-	24,24,24,24	0
57	MG	BA	3364	1/1	0.20	-	32,32,32,32	0
57	MG	BA	3358	1/1	0.15	-	38,38,38,38	0
57	MG	AA	1633	1/1	0.09	-	36,36,36,36	0
57	MG	AA	1675	1/1	0.20	-	50,50,50,50	0
57	MG	BA	3301	1/1	0.21	-	33,33,33,33	0
57	MG	BA	3065	1/1	0.28	-	24,24,24,24	0
57	MG	DA	3220	1/1	0.29	-	31,31,31,31	0
57	MG	AA	1603	1/1	0.11	-	18,18,18,18	0
57	MG	DA	3070	1/1	0.34	-	46,46,46,46	0
57	MG	CA	1685	1/1	0.10	-	33,33,33,33	0
57	MG	BA	3096	1/1	0.37	-	24,24,24,24	0
57	MG	BA	3303	1/1	0.33	-	26,26,26,26	0
57	MG	CA	1637	1/1	0.11	-	26,26,26,26	0
57	MG	DA	3109	1/1	0.08	-	33,33,33,33	0
57	MG	AA	1677	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3328	1/1	0.23	-	32,32,32,32	0
57	MG	DA	3287	1/1	0.19	-	48,48,48,48	0
57	MG	DA	3015	1/1	0.20	-	36,36,36,36	0
57	MG	BA	3160	1/1	0.17	-	30,30,30,30	0
57	MG	AA	1605	1/1	0.21	-	51,51,51,51	0
57	MG	DA	3273	1/1	0.33	-	55,55,55,55	0
57	MG	DB	207	1/1	0.14	-	27,27,27,27	0
57	MG	BA	3182	1/1	0.42	-	27,27,27,27	0
57	MG	BA	3444	1/1	0.93	-	101,101,101,101	0
57	MG	CA	1615	1/1	0.40	-	63,63,63,63	0
57	MG	DA	3086	1/1	0.38	-	25,25,25,25	0
57	MG	BA	3383	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3294	1/1	0.30	-	29,29,29,29	0
57	MG	BA	3436	1/1	0.30	-	48,48,48,48	0
57	MG	DA	3163	1/1	0.28	-	32,32,32,32	0
57	MG	BA	3168	1/1	0.12	-	33,33,33,33	0
57	MG	DA	3081	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3118	1/1	2.36	-	205,205,205,205	0
57	MG	BA	3097	1/1	0.46	-	34,34,34,34	0
57	MG	BA	3012	1/1	0.35	-	22,22,22,22	0
57	MG	BA	3231	1/1	0.36	-	54,54,54,54	0
57	MG	CA	1617	1/1	0.23	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3009	1/1	0.20	-	16,16,16,16	0
57	MG	DA	3304	1/1	0.12	-	35,35,35,35	0
57	MG	AA	1625	1/1	0.25	-	37,37,37,37	0
57	MG	BA	3252	1/1	0.17	-	25,25,25,25	0
57	MG	BB	203	1/1	0.28	-	21,21,21,21	0
57	MG	CA	1708	1/1	0.69	-	76,76,76,76	0
57	MG	AA	1664	1/1	0.56	-	77,77,77,77	0
57	MG	BA	3040	1/1	0.19	-	24,24,24,24	0
57	MG	BA	3023	1/1	0.43	-	45,45,45,45	0
57	MG	DA	3297	1/1	0.15	-	48,48,48,48	0
57	MG	AA	1707	1/1	0.21	-	20,20,20,20	0
57	MG	DA	3098	1/1	0.41	-	32,32,32,32	0
57	MG	BA	3172	1/1	0.53	-	22,22,22,22	0
57	MG	BA	3271	1/1	0.24	-	40,40,40,40	0
57	MG	BA	3163	1/1	0.19	-	21,21,21,21	0
57	MG	BA	3245	1/1	0.14	-	27,27,27,27	0
57	MG	DA	3099	1/1	0.35	-	23,23,23,23	0
57	MG	BA	3405	1/1	0.08	-	25,25,25,25	0
57	MG	DB	201	1/1	0.19	-	53,53,53,53	0
57	MG	BA	3063	1/1	0.24	-	17,17,17,17	0
57	MG	AA	1687	1/1	0.26	-	44,44,44,44	0
57	MG	DA	3137	1/1	0.17	-	30,30,30,30	0
57	MG	DA	3135	1/1	0.17	-	42,42,42,42	0
57	MG	CA	1678	1/1	0.19	-	25,25,25,25	0
57	MG	DA	3283	1/1	0.19	-	62,62,62,62	0
57	MG	BA	3214	1/1	0.07	-	29,29,29,29	0
57	MG	BA	3173	1/1	0.11	-	40,40,40,40	0
57	MG	BA	3099	1/1	0.46	-	29,29,29,29	0
57	MG	AA	1629	1/1	0.13	-	56,56,56,56	0
57	MG	DA	3082	1/1	0.27	-	21,21,21,21	0
57	MG	DA	3180	1/1	0.22	-	49,49,49,49	0
57	MG	AA	1666	1/1	0.18	-	24,24,24,24	0
57	MG	BA	3228	1/1	0.37	-	36,36,36,36	0
57	MG	BA	3227	1/1	0.31	-	21,21,21,21	0
57	MG	BA	3397	1/1	0.20	-	44,44,44,44	0
57	MG	DA	3248	1/1	0.19	-	36,36,36,36	0
57	MG	DA	3208	1/1	0.07	-	59,59,59,59	0
57	MG	DA	3264	1/1	0.08	-	25,25,25,25	0
57	MG	DA	3210	1/1	0.28	-	41,41,41,41	0
57	MG	DA	3058	1/1	0.20	-	27,27,27,27	0
57	MG	AA	1696	1/1	0.22	-	26,26,26,26	0
57	MG	DA	3233	1/1	0.13	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3069	1/1	0.50	-	30,30,30,30	0
57	MG	AA	1608	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3132	1/1	0.23	-	28,28,28,28	0
57	MG	BA	3195	1/1	0.23	-	47,47,47,47	0
57	MG	DA	3216	1/1	0.43	-	23,23,23,23	0
57	MG	DA	3144	1/1	0.34	-	44,44,44,44	0
57	MG	AA	1700	1/1	0.18	-	44,44,44,44	0
57	MG	B1	101	1/1	0.40	-	63,63,63,63	0
57	MG	DA	3280	1/1	0.14	-	44,44,44,44	0
57	MG	CA	1647	1/1	0.25	-	61,61,61,61	0
57	MG	BA	3034	1/1	0.20	-	19,19,19,19	0
57	MG	BA	3152	1/1	0.27	-	23,23,23,23	0
57	MG	BA	3108	1/1	0.25	-	35,35,35,35	0
57	MG	BA	3316	1/1	0.20	-	28,28,28,28	0
57	MG	DA	3183	1/1	0.20	-	54,54,54,54	0
57	MG	BA	3320	1/1	0.24	-	25,25,25,25	0
57	MG	DA	3201	1/1	0.40	-	32,32,32,32	0
57	MG	BA	3190	1/1	0.17	-	34,34,34,34	0
57	MG	BA	3061	1/1	0.39	-	25,25,25,25	0
57	MG	DA	3141	1/1	0.18	-	25,25,25,25	0
57	MG	DA	3073	1/1	0.49	-	49,49,49,49	0
57	MG	AA	1610	1/1	0.40	-	21,21,21,21	0
57	MG	CA	1675	1/1	0.44	-	33,33,33,33	0
57	MG	BA	3106	1/1	0.33	-	23,23,23,23	0
57	MG	BA	3053	1/1	0.44	-	63,63,63,63	0
57	MG	BA	3029	1/1	0.13	-	40,40,40,40	0
57	MG	BA	3254	1/1	0.22	-	37,37,37,37	0
57	MG	AA	1699	1/1	0.27	-	29,29,29,29	0
57	MG	DA	3186	1/1	0.08	-	29,29,29,29	0
57	MG	BA	3281	1/1	0.28	-	29,29,29,29	0
57	MG	DA	3094	1/1	0.55	-	71,71,71,71	0
57	MG	BA	3198	1/1	0.13	-	34,34,34,34	0
57	MG	CA	1701	1/1	0.23	-	25,25,25,25	0
57	MG	AA	1631	1/1	0.16	-	29,29,29,29	0
57	MG	CA	1635	1/1	0.28	-	22,22,22,22	0
57	MG	BA	3394	1/1	0.11	-	28,28,28,28	0
57	MG	BA	3415	1/1	0.21	-	36,36,36,36	0
57	MG	BA	3425	1/1	0.18	-	55,55,55,55	0
57	MG	BA	3253	1/1	0.46	-	41,41,41,41	0
57	MG	DA	3057	1/1	0.25	-	22,22,22,22	0
57	MG	BA	3398	1/1	0.18	-	34,34,34,34	0
57	MG	DA	3140	1/1	0.25	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3428	1/1	0.18	-	24,24,24,24	0
57	MG	DA	3050	1/1	0.46	-	46,46,46,46	0
57	MG	BA	3159	1/1	0.48	-	29,29,29,29	0
57	MG	BA	3207	1/1	0.20	-	74,74,74,74	0
57	MG	DA	3112	1/1	0.27	-	27,27,27,27	0
57	MG	BA	3308	1/1	0.32	-	22,22,22,22	0
57	MG	DA	3060	1/1	0.24	-	27,27,27,27	0
57	MG	BA	3137	1/1	0.42	-	46,46,46,46	0
57	MG	BA	3203	1/1	0.28	-	29,29,29,29	0
57	MG	AA	1604	1/1	0.31	-	38,38,38,38	0
57	MG	BA	3079	1/1	0.31	-	25,25,25,25	0
57	MG	BA	3113	1/1	0.45	-	32,32,32,32	0
57	MG	DB	210	1/1	0.15	-	41,41,41,41	0
57	MG	BA	3230	1/1	0.28	-	34,34,34,34	0
57	MG	BA	3404	1/1	0.08	-	53,53,53,53	0
57	MG	DA	3013	1/1	0.37	-	20,20,20,20	0
57	MG	BA	3418	1/1	0.23	-	31,31,31,31	0
57	MG	DA	3169	1/1	0.36	-	18,18,18,18	0
57	MG	AA	1647	1/1	0.23	-	45,45,45,45	0
57	MG	BA	3031	1/1	0.18	-	21,21,21,21	0
57	MG	BA	3068	1/1	0.24	-	30,30,30,30	0
57	MG	AA	1602	1/1	0.30	-	77,77,77,77	0
58	ZN	AD	301	1/1	0.58	-	192,192,192,192	0
57	MG	BA	3041	1/1	0.45	-	44,44,44,44	0
57	MG	BA	3262	1/1	0.52	-	32,32,32,32	0
57	MG	DA	3006	1/1	0.35	-	28,28,28,28	0
57	MG	DA	3021	1/1	0.23	-	34,34,34,34	0
57	MG	BA	3144	1/1	0.20	-	24,24,24,24	0
57	MG	DA	3020	1/1	0.31	-	23,23,23,23	0
57	MG	DA	3206	1/1	0.09	-	49,49,49,49	0
57	MG	CX	101	1/1	0.15	-	22,22,22,22	0
57	MG	BA	3153	1/1	0.14	-	42,42,42,42	0
57	MG	DA	3174	1/1	0.52	-	23,23,23,23	0
57	MG	BA	3385	1/1	0.14	-	54,54,54,54	0
57	MG	AA	1620	1/1	0.17	-	27,27,27,27	0
57	MG	BA	3134	1/1	0.16	-	22,22,22,22	0
57	MG	BA	3210	1/1	0.27	-	24,24,24,24	0
57	MG	DA	3214	1/1	0.34	-	29,29,29,29	0
57	MG	BA	3258	1/1	0.23	-	39,39,39,39	0
57	MG	BA	3086	1/1	1.90	-	130,130,130,130	0
57	MG	BA	3179	1/1	0.47	-	23,23,23,23	0
57	MG	BA	3007	1/1	0.35	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1626	1/1	0.25	-	35,35,35,35	0
57	MG	DA	3152	1/1	0.29	-	61,61,61,61	0
57	MG	CA	1676	1/1	0.21	-	48,48,48,48	0
57	MG	BA	3233	1/1	0.63	-	53,53,53,53	0
57	MG	BA	3103	1/1	0.28	-	21,21,21,21	0
57	MG	BA	3366	1/1	0.30	-	49,49,49,49	0
57	MG	DA	3296	1/1	0.38	-	40,40,40,40	0
57	MG	DA	3237	1/1	0.26	-	33,33,33,33	0
57	MG	BA	3434	1/1	0.26	-	28,28,28,28	0
57	MG	BA	3299	1/1	0.27	-	22,22,22,22	0
57	MG	CA	1643	1/1	0.12	-	44,44,44,44	0
57	MG	DA	3199	1/1	0.27	-	67,67,67,67	0
57	MG	CA	1601	1/1	0.23	-	39,39,39,39	0
57	MG	BA	3219	1/1	0.08	-	28,28,28,28	0
57	MG	BA	3200	1/1	0.35	-	20,20,20,20	0
57	MG	CA	1644	1/1	0.29	-	30,30,30,30	0
57	MG	BA	3251	1/1	0.23	-	23,23,23,23	0
57	MG	BA	3064	1/1	0.40	-	44,44,44,44	0
57	MG	BA	3371	1/1	0.14	-	48,48,48,48	0
57	MG	DA	3192	1/1	0.24	-	43,43,43,43	0
57	MG	CA	1603	1/1	0.19	-	49,49,49,49	0
57	MG	BA	3341	1/1	0.17	-	28,28,28,28	0
57	MG	CA	1674	1/1	0.30	-	41,41,41,41	0
57	MG	DA	3230	1/1	0.32	-	23,23,23,23	0
57	MG	CA	1654	1/1	0.15	-	17,17,17,17	0
57	MG	BA	3181	1/1	0.53	-	19,19,19,19	0
57	MG	BA	3104	1/1	0.27	-	37,37,37,37	0
57	MG	BA	3217	1/1	0.29	-	34,34,34,34	0
57	MG	CA	1709	1/1	0.36	-	28,28,28,28	0
57	MG	BA	3004	1/1	0.64	-	61,61,61,61	0
57	MG	AA	1653	1/1	0.22	-	28,28,28,28	0
57	MG	BA	3293	1/1	0.31	-	23,23,23,23	0
57	MG	BA	3339	1/1	0.28	-	29,29,29,29	0
57	MG	DA	3095	1/1	0.27	-	62,62,62,62	0
57	MG	DA	3255	1/1	0.29	-	46,46,46,46	0
57	MG	BP	201	1/1	1.51	-	205,205,205,205	0
57	MG	DA	3046	1/1	0.36	-	26,26,26,26	0
57	MG	BA	3244	1/1	0.23	-	47,47,47,47	0
57	MG	AA	1691	1/1	0.11	-	39,39,39,39	0
57	MG	BA	3201	1/1	0.09	-	24,24,24,24	0
57	MG	BA	3216	1/1	0.42	-	20,20,20,20	0
57	MG	DA	3157	1/1	0.29	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3247	1/1	0.22	-	23,23,23,23	0
57	MG	BA	3116	1/1	0.12	-	23,23,23,23	0
57	MG	BA	3288	1/1	0.19	-	18,18,18,18	0
57	MG	BA	3090	1/1	0.25	-	17,17,17,17	0
57	MG	BA	3211	1/1	0.21	-	38,38,38,38	0
57	MG	D5	101	1/1	0.17	-	38,38,38,38	0
57	MG	BA	3135	1/1	0.15	-	23,23,23,23	0
57	MG	BA	3037	1/1	0.20	-	9,9,9,9	0
57	MG	DA	3281	1/1	0.08	-	49,49,49,49	0
57	MG	BA	3377	1/1	0.09	-	23,23,23,23	0
57	MG	BA	3354	1/1	0.31	-	25,25,25,25	0
57	MG	BA	3382	1/1	0.27	-	26,26,26,26	0
57	MG	DA	3043	1/1	0.22	-	39,39,39,39	0
57	MG	DA	3130	1/1	0.30	-	34,34,34,34	0
57	MG	BA	3095	1/1	0.22	-	45,45,45,45	0
57	MG	AA	1640	1/1	0.24	-	19,19,19,19	0
57	MG	BA	3433	1/1	0.45	-	52,52,52,52	0
57	MG	BA	3453	1/1	0.25	-	41,41,41,41	0
57	MG	AA	1686	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3200	1/1	0.31	-	66,66,66,66	0
57	MG	BA	3092	1/1	0.19	-	36,36,36,36	0
57	MG	BA	3307	1/1	0.42	-	24,24,24,24	0
57	MG	DA	3146	1/1	0.25	-	60,60,60,60	0
57	MG	BA	3273	1/1	0.22	-	40,40,40,40	0
57	MG	CA	1704	1/1	0.19	-	26,26,26,26	0
57	MG	DA	3229	1/1	0.17	-	19,19,19,19	0
57	MG	BA	3196	1/1	0.12	-	27,27,27,27	0
57	MG	BA	3022	1/1	2.26	-	205,205,205,205	0
57	MG	BA	3055	1/1	0.22	-	24,24,24,24	0
57	MG	BA	3105	1/1	0.15	-	15,15,15,15	0
57	MG	BA	3002	1/1	0.18	-	39,39,39,39	0
57	MG	BA	3265	1/1	0.12	-	67,67,67,67	0
57	MG	BA	3367	1/1	0.36	-	33,33,33,33	0
57	MG	BF	301	1/1	0.25	-	62,62,62,62	0
57	MG	DA	3150	1/1	0.21	-	21,21,21,21	0
57	MG	DA	3107	1/1	0.31	-	64,64,64,64	0
57	MG	CA	1667	1/1	0.14	-	23,23,23,23	0
57	MG	AA	1654	1/1	0.23	-	29,29,29,29	0
57	MG	BA	3141	1/1	0.30	-	45,45,45,45	0
57	MG	CA	1692	1/1	0.19	-	48,48,48,48	0
57	MG	DA	3258	1/1	0.22	-	64,64,64,64	0
57	MG	BA	3424	1/1	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1605	1/1	0.39	-	62,62,62,62	0
57	MG	BA	3072	1/1	0.43	-	23,23,23,23	0
57	MG	BA	3187	1/1	0.39	-	45,45,45,45	0
57	MG	AA	1656	1/1	0.13	-	28,28,28,28	0
57	MG	CA	1703	1/1	0.43	-	34,34,34,34	0
57	MG	BA	3110	1/1	0.23	-	32,32,32,32	0
57	MG	BA	3241	1/1	0.24	-	50,50,50,50	0
57	MG	B7	101	1/1	0.17	-	12,12,12,12	0
57	MG	DA	3093	1/1	0.25	-	19,19,19,19	0
57	MG	BA	3379	1/1	0.24	-	40,40,40,40	0
57	MG	AA	1697	1/1	0.18	-	27,27,27,27	0
57	MG	BB	208	1/1	0.36	-	36,36,36,36	0
57	MG	CW	103	1/1	0.23	-	27,27,27,27	0
57	MG	DA	3083	1/1	0.09	-	30,30,30,30	0
57	MG	CA	1648	1/1	0.07	-	28,28,28,28	0
57	MG	BA	3372	1/1	0.20	-	59,59,59,59	0
57	MG	DA	3215	1/1	0.34	-	37,37,37,37	0
57	MG	AA	1678	1/1	0.11	-	33,33,33,33	0
57	MG	BA	3081	1/1	0.47	-	16,16,16,16	0
57	MG	BA	3154	1/1	0.30	-	38,38,38,38	0
57	MG	B0	101	1/1	0.34	-	30,30,30,30	0
57	MG	DA	3035	1/1	0.39	-	22,22,22,22	0
57	MG	DA	3124	1/1	0.22	-	26,26,26,26	0
57	MG	DA	3257	1/1	0.09	-	35,35,35,35	0
57	MG	BX	101	1/1	0.12	-	36,36,36,36	0
57	MG	BA	3355	1/1	0.49	-	31,31,31,31	0
57	MG	BA	3114	1/1	0.34	-	24,24,24,24	0
57	MG	DA	3171	1/1	0.47	-	27,27,27,27	0
57	MG	DA	3138	1/1	0.27	-	17,17,17,17	0
57	MG	CA	1702	1/1	0.32	-	29,29,29,29	0
57	MG	BA	3349	1/1	0.22	-	38,38,38,38	0
57	MG	BA	3083	1/1	0.13	-	22,22,22,22	0
57	MG	DA	3011	1/1	0.30	-	20,20,20,20	0
57	MG	BA	3176	1/1	0.19	-	44,44,44,44	0
57	MG	B5	103	1/1	0.19	-	20,20,20,20	0
57	MG	BA	3452	1/1	0.13	-	16,16,16,16	0
57	MG	BR	201	1/1	0.42	-	35,35,35,35	0
57	MG	BA	3289	1/1	0.33	-	38,38,38,38	0
57	MG	BA	3175	1/1	0.17	-	71,71,71,71	0
57	MG	BA	3414	1/1	0.36	-	36,36,36,36	0
57	MG	AA	1705	1/1	0.25	-	66,66,66,66	0
57	MG	DA	3134	1/1	0.14	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3193	1/1	0.29	-	27,27,27,27	0
57	MG	DA	3165	1/1	0.23	-	43,43,43,43	0
57	MG	BA	3180	1/1	0.35	-	21,21,21,21	0
57	MG	BA	3020	1/1	0.34	-	19,19,19,19	0
57	MG	DB	206	1/1	0.12	-	19,19,19,19	0
57	MG	DA	3106	1/1	0.47	-	25,25,25,25	0
58	ZN	D9	101	1/1	0.17	-	30,30,30,30	0
57	MG	DA	3189	1/1	0.19	-	34,34,34,34	0
57	MG	BA	3205	1/1	0.12	-	45,45,45,45	0
57	MG	BA	3413	1/1	0.32	-	24,24,24,24	0
57	MG	DA	3038	1/1	0.43	-	49,49,49,49	0
57	MG	AA	1632	1/1	0.42	-	57,57,57,57	0
57	MG	CA	1613	1/1	0.43	-	42,42,42,42	0
57	MG	BA	3127	1/1	0.25	-	30,30,30,30	0
57	MG	DA	3143	1/1	0.21	-	23,23,23,23	0
57	MG	BA	3309	1/1	0.07	-	20,20,20,20	0
57	MG	CA	1683	1/1	0.15	-	36,36,36,36	0
57	MG	BA	3275	1/1	0.27	-	27,27,27,27	0
57	MG	DA	3148	1/1	0.23	-	24,24,24,24	0
57	MG	DA	3167	1/1	0.38	-	38,38,38,38	0
57	MG	BP	202	1/1	0.16	-	22,22,22,22	0
57	MG	AA	1641	1/1	0.20	-	30,30,30,30	0
57	MG	BA	3235	1/1	0.18	-	51,51,51,51	0
57	MG	DA	3066	1/1	0.32	-	22,22,22,22	0
57	MG	AA	1601	1/1	0.22	-	47,47,47,47	0
57	MG	BA	3027	1/1	0.13	-	26,26,26,26	0
57	MG	BA	3199	1/1	0.30	-	23,23,23,23	0
57	MG	BA	3417	1/1	0.31	-	62,62,62,62	0
57	MG	BA	3395	1/1	0.41	-	39,39,39,39	0
57	MG	BA	3046	1/1	0.29	-	32,32,32,32	0
57	MG	DA	3166	1/1	0.12	-	22,22,22,22	0
57	MG	DA	3190	1/1	0.22	-	44,44,44,44	0
57	MG	AW	101	1/1	0.21	-	6,6,6,6	0
57	MG	DA	3101	1/1	0.27	-	35,35,35,35	0
57	MG	DA	3023	1/1	0.21	-	42,42,42,42	0
57	MG	BA	3162	1/1	0.09	-	21,21,21,21	0
57	MG	BA	3263	1/1	0.07	-	36,36,36,36	0
57	MG	CE	201	1/1	0.25	-	42,42,42,42	0
57	MG	DA	3179	1/1	0.36	-	30,30,30,30	0
57	MG	DA	3158	1/1	0.36	-	44,44,44,44	0
57	MG	CA	1646	1/1	0.20	-	59,59,59,59	0
57	MG	BA	3442	1/1	3.46	-	205,205,205,205	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3044	1/1	0.28	-	22,22,22,22	0
57	MG	CA	1619	1/1	0.12	-	34,34,34,34	0
57	MG	DA	3178	1/1	0.07	-	30,30,30,30	0
57	MG	BA	3057	1/1	0.42	-	39,39,39,39	0
57	MG	BA	3030	1/1	0.39	-	37,37,37,37	0
57	MG	BA	3128	1/1	0.39	-	33,33,33,33	0
57	MG	BA	3264	1/1	0.26	-	34,34,34,34	0
57	MG	BA	3278	1/1	0.16	-	33,33,33,33	0
57	MG	AA	1621	1/1	0.24	-	48,48,48,48	0
57	MG	BA	3223	1/1	0.27	-	49,49,49,49	0
57	MG	AA	1692	1/1	0.28	-	51,51,51,51	0
57	MG	BA	3406	1/1	0.16	-	50,50,50,50	0
57	MG	AA	1660	1/1	0.20	-	31,31,31,31	0
57	MG	BQ	202	1/1	0.39	-	30,30,30,30	0
57	MG	BD	301	1/1	0.24	-	34,34,34,34	0
57	MG	BA	3298	1/1	0.14	-	20,20,20,20	0
57	MG	DA	3181	1/1	0.23	-	36,36,36,36	0
57	MG	DA	3236	1/1	0.09	-	30,30,30,30	0
57	MG	CA	1614	1/1	0.10	-	30,30,30,30	0
57	MG	BA	3070	1/1	0.13	-	23,23,23,23	0
57	MG	BA	3374	1/1	0.19	-	51,51,51,51	0
57	MG	AA	1676	1/1	0.27	-	30,30,30,30	0
57	MG	AA	1638	1/1	0.11	-	55,55,55,55	0
57	MG	BA	3164	1/1	0.16	-	35,35,35,35	0
57	MG	DA	3164	1/1	0.40	-	83,83,83,83	0
57	MG	BA	3155	1/1	0.57	-	37,37,37,37	0
57	MG	DA	3025	1/1	0.20	-	38,38,38,38	0
57	MG	DA	3294	1/1	0.36	-	19,19,19,19	0
57	MG	CW	105	1/1	0.27	-	61,61,61,61	0
57	MG	BA	3089	1/1	0.36	-	24,24,24,24	0
57	MG	BA	3257	1/1	0.17	-	41,41,41,41	0
57	MG	BA	3432	1/1	0.58	-	70,70,70,70	0
57	MG	DA	3125	1/1	0.27	-	26,26,26,26	0
57	MG	BA	3093	1/1	0.14	-	23,23,23,23	0
57	MG	AA	1711	1/1	0.31	-	58,58,58,58	0
57	MG	BA	3347	1/1	0.10	-	28,28,28,28	0
57	MG	BA	3312	1/1	0.33	-	22,22,22,22	0
57	MG	AA	1615	1/1	0.17	-	46,46,46,46	0
57	MG	BA	3026	1/1	0.25	-	31,31,31,31	0
57	MG	BA	3411	1/1	0.40	-	53,53,53,53	0
57	MG	BA	3078	1/1	0.33	-	29,29,29,29	0
57	MG	AA	1659	1/1	0.19	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3032	1/1	0.18	-	20,20,20,20	0
57	MG	DA	3267	1/1	0.50	-	73,73,73,73	0
57	MG	BA	3005	1/1	0.22	-	23,23,23,23	0
57	MG	AA	1704	1/1	0.14	-	64,64,64,64	0
57	MG	BA	3455	1/1	0.23	-	46,46,46,46	0
57	MG	CA	1657	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3122	1/1	0.24	-	41,41,41,41	0
57	MG	AA	1698	1/1	0.33	-	37,37,37,37	0
57	MG	BA	3062	1/1	0.09	-	19,19,19,19	0
57	MG	CA	1673	1/1	0.16	-	26,26,26,26	0
57	MG	DA	3207	1/1	0.15	-	26,26,26,26	0
57	MG	DA	3017	1/1	0.34	-	21,21,21,21	0
57	MG	BA	3146	1/1	0.28	-	22,22,22,22	0
57	MG	DA	3212	1/1	0.18	-	18,18,18,18	0
57	MG	CA	1630	1/1	0.10	-	29,29,29,29	0
57	MG	BA	3403	1/1	0.23	-	48,48,48,48	0
57	MG	DA	3286	1/1	0.28	-	52,52,52,52	0
57	MG	AA	1635	1/1	0.41	-	31,31,31,31	0
57	MG	AA	1607	1/1	0.25	-	51,51,51,51	0
57	MG	CA	1662	1/1	0.35	-	26,26,26,26	0
57	MG	BA	3390	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3193	1/1	0.12	-	47,47,47,47	0
57	MG	AA	1694	1/1	0.20	-	23,23,23,23	0
57	MG	BA	3447	1/1	0.44	-	27,27,27,27	0
57	MG	BA	3212	1/1	0.40	-	30,30,30,30	0
57	MG	DA	3196	1/1	0.24	-	26,26,26,26	0
57	MG	DA	3170	1/1	0.30	-	22,22,22,22	0
57	MG	BA	3427	1/1	0.24	-	40,40,40,40	0
57	MG	BA	3329	1/1	0.07	-	26,26,26,26	0
57	MG	BA	3348	1/1	0.39	-	55,55,55,55	0
57	MG	BA	3185	1/1	0.25	-	17,17,17,17	0
57	MG	CA	1638	1/1	0.40	-	35,35,35,35	0
57	MG	DA	3079	1/1	0.22	-	45,45,45,45	0
57	MG	BA	3242	1/1	0.23	-	24,24,24,24	0
57	MG	CA	1689	1/1	0.20	-	39,39,39,39	0
57	MG	BA	3059	1/1	0.30	-	28,28,28,28	0
57	MG	BA	3109	1/1	0.27	-	21,21,21,21	0
57	MG	BA	3021	1/1	1.60	-	180,180,180,180	0
57	MG	CA	1695	1/1	0.24	-	38,38,38,38	0
57	MG	DA	3077	1/1	0.33	-	22,22,22,22	0
57	MG	BA	3011	1/1	0.24	-	6,6,6,6	0
57	MG	BA	3117	1/1	0.60	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3400	1/1	0.07	-	32,32,32,32	0
57	MG	BA	3368	1/1	0.41	-	49,49,49,49	0
57	MG	BA	3392	1/1	0.17	-	52,52,52,52	0
57	MG	BA	3335	1/1	0.08	-	47,47,47,47	0
57	MG	DB	209	1/1	0.18	-	41,41,41,41	0
57	MG	DA	3119	1/1	0.25	-	42,42,42,42	0
57	MG	DA	3117	1/1	0.21	-	42,42,42,42	0
57	MG	DA	3246	1/1	0.37	-	43,43,43,43	0
57	MG	BA	3437	1/1	0.12	-	27,27,27,27	0
57	MG	BA	3282	1/1	0.32	-	22,22,22,22	0
57	MG	DA	3291	1/1	0.16	-	31,31,31,31	0
57	MG	BA	3167	1/1	0.28	-	65,65,65,65	0
57	MG	DF	301	1/1	0.34	-	49,49,49,49	0
57	MG	DA	3226	1/1	0.27	-	32,32,32,32	0
57	MG	DA	3203	1/1	0.18	-	52,52,52,52	0
57	MG	CA	1687	1/1	0.15	-	37,37,37,37	0
57	MG	BA	3361	1/1	0.22	-	31,31,31,31	0
57	MG	DA	3172	1/1	0.12	-	30,30,30,30	0
57	MG	DA	3051	1/1	0.25	-	6,6,6,6	0
57	MG	DA	3205	1/1	0.28	-	55,55,55,55	0
57	MG	DA	3123	1/1	0.22	-	25,25,25,25	0
57	MG	CA	1688	1/1	0.09	-	35,35,35,35	0
57	MG	CA	1620	1/1	0.47	-	29,29,29,29	0
57	MG	DA	3014	1/1	0.30	-	44,44,44,44	0
57	MG	CA	1666	1/1	0.33	-	18,18,18,18	0
57	MG	DA	3292	1/1	0.10	-	17,17,17,17	0
57	MG	BA	3140	1/1	0.07	-	33,33,33,33	0
57	MG	BA	3107	1/1	0.10	-	40,40,40,40	0
57	MG	DA	3151	1/1	0.28	-	43,43,43,43	0
57	MG	DA	3008	1/1	0.24	-	6,6,6,6	0
57	MG	DA	3010	1/1	0.40	-	66,66,66,66	0
57	MG	BA	3430	1/1	0.38	-	58,58,58,58	0
58	ZN	B9	101	1/1	0.13	-	75,75,75,75	0
57	MG	DA	3221	1/1	0.29	-	38,38,38,38	0
57	MG	BA	3391	1/1	0.22	-	44,44,44,44	0
57	MG	BA	3410	1/1	0.12	-	30,30,30,30	0
57	MG	BA	3045	1/1	0.18	-	6,6,6,6	0
57	MG	DA	3240	1/1	0.14	-	35,35,35,35	0
57	MG	BA	3357	1/1	0.20	-	38,38,38,38	0
57	MG	DA	3279	1/1	0.27	-	43,43,43,43	0
57	MG	DA	3160	1/1	0.27	-	38,38,38,38	0
57	MG	BU	201	1/1	0.38	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3119	1/1	0.41	-	23,23,23,23	0
57	MG	DA	3204	1/1	0.12	-	41,41,41,41	0
57	MG	BA	3441	1/1	0.39	-	37,37,37,37	0
57	MG	BA	3350	1/1	0.24	-	37,37,37,37	0
57	MG	DD	301	1/1	0.15	-	18,18,18,18	0
57	MG	DA	3133	1/1	0.15	-	31,31,31,31	0
57	MG	AA	1702	1/1	0.11	-	26,26,26,26	0
57	MG	BA	3098	1/1	0.26	-	25,25,25,25	0
57	MG	BA	3112	1/1	0.21	-	23,23,23,23	0
57	MG	BA	3297	1/1	0.21	-	21,21,21,21	0
57	MG	AA	1628	1/1	0.45	-	43,43,43,43	0
57	MG	BA	3422	1/1	0.43	-	20,20,20,20	0
57	MG	BA	3188	1/1	0.85	-	87,87,87,87	0
57	MG	CA	1705	1/1	0.20	-	48,48,48,48	0
57	MG	BA	3369	1/1	0.13	-	63,63,63,63	0
57	MG	DA	3002	1/1	0.59	-	37,37,37,37	0
57	MG	BA	3330	1/1	0.17	-	21,21,21,21	0
57	MG	BA	3124	1/1	0.21	-	41,41,41,41	0
57	MG	DA	3111	1/1	0.55	-	76,76,76,76	0
57	MG	BA	3412	1/1	0.21	-	35,35,35,35	0
57	MG	AA	1623	1/1	0.30	-	18,18,18,18	0
57	MG	BA	3401	1/1	0.11	-	46,46,46,46	0
57	MG	DA	3097	1/1	0.26	-	21,21,21,21	0
57	MG	DA	3078	1/1	0.21	-	44,44,44,44	0
57	MG	DA	3053	1/1	0.34	-	21,21,21,21	0
57	MG	BA	3008	1/1	0.41	-	16,16,16,16	0
57	MG	DA	3039	1/1	0.27	-	18,18,18,18	0
57	MG	DA	3232	1/1	0.31	-	40,40,40,40	0
57	MG	BA	3438	1/1	0.33	-	67,67,67,67	0
57	MG	DA	3018	1/1	0.36	-	21,21,21,21	0
57	MG	DA	3030	1/1	0.18	-	46,46,46,46	0
57	MG	DA	3187	1/1	0.28	-	48,48,48,48	0
57	MG	BA	3052	1/1	0.43	-	30,30,30,30	0
57	MG	CA	1700	1/1	0.35	-	56,56,56,56	0
57	MG	BA	3142	1/1	0.27	-	25,25,25,25	0
57	MG	CA	1661	1/1	0.33	-	26,26,26,26	0
57	MG	BA	3194	1/1	0.07	-	72,72,72,72	0
57	MG	AA	1663	1/1	0.10	-	27,27,27,27	0
57	MG	DA	3145	1/1	0.74	-	57,57,57,57	0
57	MG	CA	1707	1/1	0.60	-	62,62,62,62	0
57	MG	DA	3265	1/1	0.31	-	54,54,54,54	0
57	MG	BB	205	1/1	0.24	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3149	1/1	0.26	-	27,27,27,27	0
57	MG	BA	3218	1/1	0.39	-	23,23,23,23	0
57	MG	DA	3080	1/1	0.30	-	24,24,24,24	0
57	MG	DA	3061	1/1	0.20	-	22,22,22,22	0
57	MG	BA	3431	1/1	0.32	-	53,53,53,53	0
57	MG	CA	1602	1/1	0.17	-	35,35,35,35	0
57	MG	BA	3409	1/1	0.12	-	24,24,24,24	0
57	MG	BA	3006	1/1	0.26	-	27,27,27,27	0
57	MG	BA	3014	1/1	0.36	-	24,24,24,24	0
57	MG	BB	201	1/1	0.35	-	59,59,59,59	0
57	MG	BA	3416	1/1	0.16	-	42,42,42,42	0
57	MG	DA	3298	1/1	0.15	-	33,33,33,33	0
57	MG	CA	1677	1/1	0.33	-	27,27,27,27	0
57	MG	BA	3035	1/1	0.34	-	25,25,25,25	0
57	MG	DA	3085	1/1	0.36	-	49,49,49,49	0
57	MG	AA	1708	1/1	0.14	-	46,46,46,46	0
57	MG	DA	3142	1/1	0.18	-	51,51,51,51	0
57	MG	BA	3204	1/1	0.48	-	52,52,52,52	0
57	MG	BB	206	1/1	0.29	-	31,31,31,31	0
57	MG	AA	1667	1/1	0.23	-	62,62,62,62	0
57	MG	DA	3211	1/1	0.41	-	55,55,55,55	0
57	MG	BA	3352	1/1	0.27	-	22,22,22,22	0
57	MG	DA	3126	1/1	0.21	-	6,6,6,6	0
57	MG	CW	102	1/1	0.38	-	93,93,93,93	0
57	MG	DA	3089	1/1	0.10	-	19,19,19,19	0
57	MG	DB	202	1/1	0.15	-	61,61,61,61	0
57	MG	AA	1617	1/1	0.32	-	43,43,43,43	0
57	MG	BA	3237	1/1	0.11	-	21,21,21,21	0
57	MG	DA	3213	1/1	0.26	-	28,28,28,28	0
57	MG	BA	3184	1/1	0.26	-	53,53,53,53	0
57	MG	DA	3071	1/1	0.25	-	20,20,20,20	0
57	MG	CA	1680	1/1	0.10	-	31,31,31,31	0
57	MG	DA	3004	1/1	0.14	-	21,21,21,21	0
57	MG	DA	3254	1/1	0.28	-	60,60,60,60	0
57	MG	BA	3075	1/1	0.23	-	24,24,24,24	0
57	MG	DA	3275	1/1	0.28	-	48,48,48,48	0
57	MG	BA	3292	1/1	0.34	-	24,24,24,24	0
57	MG	DA	3270	1/1	0.25	-	47,47,47,47	0
57	MG	AA	1637	1/1	0.35	-	45,45,45,45	0
57	MG	BA	3388	1/1	0.37	-	37,37,37,37	0
57	MG	CA	1631	1/1	0.29	-	34,34,34,34	0
57	MG	BA	3376	1/1	0.16	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1689	1/1	0.17	-	55,55,55,55	0
57	MG	BA	3166	1/1	0.54	-	38,38,38,38	0
58	ZN	CD	301	1/1	0.35	-	81,81,81,81	0
57	MG	BA	3344	1/1	0.18	-	24,24,24,24	0
57	MG	CA	1671	1/1	0.10	-	54,54,54,54	0
57	MG	B5	101	1/1	0.47	-	78,78,78,78	0
57	MG	BA	3189	1/1	0.08	-	14,14,14,14	0
57	MG	BA	3420	1/1	0.23	-	45,45,45,45	0
57	MG	AA	1717	1/1	0.33	-	25,25,25,25	0
57	MG	AA	1650	1/1	0.21	-	28,28,28,28	0
57	MG	AA	1616	1/1	0.24	-	30,30,30,30	0
57	MG	AA	1693	1/1	0.10	-	45,45,45,45	0
57	MG	DA	3040	1/1	0.34	-	26,26,26,26	0
57	MG	BA	3069	1/1	0.28	-	30,30,30,30	0
57	MG	AA	1662	1/1	0.12	-	22,22,22,22	0
57	MG	CA	1625	1/1	0.22	-	31,31,31,31	0
57	MG	CA	1611	1/1	0.08	-	25,25,25,25	0
57	MG	CA	1663	1/1	0.13	-	33,33,33,33	0
57	MG	DB	205	1/1	0.31	-	42,42,42,42	0
57	MG	BA	3120	1/1	0.26	-	35,35,35,35	0
57	MG	DA	3118	1/1	0.19	-	33,33,33,33	0
57	MG	CA	1642	1/1	0.13	-	37,37,37,37	0
57	MG	DA	3302	1/1	0.29	-	36,36,36,36	0
57	MG	DA	3231	1/1	0.39	-	45,45,45,45	0
57	MG	AA	1680	1/1	0.29	-	49,49,49,49	0
57	MG	DA	3269	1/1	0.27	-	47,47,47,47	0
57	MG	DA	3239	1/1	0.25	-	32,32,32,32	0
57	MG	DA	3301	1/1	0.07	-	33,33,33,33	0
57	MG	BB	207	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3087	1/1	0.34	-	23,23,23,23	0
57	MG	DA	3271	1/1	0.15	-	42,42,42,42	0
57	MG	BA	3284	1/1	0.17	-	15,15,15,15	0
57	MG	DA	3289	1/1	0.13	-	27,27,27,27	0
57	MG	CA	1698	1/1	0.19	-	33,33,33,33	0
57	MG	BA	3147	1/1	0.33	-	24,24,24,24	0
57	MG	BA	3448	1/1	0.41	-	54,54,54,54	0
57	MG	CA	1655	1/1	0.17	-	34,34,34,34	0
57	MG	BA	3032	1/1	0.24	-	6,6,6,6	0
57	MG	BA	3337	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3229	1/1	0.25	-	6,6,6,6	0
57	MG	CA	1622	1/1	0.26	-	24,24,24,24	0
57	MG	DA	3120	1/1	0.17	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3024	1/1	0.36	-	20,20,20,20	0
57	MG	DR	201	1/1	0.13	-	22,22,22,22	0
57	MG	AA	1672	1/1	0.21	-	33,33,33,33	0
57	MG	AA	1710	1/1	0.14	-	30,30,30,30	0
57	MG	BA	3285	1/1	0.11	-	6,6,6,6	0
57	MG	AA	1618	1/1	0.16	-	64,64,64,64	0
57	MG	DA	3076	1/1	0.12	-	19,19,19,19	0
57	MG	DA	3091	1/1	0.12	-	26,26,26,26	0
57	MG	DA	3114	1/1	0.33	-	30,30,30,30	0
57	MG	BA	3206	1/1	0.18	-	22,22,22,22	0
57	MG	AA	1639	1/1	0.15	-	27,27,27,27	0
57	MG	BA	3208	1/1	0.05	-	56,56,56,56	0
57	MG	BA	3115	1/1	0.25	-	19,19,19,19	0
57	MG	DA	3029	1/1	0.13	-	22,22,22,22	0
57	MG	DA	3175	1/1	0.47	-	56,56,56,56	0
57	MG	BA	3300	1/1	0.51	-	67,67,67,67	0
57	MG	DA	3259	1/1	0.19	-	47,47,47,47	0
57	MG	AA	1714	1/1	0.22	-	42,42,42,42	0
57	MG	BA	3017	1/1	0.25	-	20,20,20,20	0
57	MG	BA	3042	1/1	0.33	-	10,10,10,10	0
57	MG	DA	3059	1/1	0.24	-	26,26,26,26	0
57	MG	DA	3224	1/1	0.33	-	14,14,14,14	0
57	MG	BA	3306	1/1	0.31	-	47,47,47,47	0
57	MG	DA	3274	1/1	0.19	-	36,36,36,36	0
57	MG	BA	3362	1/1	0.25	-	30,30,30,30	0
57	MG	BA	3080	1/1	0.33	-	32,32,32,32	0
57	MG	DA	3188	1/1	0.10	-	27,27,27,27	0
57	MG	B5	102	1/1	0.36	-	40,40,40,40	0
57	MG	BA	3378	1/1	0.20	-	55,55,55,55	0
57	MG	DA	3261	1/1	0.20	-	58,58,58,58	0
57	MG	BA	3243	1/1	0.24	-	51,51,51,51	0
57	MG	BA	3451	1/1	0.12	-	23,23,23,23	0
57	MG	BA	3260	1/1	0.22	-	24,24,24,24	0
57	MG	BA	3236	1/1	0.33	-	62,62,62,62	0
57	MG	DA	3202	1/1	0.52	-	38,38,38,38	0
57	MG	CA	1665	1/1	0.24	-	30,30,30,30	0
57	MG	DA	3067	1/1	0.21	-	56,56,56,56	0
57	MG	BA	3315	1/1	0.13	-	17,17,17,17	0
57	MG	DA	3122	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3091	1/1	0.43	-	21,21,21,21	0
57	MG	BA	3259	1/1	0.17	-	37,37,37,37	0
57	MG	BA	3238	1/1	0.40	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3197	1/1	0.36	-	20,20,20,20	0
57	MG	DA	3009	1/1	0.20	-	18,18,18,18	0
57	MG	DA	3129	1/1	0.17	-	47,47,47,47	0
57	MG	BA	3126	1/1	0.30	-	66,66,66,66	0
57	MG	BA	3018	1/1	0.48	-	21,21,21,21	0
57	MG	BA	3177	1/1	0.31	-	21,21,21,21	0
57	MG	CA	1706	1/1	0.29	-	59,59,59,59	0
57	MG	BE	301	1/1	0.29	-	43,43,43,43	0
57	MG	BA	3101	1/1	0.09	-	21,21,21,21	0
57	MG	BA	3158	1/1	0.36	-	37,37,37,37	0
57	MG	DA	3277	1/1	0.19	-	57,57,57,57	0
57	MG	BA	3186	1/1	0.53	-	24,24,24,24	0
57	MG	DA	3176	1/1	0.30	-	24,24,24,24	0
57	MG	BA	3323	1/1	1.38	-	205,205,205,205	0
57	MG	DA	3278	1/1	0.26	-	59,59,59,59	0
57	MG	CA	1629	1/1	0.23	-	25,25,25,25	0
57	MG	BA	3121	1/1	0.19	-	20,20,20,20	0
57	MG	DA	3299	1/1	0.17	-	42,42,42,42	0
57	MG	CA	1610	1/1	0.28	-	30,30,30,30	0
57	MG	DA	3191	1/1	0.22	-	18,18,18,18	0
57	MG	BA	3213	1/1	0.34	-	43,43,43,43	0
57	MG	DA	3065	1/1	0.37	-	29,29,29,29	0
57	MG	BA	3038	1/1	1.42	-	163,163,163,163	0
57	MG	CA	1686	1/1	0.22	-	44,44,44,44	0
57	MG	CA	1649	1/1	0.29	-	65,65,65,65	0
57	MG	DA	3218	1/1	0.20	-	35,35,35,35	0
57	MG	CA	1626	1/1	0.47	-	67,67,67,67	0
57	MG	DA	3052	1/1	0.25	-	21,21,21,21	0
57	MG	BA	3286	1/1	0.29	-	24,24,24,24	0
57	MG	BA	3221	1/1	0.16	-	22,22,22,22	0
57	MG	DA	3041	1/1	0.12	-	19,19,19,19	0
57	MG	BA	3336	1/1	0.15	-	29,29,29,29	0
57	MG	BA	3047	1/1	0.42	-	62,62,62,62	0
57	MG	AA	1649	1/1	0.32	-	50,50,50,50	0
57	MG	DA	3290	1/1	0.56	-	50,50,50,50	0
57	MG	BA	3246	1/1	0.12	-	11,11,11,11	0
57	MG	DA	3054	1/1	0.51	-	27,27,27,27	0
57	MG	AA	1622	1/1	0.25	-	36,36,36,36	0
57	MG	DA	3056	1/1	0.24	-	30,30,30,30	0
57	MG	DA	3132	1/1	0.42	-	32,32,32,32	0
57	MG	BA	3150	1/1	0.39	-	29,29,29,29	0
57	MG	BA	3272	1/1	0.44	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3064	1/1	0.24	-	19,19,19,19	0
57	MG	AA	1609	1/1	0.22	-	48,48,48,48	0
57	MG	BA	3261	1/1	0.42	-	28,28,28,28	0
58	ZN	B5	105	1/1	0.15	-	90,90,90,90	0
57	MG	BA	3396	1/1	0.12	-	26,26,26,26	0
57	MG	BA	3321	1/1	0.34	-	22,22,22,22	0
57	MG	BA	3423	1/1	0.10	-	25,25,25,25	0
57	MG	BB	209	1/1	0.12	-	37,37,37,37	0
57	MG	DA	3300	1/1	0.15	-	38,38,38,38	0
57	MG	BA	3304	1/1	0.12	-	49,49,49,49	0
57	MG	BB	204	1/1	0.43	-	54,54,54,54	0
57	MG	DA	3045	1/1	0.42	-	59,59,59,59	0
57	MG	AA	1706	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3133	1/1	0.36	-	60,60,60,60	0
57	MG	BA	3139	1/1	0.89	-	72,72,72,72	0
57	MG	DA	3027	1/1	0.14	-	33,33,33,33	0
57	MG	DA	3012	1/1	0.48	-	28,28,28,28	0
57	MG	DA	3096	1/1	0.20	-	34,34,34,34	0
57	MG	DA	3042	1/1	0.33	-	28,28,28,28	0
57	MG	DA	3005	1/1	0.46	-	45,45,45,45	0
57	MG	BA	3458	1/1	0.48	-	47,47,47,47	0
57	MG	DA	3185	1/1	0.28	-	37,37,37,37	0
57	MG	BA	3346	1/1	0.45	-	50,50,50,50	0
57	MG	DA	3276	1/1	0.15	-	51,51,51,51	0
57	MG	B0	102	1/1	0.19	-	33,33,33,33	0
57	MG	DA	3249	1/1	0.16	-	33,33,33,33	0
57	MG	BA	3338	1/1	0.10	-	18,18,18,18	0
57	MG	BA	3123	1/1	0.25	-	43,43,43,43	0
57	MG	CA	1628	1/1	0.19	-	26,26,26,26	0
57	MG	DA	3127	1/1	0.35	-	34,34,34,34	0
57	MG	D5	102	1/1	0.43	-	44,44,44,44	0
57	MG	BA	3269	1/1	0.24	-	27,27,27,27	0
57	MG	CA	1690	1/1	0.30	-	44,44,44,44	0
57	MG	BA	3443	1/1	0.22	-	24,24,24,24	0
57	MG	DA	3272	1/1	0.21	-	40,40,40,40	0
57	MG	DA	3092	1/1	0.30	-	25,25,25,25	0
57	MG	BA	3222	1/1	0.29	-	31,31,31,31	0
57	MG	DA	3285	1/1	0.18	-	38,38,38,38	0
57	MG	CA	1632	1/1	0.35	-	18,18,18,18	0
57	MG	BA	3248	1/1	0.28	-	34,34,34,34	0
57	MG	CA	1693	1/1	0.24	-	36,36,36,36	0
57	MG	DA	3024	1/1	0.10	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3161	1/1	0.23	-	25,25,25,25	0
57	MG	AA	1715	1/1	0.10	-	62,62,62,62	0
57	MG	DA	3194	1/1	0.30	-	61,61,61,61	0
57	MG	AA	1716	1/1	0.15	-	31,31,31,31	0
57	MG	DA	3047	1/1	0.34	-	26,26,26,26	0
57	MG	DA	3266	1/1	0.27	-	46,46,46,46	0
57	MG	BA	3033	1/1	0.23	-	34,34,34,34	0
57	MG	BA	3010	1/1	0.24	-	23,23,23,23	0
57	MG	BA	3291	1/1	0.28	-	24,24,24,24	0
57	MG	DA	3139	1/1	0.23	-	58,58,58,58	0
57	MG	BA	3268	1/1	0.62	-	46,46,46,46	0
57	MG	DA	3168	1/1	0.16	-	35,35,35,35	0
57	MG	CA	1652	1/1	0.32	-	59,59,59,59	0
57	MG	DA	3251	1/1	0.40	-	53,53,53,53	0
57	MG	CA	1664	1/1	0.36	-	42,42,42,42	0
57	MG	CA	1616	1/1	0.16	-	20,20,20,20	0
57	MG	DA	3303	1/1	0.27	-	54,54,54,54	0
57	MG	BA	3426	1/1	0.12	-	26,26,26,26	0
57	MG	BA	3224	1/1	0.33	-	31,31,31,31	0
57	MG	AA	1644	1/1	0.21	-	40,40,40,40	0
57	MG	BA	3077	1/1	0.81	-	63,63,63,63	0
57	MG	AA	1611	1/1	0.78	-	58,58,58,58	0
57	MG	CA	1679	1/1	0.08	-	29,29,29,29	0
57	MG	BA	3136	1/1	0.80	-	76,76,76,76	0
57	MG	DA	3161	1/1	0.35	-	50,50,50,50	0
57	MG	BH	201	1/1	0.15	-	21,21,21,21	0
57	MG	BA	3240	1/1	0.20	-	23,23,23,23	0
57	MG	BA	3445	1/1	0.12	-	36,36,36,36	0
57	MG	AA	1646	1/1	0.16	-	49,49,49,49	0
57	MG	DA	3037	1/1	0.43	-	45,45,45,45	0
57	MG	AA	1688	1/1	0.22	-	56,56,56,56	0
57	MG	BA	3232	1/1	0.44	-	38,38,38,38	0
57	MG	CA	1623	1/1	0.33	-	59,59,59,59	0
57	MG	DA	3055	1/1	0.24	-	24,24,24,24	0
57	MG	AA	1614	1/1	0.37	-	29,29,29,29	0
57	MG	DA	3250	1/1	0.35	-	26,26,26,26	0
57	MG	DA	3048	1/1	0.24	-	6,6,6,6	0
57	MG	DA	3074	1/1	0.23	-	21,21,21,21	0
57	MG	DB	204	1/1	0.17	-	43,43,43,43	0
57	MG	BA	3025	1/1	0.34	-	31,31,31,31	0
57	MG	BA	3314	1/1	0.07	-	22,22,22,22	0
57	MG	AA	1613	1/1	0.30	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3100	1/1	0.28	-	21,21,21,21	0
57	MG	DA	3217	1/1	0.52	-	54,54,54,54	0
57	MG	BA	3360	1/1	0.17	-	27,27,27,27	0
57	MG	BA	3429	1/1	0.14	-	33,33,33,33	0
57	MG	BA	3145	1/1	0.36	-	29,29,29,29	0
57	MG	DA	3154	1/1	0.11	-	61,61,61,61	0
57	MG	DA	3245	1/1	0.26	-	52,52,52,52	0
57	MG	AA	1681	1/1	0.36	-	63,63,63,63	0
57	MG	BA	3381	1/1	0.48	-	66,66,66,66	0
57	MG	BA	3191	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3022	1/1	0.21	-	21,21,21,21	0
57	MG	AA	1606	1/1	0.22	-	42,42,42,42	0
57	MG	BA	3157	1/1	0.13	-	38,38,38,38	0
57	MG	BA	3459	1/1	0.19	-	35,35,35,35	0
57	MG	AA	1627	1/1	0.16	-	21,21,21,21	0
57	MG	DA	3049	1/1	0.23	-	15,15,15,15	0
57	MG	CA	1699	1/1	0.19	-	32,32,32,32	0
57	MG	AW	102	1/1	0.10	-	26,26,26,26	0
57	MG	BA	3277	1/1	0.24	-	29,29,29,29	0
57	MG	BA	3449	1/1	0.21	-	53,53,53,53	0
57	MG	BA	3279	1/1	0.06	-	26,26,26,26	0
57	MG	BA	3054	1/1	0.43	-	33,33,33,33	0
57	MG	CA	1691	1/1	0.53	-	67,67,67,67	0
57	MG	DA	3063	1/1	0.13	-	29,29,29,29	0
57	MG	DA	3088	1/1	0.23	-	20,20,20,20	0
57	MG	CA	1624	1/1	0.51	-	39,39,39,39	0
57	MG	BQ	203	1/1	0.22	-	27,27,27,27	0
57	MG	CA	1606	1/1	0.32	-	50,50,50,50	0
57	MG	CA	1634	1/1	0.11	-	37,37,37,37	0
57	MG	CA	1672	1/1	0.22	-	29,29,29,29	0
57	MG	AA	1658	1/1	0.14	-	23,23,23,23	0
57	MG	BA	3036	1/1	0.20	-	30,30,30,30	0
57	MG	BA	3380	1/1	0.23	-	37,37,37,37	0
57	MG	AA	1648	1/1	0.11	-	40,40,40,40	0
57	MG	BA	3408	1/1	0.34	-	57,57,57,57	0
57	MG	BA	3016	1/1	0.48	-	20,20,20,20	0
57	MG	BA	3384	1/1	0.19	-	42,42,42,42	0
57	MG	AL	201	1/1	0.40	-	29,29,29,29	0
57	MG	DA	3242	1/1	0.09	-	32,32,32,32	0
57	MG	CA	1651	1/1	0.15	-	28,28,28,28	0
57	MG	DA	3007	1/1	0.35	-	54,54,54,54	0
57	MG	BA	3440	1/1	0.41	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3305	1/1	0.35	-	41,41,41,41	0
57	MG	DA	3173	1/1	0.24	-	33,33,33,33	0
57	MG	AA	1701	1/1	0.28	-	33,33,33,33	0
57	MG	BA	3266	1/1	0.46	-	26,26,26,26	0
57	MG	CA	1640	1/1	0.60	-	61,61,61,61	0
57	MG	BA	3393	1/1	0.07	-	61,61,61,61	0
57	MG	BA	3356	1/1	0.16	-	21,21,21,21	0
57	MG	BA	3102	1/1	0.51	-	33,33,33,33	0
57	MG	DA	3256	1/1	0.25	-	62,62,62,62	0
57	MG	BA	3067	1/1	0.18	-	30,30,30,30	0
57	MG	DA	3149	1/1	0.48	-	38,38,38,38	0
57	MG	B5	104	1/1	0.19	-	33,33,33,33	0
57	MG	AA	1645	1/1	0.29	-	52,52,52,52	0
57	MG	DA	3036	1/1	0.48	-	27,27,27,27	0
57	MG	BA	3226	1/1	0.33	-	31,31,31,31	0
57	MG	DA	3156	1/1	0.75	-	58,58,58,58	0
57	MG	CA	1670	1/1	0.32	-	43,43,43,43	0
57	MG	AA	1703	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3178	1/1	0.28	-	22,22,22,22	0
57	MG	CA	1659	1/1	0.32	-	32,32,32,32	0
57	MG	BA	3280	1/1	0.15	-	19,19,19,19	0
57	MG	BA	3169	1/1	0.17	-	21,21,21,21	0
57	MG	DA	3282	1/1	0.20	-	65,65,65,65	0
57	MG	BA	3076	1/1	0.31	-	24,24,24,24	0
57	MG	DA	3241	1/1	0.07	-	26,26,26,26	0
57	MG	BA	3283	1/1	0.33	-	20,20,20,20	0
57	MG	CA	1645	1/1	0.25	-	41,41,41,41	0
57	MG	BA	3322	1/1	0.25	-	29,29,29,29	0
57	MG	DA	3243	1/1	0.12	-	44,44,44,44	0
57	MG	BA	3085	1/1	0.15	-	17,17,17,17	0
57	MG	D6	101	1/1	0.26	-	57,57,57,57	0
57	MG	BA	3387	1/1	0.20	-	46,46,46,46	0
57	MG	CA	1633	1/1	0.31	-	45,45,45,45	0
57	MG	AA	1683	1/1	0.16	-	31,31,31,31	0
57	MG	BA	3138	1/1	0.10	-	39,39,39,39	0
57	MG	BA	3454	1/1	0.21	-	25,25,25,25	0
57	MG	DA	3222	1/1	0.31	-	26,26,26,26	0
57	MG	CA	1684	1/1	0.22	-	42,42,42,42	0
57	MG	BA	3325	1/1	0.29	-	22,22,22,22	0
57	MG	DB	208	1/1	0.35	-	48,48,48,48	0
57	MG	BA	3050	1/1	0.27	-	24,24,24,24	0
57	MG	CA	1682	1/1	0.20	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3255	1/1	0.38	-	31,31,31,31	0
57	MG	CA	1608	1/1	0.66	-	52,52,52,52	0
57	MG	BA	3365	1/1	0.35	-	23,23,23,23	0
57	MG	DA	3219	1/1	0.39	-	34,34,34,34	0
57	MG	AA	1674	1/1	0.18	-	49,49,49,49	0
57	MG	BA	3056	1/1	0.42	-	26,26,26,26	0
57	MG	BA	3143	1/1	0.33	-	31,31,31,31	0
57	MG	DA	3227	1/1	0.38	-	37,37,37,37	0
57	MG	BA	3131	1/1	0.31	-	26,26,26,26	0
57	MG	DA	3197	1/1	0.25	-	27,27,27,27	0
57	MG	AA	1630	1/1	0.20	-	41,41,41,41	0
57	MG	DA	3044	1/1	0.48	-	69,69,69,69	0
57	MG	DA	3252	1/1	0.39	-	27,27,27,27	0
57	MG	AA	1684	1/1	0.14	-	31,31,31,31	0
57	MG	DA	3268	1/1	0.19	-	43,43,43,43	0
57	MG	BA	3048	1/1	0.37	-	27,27,27,27	0
57	MG	DA	3177	1/1	0.44	-	52,52,52,52	0
57	MG	BA	3419	1/1	0.37	-	44,44,44,44	0
57	MG	D6	102	1/1	0.20	-	23,23,23,23	0
57	MG	AA	1657	1/1	0.12	-	54,54,54,54	0
57	MG	BA	3003	1/1	0.10	-	25,25,25,25	0
57	MG	BA	3290	1/1	0.23	-	22,22,22,22	0
57	MG	BA	3071	1/1	0.34	-	25,25,25,25	0
57	MG	BA	3151	1/1	0.35	-	24,24,24,24	0
57	MG	AA	1670	1/1	0.25	-	30,30,30,30	0
57	MG	CA	1660	1/1	0.41	-	22,22,22,22	0
57	MG	BA	3370	1/1	0.06	-	48,48,48,48	0
57	MG	BA	3421	1/1	0.18	-	32,32,32,32	0
57	MG	DA	3235	1/1	0.18	-	24,24,24,24	0
57	MG	BA	3247	1/1	0.05	-	33,33,33,33	0
57	MG	BA	3156	1/1	0.09	-	26,26,26,26	0
57	MG	DA	3090	1/1	0.28	-	31,31,31,31	0
57	MG	DA	3105	1/1	0.33	-	30,30,30,30	0
57	MG	DA	3260	1/1	0.09	-	31,31,31,31	0
57	MG	DA	3155	1/1	0.05	-	60,60,60,60	0
57	MG	DA	3162	1/1	0.20	-	24,24,24,24	0
57	MG	DA	3019	1/1	0.40	-	35,35,35,35	0
57	MG	DA	3131	1/1	0.24	-	39,39,39,39	0
57	MG	BA	3171	1/1	0.42	-	41,41,41,41	0
57	MG	BA	3013	1/1	0.14	-	56,56,56,56	0
57	MG	BA	3334	1/1	0.18	-	24,24,24,24	0
57	MG	CA	1658	1/1	0.12	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3148	1/1	0.24	-	64,64,64,64	0
57	MG	BA	3073	1/1	0.24	-	23,23,23,23	0
57	MG	BA	3001	1/1	0.21	-	50,50,50,50	0
57	MG	DA	3244	1/1	0.23	-	26,26,26,26	0
57	MG	DA	3184	1/1	0.24	-	54,54,54,54	0
57	MG	DA	3016	1/1	0.42	-	24,24,24,24	0
57	MG	BQ	201	1/1	0.18	-	24,24,24,24	0
57	MG	BA	3446	1/1	0.63	-	60,60,60,60	0
57	MG	CA	1607	1/1	0.20	-	37,37,37,37	0
57	MG	CA	1681	1/1	0.19	-	44,44,44,44	0
57	MG	AA	1661	1/1	0.37	-	67,67,67,67	0
57	MG	BA	3318	1/1	0.34	-	41,41,41,41	0
57	MG	BA	3296	1/1	0.20	-	25,25,25,25	0
57	MG	BA	3386	1/1	0.25	-	68,68,68,68	0
57	MG	AA	1643	1/1	0.11	-	23,23,23,23	0
57	MG	BA	3267	1/1	0.22	-	19,19,19,19	0
57	MG	CA	1621	1/1	0.20	-	22,22,22,22	0
57	MG	DA	3104	1/1	0.21	-	21,21,21,21	0
57	MG	CA	1656	1/1	0.37	-	43,43,43,43	0
57	MG	DA	3068	1/1	0.25	-	19,19,19,19	0
57	MG	CA	1696	1/1	0.32	-	54,54,54,54	0
57	MG	AA	1709	1/1	0.23	-	66,66,66,66	0
57	MG	BA	3125	1/1	0.36	-	60,60,60,60	0
57	MG	BA	3340	1/1	0.24	-	29,29,29,29	0
57	MG	DA	3253	1/1	0.12	-	20,20,20,20	0
57	MG	DA	3262	1/1	0.24	-	29,29,29,29	0
57	MG	DA	3153	1/1	0.18	-	41,41,41,41	0
57	MG	BA	3066	1/1	0.16	-	14,14,14,14	0
57	MG	AA	1612	1/1	0.37	-	25,25,25,25	0
57	MG	BA	3435	1/1	0.06	-	30,30,30,30	0
57	MG	AA	1665	1/1	0.44	-	63,63,63,63	0
57	MG	BA	3094	1/1	0.28	-	34,34,34,34	0
57	MG	AA	1685	1/1	0.25	-	42,42,42,42	0
57	MG	BA	3327	1/1	0.23	-	28,28,28,28	0
57	MG	DA	3225	1/1	0.32	-	44,44,44,44	0
57	MG	BA	3287	1/1	0.20	-	20,20,20,20	0
57	MG	BA	3111	1/1	0.14	-	20,20,20,20	0
57	MG	BA	3351	1/1	0.18	-	56,56,56,56	0
57	MG	CW	101	1/1	0.24	-	22,22,22,22	0
57	MG	AA	1713	1/1	0.09	-	43,43,43,43	0
57	MG	AT	201	1/1	0.12	-	22,22,22,22	0
57	MG	BA	3389	1/1	0.22	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3084	1/1	0.64	-	61,61,61,61	0
57	MG	DA	3136	1/1	0.15	-	22,22,22,22	0
57	MG	BA	3250	1/1	0.47	-	22,22,22,22	0
57	MG	BA	3019	1/1	0.34	-	25,25,25,25	0
57	MG	DA	3121	1/1	0.31	-	57,57,57,57	0
57	MG	DA	3293	1/1	0.29	-	39,39,39,39	0
57	MG	BA	3313	1/1	0.36	-	26,26,26,26	0
57	MG	DA	3159	1/1	0.41	-	38,38,38,38	0
57	MG	AA	1636	1/1	0.20	-	62,62,62,62	0
57	MG	BA	3270	1/1	0.33	-	43,43,43,43	0
57	MG	BA	3302	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3183	1/1	0.10	-	22,22,22,22	0
57	MG	BA	3331	1/1	0.28	-	28,28,28,28	0
57	MG	DA	3075	1/1	0.23	-	27,27,27,27	0
57	MG	DA	3062	1/1	0.16	-	33,33,33,33	0
57	MG	CA	1669	1/1	0.21	-	21,21,21,21	0
57	MG	BA	3015	1/1	0.44	-	21,21,21,21	0
57	MG	BA	3375	1/1	0.39	-	36,36,36,36	0
57	MG	DA	3084	1/1	0.14	-	21,21,21,21	0
57	MG	BP	203	1/1	0.17	-	27,27,27,27	0
57	MG	DA	3003	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3130	1/1	0.34	-	35,35,35,35	0
57	MG	DA	3116	1/1	0.30	-	33,33,33,33	0
57	MG	DA	3028	1/1	0.11	-	34,34,34,34	0
57	MG	CA	1636	1/1	0.12	-	28,28,28,28	0
57	MG	CA	1604	1/1	0.22	-	38,38,38,38	0
57	MG	CA	1653	1/1	0.19	-	36,36,36,36	0
57	MG	DA	3087	1/1	0.42	-	26,26,26,26	0
57	MG	AA	1671	1/1	0.18	-	42,42,42,42	0
57	MG	DA	3031	1/1	0.27	-	24,24,24,24	0
57	MG	AA	1673	1/1	0.13	-	40,40,40,40	0
57	MG	AA	1682	1/1	0.15	-	18,18,18,18	0
57	MG	DA	3102	1/1	0.31	-	32,32,32,32	0
57	MG	DA	3103	1/1	0.48	-	19,19,19,19	0
57	MG	BA	3319	1/1	0.05	-	28,28,28,28	0
57	MG	AA	1690	1/1	0.09	-	26,26,26,26	0
57	MG	DA	3182	1/1	0.11	-	37,37,37,37	0
57	MG	BA	3192	1/1	0.27	-	27,27,27,27	0
57	MG	BA	3225	1/1	0.15	-	16,16,16,16	0
57	MG	BA	3332	1/1	0.17	-	61,61,61,61	0
57	MG	BA	3456	1/1	0.31	-	43,43,43,43	0
57	MG	DA	3228	1/1	0.22	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1612	1/1	0.50	-	55,55,55,55	0
57	MG	BA	3407	1/1	0.39	-	66,66,66,66	0
57	MG	DA	3115	1/1	0.10	-	36,36,36,36	0
57	MG	CA	1609	1/1	0.19	-	27,27,27,27	0
57	MG	CA	1641	1/1	0.06	-	18,18,18,18	0
57	MG	BA	3439	1/1	0.12	-	32,32,32,32	0
57	MG	BA	3345	1/1	0.29	-	34,34,34,34	0
57	MG	AA	1668	1/1	0.10	-	40,40,40,40	0
57	MG	BA	3174	1/1	0.16	-	53,53,53,53	0
57	MG	DA	3295	1/1	0.31	-	40,40,40,40	0
57	MG	BA	3295	1/1	0.27	-	20,20,20,20	0
57	MG	BA	3100	1/1	0.52	-	28,28,28,28	0
57	MG	BA	3249	1/1	0.27	-	46,46,46,46	0
57	MG	DA	3238	1/1	0.17	-	33,33,33,33	0
57	MG	BA	3317	1/1	0.40	-	27,27,27,27	0
57	MG	CA	1650	1/1	0.16	-	28,28,28,28	0
57	MG	AA	1624	1/1	0.31	-	33,33,33,33	0
57	MG	DA	3147	1/1	0.48	-	18,18,18,18	0
57	MG	AA	1712	1/1	0.15	-	56,56,56,56	0
57	MG	BA	3039	1/1	0.66	-	39,39,39,39	0
57	MG	BA	3311	1/1	0.17	-	31,31,31,31	0
57	MG	BA	3060	1/1	0.37	-	47,47,47,47	0
57	MG	BA	3209	1/1	0.24	-	23,23,23,23	0
57	MG	BA	3074	1/1	0.35	-	31,31,31,31	0
57	MG	BA	3276	1/1	0.28	-	21,21,21,21	0
57	MG	BA	3239	1/1	0.25	-	46,46,46,46	0
57	MG	BA	3028	1/1	0.25	-	29,29,29,29	0
57	MG	BA	3342	1/1	0.11	-	22,22,22,22	0
57	MG	DA	3288	1/1	0.24	-	60,60,60,60	0
57	MG	DA	3263	1/1	0.14	-	28,28,28,28	0
57	MG	DA	3001	1/1	0.19	-	61,61,61,61	0
57	MG	CA	1668	1/1	0.19	-	27,27,27,27	0
57	MG	BA	3326	1/1	0.20	-	21,21,21,21	0
57	MG	DA	3234	1/1	0.32	-	33,33,33,33	0
58	ZN	D5	103	1/1	0.18	-	30,30,30,30	0
57	MG	DA	3034	1/1	0.19	-	57,57,57,57	0
57	MG	DA	3223	1/1	0.22	-	32,32,32,32	0
57	MG	DA	3072	1/1	0.54	-	72,72,72,72	0
57	MG	BA	3202	1/1	0.12	-	19,19,19,19	0
57	MG	AA	1651	1/1	0.18	-	49,49,49,49	0
57	MG	BA	3310	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3373	1/1	0.17	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3170	1/1	0.20	-	40,40,40,40	0
57	MG	BA	3450	1/1	0.42	-	44,44,44,44	0
57	MG	DA	3033	1/1	0.51	-	59,59,59,59	0
57	MG	DA	3195	1/1	0.83	-	73,73,73,73	0
57	MG	DP	201	1/1	0.14	-	38,38,38,38	0
57	MG	CA	1618	1/1	0.20	-	39,39,39,39	0
57	MG	BA	3082	1/1	0.33	-	24,24,24,24	0
57	MG	AA	1619	1/1	0.45	-	66,66,66,66	0
57	MG	BA	3220	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3165	1/1	0.19	-	25,25,25,25	0
57	MG	CA	1697	1/1	0.04	-	39,39,39,39	0
57	MG	BA	3457	1/1	0.20	-	35,35,35,35	0
57	MG	DA	3128	1/1	0.26	-	24,24,24,24	0
57	MG	BA	3402	1/1	0.14	-	24,24,24,24	0
57	MG	BA	3256	1/1	0.14	-	25,25,25,25	0
57	MG	BA	3399	1/1	0.24	-	38,38,38,38	0
57	MG	BA	3324	1/1	0.12	-	25,25,25,25	0
57	MG	DA	3110	1/1	0.23	-	38,38,38,38	0
57	MG	BA	3353	1/1	0.36	-	36,36,36,36	0
57	MG	BA	3333	1/1	0.53	-	77,77,77,77	0
57	MG	AA	1634	1/1	0.41	-	41,41,41,41	0
57	MG	AA	1679	1/1	0.29	-	56,56,56,56	0
57	MG	BA	3129	1/1	0.16	-	25,25,25,25	0
57	MG	CA	1639	1/1	0.08	-	22,22,22,22	0
57	MG	BA	3359	1/1	0.20	-	44,44,44,44	0
57	MG	DA	3284	1/1	0.13	-	51,51,51,51	0
57	MG	BA	3051	1/1	0.46	-	51,51,51,51	0
57	MG	BA	3043	1/1	0.33	-	25,25,25,25	0
57	MG	DA	3108	1/1	0.51	-	47,47,47,47	0
57	MG	BA	3058	1/1	0.42	-	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.