



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:13 PM BST

PDB ID : 4V7L
Title : The structures of viomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.00 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>

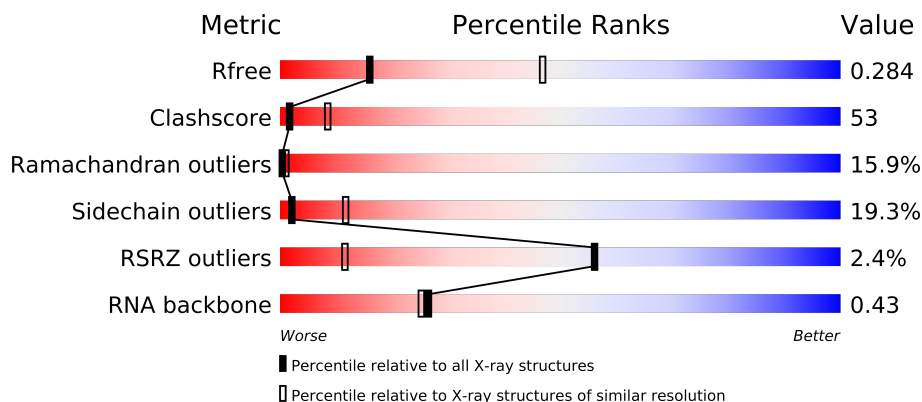
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
24	CX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	

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Mol	Chain	Length	Quality of chain
28	BB	122	
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	
40	DR	118	
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	

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Mol	Chain	Length	Quality of chain
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	
53	B4	71	
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294559 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
			32141	14306	5964	10377	1494			
1	CA	1495	Total	C	N	O	P	0	0	0
			32141	14306	5964	10377	1494			

- 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
			1005	636	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1006	637	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	0
			947	585	195	165	2			
13	CM	119	Total	C	N	O	S	0	0	0
			910	564	180	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	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 RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			
23	CW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
24	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	CONFLICT	GB CP001637.1
AY	44	U	A	CONFLICT	GB CP001637.1

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	33	G	C	CONFLICT	GB CP001637.1
CY	44	U	A	CONFLICT	GB CP001637.1

- Molecule 26 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			48	25	13	10			
26	CZ	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2800	Total	C	N	O	P	0	0	0
			60311	26841	11284	19387	2799			
27	DA	2800	Total	C	N	O	P	0	0	0
			60313	26842	11286	19386	2799			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			
28	DB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
30	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	164	Total	C	N	O	S	0	0	1
			1252	794	233	224	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1042	668	175	198	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1046	670	175	200	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
39	DQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DS	101	Total	C	N	O	0	0	1
			777	489	156	132			

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
46	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			715	448	141	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
52	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

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

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	51	Total	C	N	O	S	0	0	1
			411	253	84	70	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

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

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	400	Total	Mg	0	0
			400	400		
59	AK	2	Total	Mg	0	0
			2	2		
59	DF	1	Total	Mg	0	0
			1	1		
59	CV	2	Total	Mg	0	0
			2	2		
59	BE	1	Total	Mg	0	0
			1	1		
59	AW	7	Total	Mg	0	0
			7	7		
59	BP	1	Total	Mg	0	0
			1	1		
59	AX	7	Total	Mg	0	0
			7	7		
59	DR	1	Total	Mg	0	0
			1	1		
59	CA	92	Total	Mg	0	0
			92	92		
59	B5	1	Total	Mg	0	0
			1	1		
59	BB	1	Total	Mg	0	0
			1	1		
59	D6	1	Total	Mg	0	0
			1	1		
59	AE	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BF	2	Total 2	Mg 2	0	0
59	BX	1	Total 1	Mg 1	0	0
59	AA	133	Total 133	Mg 133	0	0
59	BQ	1	Total 1	Mg 1	0	0
59	CQ	1	Total 1	Mg 1	0	0
59	CX	3	Total 3	Mg 3	0	0
59	BU	1	Total 1	Mg 1	0	0
59	AD	1	Total 1	Mg 1	0	0
59	BN	1	Total 1	Mg 1	0	0
59	BY	1	Total 1	Mg 1	0	0
59	BR	1	Total 1	Mg 1	0	0
59	DA	275	Total 275	Mg 275	0	0
59	CE	2	Total 2	Mg 2	0	0
59	DD	3	Total 3	Mg 3	0	0
59	AL	1	Total 1	Mg 1	0	0
59	DE	3	Total 3	Mg 3	0	0
59	AH	1	Total 1	Mg 1	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	DZ	1	Total 1	Mg 1	0	0
59	AC	1	Total 1	Mg 1	0	0
59	DB	1	Total 1	Mg 1	0	0

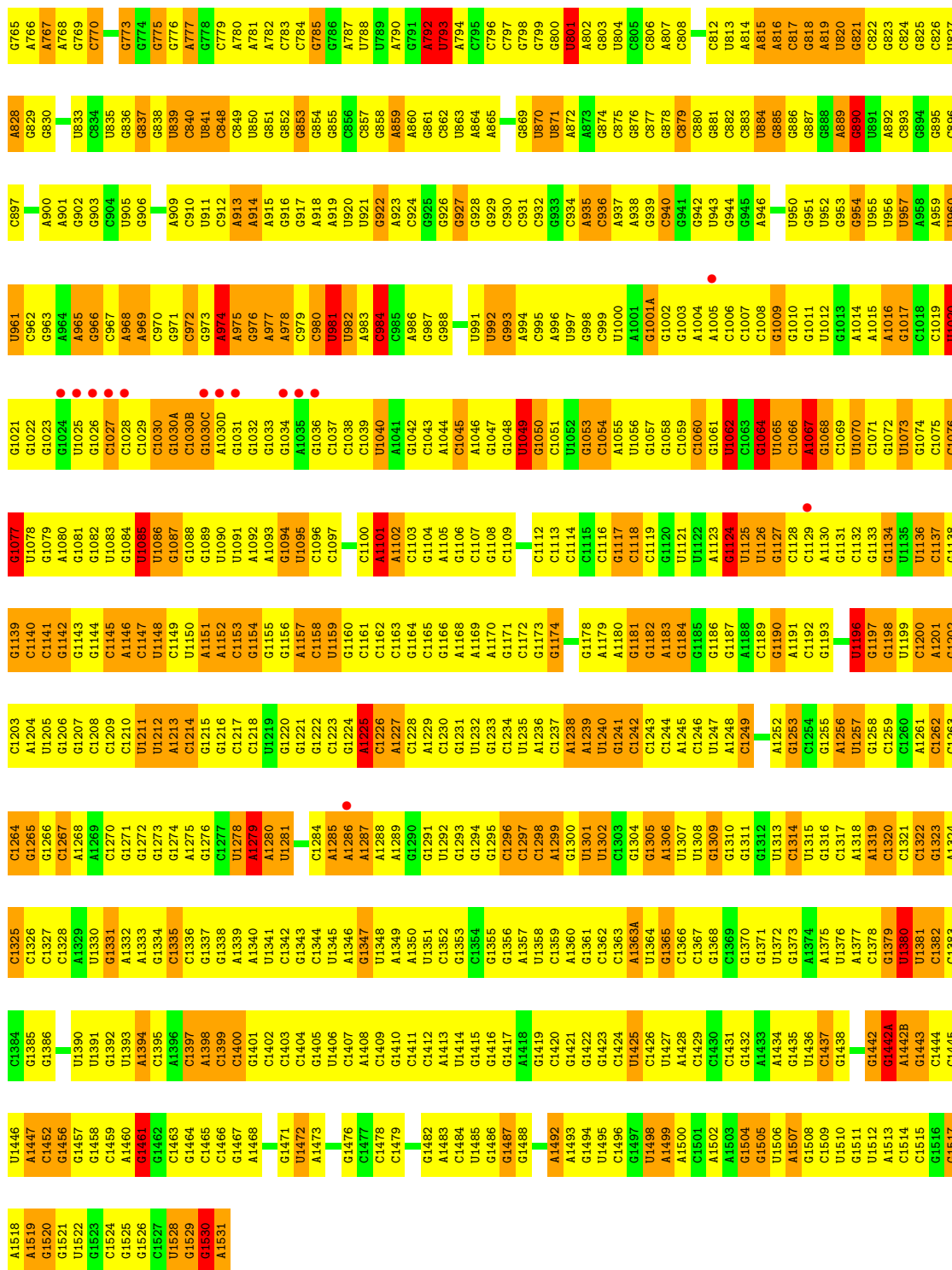
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D5	2	Total 2	Mg 2	0	0
59	BD	1	Total 1	Mg 1	0	0
59	AT	2	Total 2	Mg 2	0	0
59	B0	2	Total 2	Mg 2	0	0
59	AO	1	Total 1	Mg 1	0	0
59	AY	2	Total 2	Mg 2	0	0
59	AF	1	Total 1	Mg 1	0	0
59	BH	1	Total 1	Mg 1	0	0

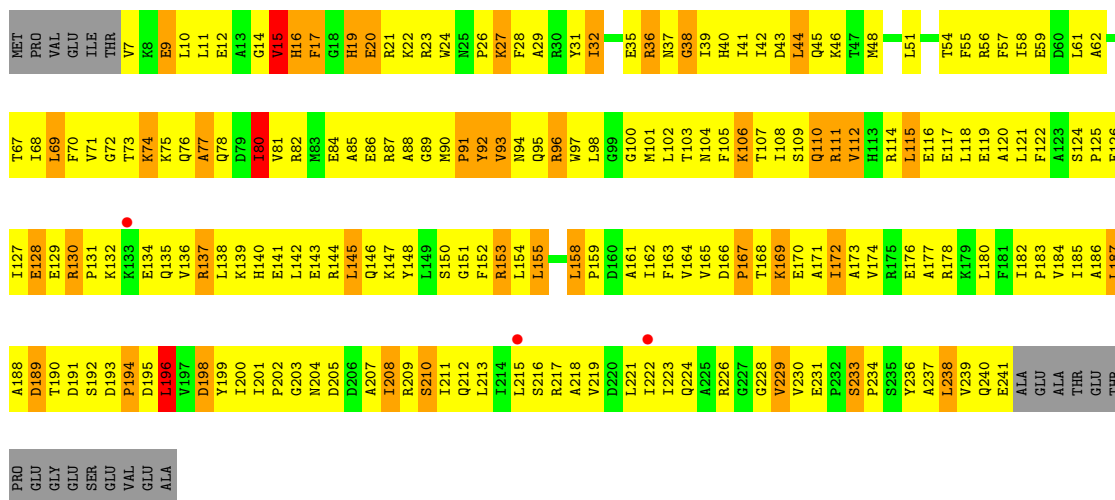
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B5	1	Total 1	Zn 1	0	0
60	B4	1	Total 1	Zn 1	0	0
60	AD	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0
60	D9	1	Total 1	Zn 1	0	0
60	D5	1	Total 1	Zn 1	0	0
60	D4	1	Total 1	Zn 1	0	0
60	CD	1	Total 1	Zn 1	0	0



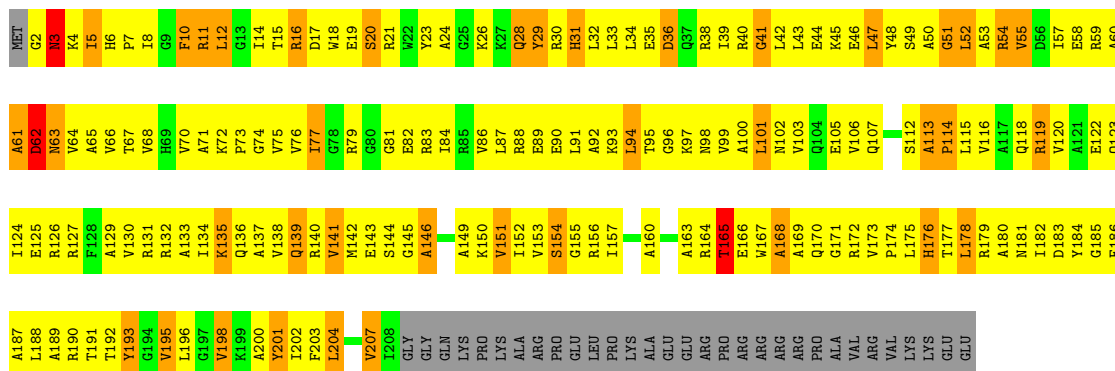
G998	G999	A938	C875	G809	C748	G688	G627	A563	C503	A430	C370	G309	G247	C188	G127	A80
G999	U1000	C940	C877	C810	C749	C689	G628	C564	C504	A431	G371	G310	C248	G189	G128	G61
U1001	G941	G878	C878	C811	G750	G690	G629	C565	G505	A432	C372	C311	U259	C189A	U129	U62
G1001A	G942	C879	C879	U813	G752	G692	G630	G566	G506	A433	A373	C312	A260	C189B	G129A	C63
G1002	U943	A763	C880	U814	A763	G693	G631	G567	C507	U434	A374	A313	U252	C189C	A310	G64
G1003	G944	A764	C881	A815	C754	A694	A632	G568	C508	A435	U375	G316	U253	U189D	G131	U65
A1004	G945	C755	C882	A816	G756	A695	C633	C569	A509	C436	G376	G317	U254	U189E	C132	G66
C1006	A1005	C756	C883	C817	C756	A696	C634	G570	A510	U437	G377	G318	G255	U189F	U133	C67
G1009	G947	U757	U884	G818	U757	G697	U636	A572	C511	A438	G378	G319	U256	G189G	A134	G68
G1010	C948	G758	C885	A819	G758	G698	G637	A573	C513	A441	G380	C320	G257	G189H	C135	G69
G1011	A949	U759	C886	U820	G759	G699	G638	A574	C514	A442	C381	A321	G258	U189I	C136	G70
G1012	U950	G760	C887	G821	G760	G700	C639	G575	C515	C443	A382	A322	G259	G189J	C137	C71
U1020	G1021	C822	A889	C823	G761	C701	A640	G576	U516	C444	A383	U523	G260	U189K	G138	C72
U1025	G1026	G823	C890	G824	C762	A702	U641	G577	C517	G445	A384	G324	U261	G189L	G139	G73
G1028	C1029	C824	U891	C825	G763	A703	A642	C578	G518	G446	C385	A325	A262	U190	A140	C76
C1029	U905	G826	A892	G827	C764	U705	C643	G579	C519	G447	C386	G326	A263	G191	A141	G77
G1030A	G1030B	U827	C894	C828	G765	A706	C644	U580	A520	G448	U387	A327	U264	G192	G142	G78
G1030C	G970	U828	C895	A828	C766	C707	C645	G581	C521	G450	G388	C328	G265	C193	A143	G
G1032	G1033	G829	C896	G829	A767	C708	U646	U582	C522	A451	A389	A329	C286	C194	G144	U
G1035	G1036	G830	C897	U831	G768	G709	A648	A583	A523	A452	C390	C330	C287	A195	G145	U
C1037	G1038	U832	C898	U831	C769	G710	G649	G584	C524	A453	G391	G331	C288	A197	G146	U
C1039	U906	G833	C899	C832	C770	G711	C650	G585	C525	C454	G392	G332	C289	G198	G147	U
U1040	U1041	U834	A900	U833	U772	A712	C651	C586	C526	C455	A393	G333	A270	G199	A148	U
A1042	A1043	U835	A901	C834	G773	G713	U652	C587	C528	C457	C395	C335	C272	G200	C	A
A1044	A1045	G836	C902	U835	G774	G714	A653	C590	C529	C458	G396	C336	A273	C201	A152	U
A1046	A1047	G837	A903	G836	G775	A715	G654	C591	G530	G460	A397	C337	A274	U202	A153	C91
A1048	A1049	G838	C904	G837	G776	C717	G657	G592	U531	A461	C398	A338	G275	U203	C92	C92
A1051	A1052	U839	C905	U838	A777	A718	U658	G593	A532	C470	G399	C339	G276	G216	G155	G93
A1053	A1054	G840	C906	U839	C778	G719	U659	G594	A533	G471	C400	U340	G277	C217	G156	U96
A1055	A1056	U841	A908	C840	C779	C719	U660	G595	U534	A472	C401	C341	G278	C218	G157	G97
A1057	A1058	U842	C909	U841	A760	G720	G660	G596	A535	G473	G402	C342	A279	C219	G158	G98
A1059	A1060	G843	C910	U842	A761	G721	G661	G597	C536	G474	C403	U343	C280	G220	U99	U99
A1061	A1062	G844	A913	G843	G722	A722	G662	U598	C537	G475	U404	A344	G281	C221	A161	A101
A1063	A1064	G845	A914	G844	G723	U723	A663	C599	C538	G476	U405	C345	A282	U222	A162	G102
A1065	A1066	G846	A915	G845	G724	G724	A664	C600	A539	A477	G406	G346	C283	U223	C163	C103
A1067	A1068	G847	A916	G846	G725	G725	A665	C601	C540	C479	G407	G347	G284	C224	U164	G104
A1069	A1070	G848	A917	G847	G726	C726	A666	A602	G541	U480	A408	G348	G285	C225	G105	G105
A1071	A1072	G849	A918	G848	G727	G727	G667	G603	C542	G481	G409	A349	G286	G226	C166	G106
A1073	A1074	G850	A919	G849	A728	A728	U668	G604	C543	A482	G410	G350	U287	G227	G107	G107
A1075	A1076	G851	A920	G850	A729	A729	U669	U605	C544	C483	A411	G351	A288	A228	G108	G108
A1077	A1078	G852	A921	G851	G730	G730	G670	G606	C545	G484	A412	C352	G289	U229	A109	A109
A1079	A1080	G853	A922	G852	G731	G731	G671	A607	C546	G485	G413	A353	C290	G230	C110	C110
A1081	A1082	G854	A923	G853	G732	C732	U672	A608	A547	U486	A414	G354	C291	G231	A172	G111
A1083	A1084	G855	A924	G854	A733	A733	G673	A609	C548	A487	A415	C355	G292	G232	U173	G112
A1085	A1086	G856	A925	G855	G734	G734	G674	G610	C549	C488	G416	A356	G293	C233	C174	G113
A1087	A1088	G857	A926	G856	G735	C735	A675	A611	C550	C489	C417	G357	U296	C234	C175	U114
A1089	A1090	G858	A927	G857	G736	G736	A676	C612	U551	G490	C418	U358	G297	C235	C176	G115
A1091	A1092	G859	A928	G858	A737	A737	U677	C613	U552	G491	C419	U359	G298	C236	C177	A116
A1093	A1094	G860	A929	G859	G738	C738	U678	A614	A553	G492	U420	A360	A298	C237	C178	G117
A1095	A1096	G861	A930	G860	G739	C739	G679	G619	C554	G493	U421	G361	A299	G238	A179	U118
A1097	A1098	G862	A931	G861	U740	U740	C680	U619	C555	U494	C422	C362	G299	G239	U180	A119
A1099	A1100	G863	A932	G862	G741	G741	C681	U620	C556	A495	C423	A363	A300	U239	A181	A120
A1101	A1102	G864	A933	G863	G742	G742	G682	A621	C557	A496	G424	U364	G302	C241	U182	G121
A1103	A1104	G865	A934	G864	G743	G743	G683	A622	C558	U497	G425	U365	G303	C242	U183	C122
A1105	A1106	G866	A935	G865	G744	C744	A684	C623	A559	A499	G426	C366	U304	A243	G184	C123
A1107	A1108	G867	A936	G866	G745	C745	U685	C624	U560	G501	U427	U367	G305	U244	A185	G124
A1109	A1110	G868	A937	G867	A746	A746	U686	G625	U561	G502	U428	U368	G306	C245	C186	U125
A1111	A1112	G869	A938	G868	A747	C747	A687	U626	C562			C369		A246	C187	G126





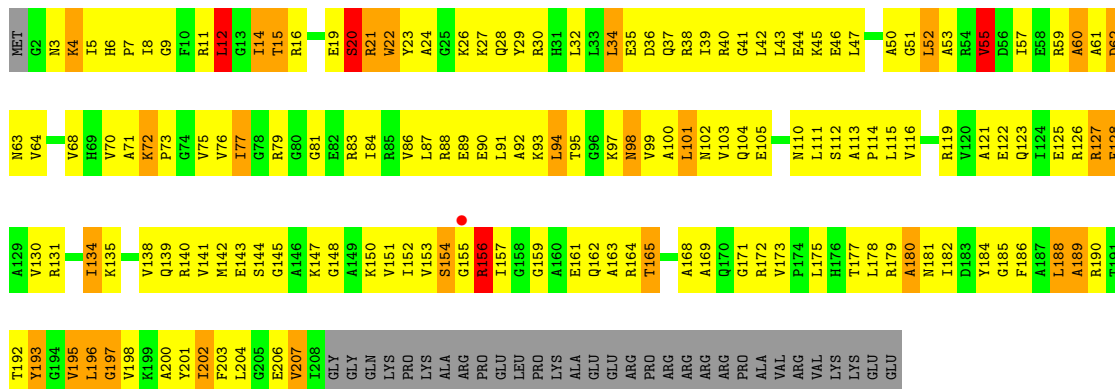
• Molecule 3: 30S ribosomal protein S3

Chain AC:



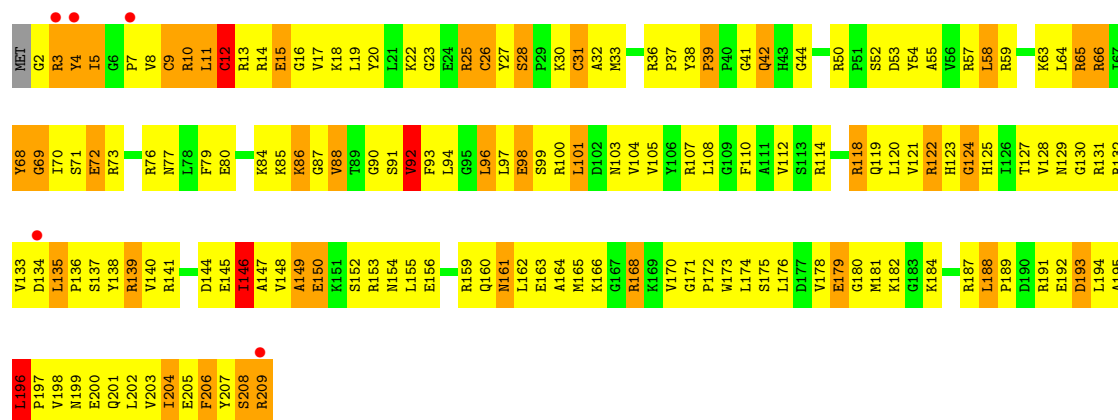
• Molecule 3: 30S ribosomal protein S3

Chain CC:



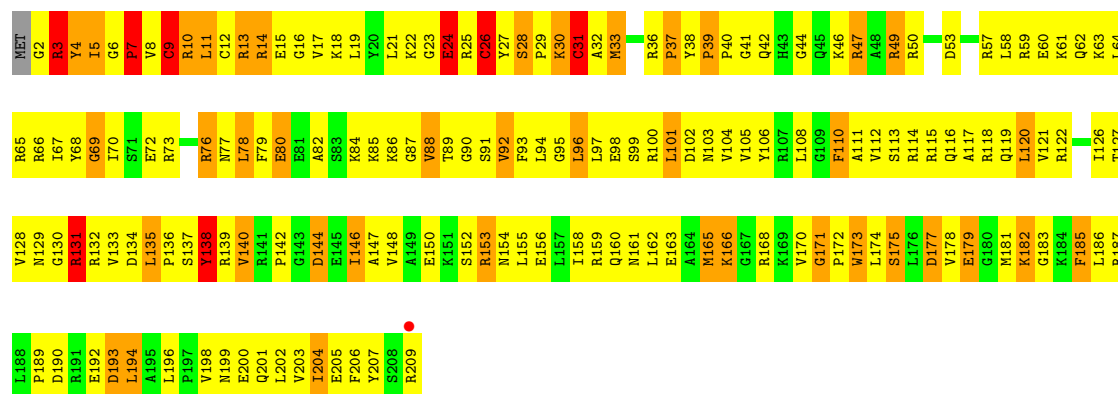
• Molecule 4: 30S ribosomal protein S4

Chain AD:



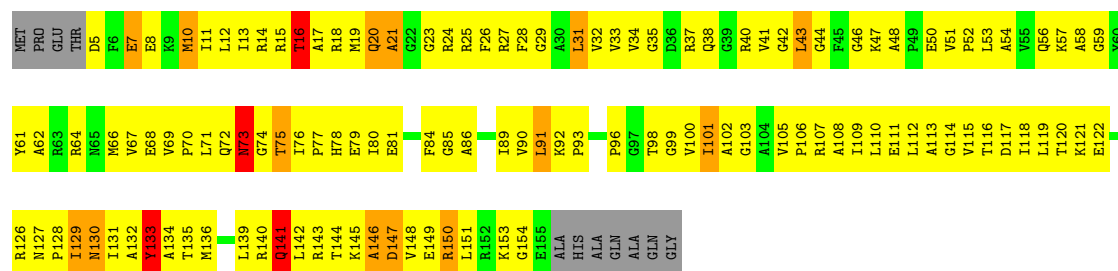
• Molecule 4: 30S ribosomal protein S4

Chain CD:



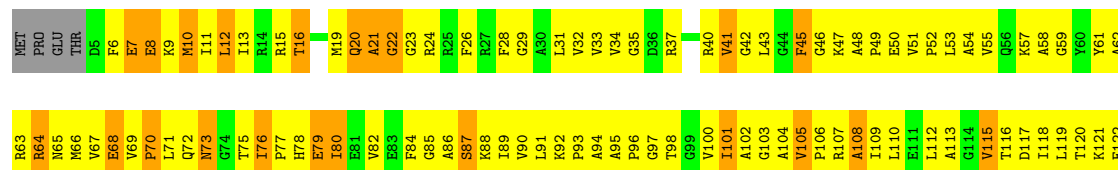
• Molecule 5: 30S ribosomal protein S5

Chain AE:

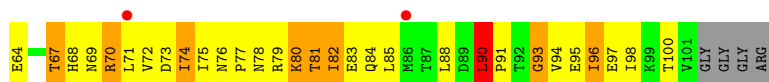


• Molecule 5: 30S ribosomal protein S5

Chain CE:

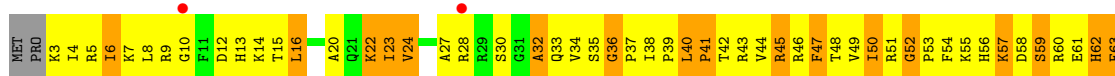






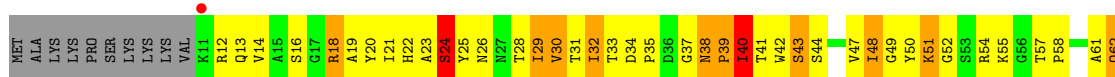
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



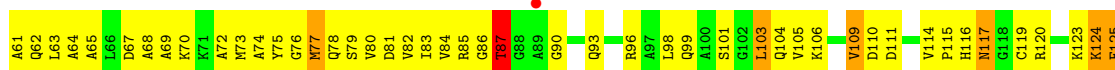
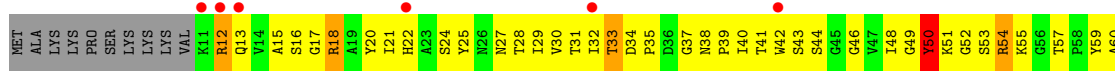
- Molecule 11: 30S ribosomal protein S11

Chain AK:



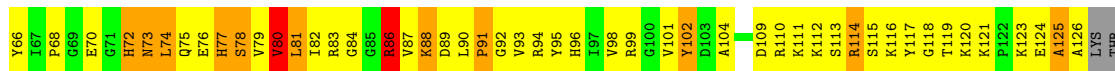
- Molecule 11: 30S ribosomal protein S11

Chain CK:



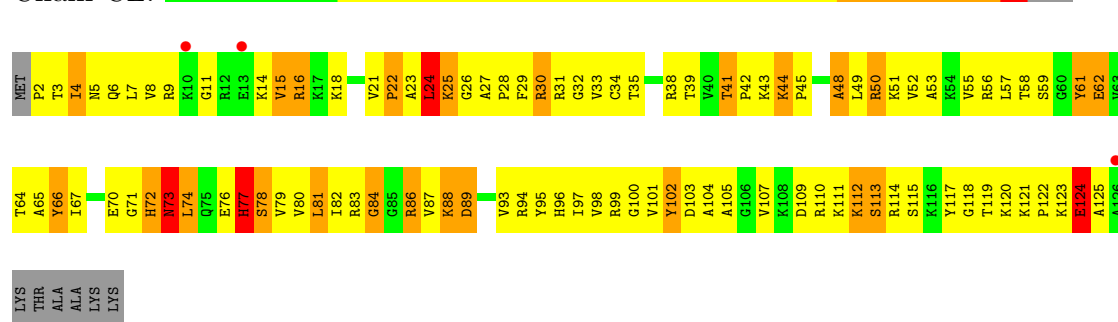
- Molecule 12: 30S ribosomal protein S12

Chain AL:



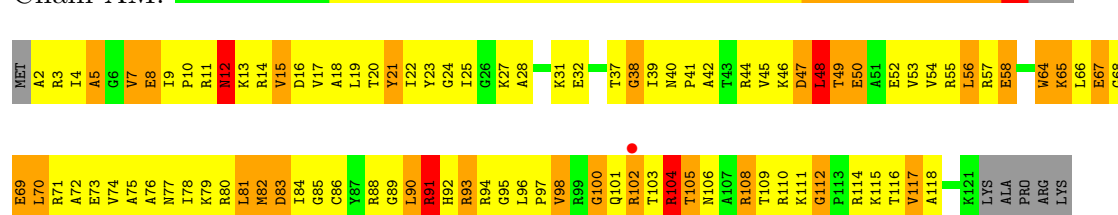
- Molecule 12: 30S ribosomal protein S12

Chain CL:



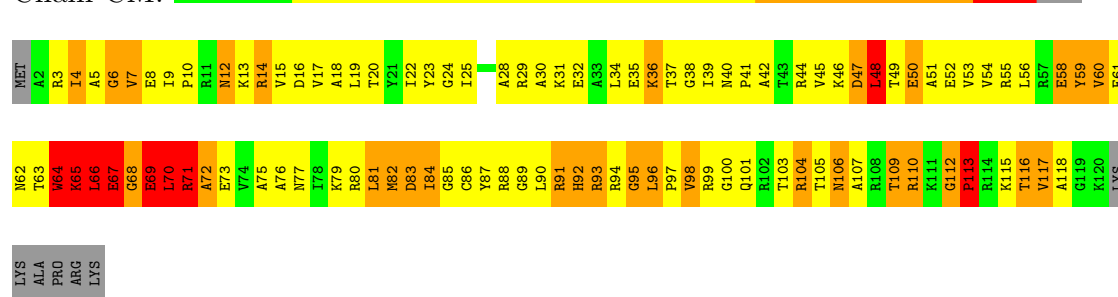
- Molecule 13: 30S ribosomal protein S13

Chain AM:



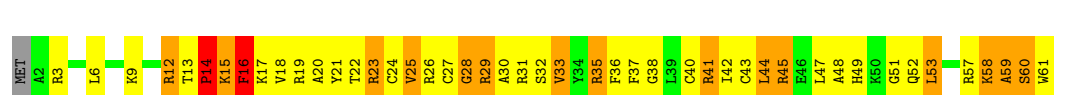
- Molecule 13: 30S ribosomal protein S13

Chain CM:



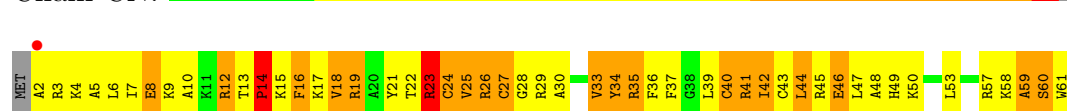
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 14: 30S ribosomal protein S14

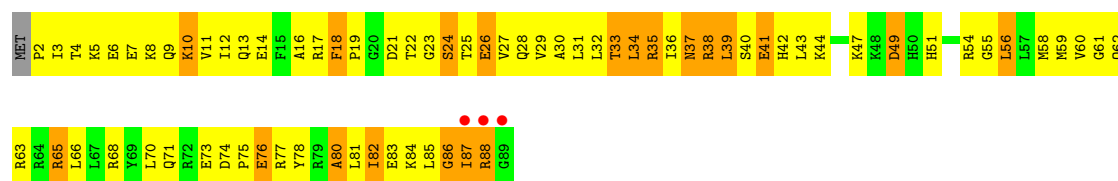
Chain CN:



- Molecule 15: 30S ribosomal protein S15

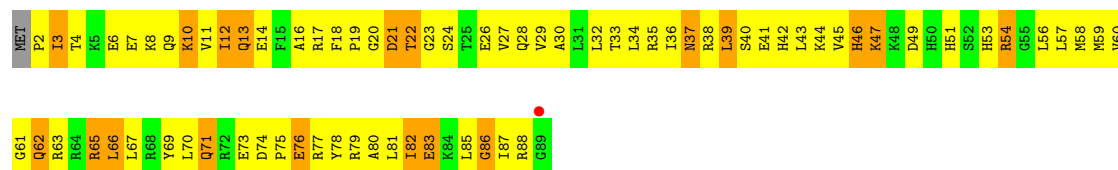
Chain AO:





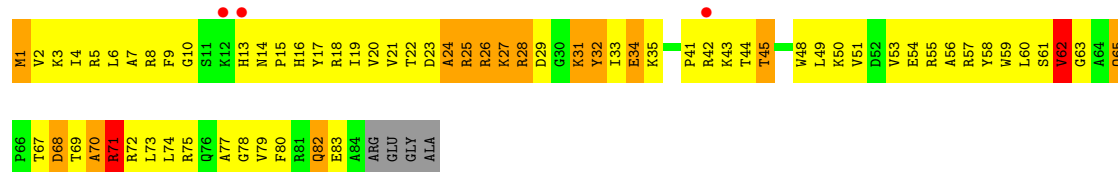
- Molecule 15: 30S ribosomal protein S15

Chain CO:



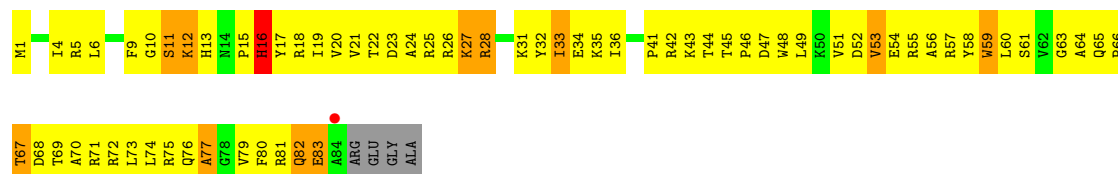
- Molecule 16: 30S ribosomal protein S16

Chain AP:



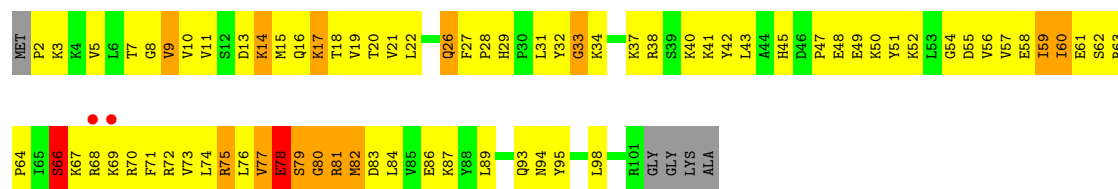
- Molecule 16: 30S ribosomal protein S16

Chain CP:



- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

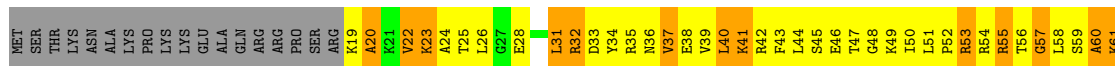
Chain CQ:





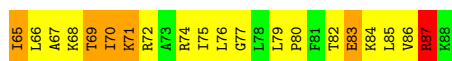
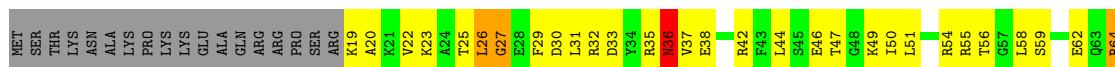
- Molecule 18: 30S ribosomal protein S18

Chain AR:



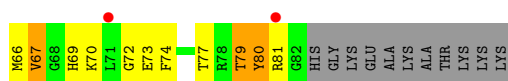
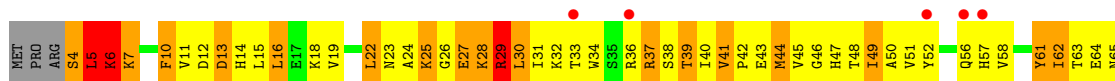
- Molecule 18: 30S ribosomal protein S18

Chain CR:



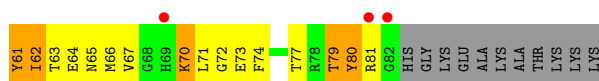
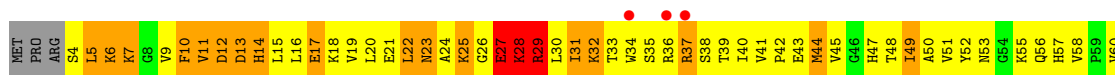
- Molecule 19: 30S ribosomal protein S19

Chain AS:



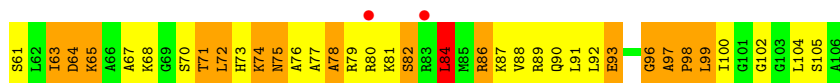
- Molecule 19: 30S ribosomal protein S19

Chain CS:



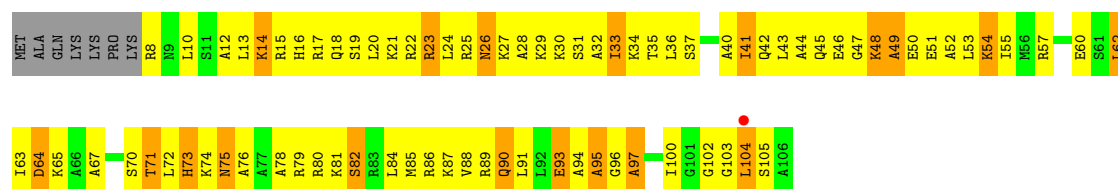
- Molecule 20: 30S ribosomal protein S20

Chain AT:



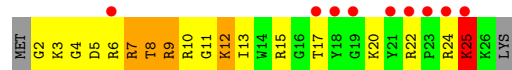
- Molecule 20: 30S ribosomal protein S20

Chain CT:



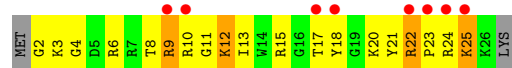
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



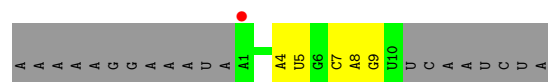
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



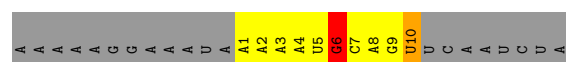
- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

Chain AV:



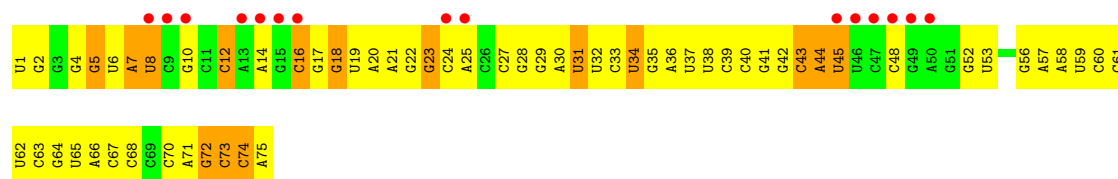
- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

Chain CV:



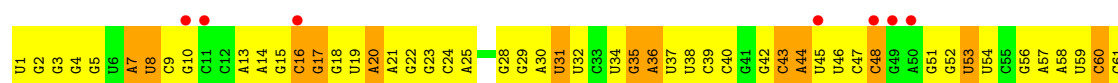
- Molecule 23: tRNA-Gln

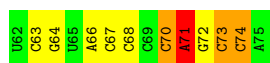
Chain AW:



- Molecule 23: tRNA-Gln

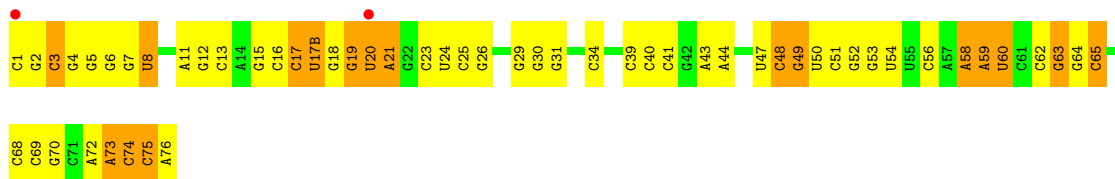
Chain CW:





- Molecule 24: tRNA-Met

Chain AX:



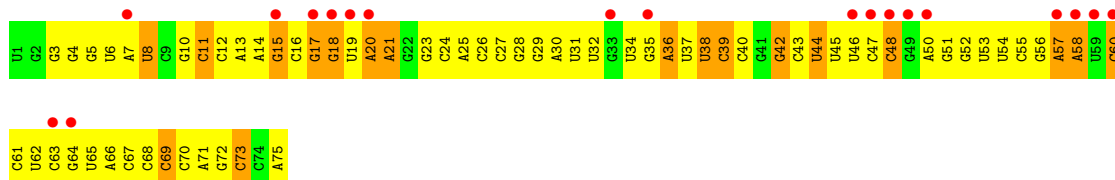
- Molecule 24: tRNA-Met

Chain CX:



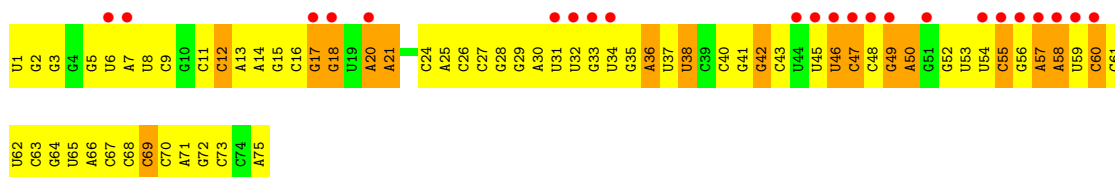
- Molecule 25: tRNA-Gln

Chain AY:



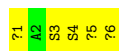
- Molecule 25: tRNA-Gln

Chain CY:



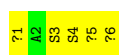
- Molecule 26: Viomycin

Chain AZ:



- Molecule 26: Viomycin

Chain CZ:



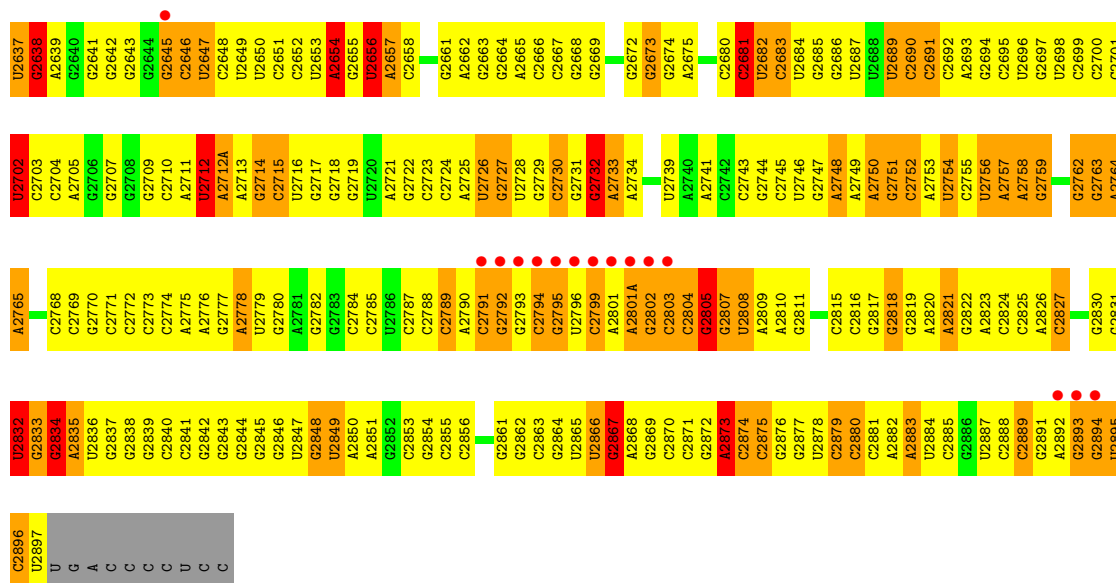






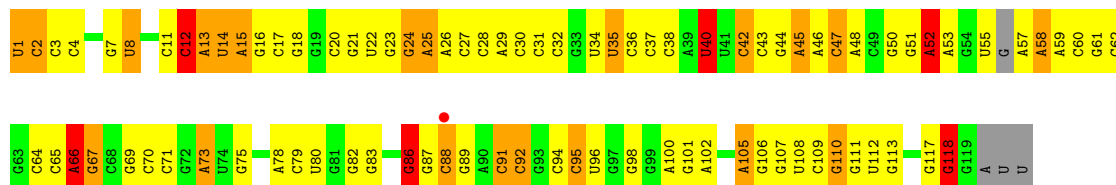


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U2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562																											
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C2142	C2143	U2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201																
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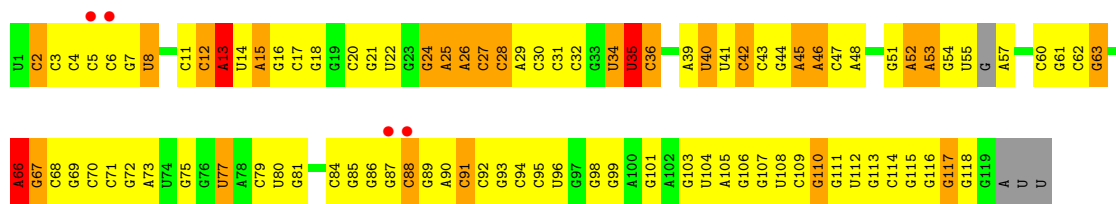
• Molecule 28: 5S ribosomal RNA

Chain BB:



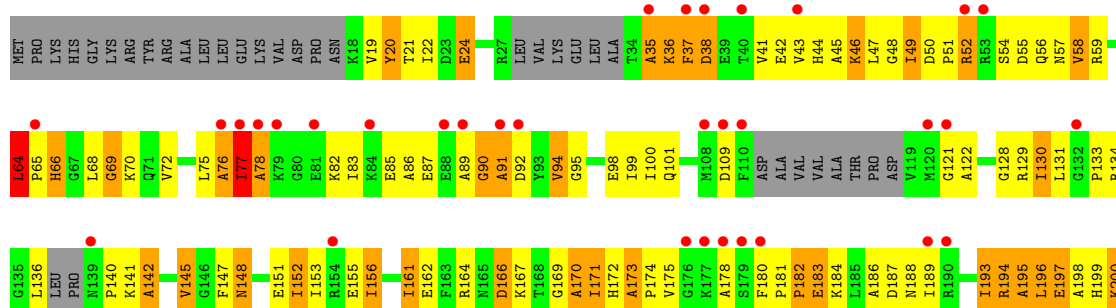
• Molecule 28: 5S ribosomal RNA

Chain DB:

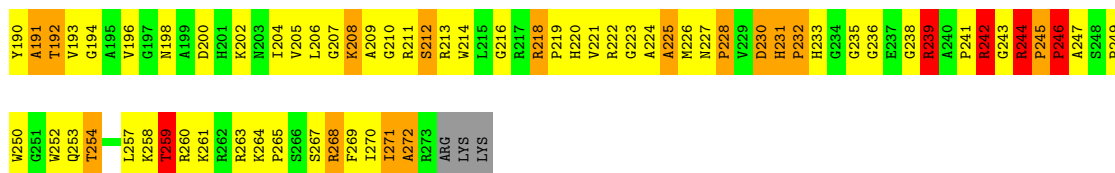


• Molecule 29: 50S ribosomal protein L1

Chain BC:

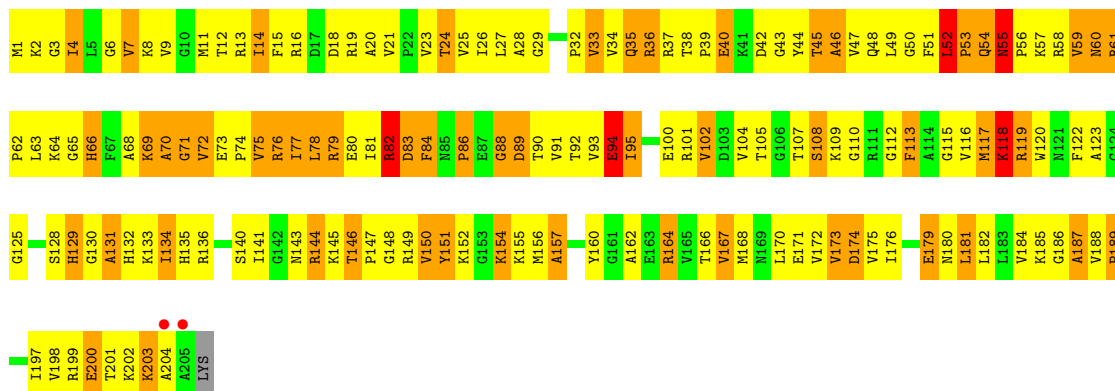






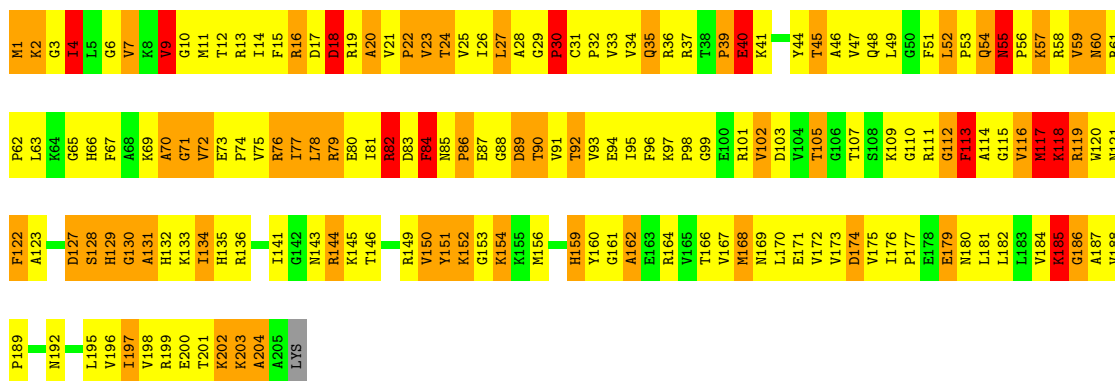
• Molecule 31: 50S ribosomal protein L3

Chain BE:



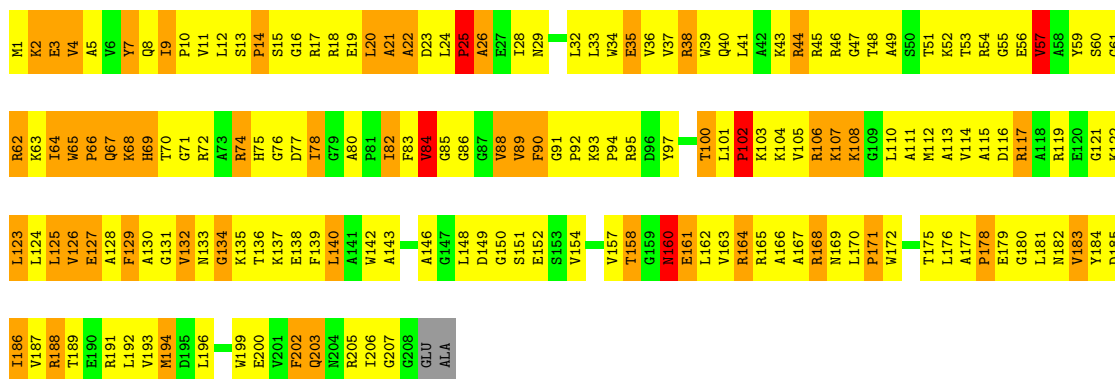
• Molecule 31: 50S ribosomal protein L3

Chain DE:



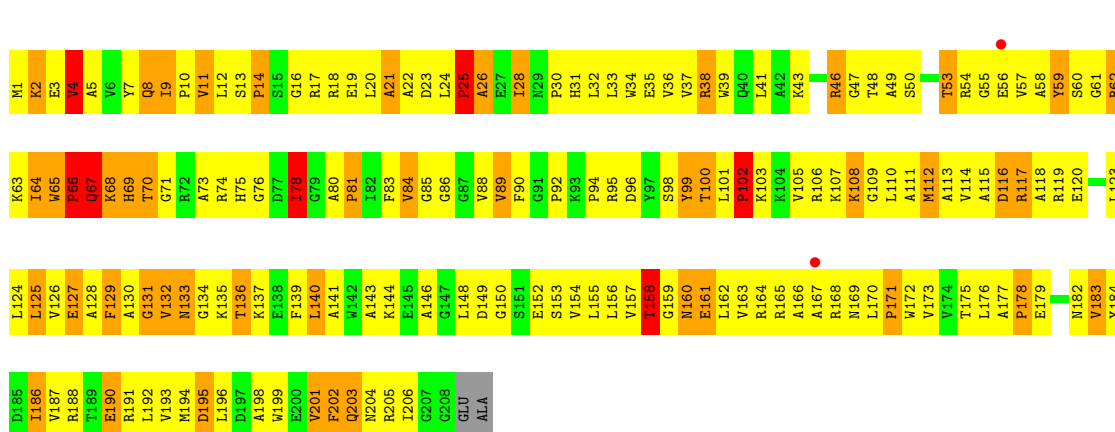
• Molecule 32: 50S ribosomal protein L4

Chain BF:



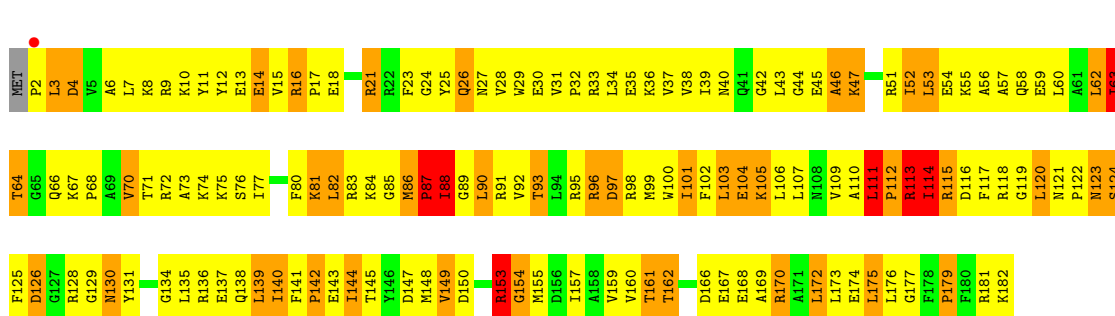
- Molecule 32: 50S ribosomal protein L4

Chain DF:



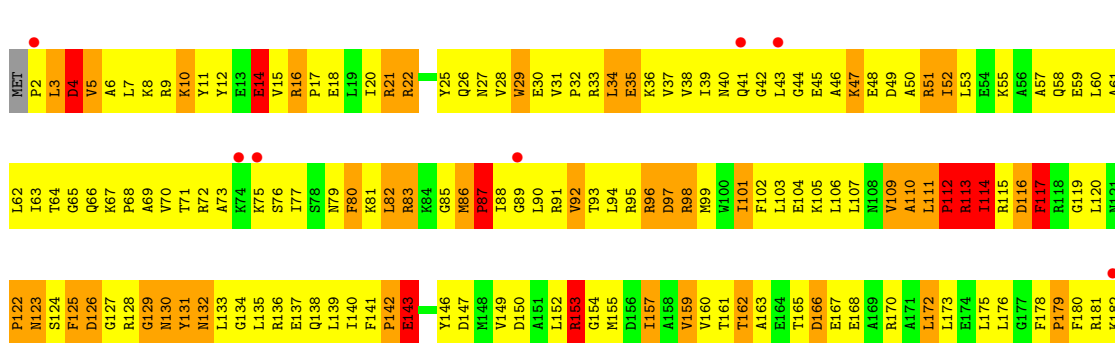
- Molecule 33: 50S ribosomal protein L5

Chain BG:



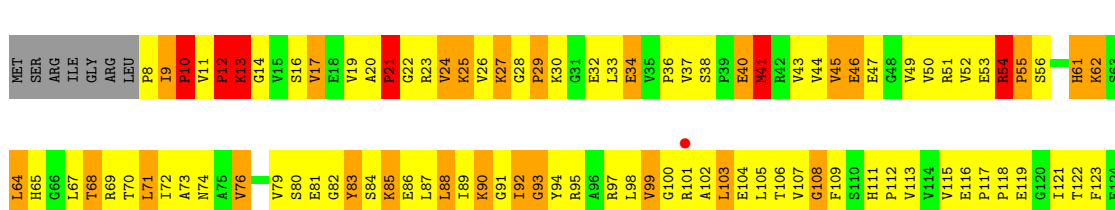
- Molecule 33: 50S ribosomal protein L5

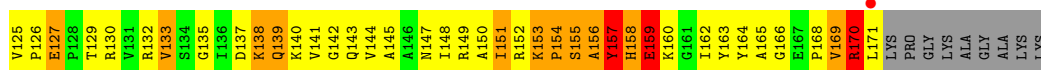
Chain DG:



- Molecule 34: 50S ribosomal protein L6

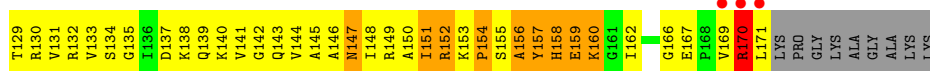
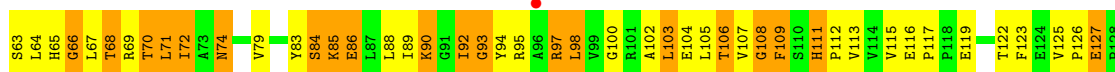
Chain BH:





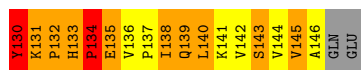
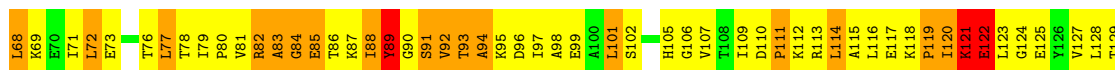
• Molecule 34: 50S ribosomal protein L6

Chain DH:



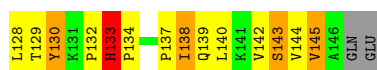
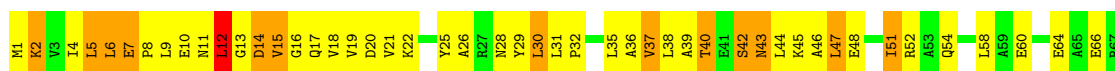
• Molecule 35: 50S ribosomal protein L9

Chain BI:



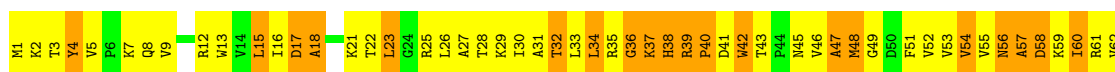
• Molecule 35: 50S ribosomal protein L9

Chain DI:



• Molecule 36: 50S ribosomal protein L13

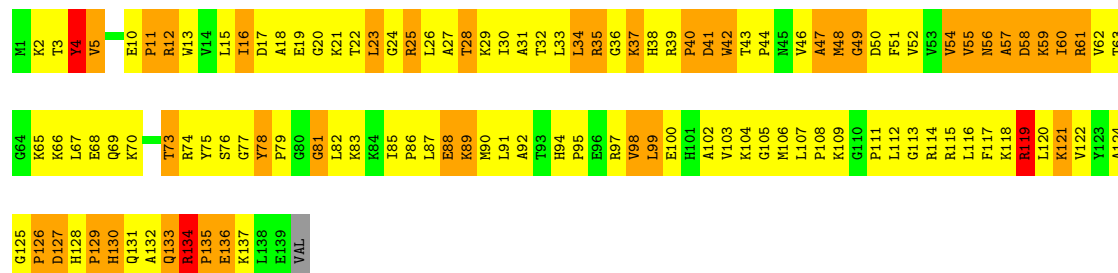
Chain BN:





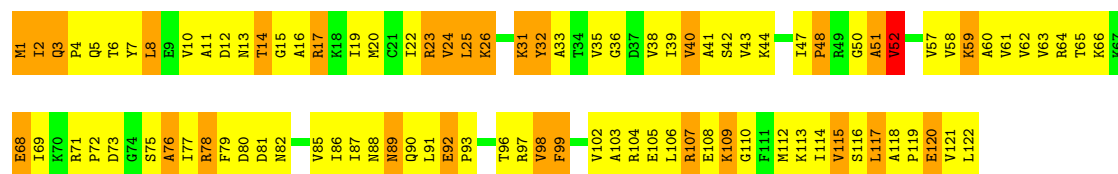
• Molecule 36: 50S ribosomal protein L13

Chain DN:



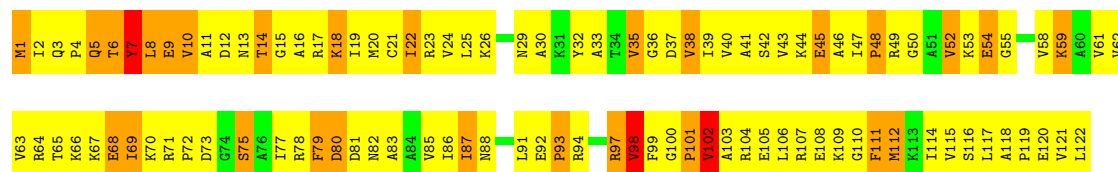
• Molecule 37: 50S ribosomal protein L14

Chain BO:



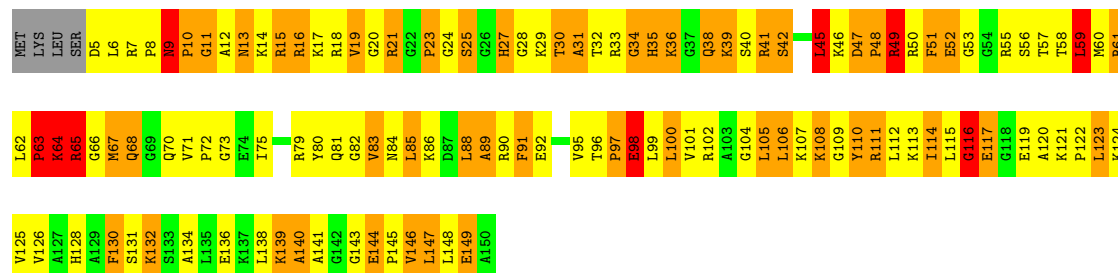
• Molecule 37: 50S ribosomal protein L14

Chain DO:



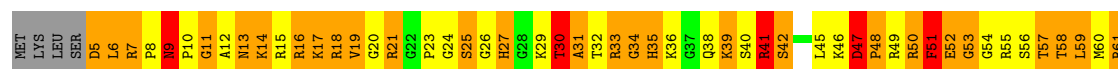
• Molecule 38: 50S ribosomal protein L15

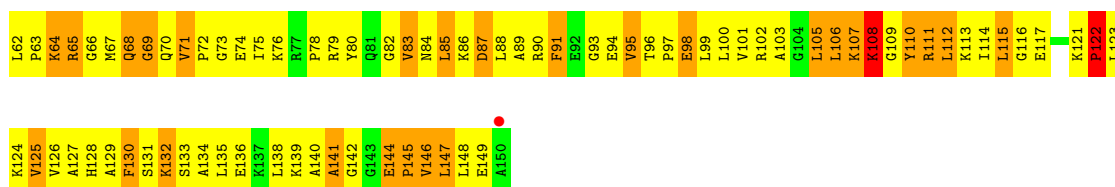
Chain BP:



• Molecule 38: 50S ribosomal protein L15

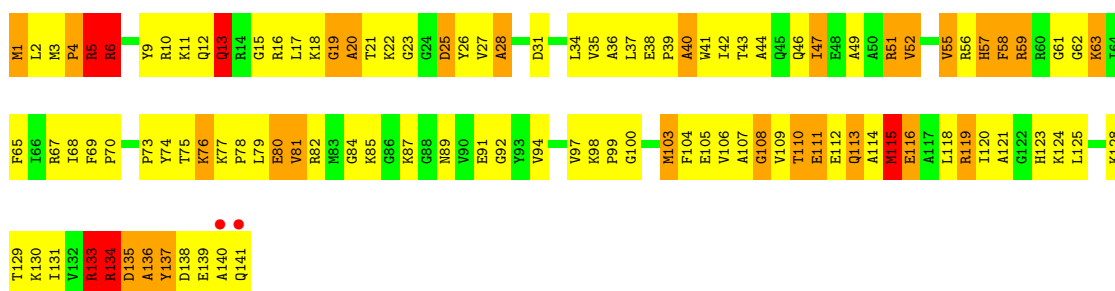
Chain DP:





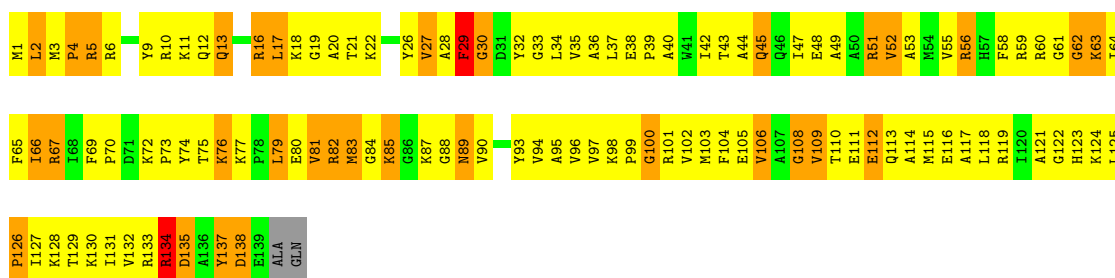
- Molecule 39: 50S ribosomal protein L16

Chain BQ:



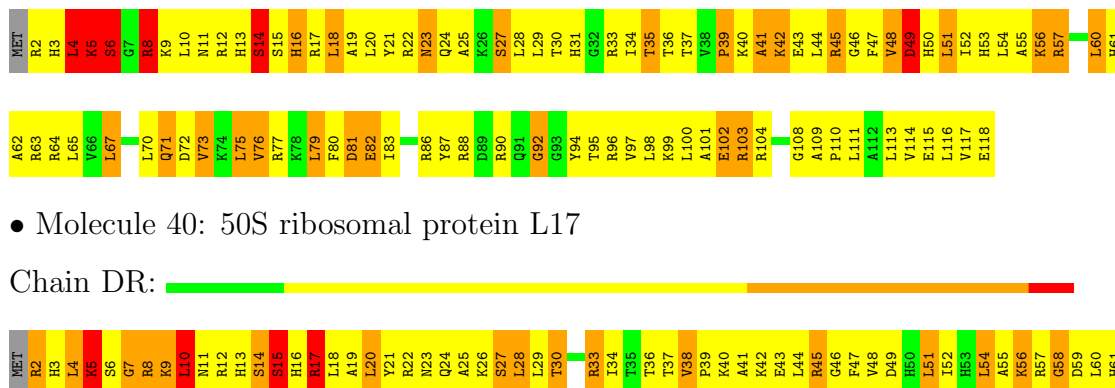
- Molecule 39: 50S ribosomal protein L16

Chain DQ:



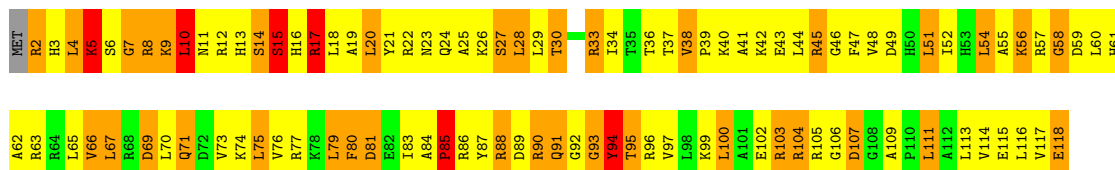
- Molecule 40: 50S ribosomal protein L17

Chain BR:



- Molecule 40: 50S ribosomal protein L17

Chain DR:



- Molecule 41: 50S ribosomal protein L18

Chain BS: 

MET	ALA	ARG	LEU	THR	ALA	TYR	GLU	ARG	ARG	K11	F12	F13	F14	R15	M16	R17	A18	K19	R20	T21	G22	R23	L24	R25	L26	F29	R30	S31	L32	K33	H34	T35	Y36	A37	Q38	T39	I40	D41	D42	E43	K44	G45	V46	T47	L48	V49	S50	A51	S52	S53	L54	A55	L56	K57	L58	R59	G60	N61
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K62	T63	E64	V65	A66	R67	Q68	V69	G70	R71	A72	L73	A74	E75	K76	A77	L78	A79	L80	G81	L82	K83	Q84	V85	L24	A86	F87	R88	R89	G90	P91	Y92	K93	Y94	H95	G96	V97	V98	K99	A100	L101	A102	E103	G104	A105	R106	E107	G108	G109	LEU	GLU	PHE
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• Molecule 41: 50S ribosomal protein L18

Chain DS: 

MET	ALA	ARG	LEU	THR	ALA	TYR	GLU	R9	L9	R10	K11	F12	F13	A14	V15	R16	A77	L78	A79	L80	G81	L82	K83	Q84	V85	L24	A86	F87	R88	R89	G90	P91	Y92	K93	L32	K33	H34	T35	Y36	A37	Q38	T39	I40	D41	D42	E43	K44	T47	L48	V49	S50	A51	S52	S53	L54	A55	L56	K57	L58	R59	G60	N61
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K62	T63	E64	V65	A66	R67	Q68	V69	G70	R71	A72	L73	A74	E75	K76	A77	L78	A79	L80	G81	L82	K83	Q84	V85	L24	A86	F87	R88	R89	G90	P91	Y92	K93	G96	R97	V98	K99	A100	L101	A102	E103	G104	A105	R106	E107	G108	G109	LEU	GLU	PHE
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• Molecule 42: 50S ribosomal protein L19

Chain BT: 

M1	N2	R3	G4	A5	L6	I7	K8	V9	G99	V10	E11	S12	R13	Y14	V15	R16	T17	D18	L19	P20	E21	F22	K23	P24	G25	D26	T27	V28	R29	V30	S31	Y32	K33	V34	E36	G37	N38	R39	T40	I42	R41	D42	Q43	D44	F45	E46	G47	I48	V49	I50	R51	I52	R53	L54	N55	F57	N58	T59	T60
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F61	T62	V63	R64	K65	V66	S67	T68	G69	V70	G71	E72	E73	R74	F75	P77	L78	H79	S80	P81	L82	R83	Q84	K85	T86	D87	V88	V89	Q90	R91	G92	R93	A94	R95	R96	A97	K98	L99	Y100	F101	I102	I103	N104	L105	S106	D107	R108	E109	I110	R111	R112	K113	L114	R115	A116	D117	R120	I121
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D122	Q123	D124	R125	A126	E127	R128	R129	A130	A131	E132	E133	E134	A135	Q136	K137	GLN	GLU	PRO	LYS	ALA	SER	GLN	GLU
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• Molecule 42: 50S ribosomal protein L19

Chain DT: 

M1	N2	R3	G4	A5	L6	I7	K8	V9	G99	V10	E11	S12	R13	Y14	V15	R16	T17	D18	L19	P20	E21	F22	K23	P24	G25	D26	T27	V28	R29	V30	S31	Y32	K33	V34	E36	G37	N38	R39	T40	I42	R41	D42	Q43	D44	F45	E46	G47	I48	V49	I50	R51	I52	R53	L54	N55	F57	N58	T59	T60
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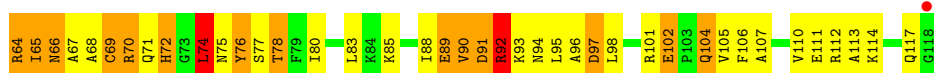
F61	T62	V63	R64	K65	V66	S67	T68	G69	V70	G71	E72	E73	R74	F75	P77	L78	H79	S80	P81	L82	R83	Q84	K85	T86	D87	V88	V89	Q90	R91	G92	R93	A94	R95	R96	A97	K98	L99	Y100	F101	I102	I103	N104	L105	S106	D107	R108	E109	I110	R111	R112	K113	L114	R115	A116	D117	R118	K119	T120
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I121	D122	Q123	D124	R125	A126	E127	R128	R129	A130	A131	E132	E133	E134	A135	Q136	K137	A138	GLN	GLU	PRO	LYS	ALA	SER	GLN	GLU
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• Molecule 43: 50S ribosomal protein L20

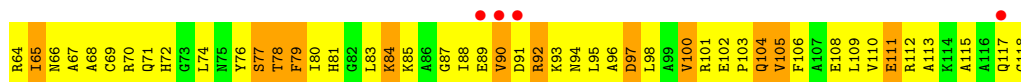
Chain BU: 

MET	F2	R3	A4	K5	T6	G7	V8	V9	R12	K13	H14	K15	K16	I17	L18	K19	L20	A21	K22	G23	Y24	W25	G26	L27	R28	S29	K30	S31	F32	R33	K34	A35	T38	L39	F40	A41	A42	G43	N44	Y45	A46	Y47	A48	H49	R50	K51	R52	R53	K54	R55	D56	R59	L60	W61	T62	V63
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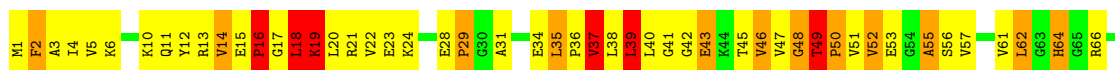
- Molecule 43: 50S ribosomal protein L20

Chain DU:



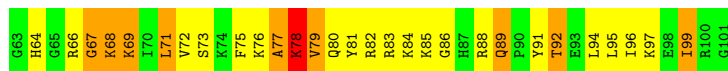
- Molecule 44: 50S ribosomal protein L21

Chain BV:



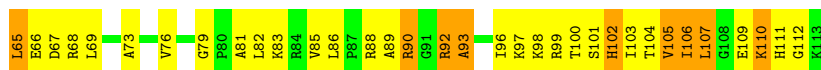
- Molecule 44: 50S ribosomal protein L21

Chain DV:



- Molecule 45: 50S ribosomal protein L22

Chain BW:



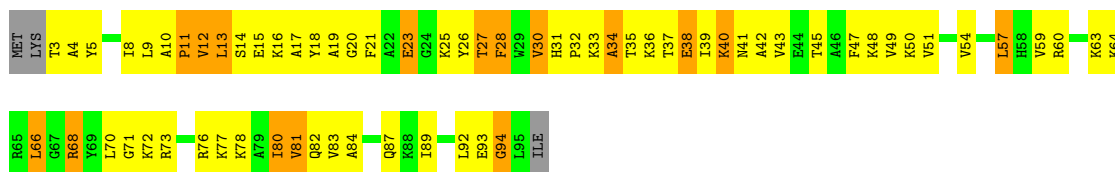
- Molecule 45: 50S ribosomal protein L22

Chain DW:



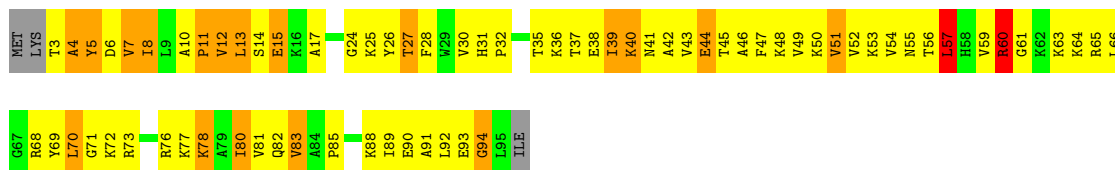
- Molecule 46: 50S ribosomal protein L23

Chain BX:



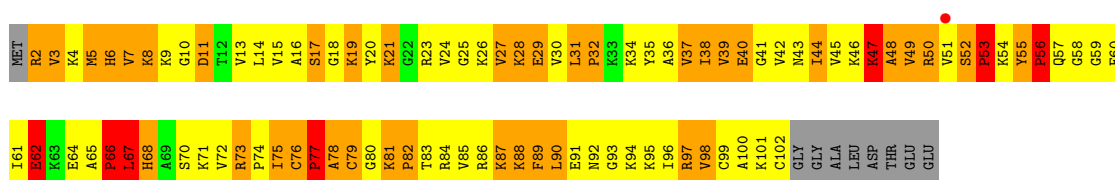
- Molecule 46: 50S ribosomal protein L23

Chain DX:



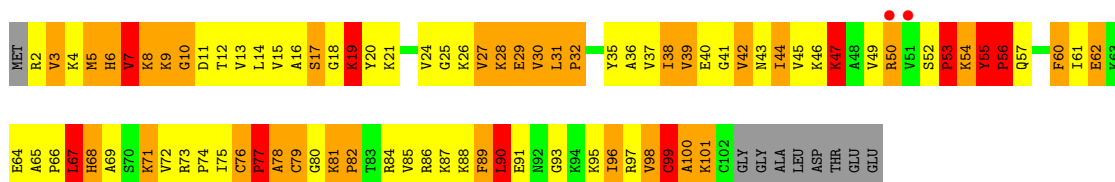
- Molecule 47: 50S ribosomal protein L24

Chain BY:



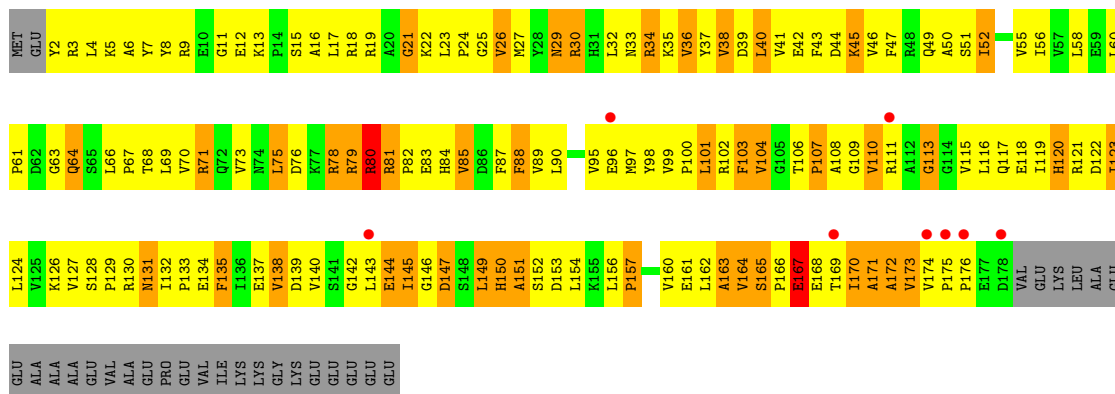
- Molecule 47: 50S ribosomal protein L24

Chain DY:



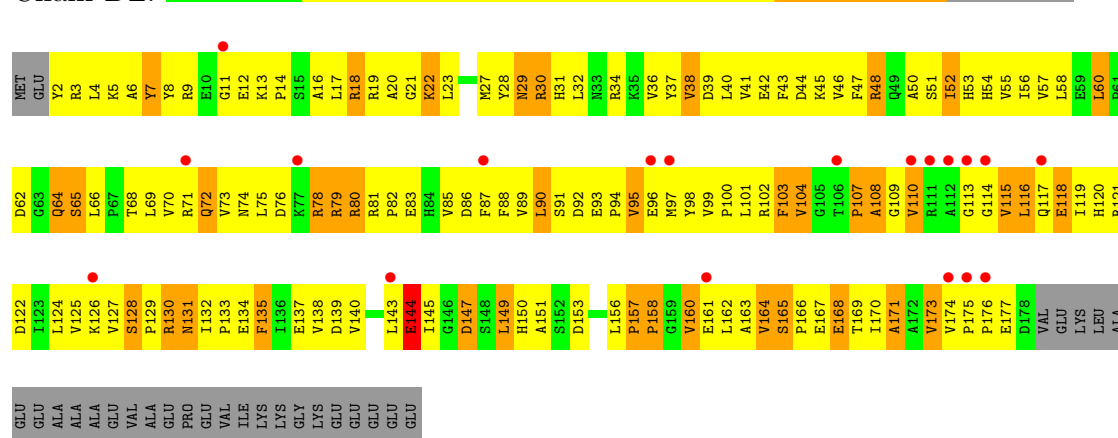
- Molecule 48: 50S ribosomal protein L25

Chain BZ:



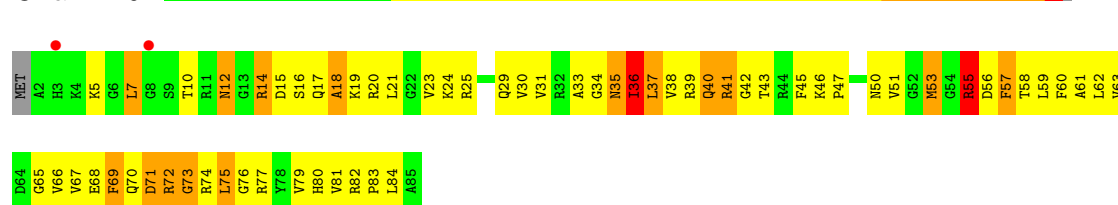
- Molecule 48: 50S ribosomal protein L25

Chain DZ:



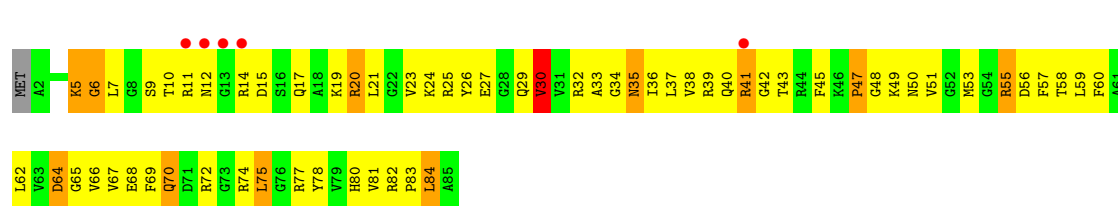
- Molecule 49: 50S ribosomal protein L27

Chain B0:



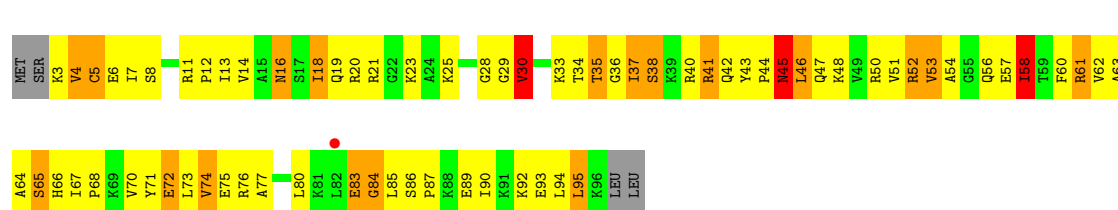
- Molecule 49: 50S ribosomal protein L27

Chain D0:



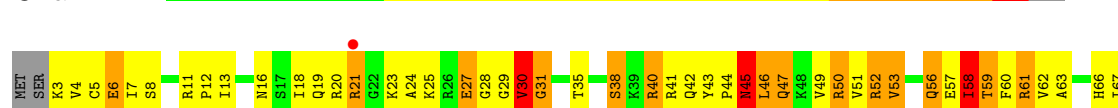
- Molecule 50: 50S ribosomal protein L28

Chain B1:



- Molecule 50: 50S ribosomal protein L28

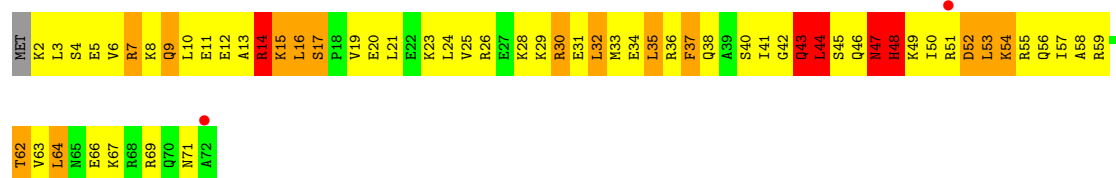
Chain D1:





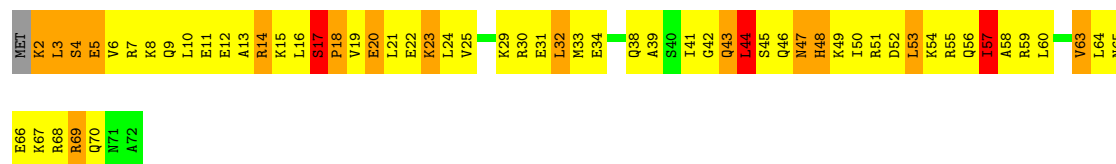
- Molecule 51: 50S ribosomal protein L29

Chain B2:



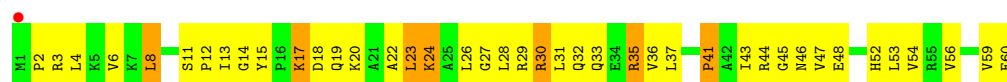
- Molecule 51: 50S ribosomal protein L29

Chain D2:



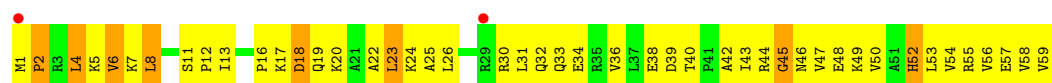
- Molecule 52: 50S ribosomal protein L30

Chain B3:



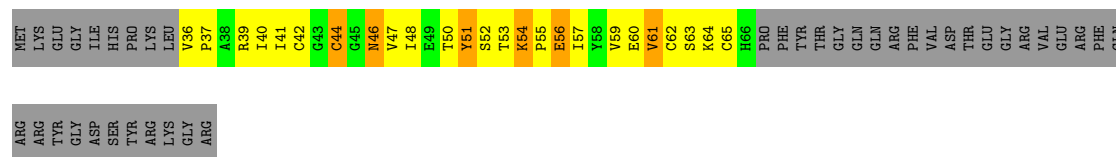
- Molecule 52: 50S ribosomal protein L30

Chain D3:



- Molecule 53: 50S ribosomal protein L31

Chain B4:



- Molecule 53: 50S ribosomal protein L31

Chain D4:



TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

- Molecule 54: 50S ribosomal protein L32

Chain B5: 

MET A2 K3 H4 P5 V6 P7 K8 K9 K10 T11 T12 S12 R16 D17 A18 R19 R20 R25 P28 T29 T30 L30 V31 P32 C33 P34 E35 C36 K37 A38 P39 K40 P41 P42 H43 T44 V45 C46 E48 C49 G50 Y51 Y52 A53 K56 V57 L58 E59 V60

- Molecule 54: 50S ribosomal protein L32

Chain D5: 

MET A2 K3 H4 P5 V6 P7 K8 K9 K10 T11 T12 S12 R16 D17 A18 R19 R20 R25 P28 T29 T30 L30 V31 P32 C33 P34 E35 C36 K37 A38 P39 K40 P41 P42 H43 T44 V45 C46 E48 C49 G50 Y51 Y52 A53 K56 V57 L58 E59 V60

- Molecule 55: 50S ribosomal protein L33

Chain B6: 

MET ALA S3 E4 V5 R6 L7 K8 K9 L10 L11 L12 E12 C13 T14 E15 C16 R17 R18 R19 R20 Y21 Y22 T23 T24 E24 K25 N26 R27 R28 N29 T30 P31 N32 K33 L34 E35 R36 R37 K38 Y39 C40 P41 P42 H43 T44 V45 C46 E48 C49 G50 Y51 Y52 A53 K56 V57 L58 E59 V60

- Molecule 55: 50S ribosomal protein L33

Chain D6: 

MET ALA SER GLU VAL ARG ARG ILE K8 K9 L10 L11 L12 E12 C13 T14 E15 C16 R17 R18 R19 R20 Y21 Y22 T23 T24 E24 K25 N26 R27 R28 N29 T30 P31 N32 K33 L34 E35 R36 R37 K38 Y39 C40 P41 P42 H43 T44 V45 C46 E48 C49 G50 Y51 Y52 A53 K56 V57 L58 E59 V60

- Molecule 56: 50S ribosomal protein L34

Chain B7: 

M1 R2 T3 T4 W5 Q6 P7 N8 R9 R10 R11 K12 R13 H16 G17 A20 R21 R22 R23 T24 R28 R29 V30 L31 K32 R33 R34 R35 Q36 K37 G38 R39 L42 A45 V46 R47 K48 R49

- Molecule 56: 50S ribosomal protein L34

Chain D7: 

M1 T4 W5 Q6 P7 N8 R9 R10 R11 K12 R13 H16 G17 A20 R21 R22 R23 T24 R28 R29 V30 L31 K32 R33 R34 R35 Q36 K37 G38 R39 L42 A45 V46 R47 K48 R49

- Molecule 57: 50S ribosomal protein L35

Chain B8: 

MET P2 K3 M4 K5 T6 H7 K8 G9 A10 K11 K12 R13 H16 G17 A20 R21 R22 R23 T24 R28 R29 V30 L31 K32 R33 R34 R35 Q36 K37 G38 R39 L42 A45 V46 R47 K48 R49

Y64 E65

- Molecule 57: 50S ribosomal protein L35

Chain D8: 



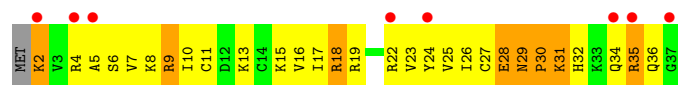
- Molecule 58: 50S ribosomal protein L36

Chain B9: 



- Molecule 58: 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	210.23Å 448.51Å 633.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.1 (49.93-3.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.272 0.253 , 0.284	Depositor DCC
R_{free} test set	55515 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 1109073 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	294559	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, DPP, MG, KBE, UAL, 5OH

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	0.52	0/35980	0.82	47/56157 (0.1%)
1	CA	0.50	0/35980	0.82	32/56157 (0.1%)
2	AB	0.38	0/1936	0.73	0/2611
2	CB	0.37	0/1936	0.71	0/2611
3	AC	0.37	0/1637	0.74	1/2207 (0.0%)
3	CC	0.37	0/1637	0.73	0/2207
4	AD	0.45	0/1733	0.76	1/2318 (0.0%)
4	CD	0.44	0/1733	0.80	2/2318 (0.1%)
5	AE	0.43	0/1163	0.77	0/1566
5	CE	0.43	0/1163	0.77	0/1566
6	AF	0.41	0/856	0.71	0/1154
6	CF	0.41	0/856	0.72	0/1154
7	AG	0.39	0/1276	0.75	1/1709 (0.1%)
7	CG	0.40	0/1276	0.69	0/1709
8	AH	0.42	0/1136	0.76	0/1527
8	CH	0.40	0/1136	0.73	0/1527
9	AI	0.36	0/1023	0.71	0/1371
9	CI	0.37	0/1024	0.68	0/1372
10	AJ	0.37	0/808	0.68	0/1087
10	CJ	0.39	0/808	0.72	0/1087
11	AK	0.40	0/900	0.77	1/1213 (0.1%)
11	CK	0.41	0/900	0.77	1/1213 (0.1%)
12	AL	0.47	0/987	0.89	0/1322
12	CL	0.43	0/987	0.79	0/1322
13	AM	0.44	0/957	0.80	0/1284
13	CM	0.89	5/920 (0.5%)	1.22	13/1241 (1.0%)
14	AN	0.43	0/501	0.73	0/664
14	CN	0.42	0/501	0.72	1/664 (0.2%)
15	AO	0.43	0/745	0.71	0/992
15	CO	0.41	0/745	0.67	0/992
16	AP	0.43	0/717	0.78	1/965 (0.1%)
16	CP	0.40	0/717	0.70	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	0/837	0.77	0/1119
17	CQ	0.40	0/837	0.74	0/1119
18	AR	0.45	0/579	0.82	0/768
18	CR	0.44	0/579	0.82	0/768
19	AS	0.41	0/643	0.71	0/867
19	CS	0.39	0/643	0.69	0/867
20	AT	0.38	0/765	0.80	0/1007
20	CT	0.39	0/765	0.77	0/1007
21	AU	0.46	0/213	0.77	0/279
21	CU	0.36	0/213	0.66	0/279
22	AV	0.56	0/239	0.66	0/371
22	CV	0.49	0/239	0.81	1/371 (0.3%)
23	AW	0.50	0/1778	0.76	0/2768
23	CW	0.43	0/1778	0.74	0/2768
24	AX	0.50	0/1832	0.74	0/2855
24	CX	0.49	0/1832	0.73	1/2855 (0.0%)
25	AY	0.36	0/1776	0.71	0/2766
25	CY	0.39	0/1776	0.73	0/2766
26	AZ	0.95	0/11	0.62	0/13
26	CZ	1.05	0/11	0.87	0/13
27	BA	0.64	0/67544	0.87	94/105433 (0.1%)
27	DA	0.55	0/67547	0.85	93/105438 (0.1%)
28	BB	0.58	0/2826	0.85	4/4406 (0.1%)
28	DB	0.50	0/2826	0.85	4/4406 (0.1%)
29	BC	0.29	0/1145	0.64	0/1556
29	DC	0.30	0/1145	0.67	0/1556
30	BD	0.60	2/2155 (0.1%)	0.94	3/2907 (0.1%)
30	DD	0.52	0/2155	0.90	5/2907 (0.2%)
31	BE	0.55	0/1597	0.92	0/2155
31	DE	0.46	0/1597	0.89	3/2155 (0.1%)
32	BF	0.50	0/1659	0.83	0/2246
32	DF	0.44	0/1659	0.81	1/2246 (0.0%)
33	BG	0.52	1/1499 (0.1%)	0.91	5/2016 (0.2%)
33	DG	0.50	1/1499 (0.1%)	0.89	5/2016 (0.2%)
34	BH	0.54	1/1277 (0.1%)	0.89	3/1729 (0.2%)
34	DH	0.35	0/1246	0.76	0/1684
35	BI	0.37	0/1057	0.81	0/1453
35	DI	0.38	0/1061	0.81	0/1458
36	BN	0.54	0/1132	0.89	2/1527 (0.1%)
36	DN	0.41	0/1132	0.79	0/1527
37	BO	0.50	0/943	0.90	4/1269 (0.3%)
37	DO	0.48	0/943	0.79	0/1269
38	BP	0.60	0/1131	1.14	9/1504 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.49	0/1131	0.97	5/1504 (0.3%)
39	BQ	0.52	0/1143	0.79	0/1527
39	DQ	0.41	0/1128	0.73	0/1508
40	BR	0.53	0/974	0.94	6/1302 (0.5%)
40	DR	0.45	0/974	0.87	2/1302 (0.2%)
41	BS	0.50	0/779	1.01	4/1038 (0.4%)
41	DS	0.42	0/785	0.92	3/1048 (0.3%)
42	BT	0.54	0/1156	0.99	5/1544 (0.3%)
42	DT	0.48	0/1156	0.89	2/1544 (0.1%)
43	BU	0.57	0/975	0.86	2/1297 (0.2%)
43	DU	0.42	0/975	0.84	3/1297 (0.2%)
44	BV	0.51	0/790	0.95	3/1057 (0.3%)
44	DV	0.42	0/790	0.82	0/1057
45	BW	0.52	0/907	0.88	2/1216 (0.2%)
45	DW	0.50	0/907	0.85	0/1216
46	BX	0.53	0/740	0.89	0/995
46	DX	0.48	0/740	0.81	1/995 (0.1%)
47	BY	0.56	0/789	1.06	3/1053 (0.3%)
47	DY	0.48	0/789	0.93	3/1053 (0.3%)
48	BZ	0.42	0/1436	0.74	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.53	0/671	0.81	1/892 (0.1%)
49	D0	0.45	0/671	0.73	0/892
50	B1	0.49	0/722	0.82	0/964
50	D1	0.47	0/739	0.79	0/983
51	B2	0.55	0/600	0.86	1/793 (0.1%)
51	D2	0.42	0/600	0.74	0/793
52	B3	0.52	0/473	0.84	0/636
52	D3	0.41	0/473	0.81	0/636
53	B4	0.42	0/229	0.86	0/311
53	D4	0.50	0/229	1.01	2/311 (0.6%)
54	B5	0.53	0/473	0.95	2/639 (0.3%)
54	D5	0.46	0/473	0.79	0/639
55	B6	0.75	0/418	1.17	3/562 (0.5%)
55	D6	0.80	1/397 (0.3%)	1.20	4/531 (0.8%)
56	B7	0.59	0/427	0.92	1/563 (0.2%)
56	D7	0.50	0/427	0.85	0/563
57	B8	0.59	0/516	1.01	1/681 (0.1%)
57	D8	0.50	0/516	0.95	3/681 (0.4%)
58	B9	0.54	0/302	0.88	0/397
58	D9	0.33	0/302	0.74	0/397
All	All	0.54	11/318953 (0.0%)	0.84	400/477060 (0.1%)

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	90
1	CA	1	81
13	CM	0	1
22	CV	0	2
23	AW	0	1
23	CW	0	2
27	BA	0	223
27	DA	0	164
28	BB	0	6
28	DB	0	6
30	DD	0	1
36	DN	0	1
47	BY	0	1
54	D5	0	1
55	B6	0	1
55	D6	0	1
All	All	1	582

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	CM	113	PRO	N-CD	-7.63	1.37	1.47
55	D6	46	HIS	C-N	-6.65	1.18	1.34
34	BH	11	VAL	C-N	6.53	1.46	1.34
13	CM	65	LYS	C-N	6.24	1.48	1.34
33	BG	111	LEU	C-N	5.78	1.45	1.34

The worst 5 of 400 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	CM	70	LEU	N-CA-C	-12.04	78.50	111.00
27	BA	2424	C	N1-C1'-C2'	-11.64	98.86	114.00
55	B6	46	HIS	N-CA-C	11.54	142.16	111.00
38	BP	52	GLU	N-CA-C	11.01	140.73	111.00
27	DA	1782	C	N1-C1'-C2'	-10.49	100.36	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	CA	517	G	C3'

5 of 582 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	34	C	Sidechain
1	AA	49	U	Sidechain
1	AA	52	G	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	32141	0	16225	1913	0
1	CA	32141	0	16225	2200	0
2	AB	1901	0	1951	267	0
2	CB	1901	0	1951	267	0
3	AC	1613	0	1677	233	0
3	CC	1613	0	1677	215	0
4	AD	1703	0	1764	222	0
4	CD	1703	0	1764	256	0
5	AE	1147	0	1207	175	0
5	CE	1147	0	1207	184	0
6	AF	843	0	857	110	0
6	CF	843	0	857	121	0
7	AG	1257	0	1296	180	0
7	CG	1257	0	1296	149	0
8	AH	1116	0	1177	206	0
8	CH	1116	0	1177	178	0
9	AI	1005	0	1032	145	0
9	CI	1006	0	1034	145	0
10	AJ	795	0	840	164	0
10	CJ	795	0	840	157	0
11	AK	885	0	904	123	0
11	CK	885	0	904	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1057	167	0
12	CL	971	0	1057	185	0
13	AM	947	0	999	196	0
13	CM	910	0	931	185	0
14	AN	492	0	533	99	0
14	CN	492	0	533	106	0
15	AO	734	0	771	116	0
15	CO	734	0	771	104	0
16	AP	701	0	720	113	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	109	0
17	CQ	824	0	891	121	0
18	AR	574	0	644	90	0
18	CR	574	0	644	73	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	118	0
20	CT	763	0	861	132	0
21	AU	209	0	221	24	0
21	CU	209	0	221	33	0
22	AV	213	0	110	6	0
22	CV	213	0	110	12	0
23	AW	1593	0	810	80	0
23	CW	1593	0	810	75	0
24	AX	1640	0	837	69	0
24	CX	1640	0	837	73	0
25	AY	1591	0	810	83	0
25	CY	1591	0	810	87	0
26	AZ	48	0	40	12	0
26	CZ	48	0	40	19	0
27	BA	60311	0	30410	3523	0
27	DA	60313	0	30409	3995	0
28	BB	2528	0	1285	121	0
28	DB	2528	0	1285	141	0
29	BC	1142	0	865	101	0
29	DC	1142	0	865	133	0
30	BD	2105	0	2182	414	0
30	DD	2105	0	2182	386	0
31	BE	1564	0	1629	294	0
31	DE	1564	0	1629	325	0
32	BF	1624	0	1677	321	0
32	DF	1624	0	1677	262	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BG	1474	0	1535	226	0
33	DG	1474	0	1535	259	0
34	BH	1252	0	1316	235	0
34	DH	1223	0	1282	194	0
35	BI	1042	0	1031	193	0
35	DI	1046	0	1035	152	0
36	BN	1105	0	1180	171	0
36	DN	1105	0	1180	214	0
37	BO	933	0	996	170	0
37	DO	933	0	996	165	0
38	BP	1114	0	1187	295	0
38	DP	1114	0	1187	327	0
39	BQ	1122	0	1179	176	0
39	DQ	1107	0	1166	203	0
40	BR	960	0	1021	164	0
40	DR	960	0	1021	179	0
41	BS	771	0	832	160	0
41	DS	777	0	825	148	0
42	BT	1142	0	1202	279	0
42	DT	1142	0	1202	273	0
43	BU	958	0	1015	185	0
43	DU	958	0	1015	196	0
44	BV	779	0	852	166	0
44	DV	779	0	852	168	0
45	BW	896	0	953	103	0
45	DW	896	0	953	157	0
46	BX	726	0	778	103	0
46	DX	726	0	778	127	0
47	BY	776	0	870	215	0
47	DY	776	0	870	191	0
48	BZ	1404	0	1432	184	0
48	DZ	1404	0	1432	221	0
49	B0	662	0	688	89	0
49	D0	662	0	688	103	0
50	B1	715	0	766	118	0
50	D1	732	0	808	98	0
51	B2	598	0	653	112	0
51	D2	598	0	653	84	0
52	B3	468	0	523	56	0
52	D3	468	0	523	84	0
53	B4	226	0	226	40	0
53	D4	226	0	227	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B5	459	0	476	76	0
54	D5	459	0	476	70	0
55	B6	411	0	403	122	0
55	D6	390	0	403	103	0
56	B7	419	0	467	49	0
56	D7	419	0	467	80	0
57	B8	508	0	576	122	0
57	D8	508	0	576	135	0
58	B9	299	0	323	50	0
58	D9	299	0	323	49	0
59	AA	133	0	0	0	0
59	AC	1	0	0	0	0
59	AD	1	0	0	0	0
59	AE	1	0	0	0	0
59	AF	1	0	0	0	0
59	AH	1	0	0	0	0
59	AK	2	0	0	0	0
59	AL	1	0	0	0	0
59	AO	1	0	0	0	0
59	AT	2	0	0	0	0
59	AW	7	0	0	0	0
59	AX	7	0	0	0	0
59	AY	2	0	0	0	0
59	B0	2	0	0	0	0
59	B5	1	0	0	0	0
59	BA	400	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	2	0	0	0	0
59	BH	1	0	0	0	0
59	BN	1	0	0	0	0
59	BP	1	0	0	0	0
59	BQ	1	0	0	0	0
59	BR	1	0	0	0	0
59	BU	1	0	0	0	0
59	BX	1	0	0	0	0
59	BY	1	0	0	1	0
59	BZ	1	0	0	0	0
59	CA	92	0	0	0	0
59	CE	2	0	0	0	0
59	CQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CV	2	0	0	0	0
59	CX	3	0	0	0	0
59	D5	2	0	0	0	0
59	D6	1	0	0	0	0
59	DA	275	0	0	0	0
59	DB	1	0	0	0	0
59	DD	3	0	0	0	0
59	DE	3	0	0	0	0
59	DF	1	0	0	0	0
59	DR	1	0	0	0	0
59	DZ	1	0	0	0	0
60	AD	1	0	0	1	0
60	B4	1	0	0	0	0
60	B5	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	1	0
60	D4	1	0	0	0	0
60	D5	1	0	0	0	0
60	D9	1	0	0	0	0
All	All	294559	0	198754	25938	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 53.

The worst 5 of 25938 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:BP:59:LEU:HA	38:BP:61:ARG:CZ	1.58	1.32
30:DD:231:HIS:ND1	30:DD:232:PRO:HD2	1.55	1.20
1:CA:1363(A):A:H1'	1:CA:1365:G:N7	1.57	1.19
40:BR:100:LEU:HD21	40:BR:113:LEU:HD13	1.24	1.19
27:BA:2787:C:H1'	31:BE:61:ARG:HG3	1.25	1.18

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%)	126 (54%)	73 (31%)	34 (15%)	0	1
2	CB	233/256 (91%)	151 (65%)	50 (22%)	32 (14%)	0	2
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	2
3	CC	205/239 (86%)	121 (59%)	59 (29%)	25 (12%)	1	2
4	AD	206/209 (99%)	129 (63%)	52 (25%)	25 (12%)	1	2
4	CD	206/209 (99%)	126 (61%)	51 (25%)	29 (14%)	0	2
5	AE	149/162 (92%)	94 (63%)	38 (26%)	17 (11%)	1	3
5	CE	149/162 (92%)	103 (69%)	27 (18%)	19 (13%)	0	2
6	AF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	1	4
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	2	9
7	AG	153/156 (98%)	101 (66%)	39 (26%)	13 (8%)	1	6
7	CG	153/156 (98%)	102 (67%)	38 (25%)	13 (8%)	1	6
8	AH	136/138 (99%)	98 (72%)	27 (20%)	11 (8%)	1	7
8	CH	136/138 (99%)	81 (60%)	38 (28%)	17 (12%)	1	2
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	1	4
9	CI	125/128 (98%)	82 (66%)	26 (21%)	17 (14%)	0	2
10	AJ	97/105 (92%)	64 (66%)	26 (27%)	7 (7%)	2	8
10	CJ	97/105 (92%)	55 (57%)	28 (29%)	14 (14%)	0	1
11	AK	117/129 (91%)	70 (60%)	34 (29%)	13 (11%)	1	3
11	CK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	10
12	AL	123/132 (93%)	75 (61%)	25 (20%)	23 (19%)	0	1
12	CL	123/132 (93%)	76 (62%)	24 (20%)	23 (19%)	0	1
13	AM	118/126 (94%)	64 (54%)	33 (28%)	21 (18%)	0	1
13	CM	117/126 (93%)	64 (55%)	29 (25%)	24 (20%)	0	0
14	AN	58/61 (95%)	29 (50%)	19 (33%)	10 (17%)	0	1
14	CN	58/61 (95%)	35 (60%)	12 (21%)	11 (19%)	0	0
15	AO	86/89 (97%)	56 (65%)	19 (22%)	11 (13%)	0	2
15	CO	86/89 (97%)	49 (57%)	28 (33%)	9 (10%)	1	3
16	AP	82/88 (93%)	49 (60%)	21 (26%)	12 (15%)	0	1
16	CP	82/88 (93%)	45 (55%)	28 (34%)	9 (11%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	98/105 (93%)	73 (74%)	15 (15%)	10 (10%)	1	4
17	CQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	2	14
18	AR	68/88 (77%)	35 (52%)	21 (31%)	12 (18%)	0	1
18	CR	68/88 (77%)	41 (60%)	16 (24%)	11 (16%)	0	1
19	AS	77/93 (83%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/93 (83%)	46 (60%)	18 (23%)	13 (17%)	0	1
20	AT	97/106 (92%)	59 (61%)	20 (21%)	18 (19%)	0	1
20	CT	97/106 (92%)	52 (54%)	36 (37%)	9 (9%)	1	5
21	AU	23/27 (85%)	16 (70%)	4 (17%)	3 (13%)	0	2
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
26	AZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
26	CZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
29	BC	183/229 (80%)	69 (38%)	49 (27%)	65 (36%)	0	0
29	DC	183/229 (80%)	69 (38%)	59 (32%)	55 (30%)	0	0
30	BD	270/276 (98%)	172 (64%)	66 (24%)	32 (12%)	1	2
30	DD	270/276 (98%)	180 (67%)	57 (21%)	33 (12%)	1	2
31	BE	203/206 (98%)	130 (64%)	38 (19%)	35 (17%)	0	1
31	DE	203/206 (98%)	125 (62%)	34 (17%)	44 (22%)	0	0
32	BF	206/210 (98%)	137 (66%)	31 (15%)	38 (18%)	0	1
32	DF	206/210 (98%)	125 (61%)	40 (19%)	41 (20%)	0	0
33	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	2
33	DG	179/182 (98%)	109 (61%)	42 (24%)	28 (16%)	0	1
34	BH	162/180 (90%)	87 (54%)	43 (26%)	32 (20%)	0	0
34	DH	158/180 (88%)	88 (56%)	35 (22%)	35 (22%)	0	0
35	BI	144/148 (97%)	73 (51%)	33 (23%)	38 (26%)	0	0
35	DI	144/148 (97%)	80 (56%)	41 (28%)	23 (16%)	0	1
36	BN	137/140 (98%)	91 (66%)	27 (20%)	19 (14%)	0	2
36	DN	137/140 (98%)	82 (60%)	28 (20%)	27 (20%)	0	0
37	BO	120/122 (98%)	84 (70%)	25 (21%)	11 (9%)	1	5
37	DO	120/122 (98%)	80 (67%)	23 (19%)	17 (14%)	0	1
38	BP	144/150 (96%)	71 (49%)	42 (29%)	31 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DP	144/150 (96%)	72 (50%)	36 (25%)	36 (25%)	0	0
39	BQ	139/141 (99%)	98 (70%)	21 (15%)	20 (14%)	0	1
39	DQ	137/141 (97%)	88 (64%)	29 (21%)	20 (15%)	0	1
40	BR	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	2
40	DR	115/118 (98%)	66 (57%)	31 (27%)	18 (16%)	0	1
41	BS	97/112 (87%)	45 (46%)	24 (25%)	28 (29%)	0	0
41	DS	99/112 (88%)	51 (52%)	14 (14%)	34 (34%)	0	0
42	BT	136/146 (93%)	78 (57%)	26 (19%)	32 (24%)	0	0
42	DT	136/146 (93%)	68 (50%)	32 (24%)	36 (26%)	0	0
43	BU	115/118 (98%)	70 (61%)	27 (24%)	18 (16%)	0	1
43	DU	115/118 (98%)	69 (60%)	30 (26%)	16 (14%)	0	2
44	BV	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	2
44	DV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
45	BW	111/113 (98%)	77 (69%)	23 (21%)	11 (10%)	1	4
45	DW	111/113 (98%)	71 (64%)	29 (26%)	11 (10%)	1	4
46	BX	91/96 (95%)	67 (74%)	16 (18%)	8 (9%)	1	5
46	DX	91/96 (95%)	60 (66%)	17 (19%)	14 (15%)	0	1
47	BY	99/110 (90%)	42 (42%)	22 (22%)	35 (35%)	0	0
47	DY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
48	BZ	175/206 (85%)	99 (57%)	49 (28%)	27 (15%)	0	1
48	DZ	175/206 (85%)	97 (55%)	51 (29%)	27 (15%)	0	1
49	B0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	1	4
49	D0	82/85 (96%)	61 (74%)	14 (17%)	7 (8%)	1	6
50	B1	92/98 (94%)	60 (65%)	20 (22%)	12 (13%)	0	2
50	D1	92/98 (94%)	65 (71%)	16 (17%)	11 (12%)	1	2
51	B2	69/72 (96%)	46 (67%)	14 (20%)	9 (13%)	0	2
51	D2	69/72 (96%)	37 (54%)	20 (29%)	12 (17%)	0	1
52	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	6	31
52	D3	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	6	31
53	B4	29/71 (41%)	18 (62%)	6 (21%)	5 (17%)	0	1
53	D4	29/71 (41%)	17 (59%)	9 (31%)	3 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B5	57/60 (95%)	34 (60%)	13 (23%)	10 (18%)	0	1
54	D5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	1
55	B6	49/54 (91%)	17 (35%)	14 (29%)	18 (37%)	0	0
55	D6	44/54 (82%)	16 (36%)	11 (25%)	17 (39%)	0	0
56	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	6
56	D7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	6
57	B8	62/65 (95%)	34 (55%)	19 (31%)	9 (14%)	0	1
57	D8	62/65 (95%)	32 (52%)	15 (24%)	15 (24%)	0	0
58	B9	34/37 (92%)	25 (74%)	8 (24%)	1 (3%)	7	35
58	D9	34/37 (92%)	18 (53%)	13 (38%)	3 (9%)	1	5
All	All	11702/12598 (93%)	7090 (61%)	2747 (24%)	1865 (16%)	0	1

5 of 1865 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	96	ARG
2	AB	101	MET

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%)	169 (84%)	33 (16%)	3	17
2	CB	202/220 (92%)	174 (86%)	28 (14%)	5	23
3	AC	160/188 (85%)	129 (81%)	31 (19%)	2	11
3	CC	160/188 (85%)	140 (88%)	20 (12%)	7	28
4	AD	180/181 (99%)	147 (82%)	33 (18%)	2	13
4	CD	180/181 (99%)	147 (82%)	33 (18%)	2	13
5	AE	115/123 (94%)	101 (88%)	14 (12%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CE	115/123 (94%)	96 (84%)	19 (16%)	3	16
6	AF	90/90 (100%)	80 (89%)	10 (11%)	9	34
6	CF	90/90 (100%)	78 (87%)	12 (13%)	6	25
7	AG	126/127 (99%)	106 (84%)	20 (16%)	4	17
7	CG	126/127 (99%)	106 (84%)	20 (16%)	4	17
8	AH	119/119 (100%)	96 (81%)	23 (19%)	2	12
8	CH	119/119 (100%)	105 (88%)	14 (12%)	8	30
9	AI	97/99 (98%)	80 (82%)	17 (18%)	3	14
9	CI	97/99 (98%)	85 (88%)	12 (12%)	7	28
10	AJ	88/92 (96%)	68 (77%)	20 (23%)	1	6
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	4	17
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	14
11	CK	90/99 (91%)	78 (87%)	12 (13%)	6	25
12	AL	104/109 (95%)	87 (84%)	17 (16%)	3	17
12	CL	104/109 (95%)	90 (86%)	14 (14%)	6	24
13	AM	94/101 (93%)	75 (80%)	19 (20%)	2	10
13	CM	88/101 (87%)	69 (78%)	19 (22%)	1	8
14	AN	49/50 (98%)	39 (80%)	10 (20%)	2	9
14	CN	49/50 (98%)	37 (76%)	12 (24%)	1	5
15	AO	79/80 (99%)	63 (80%)	16 (20%)	2	9
15	CO	79/80 (99%)	65 (82%)	14 (18%)	3	14
16	AP	72/74 (97%)	63 (88%)	9 (12%)	7	28
16	CP	72/74 (97%)	60 (83%)	12 (17%)	3	16
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	4	20
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	10	36
18	AR	61/77 (79%)	53 (87%)	8 (13%)	6	25
18	CR	61/77 (79%)	55 (90%)	6 (10%)	12	41
19	AS	69/80 (86%)	53 (77%)	16 (23%)	1	6
19	CS	69/80 (86%)	51 (74%)	18 (26%)	1	4
20	AT	76/82 (93%)	63 (83%)	13 (17%)	3	15
20	CT	76/82 (93%)	65 (86%)	11 (14%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	19/22 (86%)	16 (84%)	3 (16%)	4	18
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	74
26	AZ	2/2 (100%)	2 (100%)	0	100	100
26	CZ	2/2 (100%)	2 (100%)	0	100	100
29	BC	61/181 (34%)	56 (92%)	5 (8%)	17	52
29	DC	61/181 (34%)	51 (84%)	10 (16%)	3	16
30	BD	213/218 (98%)	162 (76%)	51 (24%)	1	5
30	DD	213/218 (98%)	173 (81%)	40 (19%)	2	12
31	BE	165/166 (99%)	127 (77%)	38 (23%)	1	6
31	DE	165/166 (99%)	121 (73%)	44 (27%)	1	4
32	BF	165/166 (99%)	136 (82%)	29 (18%)	3	14
32	DF	165/166 (99%)	138 (84%)	27 (16%)	3	16
33	BG	155/156 (99%)	117 (76%)	38 (24%)	1	5
33	DG	155/156 (99%)	125 (81%)	30 (19%)	2	11
34	BH	136/148 (92%)	111 (82%)	25 (18%)	2	13
34	DH	132/148 (89%)	111 (84%)	21 (16%)	4	17
35	BI	102/124 (82%)	79 (78%)	23 (22%)	1	7
35	DI	103/124 (83%)	85 (82%)	18 (18%)	3	14
36	BN	117/119 (98%)	88 (75%)	29 (25%)	1	4
36	DN	117/119 (98%)	92 (79%)	25 (21%)	1	8
37	BO	100/100 (100%)	81 (81%)	19 (19%)	2	12
37	DO	100/100 (100%)	75 (75%)	25 (25%)	1	4
38	BP	112/116 (97%)	76 (68%)	36 (32%)	0	2
38	DP	112/116 (97%)	79 (70%)	33 (30%)	0	2
39	BQ	111/111 (100%)	85 (77%)	26 (23%)	1	5
39	DQ	110/111 (99%)	91 (83%)	19 (17%)	3	14
40	BR	100/101 (99%)	77 (77%)	23 (23%)	1	6
40	DR	100/101 (99%)	67 (67%)	33 (33%)	0	2
41	BS	77/88 (88%)	60 (78%)	17 (22%)	1	7
41	DS	76/88 (86%)	62 (82%)	14 (18%)	2	13
42	BT	120/127 (94%)	81 (68%)	39 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	120/127 (94%)	88 (73%)	32 (27%)	1	4
43	BU	92/94 (98%)	71 (77%)	21 (23%)	1	6
43	DU	92/94 (98%)	81 (88%)	11 (12%)	7	30
44	BV	82/82 (100%)	59 (72%)	23 (28%)	0	3
44	DV	82/82 (100%)	60 (73%)	22 (27%)	1	4
45	BW	91/92 (99%)	74 (81%)	17 (19%)	2	12
45	DW	91/92 (99%)	72 (79%)	19 (21%)	1	8
46	BX	74/78 (95%)	60 (81%)	14 (19%)	2	12
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	8
47	BY	84/91 (92%)	62 (74%)	22 (26%)	1	4
47	DY	84/91 (92%)	63 (75%)	21 (25%)	1	4
48	BZ	155/179 (87%)	127 (82%)	28 (18%)	2	13
48	DZ	155/179 (87%)	135 (87%)	20 (13%)	6	26
49	B0	66/67 (98%)	53 (80%)	13 (20%)	2	11
49	D0	66/67 (98%)	58 (88%)	8 (12%)	7	29
50	B1	74/83 (89%)	56 (76%)	18 (24%)	1	5
50	D1	78/83 (94%)	63 (81%)	15 (19%)	2	12
51	B2	66/67 (98%)	50 (76%)	16 (24%)	1	5
51	D2	66/67 (98%)	53 (80%)	13 (20%)	2	11
52	B3	51/52 (98%)	42 (82%)	9 (18%)	3	14
52	D3	51/52 (98%)	44 (86%)	7 (14%)	5	24
53	B4	27/63 (43%)	23 (85%)	4 (15%)	4	21
53	D4	27/63 (43%)	25 (93%)	2 (7%)	20	58
54	B5	51/52 (98%)	39 (76%)	12 (24%)	1	5
54	D5	51/52 (98%)	42 (82%)	9 (18%)	3	14
55	B6	43/52 (83%)	30 (70%)	13 (30%)	0	2
55	D6	44/52 (85%)	28 (64%)	16 (36%)	0	1
56	B7	41/42 (98%)	34 (83%)	7 (17%)	3	15
56	D7	41/42 (98%)	36 (88%)	5 (12%)	7	29
57	B8	53/55 (96%)	44 (83%)	9 (17%)	3	15
57	D8	53/55 (96%)	39 (74%)	14 (26%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	B9	33/34 (97%)	24 (73%)	9 (27%)	0 3
58	D9	33/34 (97%)	28 (85%)	5 (15%)	4 20
All	All	9600/10432 (92%)	7750 (81%)	1850 (19%)	2 12

5 of 1850 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BY	97	ARG
4	CD	78	LEU
46	DX	68	ARG
48	BZ	153	ASP
55	B6	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 293 such sidechains are listed below:

Mol	Chain	Res	Type
48	BZ	33	ASN
3	CC	28	GLN
48	DZ	72	GLN
49	B0	29	GLN
55	B6	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1509 (98%)	351 (23%)	136 (9%)
1	CA	1493/1509 (98%)	365 (24%)	120 (8%)
22	AV	9/30 (30%)	0	0
22	CV	9/30 (30%)	0	0
23	AW	74/75 (98%)	17 (22%)	2 (2%)
23	CW	74/75 (98%)	16 (21%)	4 (5%)
24	AX	76/77 (98%)	19 (25%)	1 (1%)
24	CX	76/77 (98%)	19 (25%)	0
25	AY	74/75 (98%)	23 (31%)	1 (1%)
25	CY	74/75 (98%)	22 (29%)	1 (1%)
27	BA	2792/2915 (95%)	798 (28%)	220 (7%)
27	DA	2793/2915 (95%)	905 (32%)	280 (10%)
28	BB	116/122 (95%)	26 (22%)	5 (4%)
28	DB	116/122 (95%)	28 (24%)	8 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9269/9606 (96%)	2589 (27%)	778 (8%)

5 of 2589 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G
1	AA	32	A

5 of 778 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2792	G
1	CA	967	C
27	DA	2296	U
28	BB	25	A
1	CA	389	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	KBE	AZ	1	26	8,8,9	8.22	1 (12%)	6,8,10	0.79	0
26	DPP	AZ	2	26	5,5,6	7.06	1 (20%)	3,5,7	1.93	1 (33%)
26	UAL	AZ	5	26	7,8,9	2.19	3 (42%)	6,9,11	0.83	0
26	5OH	AZ	6	26	12,12,13	5.41	4 (33%)	13,16,18	0.81	0
26	KBE	CZ	1	26	8,8,9	5.99	1 (12%)	6,8,10	0.57	0
26	DPP	CZ	2	26	5,5,6	8.82	1 (20%)	3,5,7	2.13	1 (33%)
26	UAL	CZ	5	26	7,8,9	3.61	3 (42%)	6,9,11	3.33	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	5OH	CZ	6	26	12,12,13	6.58	3 (25%)	13,16,18	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	KBE	AZ	1	26	-	0/6/7/8	0/0/0/0
26	DPP	AZ	2	26	-	0/2/4/6	0/0/0/0
26	UAL	AZ	5	26	-	0/3/7/9	0/0/0/0
26	5OH	AZ	6	26	-	0/2/18/20	0/1/1/1
26	KBE	CZ	1	26	-	0/6/7/8	0/0/0/0
26	DPP	CZ	2	26	-	0/2/4/6	0/0/0/0
26	UAL	CZ	5	26	-	0/3/7/9	0/0/0/0
26	5OH	CZ	6	26	-	0/2/18/20	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AZ	1	KBE	O-C	23.23	1.27	1.11
26	CZ	6	5OH	O-C	22.05	1.26	1.11
26	CZ	2	DPP	O-C	19.62	1.24	1.11
26	AZ	6	5OH	O-C	17.55	1.23	1.11
26	CZ	1	KBE	O-C	16.87	1.23	1.11

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CZ	5	UAL	O2-C1-N2	-6.71	111.92	123.27
26	CZ	2	DPP	C-CA-N	-3.49	110.34	113.83
26	AZ	2	DPP	C-CA-N	-2.90	110.94	113.83
26	CZ	5	UAL	N2-C1-N1	2.69	121.55	115.64
26	CZ	5	UAL	O2-C1-N1	2.59	126.51	120.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 973 ligands modelled in this entry, 973 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%)	-0.28	22 (1%) 70 16	48, 83, 149, 196	0
1	CA	1495/1509 (99%)	-0.24	22 (1%) 70 16	59, 91, 155, 196	0
2	AB	235/256 (91%)	0.04	3 (1%) 74 19	80, 114, 144, 161	0
2	CB	235/256 (91%)	0.02	3 (1%) 74 19	81, 118, 152, 171	0
3	AC	207/239 (86%)	-0.09	0 100 100	76, 101, 140, 153	0
3	CC	207/239 (86%)	0.01	1 (0%) 88 36	89, 109, 136, 147	0
4	AD	208/209 (99%)	-0.06	5 (2%) 56 11	65, 84, 101, 114	0
4	CD	208/209 (99%)	-0.23	1 (0%) 88 36	55, 77, 98, 107	0
5	AE	151/162 (93%)	-0.19	0 100 100	59, 81, 107, 122	0
5	CE	151/162 (93%)	-0.03	0 100 100	72, 88, 109, 145	0
6	AF	101/101 (100%)	-0.24	0 100 100	63, 84, 93, 110	0
6	CF	101/101 (100%)	-0.10	0 100 100	76, 88, 101, 134	0
7	AG	155/156 (99%)	-0.10	5 (3%) 45 9	74, 94, 129, 151	0
7	CG	155/156 (99%)	-0.04	7 (4%) 32 7	84, 103, 128, 140	0
8	AH	138/138 (100%)	-0.29	0 100 100	69, 84, 96, 107	0
8	CH	138/138 (100%)	-0.17	0 100 100	74, 91, 102, 117	0
9	AI	127/128 (99%)	0.14	3 (2%) 56 11	76, 115, 136, 144	0
9	CI	127/128 (99%)	0.07	2 (1%) 68 16	89, 121, 139, 143	0
10	AJ	99/105 (94%)	0.43	4 (4%) 36 7	80, 127, 152, 164	0
10	CJ	99/105 (94%)	0.51	6 (6%) 21 5	88, 125, 148, 154	0
11	AK	119/129 (92%)	0.20	2 (1%) 67 15	55, 79, 107, 127	0
11	CK	119/129 (92%)	0.08	8 (6%) 17 4	69, 88, 108, 124	0
12	AL	125/132 (94%)	-0.12	0 100 100	55, 69, 91, 126	0
12	CL	125/132 (94%)	0.09	3 (2%) 56 11	66, 82, 98, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	120/126 (95%)	-0.18	1 (0%) 83 26	58, 86, 98, 107	0
13	CM	119/126 (94%)	-0.15	0 100 100	80, 108, 125, 136	0
14	AN	60/61 (98%)	-0.08	0 100 100	76, 92, 110, 122	0
14	CN	60/61 (98%)	0.14	1 (1%) 67 15	90, 105, 120, 123	0
15	AO	88/89 (98%)	-0.04	3 (3%) 43 8	64, 76, 99, 114	0
15	CO	88/89 (98%)	0.10	1 (1%) 77 21	71, 84, 106, 117	0
16	AP	84/88 (95%)	-0.05	3 (3%) 41 8	68, 86, 108, 124	0
16	CP	84/88 (95%)	0.13	1 (1%) 75 20	71, 81, 105, 136	0
17	AQ	100/105 (95%)	0.09	2 (2%) 62 12	62, 79, 95, 99	0
17	CQ	100/105 (95%)	-0.19	0 100 100	64, 85, 100, 103	0
18	AR	70/88 (79%)	-0.11	0 100 100	67, 83, 106, 134	0
18	CR	70/88 (79%)	-0.04	0 100 100	73, 86, 107, 134	0
19	AS	79/93 (84%)	0.58	7 (8%) 10 3	87, 105, 127, 134	0
19	CS	79/93 (84%)	0.44	6 (7%) 14 3	101, 122, 143, 154	0
20	AT	99/106 (93%)	0.00	2 (2%) 62 12	71, 89, 118, 130	0
20	CT	99/106 (93%)	-0.13	1 (1%) 79 22	74, 90, 114, 125	0
21	AU	25/27 (92%)	1.59	9 (36%) 1 0	86, 92, 100, 118	0
21	CU	25/27 (92%)	1.78	8 (32%) 1 0	89, 104, 117, 119	0
22	AV	10/30 (33%)	0.36	1 (10%) 8 2	63, 73, 124, 133	0
22	CV	10/30 (33%)	-0.03	0 100 100	68, 85, 125, 130	0
23	AW	75/75 (100%)	0.52	15 (20%) 2 1	46, 119, 161, 185	0
23	CW	75/75 (100%)	0.28	7 (9%) 9 2	79, 141, 174, 184	0
24	AX	77/77 (100%)	-0.10	2 (2%) 53 10	48, 89, 121, 130	0
24	CX	77/77 (100%)	-0.13	1 (1%) 74 19	69, 98, 125, 132	0
25	AY	75/75 (100%)	0.99	19 (25%) 1 1	51, 157, 193, 194	0
25	CY	75/75 (100%)	1.16	23 (30%) 1 0	67, 167, 194, 194	0
26	AZ	2/6 (33%)	0.05	0 100 100	85, 85, 85, 88	0
26	CZ	2/6 (33%)	0.45	0 100 100	99, 99, 99, 100	0
27	BA	2800/2915 (96%)	-0.32	38 (1%) 72 18	30, 56, 157, 198	0
27	DA	2800/2915 (96%)	-0.21	53 (1%) 64 13	49, 77, 168, 197	0
28	BB	118/122 (96%)	-0.41	1 (0%) 83 26	47, 76, 119, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	118/122 (96%)	-0.15	4 (3%) 43 8	80, 104, 136, 162	0
29	BC	191/229 (83%)	0.90	33 (17%) 2 1	130, 167, 187, 195	0
29	DC	191/229 (83%)	1.15	48 (25%) 1 1	122, 173, 188, 191	0
30	BD	272/276 (98%)	-0.23	1 (0%) 90 41	32, 52, 68, 79	0
30	DD	272/276 (98%)	-0.21	0 100 100	46, 61, 78, 92	0
31	BE	205/206 (99%)	-0.14	2 (0%) 79 22	33, 58, 93, 104	0
31	DE	205/206 (99%)	-0.04	0 100 100	57, 84, 112, 121	0
32	BF	208/210 (99%)	-0.27	0 100 100	29, 60, 125, 149	0
32	DF	208/210 (99%)	0.04	2 (0%) 79 22	54, 86, 132, 152	0
33	BG	181/182 (99%)	-0.11	1 (0%) 86 32	64, 83, 116, 146	0
33	DG	181/182 (99%)	0.13	7 (3%) 37 7	79, 106, 132, 153	0
34	BH	164/180 (91%)	0.11	2 (1%) 75 20	68, 97, 124, 142	0
34	DH	160/180 (88%)	0.55	14 (8%) 10 3	110, 139, 159, 163	0
35	BI	146/148 (98%)	-0.23	0 100 100	62, 119, 140, 144	0
35	DI	146/148 (98%)	-0.12	0 100 100	67, 105, 128, 136	0
36	BN	139/140 (99%)	-0.32	1 (0%) 84 28	42, 57, 86, 104	0
36	DN	139/140 (99%)	-0.21	0 100 100	65, 91, 115, 124	0
37	BO	122/122 (100%)	-0.41	0 100 100	38, 57, 75, 88	0
37	DO	122/122 (100%)	-0.19	0 100 100	60, 77, 93, 100	0
38	BP	146/150 (97%)	0.15	0 100 100	37, 69, 102, 156	0
38	DP	146/150 (97%)	0.23	1 (0%) 84 28	61, 93, 122, 148	0
39	BQ	141/141 (100%)	-0.17	2 (1%) 72 18	42, 60, 92, 118	0
39	DQ	139/141 (98%)	-0.15	0 100 100	68, 90, 120, 134	0
40	BR	117/118 (99%)	-0.28	0 100 100	35, 52, 69, 82	0
40	DR	117/118 (99%)	-0.07	0 100 100	58, 71, 83, 96	0
41	BS	99/112 (88%)	-0.13	0 100 100	48, 76, 94, 105	0
41	DS	101/112 (90%)	0.17	3 (2%) 48 9	69, 100, 117, 122	0
42	BT	138/146 (94%)	-0.03	6 (4%) 34 7	51, 70, 126, 152	0
42	DT	138/146 (94%)	0.04	6 (4%) 34 7	61, 90, 149, 175	0
43	BU	117/118 (99%)	-0.18	1 (0%) 81 24	37, 49, 73, 95	0
43	DU	117/118 (99%)	0.20	4 (3%) 43 8	60, 91, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	101/101 (100%)	-0.32	0 100 100	35, 65, 90, 116	0
44	DV	101/101 (100%)	0.06	1 (0%) 79 22	59, 106, 121, 129	0
45	BW	113/113 (100%)	-0.23	0 100 100	32, 46, 76, 136	0
45	DW	113/113 (100%)	-0.23	0 100 100	43, 64, 95, 130	0
46	BX	93/96 (96%)	-0.24	0 100 100	43, 53, 70, 91	0
46	DX	93/96 (96%)	-0.22	0 100 100	56, 71, 89, 95	0
47	BY	101/110 (91%)	-0.13	1 (0%) 79 22	58, 78, 145, 163	0
47	DY	101/110 (91%)	0.17	2 (1%) 62 12	73, 94, 149, 156	0
48	BZ	177/206 (85%)	0.29	8 (4%) 32 7	65, 107, 169, 177	0
48	DZ	177/206 (85%)	0.76	19 (10%) 6 2	104, 130, 177, 191	0
49	B0	84/85 (98%)	-0.03	2 (2%) 56 11	43, 56, 83, 103	0
49	D0	84/85 (98%)	0.33	5 (5%) 21 5	71, 83, 100, 118	0
50	B1	94/98 (95%)	-0.18	1 (1%) 77 21	44, 61, 92, 109	0
50	D1	94/98 (95%)	0.14	2 (2%) 60 12	54, 70, 94, 110	0
51	B2	71/72 (98%)	-0.24	2 (2%) 50 10	46, 66, 86, 117	0
51	D2	71/72 (98%)	-0.18	0 100 100	65, 86, 103, 107	0
52	B3	60/60 (100%)	-0.20	1 (1%) 67 15	43, 58, 85, 110	0
52	D3	60/60 (100%)	0.08	2 (3%) 44 8	75, 90, 112, 116	0
53	B4	31/71 (43%)	-0.30	0 100 100	92, 107, 120, 126	0
53	D4	31/71 (43%)	-0.21	0 100 100	108, 119, 128, 135	0
54	B5	59/60 (98%)	-0.23	1 (1%) 67 15	33, 51, 115, 135	0
54	D5	59/60 (98%)	-0.09	3 (5%) 27 6	60, 71, 143, 177	0
55	B6	51/54 (94%)	0.03	2 (3%) 37 7	59, 83, 106, 112	0
55	D6	46/54 (85%)	0.42	3 (6%) 18 4	56, 103, 116, 117	0
56	B7	49/49 (100%)	0.02	0 100 100	28, 44, 84, 115	0
56	D7	49/49 (100%)	0.42	2 (4%) 35 7	46, 59, 90, 101	0
57	B8	64/65 (98%)	-0.11	0 100 100	40, 56, 73, 97	0
57	D8	64/65 (98%)	0.02	0 100 100	60, 74, 87, 118	0
58	B9	36/37 (97%)	0.30	0 100 100	46, 63, 80, 93	0
58	D9	36/37 (97%)	0.82	8 (22%) 1 1	88, 122, 133, 137	0
All	All	21214/22204 (95%)	-0.09	505 (2%) 56 11	28, 83, 154, 198	0

The worst 5 of 505 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	BA	2802	G	14.6
27	DA	2802	G	10.4
48	DZ	111	ARG	10.3
27	BA	2801	A	9.0
27	DA	896	A	9.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
26	DPP	CZ	2	6/7	0.16	-	94,96,97,97	0
26	UAL	AZ	5	9/10	0.20	-	81,82,83,84	0
26	DPP	AZ	2	6/7	0.14	-	79,82,82,84	0
26	UAL	CZ	5	9/10	0.37	-	97,99,99,99	0
26	5OH	AZ	6	12/13	0.17	-	84,89,92,94	0
26	KBE	AZ	1	9/10	0.39	-	78,79,82,82	0
26	5OH	CZ	6	12/13	0.29	-	99,101,102,102	0
26	KBE	CZ	1	9/10	0.34	-	89,91,93,94	0

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
59	MG	AA	1631	1/1	0.06	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3191	1/1	0.09	-	77,77,77,77	0
59	MG	DA	3147	1/1	0.32	-	44,44,44,44	0
59	MG	CA	1691	1/1	0.16	-	55,55,55,55	0
59	MG	BA	3238	1/1	0.11	-	26,26,26,26	0
59	MG	CA	1673	1/1	0.26	-	71,71,71,71	0
59	MG	BA	3209	1/1	0.10	-	27,27,27,27	0
59	MG	AA	1674	1/1	0.05	-	42,42,42,42	0
59	MG	BY	201	1/1	0.17	-	32,32,32,32	0
59	MG	AA	1733	1/1	0.14	-	30,30,30,30	0
59	MG	DA	3020	1/1	0.24	-	45,45,45,45	0
59	MG	BA	3167	1/1	0.19	-	31,31,31,31	0
59	MG	DA	3220	1/1	0.19	-	64,64,64,64	0
59	MG	BA	3270	1/1	0.20	-	64,64,64,64	0
59	MG	BA	3282	1/1	0.18	-	48,48,48,48	0
59	MG	AA	1604	1/1	0.33	-	56,56,56,56	0
59	MG	BA	3244	1/1	0.17	-	31,31,31,31	0
59	MG	BA	3034	1/1	0.32	-	37,37,37,37	0
59	MG	DA	3058	1/1	0.07	-	33,33,33,33	0
59	MG	DA	3201	1/1	0.11	-	33,33,33,33	0
59	MG	CA	1631	1/1	0.43	-	45,45,45,45	0
59	MG	AA	1713	1/1	0.17	-	57,57,57,57	0
59	MG	DA	3233	1/1	0.36	-	58,58,58,58	0
59	MG	DA	3070	1/1	0.15	-	10,10,10,10	0
59	MG	BA	3134	1/1	0.57	-	39,39,39,39	0
59	MG	BA	3204	1/1	0.10	-	2,2,2,2	0
59	MG	DA	3174	1/1	0.05	-	47,47,47,47	0
59	MG	BA	3263	1/1	0.17	-	37,37,37,37	0
59	MG	BA	3009	1/1	0.23	-	30,30,30,30	0
59	MG	BA	3024	1/1	0.15	-	22,22,22,22	0
59	MG	CV	102	1/1	0.35	-	44,44,44,44	0
59	MG	CA	1601	1/1	0.14	-	29,29,29,29	0
59	MG	B0	102	1/1	0.32	-	49,49,49,49	0
59	MG	BA	3073	1/1	0.13	-	10,10,10,10	0
59	MG	BA	3199	1/1	0.21	-	54,54,54,54	0
59	MG	DA	3046	1/1	0.18	-	15,15,15,15	0
59	MG	DA	3067	1/1	0.27	-	50,50,50,50	0
59	MG	CA	1640	1/1	0.10	-	47,47,47,47	0
59	MG	CA	1663	1/1	0.19	-	50,50,50,50	0
59	MG	BA	3397	1/1	0.31	-	66,66,66,66	0
59	MG	BA	3127	1/1	0.30	-	48,48,48,48	0
59	MG	BA	3005	1/1	0.07	-	17,17,17,17	0
59	MG	BA	3193	1/1	0.25	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3157	1/1	0.41	-	62,62,62,62	0
59	MG	DA	3257	1/1	0.47	-	40,40,40,40	0
59	MG	CX	102	1/1	0.46	-	78,78,78,78	0
59	MG	DA	3263	1/1	0.48	-	62,62,62,62	0
59	MG	BA	3095	1/1	0.23	-	30,30,30,30	0
59	MG	CA	1610	1/1	0.32	-	27,27,27,27	0
59	MG	BA	3086	1/1	0.51	-	46,46,46,46	0
59	MG	AA	1718	1/1	0.11	-	36,36,36,36	0
59	MG	BA	3046	1/1	0.13	-	30,30,30,30	0
59	MG	BA	3004	1/1	0.51	-	81,81,81,81	0
59	MG	BA	3294	1/1	1.02	-	72,72,72,72	0
59	MG	AA	1655	1/1	0.35	-	28,28,28,28	0
59	MG	DA	3255	1/1	0.13	-	13,13,13,13	0
59	MG	BA	3324	1/1	0.37	-	35,35,35,35	0
59	MG	DA	3235	1/1	0.22	-	68,68,68,68	0
59	MG	CA	1685	1/1	0.09	-	36,36,36,36	0
59	MG	DA	3130	1/1	0.32	-	27,27,27,27	0
59	MG	DA	3073	1/1	0.21	-	18,18,18,18	0
59	MG	AL	201	1/1	0.35	-	44,44,44,44	0
60	ZN	B5	102	1/1	0.06	-	75,75,75,75	0
59	MG	BA	3355	1/1	0.13	-	33,33,33,33	0
59	MG	BA	3120	1/1	0.23	-	49,49,49,49	0
59	MG	BA	3223	1/1	0.26	-	46,46,46,46	0
59	MG	BA	3206	1/1	0.16	-	36,36,36,36	0
59	MG	CA	1623	1/1	0.19	-	91,91,91,91	0
59	MG	DF	301	1/1	0.07	-	31,31,31,31	0
59	MG	DA	3132	1/1	0.19	-	60,60,60,60	0
59	MG	BA	3015	1/1	0.31	-	25,25,25,25	0
59	MG	AW	102	1/1	0.11	-	53,53,53,53	0
59	MG	BF	302	1/1	0.23	-	26,26,26,26	0
59	MG	AA	1726	1/1	0.25	-	32,32,32,32	0
59	MG	BA	3012	1/1	0.27	-	31,31,31,31	0
59	MG	BA	3205	1/1	0.24	-	86,86,86,86	0
59	MG	AA	1634	1/1	0.15	-	72,72,72,72	0
59	MG	BA	3100	1/1	0.24	-	22,22,22,22	0
59	MG	AA	1680	1/1	0.31	-	63,63,63,63	0
59	MG	CA	1674	1/1	0.36	-	63,63,63,63	0
59	MG	BA	3260	1/1	0.17	-	58,58,58,58	0
59	MG	DA	3167	1/1	0.14	-	42,42,42,42	0
59	MG	BA	3311	1/1	0.68	-	54,54,54,54	0
59	MG	DB	201	1/1	0.14	-	44,44,44,44	0
59	MG	AY	102	1/1	0.51	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1612	1/1	0.08	-	32,32,32,32	0
59	MG	AA	1727	1/1	0.52	-	71,71,71,71	0
59	MG	BA	3356	1/1	0.13	-	41,41,41,41	0
59	MG	DA	3215	1/1	0.55	-	63,63,63,63	0
59	MG	BA	3266	1/1	0.31	-	27,27,27,27	0
59	MG	BA	3297	1/1	0.68	-	95,95,95,95	0
59	MG	BA	3379	1/1	0.35	-	52,52,52,52	0
59	MG	BA	3022	1/1	0.14	-	12,12,12,12	0
59	MG	AA	1610	1/1	0.09	-	29,29,29,29	0
59	MG	BA	3075	1/1	0.22	-	32,32,32,32	0
59	MG	DA	3081	1/1	0.23	-	48,48,48,48	0
59	MG	BA	3188	1/1	0.42	-	22,22,22,22	0
59	MG	DA	3219	1/1	0.17	-	40,40,40,40	0
59	MG	DA	3126	1/1	0.45	-	48,48,48,48	0
59	MG	BA	3345	1/1	0.21	-	31,31,31,31	0
59	MG	BA	3233	1/1	0.16	-	32,32,32,32	0
59	MG	DA	3038	1/1	0.16	-	25,25,25,25	0
59	MG	DA	3228	1/1	0.06	-	16,16,16,16	0
59	MG	DA	3080	1/1	0.14	-	41,41,41,41	0
59	MG	DA	3270	1/1	0.22	-	61,61,61,61	0
59	MG	AA	1658	1/1	0.56	-	42,42,42,42	0
59	MG	BA	3067	1/1	0.34	-	36,36,36,36	0
59	MG	DA	3229	1/1	0.20	-	76,76,76,76	0
59	MG	BA	3396	1/1	0.15	-	37,37,37,37	0
59	MG	BA	3007	1/1	0.58	-	39,39,39,39	0
59	MG	BA	3175	1/1	0.18	-	43,43,43,43	0
59	MG	BA	3114	1/1	0.33	-	53,53,53,53	0
59	MG	AA	1621	1/1	0.25	-	54,54,54,54	0
59	MG	CA	1618	1/1	0.48	-	69,69,69,69	0
59	MG	BA	3398	1/1	0.42	-	66,66,66,66	0
59	MG	CA	1611	1/1	0.12	-	38,38,38,38	0
59	MG	DA	3031	1/1	0.13	-	31,31,31,31	0
59	MG	DA	3075	1/1	0.14	-	32,32,32,32	0
59	MG	BA	3312	1/1	0.10	-	42,42,42,42	0
59	MG	BA	3372	1/1	0.18	-	26,26,26,26	0
59	MG	BA	3069	1/1	0.22	-	20,20,20,20	0
59	MG	DA	3135	1/1	0.25	-	58,58,58,58	0
59	MG	AX	105	1/1	0.44	-	82,82,82,82	0
59	MG	DA	3144	1/1	0.59	-	57,57,57,57	0
59	MG	BA	3299	1/1	1.26	-	85,85,85,85	0
59	MG	BA	3085	1/1	0.38	-	18,18,18,18	0
59	MG	DA	3071	1/1	0.13	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3247	1/1	0.28	-	82,82,82,82	0
59	MG	BA	3138	1/1	0.13	-	17,17,17,17	0
59	MG	BA	3208	1/1	0.19	-	54,54,54,54	0
59	MG	DA	3050	1/1	0.37	-	70,70,70,70	0
59	MG	CA	1666	1/1	0.07	-	68,68,68,68	0
59	MG	BA	3329	1/1	0.10	-	48,48,48,48	0
59	MG	BA	3162	1/1	0.56	-	66,66,66,66	0
59	MG	BA	3176	1/1	0.25	-	27,27,27,27	0
59	MG	AA	1666	1/1	0.70	-	75,75,75,75	0
59	MG	BA	3328	1/1	0.20	-	35,35,35,35	0
59	MG	BA	3078	1/1	0.11	-	20,20,20,20	0
59	MG	BA	3107	1/1	0.16	-	13,13,13,13	0
59	MG	BA	3182	1/1	0.27	-	81,81,81,81	0
59	MG	BA	3079	1/1	0.15	-	23,23,23,23	0
59	MG	DA	3043	1/1	0.30	-	48,48,48,48	0
59	MG	DA	3097	1/1	0.40	-	65,65,65,65	0
59	MG	BA	3051	1/1	0.22	-	1,1,1,1	0
59	MG	BA	3228	1/1	0.44	-	21,21,21,21	0
59	MG	CA	1606	1/1	0.63	-	52,52,52,52	0
59	MG	BA	3251	1/1	0.27	-	34,34,34,34	0
59	MG	AA	1608	1/1	0.07	-	26,26,26,26	0
59	MG	BA	3119	1/1	0.15	-	20,20,20,20	0
59	MG	BA	3219	1/1	0.23	-	43,43,43,43	0
59	MG	BA	3241	1/1	0.20	-	38,38,38,38	0
59	MG	DA	3072	1/1	0.24	-	28,28,28,28	0
59	MG	AA	1689	1/1	0.18	-	73,73,73,73	0
59	MG	AA	1724	1/1	0.28	-	56,56,56,56	0
59	MG	BA	3310	1/1	0.35	-	55,55,55,55	0
59	MG	BA	3289	1/1	0.21	-	36,36,36,36	0
59	MG	BA	3291	1/1	0.11	-	42,42,42,42	0
59	MG	BA	3125	1/1	0.43	-	43,43,43,43	0
59	MG	BA	3043	1/1	0.29	-	22,22,22,22	0
59	MG	BA	3259	1/1	0.12	-	35,35,35,35	0
59	MG	BA	3395	1/1	0.18	-	46,46,46,46	0
59	MG	CA	1669	1/1	0.18	-	36,36,36,36	0
59	MG	BA	3190	1/1	0.15	-	29,29,29,29	0
59	MG	BA	3348	1/1	0.38	-	62,62,62,62	0
59	MG	CA	1667	1/1	0.25	-	37,37,37,37	0
59	MG	CA	1622	1/1	0.28	-	49,49,49,49	0
59	MG	DA	3183	1/1	0.11	-	100,100,100,100	0
59	MG	BA	3293	1/1	0.69	-	44,44,44,44	0
59	MG	AA	1675	1/1	0.45	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1620	1/1	0.37	-	45,45,45,45	0
59	MG	BA	3200	1/1	0.16	-	51,51,51,51	0
59	MG	AA	1699	1/1	0.35	-	61,61,61,61	0
59	MG	DA	3212	1/1	0.43	-	61,61,61,61	0
59	MG	BA	3037	1/1	0.46	-	27,27,27,27	0
59	MG	BA	3080	1/1	0.13	-	26,26,26,26	0
59	MG	DA	3241	1/1	0.23	-	42,42,42,42	0
59	MG	DA	3076	1/1	0.25	-	48,48,48,48	0
59	MG	AA	1672	1/1	0.16	-	51,51,51,51	0
59	MG	BA	3383	1/1	0.28	-	36,36,36,36	0
59	MG	CA	1681	1/1	0.06	-	58,58,58,58	0
59	MG	BA	3013	1/1	0.17	-	6,6,6,6	0
59	MG	BA	3261	1/1	0.17	-	53,53,53,53	0
59	MG	DA	3205	1/1	0.21	-	27,27,27,27	0
59	MG	BA	3149	1/1	0.41	-	31,31,31,31	0
59	MG	AA	1715	1/1	0.10	-	34,34,34,34	0
59	MG	AA	1677	1/1	0.41	-	75,75,75,75	0
59	MG	BA	3314	1/1	0.17	-	68,68,68,68	0
59	MG	BA	3110	1/1	0.16	-	39,39,39,39	0
59	MG	BA	3108	1/1	0.15	-	44,44,44,44	0
59	MG	DA	3227	1/1	0.31	-	72,72,72,72	0
59	MG	BA	3117	1/1	0.20	-	38,38,38,38	0
59	MG	DA	3148	1/1	0.60	-	40,40,40,40	0
59	MG	AD	301	1/1	0.13	-	49,49,49,49	0
59	MG	DA	3074	1/1	0.41	-	59,59,59,59	0
59	MG	AA	1628	1/1	0.37	-	46,46,46,46	0
59	MG	DA	3082	1/1	0.49	-	37,37,37,37	0
59	MG	DA	3197	1/1	0.24	-	84,84,84,84	0
59	MG	DA	3027	1/1	0.40	-	28,28,28,28	0
59	MG	BA	3265	1/1	0.22	-	28,28,28,28	0
59	MG	DA	3007	1/1	0.29	-	42,42,42,42	0
59	MG	BA	3056	1/1	0.74	-	59,59,59,59	0
59	MG	DA	3253	1/1	0.21	-	46,46,46,46	0
59	MG	BA	3302	1/1	0.16	-	42,42,42,42	0
59	MG	DA	3260	1/1	0.20	-	35,35,35,35	0
60	ZN	D4	101	1/1	0.11	-	147,147,147,147	0
59	MG	CA	1633	1/1	0.25	-	38,38,38,38	0
59	MG	BA	3150	1/1	0.14	-	33,33,33,33	0
59	MG	DA	3169	1/1	0.10	-	37,37,37,37	0
59	MG	AA	1611	1/1	0.12	-	52,52,52,52	0
59	MG	DA	3021	1/1	0.15	-	28,28,28,28	0
59	MG	DA	3133	1/1	0.23	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3101	1/1	0.14	-	25,25,25,25	0
59	MG	AA	1657	1/1	0.14	-	53,53,53,53	0
59	MG	BA	3010	1/1	0.30	-	29,29,29,29	0
59	MG	AA	1629	1/1	0.11	-	78,78,78,78	0
59	MG	BA	3170	1/1	0.22	-	57,57,57,57	0
59	MG	DA	3218	1/1	0.76	-	75,75,75,75	0
59	MG	AA	1696	1/1	0.16	-	34,34,34,34	0
59	MG	BA	3020	1/1	0.19	-	22,22,22,22	0
59	MG	BA	3304	1/1	0.44	-	22,22,22,22	0
59	MG	BA	3060	1/1	0.12	-	13,13,13,13	0
59	MG	BA	3203	1/1	0.15	-	38,38,38,38	0
59	MG	AA	1695	1/1	0.18	-	55,55,55,55	0
59	MG	BA	3083	1/1	0.16	-	6,6,6,6	0
59	MG	BA	3128	1/1	0.36	-	34,34,34,34	0
59	MG	CA	1644	1/1	0.77	-	68,68,68,68	0
59	MG	AW	101	1/1	0.42	-	135,135,135,135	0
59	MG	AA	1728	1/1	0.12	-	59,59,59,59	0
59	MG	BA	3144	1/1	0.12	-	37,37,37,37	0
59	MG	BA	3231	1/1	0.08	-	54,54,54,54	0
59	MG	BA	3335	1/1	0.42	-	52,52,52,52	0
59	MG	BP	201	1/1	0.11	-	21,21,21,21	0
59	MG	AA	1702	1/1	0.49	-	59,59,59,59	0
59	MG	BA	3087	1/1	0.21	-	39,39,39,39	0
59	MG	AA	1729	1/1	0.24	-	57,57,57,57	0
59	MG	AA	1654	1/1	0.20	-	100,100,100,100	0
59	MG	BA	3369	1/1	0.24	-	38,38,38,38	0
59	MG	CA	1602	1/1	0.33	-	46,46,46,46	0
59	MG	CA	1678	1/1	0.18	-	45,45,45,45	0
59	MG	BA	3246	1/1	0.44	-	46,46,46,46	0
59	MG	BA	3070	1/1	0.07	-	14,14,14,14	0
59	MG	CA	1670	1/1	0.27	-	67,67,67,67	0
59	MG	AA	1684	1/1	0.08	-	42,42,42,42	0
59	MG	DA	3118	1/1	0.17	-	41,41,41,41	0
59	MG	CA	1609	1/1	0.36	-	52,52,52,52	0
59	MG	AA	1636	1/1	0.25	-	21,21,21,21	0
59	MG	DA	3030	1/1	0.10	-	17,17,17,17	0
59	MG	DA	3064	1/1	0.17	-	48,48,48,48	0
59	MG	DA	3273	1/1	0.94	-	106,106,106,106	0
59	MG	AA	1708	1/1	0.04	-	64,64,64,64	0
59	MG	DA	3142	1/1	0.13	-	44,44,44,44	0
59	MG	D6	101	1/1	0.24	-	37,37,37,37	0
59	MG	DA	3041	1/1	0.29	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3360	1/1	0.46	-	68,68,68,68	0
59	MG	AA	1602	1/1	0.15	-	44,44,44,44	0
59	MG	AA	1731	1/1	0.18	-	22,22,22,22	0
59	MG	CA	1652	1/1	0.34	-	86,86,86,86	0
59	MG	DA	3184	1/1	0.13	-	50,50,50,50	0
59	MG	AA	1663	1/1	0.36	-	53,53,53,53	0
59	MG	DA	3236	1/1	0.95	-	91,91,91,91	0
59	MG	CA	1655	1/1	0.34	-	41,41,41,41	0
59	MG	DA	3250	1/1	0.46	-	61,61,61,61	0
59	MG	DA	3158	1/1	0.34	-	38,38,38,38	0
59	MG	DA	3164	1/1	0.31	-	51,51,51,51	0
59	MG	DA	3069	1/1	0.63	-	78,78,78,78	0
59	MG	AA	1644	1/1	0.23	-	48,48,48,48	0
59	MG	DA	3266	1/1	0.43	-	72,72,72,72	0
59	MG	CA	1686	1/1	0.23	-	64,64,64,64	0
59	MG	DD	303	1/1	0.43	-	95,95,95,95	0
59	MG	BA	3124	1/1	0.17	-	27,27,27,27	0
59	MG	BA	3156	1/1	0.28	-	25,25,25,25	0
59	MG	DA	3209	1/1	0.44	-	69,69,69,69	0
59	MG	CA	1630	1/1	0.33	-	55,55,55,55	0
59	MG	AA	1685	1/1	0.40	-	50,50,50,50	0
59	MG	DA	3083	1/1	0.32	-	35,35,35,35	0
59	MG	BA	3133	1/1	0.17	-	20,20,20,20	0
59	MG	CX	101	1/1	0.14	-	42,42,42,42	0
59	MG	DA	3196	1/1	0.38	-	48,48,48,48	0
59	MG	BA	3186	1/1	0.18	-	30,30,30,30	0
59	MG	BA	3296	1/1	0.28	-	61,61,61,61	0
59	MG	BA	3215	1/1	0.13	-	12,12,12,12	0
59	MG	BA	3047	1/1	0.19	-	30,30,30,30	0
59	MG	AA	1678	1/1	0.19	-	52,52,52,52	0
59	MG	BA	3250	1/1	0.10	-	21,21,21,21	0
59	MG	BA	3384	1/1	0.07	-	39,39,39,39	0
59	MG	AA	1627	1/1	0.36	-	55,55,55,55	0
59	MG	BA	3221	1/1	0.19	-	25,25,25,25	0
60	ZN	B4	101	1/1	0.06	-	117,117,117,117	0
59	MG	DA	3092	1/1	0.34	-	51,51,51,51	0
59	MG	CA	1687	1/1	0.11	-	56,56,56,56	0
59	MG	BA	3001	1/1	0.16	-	72,72,72,72	0
59	MG	BA	3129	1/1	0.14	-	27,27,27,27	0
59	MG	AA	1703	1/1	0.07	-	41,41,41,41	0
59	MG	DA	3114	1/1	0.07	-	42,42,42,42	0
59	MG	BA	3274	1/1	0.15	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	ZN	D9	101	1/1	0.03	-	109,109,109,109	0
59	MG	CA	1677	1/1	0.11	-	53,53,53,53	0
59	MG	BA	3386	1/1	0.18	-	20,20,20,20	0
59	MG	AA	1649	1/1	0.34	-	71,71,71,71	0
59	MG	CA	1646	1/1	0.24	-	40,40,40,40	0
59	MG	DA	3116	1/1	0.14	-	43,43,43,43	0
59	MG	BA	3109	1/1	0.12	-	34,34,34,34	0
59	MG	AA	1676	1/1	0.16	-	77,77,77,77	0
59	MG	AA	1721	1/1	0.15	-	54,54,54,54	0
59	MG	BA	3224	1/1	0.29	-	63,63,63,63	0
59	MG	BA	3017	1/1	0.17	-	14,14,14,14	0
59	MG	DA	3232	1/1	0.29	-	80,80,80,80	0
59	MG	DA	3261	1/1	0.30	-	50,50,50,50	0
59	MG	AW	105	1/1	0.28	-	41,41,41,41	0
59	MG	DA	3033	1/1	0.10	-	10,10,10,10	0
59	MG	DA	3208	1/1	0.34	-	62,62,62,62	0
59	MG	BN	201	1/1	0.35	-	67,67,67,67	0
59	MG	BA	3168	1/1	0.15	-	37,37,37,37	0
59	MG	DA	3077	1/1	0.36	-	73,73,73,73	0
59	MG	DA	3243	1/1	0.34	-	35,35,35,35	0
59	MG	DA	3258	1/1	0.18	-	29,29,29,29	0
59	MG	DA	3230	1/1	0.39	-	46,46,46,46	0
59	MG	AT	202	1/1	0.45	-	70,70,70,70	0
59	MG	BA	3317	1/1	0.41	-	50,50,50,50	0
59	MG	DA	3108	1/1	0.43	-	51,51,51,51	0
59	MG	CA	1607	1/1	0.38	-	36,36,36,36	0
59	MG	BA	3346	1/1	0.33	-	35,35,35,35	0
59	MG	AA	1630	1/1	0.08	-	26,26,26,26	0
59	MG	DZ	301	1/1	0.18	-	55,55,55,55	0
59	MG	BA	3316	1/1	0.37	-	68,68,68,68	0
59	MG	BA	3359	1/1	0.26	-	51,51,51,51	0
59	MG	BR	201	1/1	0.44	-	41,41,41,41	0
59	MG	BA	3269	1/1	0.88	-	83,83,83,83	0
59	MG	D5	102	1/1	0.23	-	91,91,91,91	0
59	MG	CA	1625	1/1	0.54	-	54,54,54,54	0
59	MG	AA	1716	1/1	0.22	-	44,44,44,44	0
59	MG	DA	3023	1/1	0.05	-	33,33,33,33	0
59	MG	DA	3206	1/1	0.21	-	27,27,27,27	0
59	MG	BA	3105	1/1	0.19	-	14,14,14,14	0
59	MG	DA	3182	1/1	0.17	-	33,33,33,33	0
59	MG	BA	3201	1/1	0.18	-	111,111,111,111	0
59	MG	BE	301	1/1	0.18	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3063	1/1	0.17	-	19,19,19,19	0
59	MG	BA	3115	1/1	0.24	-	22,22,22,22	0
59	MG	BA	3093	1/1	0.10	-	10,10,10,10	0
59	MG	CA	1627	1/1	0.15	-	62,62,62,62	0
59	MG	DA	3131	1/1	0.18	-	38,38,38,38	0
59	MG	AX	101	1/1	0.34	-	57,57,57,57	0
59	MG	DA	3185	1/1	0.07	-	42,42,42,42	0
59	MG	BA	3267	1/1	0.10	-	31,31,31,31	0
59	MG	DA	3003	1/1	0.19	-	36,36,36,36	0
59	MG	AA	1616	1/1	0.09	-	16,16,16,16	0
59	MG	DA	3137	1/1	0.11	-	28,28,28,28	0
59	MG	DA	3056	1/1	0.14	-	31,31,31,31	0
59	MG	BA	3030	1/1	0.10	-	18,18,18,18	0
59	MG	AA	1732	1/1	0.16	-	32,32,32,32	0
59	MG	BA	3279	1/1	0.16	-	62,62,62,62	0
59	MG	AA	1714	1/1	0.33	-	66,66,66,66	0
59	MG	AA	1646	1/1	0.24	-	61,61,61,61	0
59	MG	BA	3178	1/1	0.34	-	11,11,11,11	0
59	MG	BA	3353	1/1	0.31	-	50,50,50,50	0
59	MG	CA	1684	1/1	0.43	-	49,49,49,49	0
59	MG	CA	1659	1/1	0.12	-	64,64,64,64	0
59	MG	BA	3191	1/1	0.18	-	31,31,31,31	0
59	MG	DA	3200	1/1	0.26	-	46,46,46,46	0
59	MG	BA	3214	1/1	0.29	-	87,87,87,87	0
59	MG	BZ	301	1/1	0.16	-	42,42,42,42	0
59	MG	AA	1698	1/1	0.14	-	49,49,49,49	0
59	MG	AA	1626	1/1	0.10	-	48,48,48,48	0
59	MG	BA	3147	1/1	0.23	-	33,33,33,33	0
59	MG	BA	3035	1/1	0.14	-	22,22,22,22	0
59	MG	DA	3052	1/1	0.13	-	30,30,30,30	0
59	MG	AW	104	1/1	0.12	-	57,57,57,57	0
59	MG	BA	3135	1/1	0.24	-	38,38,38,38	0
59	MG	BA	3025	1/1	0.18	-	20,20,20,20	0
59	MG	BA	3245	1/1	0.66	-	48,48,48,48	0
59	MG	AW	103	1/1	0.45	-	73,73,73,73	0
59	MG	BA	3040	1/1	0.06	-	9,9,9,9	0
59	MG	BA	3065	1/1	0.07	-	13,13,13,13	0
59	MG	DA	3028	1/1	0.30	-	35,35,35,35	0
59	MG	BA	3285	1/1	0.13	-	28,28,28,28	0
59	MG	BA	3368	1/1	0.12	-	24,24,24,24	0
59	MG	BA	3281	1/1	0.25	-	41,41,41,41	0
59	MG	DA	3008	1/1	0.07	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3377	1/1	0.35	-	43,43,43,43	0
59	MG	DA	3203	1/1	0.93	-	97,97,97,97	0
59	MG	DA	3166	1/1	0.12	-	41,41,41,41	0
59	MG	BA	3126	1/1	0.28	-	52,52,52,52	0
59	MG	AA	1725	1/1	0.26	-	84,84,84,84	0
59	MG	DA	3239	1/1	0.94	-	78,78,78,78	0
59	MG	BA	3248	1/1	0.16	-	37,37,37,37	0
59	MG	DA	3244	1/1	0.18	-	33,33,33,33	0
59	MG	BA	3181	1/1	0.09	-	46,46,46,46	0
59	MG	BA	3357	1/1	0.24	-	54,54,54,54	0
59	MG	BA	3045	1/1	0.11	-	23,23,23,23	0
59	MG	BA	3341	1/1	0.33	-	86,86,86,86	0
59	MG	D5	101	1/1	0.13	-	28,28,28,28	0
59	MG	DA	3225	1/1	0.64	-	55,55,55,55	0
59	MG	CA	1634	1/1	0.04	-	17,17,17,17	0
59	MG	DA	3223	1/1	0.20	-	61,61,61,61	0
59	MG	BA	3077	1/1	0.07	-	23,23,23,23	0
59	MG	DA	3150	1/1	0.17	-	43,43,43,43	0
59	MG	AA	1690	1/1	0.22	-	40,40,40,40	0
59	MG	BA	3273	1/1	0.13	-	26,26,26,26	0
59	MG	DA	3010	1/1	0.28	-	39,39,39,39	0
59	MG	BA	3096	1/1	0.09	-	17,17,17,17	0
59	MG	DA	3198	1/1	0.47	-	56,56,56,56	0
59	MG	DA	3106	1/1	0.24	-	51,51,51,51	0
59	MG	BA	3268	1/1	0.46	-	44,44,44,44	0
59	MG	AA	1613	1/1	0.07	-	51,51,51,51	0
59	MG	DA	3264	1/1	0.26	-	41,41,41,41	0
59	MG	BA	3330	1/1	0.06	-	21,21,21,21	0
59	MG	BA	3184	1/1	0.36	-	56,56,56,56	0
59	MG	BA	3160	1/1	0.23	-	13,13,13,13	0
59	MG	DA	3204	1/1	0.11	-	41,41,41,41	0
59	MG	BA	3230	1/1	0.18	-	48,48,48,48	0
59	MG	AA	1704	1/1	0.05	-	40,40,40,40	0
59	MG	CA	1614	1/1	0.16	-	49,49,49,49	0
59	MG	DA	3111	1/1	0.49	-	71,71,71,71	0
59	MG	DA	3025	1/1	0.17	-	5,5,5,5	0
59	MG	DA	3011	1/1	0.33	-	37,37,37,37	0
59	MG	BA	3217	1/1	0.14	-	11,11,11,11	0
59	MG	BA	3141	1/1	0.23	-	1,1,1,1	0
59	MG	DA	3018	1/1	0.12	-	14,14,14,14	0
59	MG	CA	1680	1/1	0.19	-	59,59,59,59	0
59	MG	DA	3101	1/1	0.08	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3141	1/1	0.13	-	46,46,46,46	0
59	MG	DA	3173	1/1	0.22	-	57,57,57,57	0
59	MG	CA	1636	1/1	0.12	-	55,55,55,55	0
59	MG	AA	1639	1/1	0.15	-	54,54,54,54	0
60	ZN	B9	101	1/1	0.06	-	64,64,64,64	0
59	MG	DA	3112	1/1	0.19	-	70,70,70,70	0
59	MG	CA	1635	1/1	0.28	-	32,32,32,32	0
59	MG	DA	3179	1/1	0.11	-	33,33,33,33	0
59	MG	BA	3284	1/1	0.33	-	33,33,33,33	0
59	MG	DA	3175	1/1	0.57	-	53,53,53,53	0
59	MG	BA	3220	1/1	0.52	-	52,52,52,52	0
59	MG	DA	3252	1/1	0.31	-	47,47,47,47	0
59	MG	CA	1671	1/1	0.25	-	54,54,54,54	0
59	MG	BA	3068	1/1	0.19	-	15,15,15,15	0
59	MG	DA	3249	1/1	0.42	-	54,54,54,54	0
59	MG	DA	3178	1/1	0.58	-	36,36,36,36	0
59	MG	BA	3307	1/1	0.41	-	64,64,64,64	0
59	MG	DA	3207	1/1	0.86	-	69,69,69,69	0
59	MG	CE	202	1/1	0.09	-	40,40,40,40	0
59	MG	B5	101	1/1	0.41	-	37,37,37,37	0
59	MG	DA	3214	1/1	0.14	-	34,34,34,34	0
59	MG	BA	3187	1/1	0.38	-	35,35,35,35	0
59	MG	BD	301	1/1	0.12	-	13,13,13,13	0
59	MG	BA	3049	1/1	0.11	-	12,12,12,12	0
59	MG	BA	3050	1/1	0.30	-	4,4,4,4	0
59	MG	AW	106	1/1	0.50	-	94,94,94,94	0
59	MG	BA	3249	1/1	0.61	-	50,50,50,50	0
59	MG	AE	201	1/1	0.22	-	87,87,87,87	0
59	MG	BA	3023	1/1	0.19	-	23,23,23,23	0
59	MG	CA	1651	1/1	0.16	-	50,50,50,50	0
59	MG	AA	1683	1/1	0.12	-	31,31,31,31	0
59	MG	DA	3256	1/1	0.11	-	27,27,27,27	0
59	MG	BA	3019	1/1	0.33	-	21,21,21,21	0
59	MG	DA	3145	1/1	0.33	-	45,45,45,45	0
59	MG	BA	3213	1/1	0.54	-	54,54,54,54	0
59	MG	CA	1664	1/1	0.34	-	44,44,44,44	0
59	MG	BA	3253	1/1	0.23	-	56,56,56,56	0
59	MG	DA	3222	1/1	0.07	-	50,50,50,50	0
59	MG	DA	3123	1/1	0.23	-	32,32,32,32	0
59	MG	DA	3194	1/1	0.27	-	52,52,52,52	0
59	MG	BA	3059	1/1	0.05	-	33,33,33,33	0
59	MG	CA	1626	1/1	0.31	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3136	1/1	0.30	-	47,47,47,47	0
59	MG	AA	1701	1/1	0.25	-	36,36,36,36	0
59	MG	BA	3042	1/1	0.19	-	22,22,22,22	0
59	MG	BA	3347	1/1	0.84	-	78,78,78,78	0
59	MG	BA	3276	1/1	0.22	-	45,45,45,45	0
59	MG	BA	3198	1/1	0.06	-	16,16,16,16	0
59	MG	DA	3105	1/1	0.24	-	28,28,28,28	0
59	MG	BA	3090	1/1	0.12	-	32,32,32,32	0
59	MG	AA	1706	1/1	0.27	-	43,43,43,43	0
59	MG	CA	1603	1/1	0.45	-	113,113,113,113	0
59	MG	CA	1662	1/1	0.07	-	23,23,23,23	0
59	MG	DA	3242	1/1	0.17	-	34,34,34,34	0
59	MG	DA	3269	1/1	0.21	-	43,43,43,43	0
60	ZN	CD	301	1/1	0.24	-	61,61,61,61	0
59	MG	AT	201	1/1	0.11	-	92,92,92,92	0
59	MG	AA	1656	1/1	0.20	-	42,42,42,42	0
59	MG	AA	1653	1/1	0.18	-	47,47,47,47	0
59	MG	BA	3192	1/1	0.23	-	29,29,29,29	0
59	MG	BA	3148	1/1	0.15	-	27,27,27,27	0
59	MG	AA	1673	1/1	0.20	-	35,35,35,35	0
59	MG	BA	3011	1/1	0.12	-	31,31,31,31	0
59	MG	BA	3275	1/1	0.16	-	93,93,93,93	0
59	MG	BA	3211	1/1	0.14	-	16,16,16,16	0
59	MG	AX	104	1/1	0.24	-	45,45,45,45	0
59	MG	DA	3271	1/1	0.16	-	80,80,80,80	0
59	MG	DA	3066	1/1	0.23	-	31,31,31,31	0
59	MG	BA	3106	1/1	0.28	-	29,29,29,29	0
59	MG	BA	3055	1/1	0.18	-	21,21,21,21	0
59	MG	DA	3128	1/1	0.14	-	26,26,26,26	0
59	MG	DA	3015	1/1	0.43	-	37,37,37,37	0
59	MG	BA	3295	1/1	0.37	-	47,47,47,47	0
59	MG	BF	301	1/1	0.12	-	37,37,37,37	0
59	MG	CA	1605	1/1	0.54	-	99,99,99,99	0
59	MG	BA	3146	1/1	0.35	-	12,12,12,12	0
59	MG	BA	3174	1/1	0.14	-	43,43,43,43	0
59	MG	BA	3033	1/1	0.23	-	26,26,26,26	0
59	MG	CA	1657	1/1	0.51	-	62,62,62,62	0
59	MG	BA	3194	1/1	0.29	-	33,33,33,33	0
59	MG	BA	3179	1/1	0.34	-	31,31,31,31	0
59	MG	CA	1653	1/1	0.13	-	46,46,46,46	0
59	MG	BA	3243	1/1	0.30	-	35,35,35,35	0
59	MG	DA	3022	1/1	0.14	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DE	301	1/1	0.14	-	43,43,43,43	0
59	MG	BA	3218	1/1	0.13	-	21,21,21,21	0
59	MG	CA	1613	1/1	0.06	-	66,66,66,66	0
59	MG	AW	107	1/1	0.20	-	41,41,41,41	0
59	MG	BA	3235	1/1	0.45	-	51,51,51,51	0
59	MG	BA	3151	1/1	0.30	-	22,22,22,22	0
59	MG	DA	3193	1/1	0.16	-	40,40,40,40	0
59	MG	BA	3290	1/1	0.25	-	69,69,69,69	0
59	MG	DA	3104	1/1	0.12	-	36,36,36,36	0
59	MG	DA	3171	1/1	0.43	-	75,75,75,75	0
59	MG	DA	3001	1/1	0.05	-	25,25,25,25	0
59	MG	CE	201	1/1	0.09	-	71,71,71,71	0
59	MG	BA	3394	1/1	0.17	-	49,49,49,49	0
59	MG	BA	3132	1/1	0.16	-	87,87,87,87	0
59	MG	BA	3365	1/1	0.20	-	36,36,36,36	0
59	MG	DA	3045	1/1	0.13	-	41,41,41,41	0
59	MG	BA	3255	1/1	0.10	-	22,22,22,22	0
59	MG	DA	3115	1/1	0.14	-	59,59,59,59	0
59	MG	BA	3375	1/1	0.20	-	38,38,38,38	0
59	MG	DA	3265	1/1	0.42	-	51,51,51,51	0
59	MG	DA	3125	1/1	0.34	-	59,59,59,59	0
59	MG	AA	1603	1/1	0.54	-	58,58,58,58	0
59	MG	AA	1643	1/1	0.19	-	51,51,51,51	0
59	MG	AA	1664	1/1	0.11	-	20,20,20,20	0
59	MG	BA	3044	1/1	0.28	-	28,28,28,28	0
59	MG	BA	3363	1/1	0.23	-	56,56,56,56	0
59	MG	AA	1638	1/1	0.14	-	50,50,50,50	0
59	MG	DA	3151	1/1	0.12	-	14,14,14,14	0
59	MG	BA	3378	1/1	0.30	-	25,25,25,25	0
59	MG	CA	1648	1/1	0.17	-	56,56,56,56	0
59	MG	BH	201	1/1	0.11	-	71,71,71,71	0
59	MG	CA	1682	1/1	0.45	-	61,61,61,61	0
59	MG	DA	3268	1/1	0.19	-	47,47,47,47	0
59	MG	AA	1670	1/1	0.23	-	36,36,36,36	0
59	MG	BA	3166	1/1	0.18	-	35,35,35,35	0
59	MG	BA	3308	1/1	0.82	-	49,49,49,49	0
59	MG	DA	3034	1/1	0.06	-	30,30,30,30	0
59	MG	BA	3315	1/1	0.33	-	46,46,46,46	0
59	MG	BA	3374	1/1	0.40	-	31,31,31,31	0
59	MG	DA	3088	1/1	0.14	-	36,36,36,36	0
59	MG	DA	3087	1/1	0.86	-	59,59,59,59	0
59	MG	BA	3323	1/1	0.14	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	CA	1656	1/1	0.19	-	51,51,51,51	0
59	MG	DA	3139	1/1	0.07	-	18,18,18,18	0
59	MG	BA	3339	1/1	0.37	-	66,66,66,66	0
59	MG	BA	3252	1/1	0.13	-	18,18,18,18	0
59	MG	AA	1679	1/1	0.07	-	27,27,27,27	0
59	MG	BA	3111	1/1	0.23	-	28,28,28,28	0
59	MG	BA	3145	1/1	0.29	-	13,13,13,13	0
59	MG	AA	1692	1/1	0.09	-	55,55,55,55	0
59	MG	AA	1618	1/1	0.20	-	22,22,22,22	0
59	MG	AC	301	1/1	0.15	-	64,64,64,64	0
59	MG	BA	3159	1/1	0.17	-	46,46,46,46	0
59	MG	DA	3165	1/1	0.05	-	49,49,49,49	0
59	MG	BA	3382	1/1	0.31	-	37,37,37,37	0
59	MG	BA	3099	1/1	0.81	-	51,51,51,51	0
59	MG	AX	103	1/1	0.12	-	32,32,32,32	0
60	ZN	AD	302	1/1	0.23	-	67,67,67,67	0
59	MG	DA	3163	1/1	0.37	-	62,62,62,62	0
59	MG	BA	3152	1/1	0.36	-	18,18,18,18	0
59	MG	AA	1688	1/1	0.25	-	47,47,47,47	0
59	MG	CA	1612	1/1	0.44	-	80,80,80,80	0
59	MG	BA	3088	1/1	0.28	-	22,22,22,22	0
59	MG	BA	3072	1/1	0.21	-	16,16,16,16	0
59	MG	BA	3393	1/1	0.13	-	40,40,40,40	0
59	MG	BA	3154	1/1	0.27	-	44,44,44,44	0
59	MG	DA	3226	1/1	0.62	-	70,70,70,70	0
59	MG	BA	3343	1/1	0.21	-	34,34,34,34	0
59	MG	CA	1615	1/1	0.52	-	51,51,51,51	0
59	MG	BA	3165	1/1	0.58	-	60,60,60,60	0
59	MG	DA	3103	1/1	0.08	-	38,38,38,38	0
59	MG	AA	1648	1/1	0.19	-	48,48,48,48	0
59	MG	BA	3021	1/1	0.23	-	3,3,3,3	0
59	MG	DA	3086	1/1	0.16	-	26,26,26,26	0
59	MG	BA	3195	1/1	0.14	-	79,79,79,79	0
59	MG	AA	1730	1/1	0.54	-	60,60,60,60	0
59	MG	DA	3254	1/1	0.20	-	54,54,54,54	0
59	MG	BA	3303	1/1	0.84	-	91,91,91,91	0
59	MG	DA	3172	1/1	0.32	-	55,55,55,55	0
59	MG	BA	3038	1/1	0.23	-	20,20,20,20	0
59	MG	AA	1659	1/1	0.20	-	73,73,73,73	0
59	MG	CA	1621	1/1	0.38	-	42,42,42,42	0
59	MG	BA	3027	1/1	0.22	-	35,35,35,35	0
59	MG	DA	3146	1/1	0.20	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1608	1/1	0.61	-	57,57,57,57	0
59	MG	DA	3039	1/1	0.32	-	58,58,58,58	0
59	MG	BA	3062	1/1	0.12	-	14,14,14,14	0
59	MG	BA	3385	1/1	0.07	-	32,32,32,32	0
59	MG	BA	3332	1/1	0.42	-	105,105,105,105	0
59	MG	DA	3044	1/1	0.10	-	22,22,22,22	0
59	MG	DA	3117	1/1	0.10	-	32,32,32,32	0
59	MG	BA	3002	1/1	0.15	-	59,59,59,59	0
59	MG	BA	3283	1/1	0.25	-	46,46,46,46	0
59	MG	BA	3226	1/1	0.10	-	33,33,33,33	0
59	MG	DA	3085	1/1	0.19	-	22,22,22,22	0
59	MG	DA	3177	1/1	0.41	-	29,29,29,29	0
59	MG	AA	1650	1/1	0.19	-	26,26,26,26	0
59	MG	DA	3143	1/1	0.25	-	30,30,30,30	0
59	MG	DA	3259	1/1	0.32	-	43,43,43,43	0
59	MG	AA	1662	1/1	0.19	-	23,23,23,23	0
59	MG	BA	3185	1/1	0.29	-	62,62,62,62	0
59	MG	DA	3084	1/1	0.15	-	48,48,48,48	0
59	MG	DA	3272	1/1	0.45	-	60,60,60,60	0
59	MG	DA	3202	1/1	0.08	-	34,34,34,34	0
59	MG	CA	1649	1/1	0.10	-	48,48,48,48	0
59	MG	DA	3002	1/1	0.24	-	31,31,31,31	0
59	MG	AA	1723	1/1	0.18	-	36,36,36,36	0
59	MG	DA	3122	1/1	0.22	-	31,31,31,31	0
59	MG	BA	3210	1/1	0.24	-	57,57,57,57	0
59	MG	DA	3120	1/1	0.20	-	55,55,55,55	0
59	MG	BA	3351	1/1	0.30	-	60,60,60,60	0
59	MG	DA	3061	1/1	0.30	-	28,28,28,28	0
59	MG	BA	3300	1/1	0.11	-	40,40,40,40	0
59	MG	DA	3267	1/1	0.27	-	53,53,53,53	0
59	MG	CA	1629	1/1	0.27	-	52,52,52,52	0
59	MG	BQ	201	1/1	0.14	-	48,48,48,48	0
59	MG	BA	3280	1/1	0.38	-	54,54,54,54	0
59	MG	CA	1690	1/1	0.18	-	46,46,46,46	0
59	MG	BU	201	1/1	0.28	-	22,22,22,22	0
59	MG	BA	3287	1/1	0.42	-	56,56,56,56	0
59	MG	DA	3138	1/1	0.11	-	19,19,19,19	0
59	MG	BA	3239	1/1	0.15	-	25,25,25,25	0
59	MG	BA	3391	1/1	0.14	-	31,31,31,31	0
59	MG	CA	1643	1/1	0.63	-	51,51,51,51	0
59	MG	BA	3136	1/1	0.06	-	30,30,30,30	0
59	MG	DA	3246	1/1	0.13	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DD	301	1/1	0.52	-	110,110,110,110	0
59	MG	BA	3123	1/1	0.19	-	45,45,45,45	0
59	MG	DA	3009	1/1	0.14	-	20,20,20,20	0
59	MG	DA	3059	1/1	0.03	-	28,28,28,28	0
59	MG	BA	3036	1/1	0.29	-	20,20,20,20	0
59	MG	CA	1641	1/1	0.14	-	28,28,28,28	0
59	MG	BA	3362	1/1	0.35	-	51,51,51,51	0
59	MG	CA	1679	1/1	0.17	-	46,46,46,46	0
59	MG	AX	102	1/1	0.10	-	51,51,51,51	0
59	MG	BA	3076	1/1	0.38	-	34,34,34,34	0
59	MG	BA	3008	1/1	0.19	-	13,13,13,13	0
59	MG	CA	1624	1/1	0.14	-	24,24,24,24	0
59	MG	BA	3257	1/1	0.18	-	21,21,21,21	0
59	MG	BX	101	1/1	0.48	-	53,53,53,53	0
59	MG	DA	3047	1/1	0.14	-	25,25,25,25	0
59	MG	DA	3168	1/1	0.25	-	43,43,43,43	0
59	MG	CA	1688	1/1	0.18	-	59,59,59,59	0
59	MG	DA	3248	1/1	0.47	-	60,60,60,60	0
59	MG	BA	3364	1/1	0.12	-	8,8,8,8	0
59	MG	BA	3301	1/1	0.10	-	21,21,21,21	0
59	MG	BA	3016	1/1	0.41	-	27,27,27,27	0
59	MG	AA	1623	1/1	0.18	-	27,27,27,27	0
59	MG	BA	3161	1/1	0.42	-	16,16,16,16	0
59	MG	AA	1637	1/1	0.15	-	40,40,40,40	0
59	MG	DA	3014	1/1	0.19	-	79,79,79,79	0
59	MG	DA	3180	1/1	0.47	-	27,27,27,27	0
59	MG	BA	3334	1/1	0.14	-	32,32,32,32	0
59	MG	BA	3052	1/1	0.43	-	37,37,37,37	0
59	MG	BA	3240	1/1	0.14	-	60,60,60,60	0
59	MG	BA	3061	1/1	0.29	-	21,21,21,21	0
59	MG	AA	1605	1/1	0.19	-	54,54,54,54	0
59	MG	DA	3013	1/1	0.39	-	32,32,32,32	0
59	MG	AA	1606	1/1	0.13	-	63,63,63,63	0
59	MG	AA	1712	1/1	0.40	-	53,53,53,53	0
59	MG	DA	3176	1/1	0.13	-	51,51,51,51	0
59	MG	BA	3153	1/1	0.14	-	37,37,37,37	0
59	MG	AA	1686	1/1	0.13	-	58,58,58,58	0
59	MG	BA	3390	1/1	0.15	-	53,53,53,53	0
59	MG	CA	1661	1/1	0.46	-	42,42,42,42	0
59	MG	DA	3016	1/1	0.11	-	54,54,54,54	0
59	MG	DA	3154	1/1	0.06	-	64,64,64,64	0
59	MG	BA	3222	1/1	0.17	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3236	1/1	0.18	-	23,23,23,23	0
59	MG	CA	1632	1/1	0.31	-	47,47,47,47	0
59	MG	BA	3225	1/1	0.18	-	43,43,43,43	0
59	MG	AA	1682	1/1	0.11	-	53,53,53,53	0
59	MG	AH	201	1/1	0.25	-	31,31,31,31	0
59	MG	DA	3234	1/1	0.39	-	84,84,84,84	0
59	MG	DA	3188	1/1	0.23	-	40,40,40,40	0
59	MG	DA	3095	1/1	1.08	-	64,64,64,64	0
59	MG	BA	3092	1/1	0.07	-	20,20,20,20	0
59	MG	DA	3004	1/1	0.22	-	54,54,54,54	0
59	MG	BA	3157	1/1	0.10	-	42,42,42,42	0
59	MG	DA	3068	1/1	0.27	-	60,60,60,60	0
59	MG	BA	3137	1/1	0.20	-	34,34,34,34	0
59	MG	BA	3183	1/1	0.21	-	37,37,37,37	0
59	MG	DA	3152	1/1	0.38	-	54,54,54,54	0
59	MG	BA	3207	1/1	0.17	-	24,24,24,24	0
59	MG	AA	1711	1/1	0.22	-	68,68,68,68	0
59	MG	DR	201	1/1	0.28	-	65,65,65,65	0
59	MG	BA	3320	1/1	1.54	-	89,89,89,89	0
59	MG	BA	3262	1/1	0.20	-	27,27,27,27	0
59	MG	BA	3039	1/1	0.23	-	18,18,18,18	0
59	MG	BA	3026	1/1	0.29	-	29,29,29,29	0
59	MG	DA	3036	1/1	0.33	-	31,31,31,31	0
59	MG	DA	3049	1/1	0.15	-	41,41,41,41	0
59	MG	BA	3102	1/1	0.26	-	49,49,49,49	0
59	MG	BA	3130	1/1	0.08	-	13,13,13,13	0
59	MG	DA	3189	1/1	1.08	-	92,92,92,92	0
59	MG	BA	3286	1/1	0.17	-	26,26,26,26	0
59	MG	BA	3058	1/1	0.18	-	20,20,20,20	0
59	MG	CA	1642	1/1	0.24	-	29,29,29,29	0
59	MG	DA	3113	1/1	0.25	-	49,49,49,49	0
59	MG	BA	3057	1/1	0.12	-	23,23,23,23	0
59	MG	BA	3104	1/1	0.37	-	52,52,52,52	0
59	MG	AA	1641	1/1	0.18	-	62,62,62,62	0
59	MG	BA	3373	1/1	0.36	-	55,55,55,55	0
59	MG	AA	1609	1/1	0.09	-	23,23,23,23	0
59	MG	AA	1694	1/1	0.24	-	24,24,24,24	0
59	MG	AA	1619	1/1	0.58	-	47,47,47,47	0
59	MG	BA	3277	1/1	0.34	-	60,60,60,60	0
59	MG	BA	3272	1/1	0.27	-	30,30,30,30	0
59	MG	DA	3079	1/1	0.25	-	16,16,16,16	0
59	MG	BA	3306	1/1	0.14	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3118	1/1	0.21	-	18,18,18,18	0
59	MG	BA	3309	1/1	0.04	-	41,41,41,41	0
59	MG	BA	3139	1/1	0.12	-	15,15,15,15	0
59	MG	BA	3094	1/1	0.13	-	12,12,12,12	0
59	MG	BA	3189	1/1	0.27	-	18,18,18,18	0
59	MG	BA	3258	1/1	0.13	-	26,26,26,26	0
59	MG	BA	3392	1/1	0.28	-	63,63,63,63	0
59	MG	AA	1617	1/1	0.09	-	48,48,48,48	0
59	MG	DA	3035	1/1	0.58	-	63,63,63,63	0
59	MG	DA	3275	1/1	0.25	-	54,54,54,54	0
59	MG	BA	3064	1/1	0.26	-	32,32,32,32	0
59	MG	BA	3376	1/1	0.89	-	66,66,66,66	0
59	MG	AA	1687	1/1	0.05	-	27,27,27,27	0
59	MG	BA	3031	1/1	0.19	-	12,12,12,12	0
59	MG	DA	3238	1/1	0.53	-	101,101,101,101	0
59	MG	BA	3340	1/1	0.16	-	42,42,42,42	0
59	MG	DA	3119	1/1	0.61	-	62,62,62,62	0
59	MG	BA	3089	1/1	0.14	-	55,55,55,55	0
59	MG	BA	3371	1/1	0.30	-	57,57,57,57	0
59	MG	DA	3160	1/1	0.31	-	28,28,28,28	0
59	MG	AA	1651	1/1	0.27	-	37,37,37,37	0
59	MG	BA	3321	1/1	0.21	-	51,51,51,51	0
59	MG	CA	1637	1/1	0.06	-	29,29,29,29	0
59	MG	BA	3331	1/1	0.11	-	52,52,52,52	0
59	MG	AA	1668	1/1	0.20	-	194,194,194,194	0
59	MG	BA	3333	1/1	0.63	-	55,55,55,55	0
59	MG	DA	3274	1/1	0.18	-	62,62,62,62	0
59	MG	BA	3018	1/1	0.24	-	23,23,23,23	0
59	MG	AA	1717	1/1	0.16	-	50,50,50,50	0
59	MG	AA	1624	1/1	0.20	-	54,54,54,54	0
59	MG	BA	3400	1/1	0.21	-	39,39,39,39	0
59	MG	BA	3074	1/1	0.14	-	12,12,12,12	0
59	MG	AK	201	1/1	0.27	-	66,66,66,66	0
59	MG	BA	3326	1/1	0.11	-	35,35,35,35	0
59	MG	DA	3134	1/1	0.23	-	42,42,42,42	0
59	MG	AA	1632	1/1	0.35	-	53,53,53,53	0
59	MG	BA	3098	1/1	0.25	-	18,18,18,18	0
59	MG	AA	1709	1/1	0.07	-	44,44,44,44	0
59	MG	CA	1692	1/1	0.34	-	73,73,73,73	0
59	MG	BA	3389	1/1	0.20	-	44,44,44,44	0
59	MG	DA	3090	1/1	0.13	-	24,24,24,24	0
59	MG	AA	1665	1/1	0.28	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3305	1/1	0.22	-	32,32,32,32	0
59	MG	DA	3110	1/1	0.12	-	38,38,38,38	0
59	MG	DA	3237	1/1	0.10	-	39,39,39,39	0
59	MG	DA	3063	1/1	0.14	-	53,53,53,53	0
59	MG	BA	3256	1/1	0.15	-	56,56,56,56	0
59	MG	BA	3264	1/1	0.25	-	34,34,34,34	0
59	MG	DA	3217	1/1	0.39	-	85,85,85,85	0
59	MG	BA	3081	1/1	0.31	-	6,6,6,6	0
59	MG	DA	3107	1/1	0.10	-	32,32,32,32	0
59	MG	BA	3164	1/1	0.49	-	37,37,37,37	0
59	MG	DA	3055	1/1	0.35	-	42,42,42,42	0
59	MG	BA	3229	1/1	0.35	-	37,37,37,37	0
59	MG	BA	3091	1/1	0.34	-	34,34,34,34	0
59	MG	DA	3216	1/1	0.26	-	35,35,35,35	0
59	MG	BA	3122	1/1	0.24	-	38,38,38,38	0
59	MG	DA	3187	1/1	0.47	-	51,51,51,51	0
59	MG	BA	3113	1/1	0.35	-	34,34,34,34	0
59	MG	AA	1700	1/1	0.29	-	58,58,58,58	0
59	MG	CX	103	1/1	0.21	-	50,50,50,50	0
59	MG	DA	3093	1/1	0.29	-	40,40,40,40	0
59	MG	BA	3298	1/1	1.48	-	178,178,178,178	0
59	MG	BA	3142	1/1	0.19	-	18,18,18,18	0
59	MG	BA	3352	1/1	0.41	-	51,51,51,51	0
59	MG	DA	3062	1/1	0.16	-	24,24,24,24	0
59	MG	CA	1650	1/1	0.38	-	69,69,69,69	0
59	MG	AA	1647	1/1	0.28	-	80,80,80,80	0
59	MG	BA	3006	1/1	0.30	-	16,16,16,16	0
59	MG	BA	3237	1/1	0.47	-	32,32,32,32	0
59	MG	AA	1640	1/1	0.35	-	37,37,37,37	0
59	MG	DA	3017	1/1	0.24	-	16,16,16,16	0
59	MG	BA	3116	1/1	0.21	-	54,54,54,54	0
59	MG	CA	1628	1/1	0.09	-	27,27,27,27	0
59	MG	AA	1669	1/1	0.14	-	36,36,36,36	0
59	MG	BA	3029	1/1	0.12	-	23,23,23,23	0
59	MG	BA	3082	1/1	0.12	-	15,15,15,15	0
59	MG	DA	3153	1/1	0.20	-	28,28,28,28	0
59	MG	DA	3195	1/1	0.25	-	38,38,38,38	0
59	MG	AA	1607	1/1	0.42	-	43,43,43,43	0
59	MG	AA	1652	1/1	0.38	-	55,55,55,55	0
59	MG	AA	1614	1/1	0.23	-	45,45,45,45	0
59	MG	AF	201	1/1	0.13	-	39,39,39,39	0
59	MG	BA	3399	1/1	0.20	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1681	1/1	0.09	-	30,30,30,30	0
59	MG	AX	106	1/1	0.15	-	43,43,43,43	0
59	MG	DA	3245	1/1	0.31	-	86,86,86,86	0
59	MG	BA	3313	1/1	0.40	-	55,55,55,55	0
59	MG	CA	1668	1/1	0.07	-	42,42,42,42	0
59	MG	BB	201	1/1	0.06	-	18,18,18,18	0
59	MG	BA	3197	1/1	0.34	-	45,45,45,45	0
59	MG	BA	3318	1/1	0.31	-	41,41,41,41	0
59	MG	CV	101	1/1	0.23	-	36,36,36,36	0
59	MG	DA	3096	1/1	0.18	-	38,38,38,38	0
59	MG	AO	101	1/1	0.11	-	62,62,62,62	0
59	MG	DA	3192	1/1	0.21	-	39,39,39,39	0
59	MG	AA	1697	1/1	0.33	-	73,73,73,73	0
59	MG	BA	3367	1/1	0.44	-	35,35,35,35	0
59	MG	DA	3221	1/1	0.35	-	59,59,59,59	0
59	MG	BA	3202	1/1	0.11	-	28,28,28,28	0
59	MG	DA	3127	1/1	0.26	-	48,48,48,48	0
59	MG	CA	1658	1/1	0.13	-	40,40,40,40	0
59	MG	AA	1622	1/1	0.24	-	44,44,44,44	0
59	MG	DA	3155	1/1	0.14	-	56,56,56,56	0
59	MG	BA	3336	1/1	0.24	-	23,23,23,23	0
59	MG	BA	3227	1/1	0.12	-	69,69,69,69	0
59	MG	AA	1722	1/1	0.13	-	35,35,35,35	0
59	MG	DA	3098	1/1	0.13	-	37,37,37,37	0
59	MG	CA	1654	1/1	0.11	-	63,63,63,63	0
59	MG	AA	1625	1/1	0.16	-	32,32,32,32	0
59	MG	BA	3155	1/1	0.07	-	9,9,9,9	0
59	MG	CA	1665	1/1	0.27	-	34,34,34,34	0
59	MG	BA	3103	1/1	0.58	-	65,65,65,65	0
59	MG	AA	1691	1/1	0.44	-	56,56,56,56	0
59	MG	DA	3224	1/1	0.12	-	53,53,53,53	0
59	MG	BA	3278	1/1	0.32	-	50,50,50,50	0
59	MG	BA	3216	1/1	0.37	-	42,42,42,42	0
59	MG	DA	3109	1/1	0.58	-	65,65,65,65	0
59	MG	BA	3247	1/1	0.08	-	29,29,29,29	0
59	MG	DE	302	1/1	0.62	-	65,65,65,65	0
59	MG	AA	1645	1/1	0.32	-	64,64,64,64	0
59	MG	BA	3097	1/1	0.11	-	21,21,21,21	0
59	MG	AA	1693	1/1	0.13	-	41,41,41,41	0
59	MG	BA	3327	1/1	0.35	-	44,44,44,44	0
59	MG	BA	3337	1/1	0.28	-	61,61,61,61	0
59	MG	DA	3054	1/1	0.10	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1616	1/1	0.25	-	46,46,46,46	0
59	MG	DA	3149	1/1	0.28	-	42,42,42,42	0
59	MG	AY	101	1/1	0.19	-	71,71,71,71	0
59	MG	DA	3006	1/1	0.25	-	20,20,20,20	0
59	MG	DA	3186	1/1	0.16	-	41,41,41,41	0
59	MG	BA	3271	1/1	0.30	-	64,64,64,64	0
59	MG	BA	3242	1/1	0.50	-	44,44,44,44	0
59	MG	DA	3094	1/1	0.26	-	27,27,27,27	0
59	MG	BA	3158	1/1	0.10	-	40,40,40,40	0
59	MG	BA	3212	1/1	0.18	-	25,25,25,25	0
59	MG	CA	1645	1/1	0.05	-	27,27,27,27	0
59	MG	BA	3338	1/1	0.08	-	60,60,60,60	0
59	MG	BA	3171	1/1	0.33	-	51,51,51,51	0
59	MG	BA	3032	1/1	0.13	-	21,21,21,21	0
59	MG	CA	1683	1/1	0.52	-	55,55,55,55	0
59	MG	BA	3380	1/1	0.13	-	47,47,47,47	0
59	MG	DA	3019	1/1	0.17	-	13,13,13,13	0
59	MG	DD	302	1/1	0.46	-	34,34,34,34	0
59	MG	BA	3370	1/1	0.16	-	28,28,28,28	0
59	MG	BA	3173	1/1	0.14	-	17,17,17,17	0
59	MG	BA	3388	1/1	0.15	-	13,13,13,13	0
59	MG	BA	3177	1/1	0.20	-	65,65,65,65	0
59	MG	BA	3254	1/1	0.10	-	43,43,43,43	0
59	MG	DA	3089	1/1	0.30	-	26,26,26,26	0
59	MG	AA	1707	1/1	0.52	-	59,59,59,59	0
59	MG	BA	3071	1/1	0.04	-	42,42,42,42	0
59	MG	BA	3131	1/1	0.83	-	68,68,68,68	0
59	MG	DA	3024	1/1	0.12	-	29,29,29,29	0
59	MG	AA	1710	1/1	0.61	-	113,113,113,113	0
59	MG	BA	3028	1/1	0.22	-	41,41,41,41	0
59	MG	BA	3180	1/1	0.31	-	22,22,22,22	0
59	MG	DA	3231	1/1	0.19	-	43,43,43,43	0
59	MG	DA	3162	1/1	0.08	-	40,40,40,40	0
59	MG	AA	1661	1/1	0.12	-	34,34,34,34	0
59	MG	AA	1635	1/1	0.19	-	46,46,46,46	0
59	MG	BA	3288	1/1	0.15	-	33,33,33,33	0
59	MG	B0	101	1/1	0.22	-	58,58,58,58	0
59	MG	DA	3262	1/1	0.08	-	58,58,58,58	0
59	MG	BA	3361	1/1	0.11	-	25,25,25,25	0
59	MG	AA	1671	1/1	0.20	-	83,83,83,83	0
59	MG	DA	3140	1/1	0.43	-	38,38,38,38	0
59	MG	DA	3099	1/1	0.27	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3102	1/1	0.10	-	84,84,84,84	0
59	MG	CA	1672	1/1	0.28	-	45,45,45,45	0
59	MG	DA	3156	1/1	0.26	-	28,28,28,28	0
59	MG	BA	3292	1/1	0.35	-	40,40,40,40	0
59	MG	CA	1647	1/1	0.42	-	51,51,51,51	0
59	MG	DA	3078	1/1	0.20	-	58,58,58,58	0
59	MG	AA	1615	1/1	0.18	-	42,42,42,42	0
59	MG	DA	3161	1/1	0.46	-	32,32,32,32	0
59	MG	CA	1689	1/1	0.20	-	63,63,63,63	0
59	MG	CA	1604	1/1	0.10	-	21,21,21,21	0
59	MG	BA	3048	1/1	0.08	-	6,6,6,6	0
59	MG	DA	3057	1/1	0.11	-	21,21,21,21	0
59	MG	CA	1617	1/1	0.24	-	39,39,39,39	0
59	MG	DA	3240	1/1	0.20	-	49,49,49,49	0
59	MG	BA	3041	1/1	0.17	-	20,20,20,20	0
59	MG	BA	3003	1/1	0.42	-	42,42,42,42	0
60	ZN	D5	103	1/1	0.04	-	92,92,92,92	0
59	MG	DA	3005	1/1	0.28	-	50,50,50,50	0
59	MG	DA	3199	1/1	0.44	-	38,38,38,38	0
59	MG	BA	3053	1/1	0.18	-	11,11,11,11	0
59	MG	BA	3232	1/1	0.33	-	25,25,25,25	0
59	MG	CA	1638	1/1	0.19	-	46,46,46,46	0
59	MG	BA	3169	1/1	0.07	-	51,51,51,51	0
59	MG	BA	3172	1/1	0.36	-	40,40,40,40	0
59	MG	BA	3234	1/1	0.28	-	35,35,35,35	0
59	MG	BA	3112	1/1	0.15	-	52,52,52,52	0
59	MG	BA	3319	1/1	0.42	-	25,25,25,25	0
59	MG	BA	3366	1/1	0.40	-	64,64,64,64	0
59	MG	AA	1720	1/1	0.14	-	52,52,52,52	0
59	MG	BA	3014	1/1	0.22	-	63,63,63,63	0
59	MG	BA	3066	1/1	0.25	-	20,20,20,20	0
59	MG	AA	1719	1/1	0.24	-	58,58,58,58	0
59	MG	CA	1676	1/1	0.15	-	55,55,55,55	0
59	MG	CA	1619	1/1	0.47	-	80,80,80,80	0
59	MG	BA	3322	1/1	0.68	-	147,147,147,147	0
59	MG	BA	3054	1/1	0.14	-	22,22,22,22	0
59	MG	DA	3042	1/1	0.25	-	41,41,41,41	0
59	MG	AK	202	1/1	0.27	-	90,90,90,90	0
59	MG	DA	3210	1/1	0.46	-	57,57,57,57	0
59	MG	AA	1601	1/1	0.07	-	38,38,38,38	0
59	MG	DA	3091	1/1	0.17	-	67,67,67,67	0
59	MG	DA	3181	1/1	0.26	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3211	1/1	1.05	-	78,78,78,78	0
59	MG	AA	1642	1/1	0.27	-	55,55,55,55	0
59	MG	BA	3354	1/1	0.10	-	41,41,41,41	0
59	MG	DA	3124	1/1	0.05	-	43,43,43,43	0
59	MG	DA	3040	1/1	0.07	-	34,34,34,34	0
59	MG	AA	1633	1/1	0.09	-	37,37,37,37	0
59	MG	DA	3053	1/1	0.14	-	47,47,47,47	0
59	MG	AA	1660	1/1	0.41	-	40,40,40,40	0
59	MG	BA	3084	1/1	0.27	-	19,19,19,19	0
59	MG	BA	3121	1/1	0.10	-	38,38,38,38	0
59	MG	BA	3358	1/1	0.08	-	49,49,49,49	0
59	MG	DA	3251	1/1	0.16	-	44,44,44,44	0
59	MG	CQ	201	1/1	0.10	-	94,94,94,94	0
59	MG	BA	3350	1/1	0.11	-	20,20,20,20	0
59	MG	BA	3140	1/1	0.05	-	30,30,30,30	0
59	MG	BA	3381	1/1	0.17	-	43,43,43,43	0
59	MG	BA	3196	1/1	0.32	-	49,49,49,49	0
59	MG	BA	3344	1/1	0.08	-	37,37,37,37	0
59	MG	AA	1667	1/1	0.35	-	59,59,59,59	0
59	MG	DA	3170	1/1	0.12	-	52,52,52,52	0
59	MG	BA	3325	1/1	0.19	-	61,61,61,61	0
59	MG	DA	3190	1/1	0.13	-	33,33,33,33	0
59	MG	DA	3213	1/1	0.57	-	62,62,62,62	0
59	MG	DA	3026	1/1	0.13	-	36,36,36,36	0
59	MG	BA	3387	1/1	0.15	-	46,46,46,46	0
59	MG	DE	303	1/1	0.10	-	32,32,32,32	0
59	MG	DA	3129	1/1	0.40	-	35,35,35,35	0
59	MG	BA	3342	1/1	0.19	-	21,21,21,21	0
59	MG	DA	3065	1/1	0.27	-	51,51,51,51	0
59	MG	DA	3037	1/1	0.22	-	26,26,26,26	0
59	MG	DA	3032	1/1	0.08	-	9,9,9,9	0
59	MG	BA	3349	1/1	0.19	-	53,53,53,53	0
59	MG	CA	1639	1/1	0.33	-	74,74,74,74	0
59	MG	DA	3121	1/1	0.15	-	37,37,37,37	0
59	MG	CA	1660	1/1	0.11	-	45,45,45,45	0
59	MG	DA	3100	1/1	0.47	-	57,57,57,57	0
59	MG	DA	3012	1/1	0.20	-	33,33,33,33	0
59	MG	DA	3029	1/1	0.31	-	34,34,34,34	0
59	MG	DA	3048	1/1	0.20	-	48,48,48,48	0
59	MG	BA	3163	1/1	0.09	-	22,22,22,22	0
59	MG	DA	3159	1/1	0.10	-	16,16,16,16	0
59	MG	AX	107	1/1	0.50	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1620	1/1	0.39	-	40,40,40,40	0
59	MG	BA	3143	1/1	0.24	-	37,37,37,37	0
59	MG	DA	3051	1/1	0.46	-	51,51,51,51	0
59	MG	AA	1705	1/1	0.12	-	47,47,47,47	0
59	MG	CA	1675	1/1	0.53	-	150,150,150,150	0
59	MG	DA	3060	1/1	0.10	-	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.