



wwPDB X-ray Structure Validation Summary Report ⓘ

May 19, 2020 – 07:47 am BST

PDB ID : 4V8H
Title : Crystal structure of HPF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

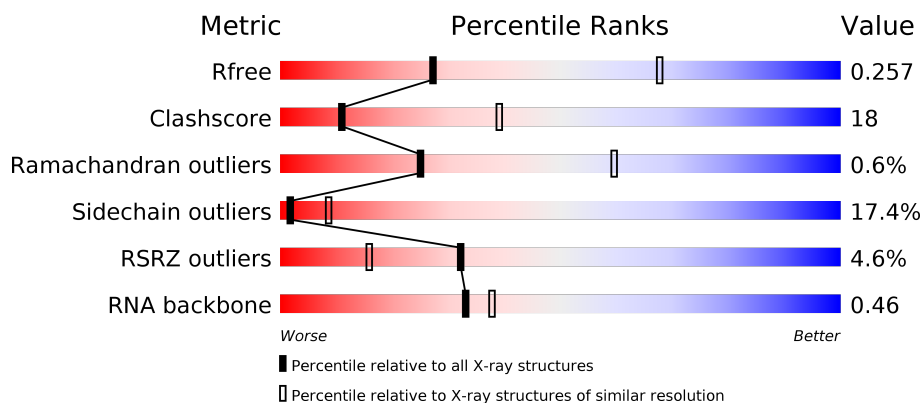
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
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	

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Mol	Chain	Length	Quality of chain
15	CO	89	% 51% 39% 8% ..
16	AP	88	9% 43% 41% 9% 7%
16	CP	88	5% 39% 43% 11% 7%
17	AQ	105	% 44% 44% 7% 6%
17	CQ	105	% 43% 45% 7% 6%
18	AR	88	2% 52% 22% .. 23%
18	CR	88	% 53% 20% . 23%
19	AS	93	40% 48% 20% 17% . 13%
19	CS	93	47% 45% 34% 8% 13%
20	AT	106	41% 36% 6% 18%
20	CT	106	42% 42% 6% . 8%
21	AU	27	52% 22% 48% 15% 15%
21	CU	27	67% 19% 44% 22% 15%
22	AX	101	4% 62% 23% 9% 6%
22	CX	101	17% 66% 24% . 6%
23	BA	2913	2% 28% 41% 21% 6% .
23	DA	2913	3% 31% 40% 20% 5% .
24	BB	122	28% 39% 27% . .
24	DB	122	% 28% 51% 15% 5% .
25	BD	276	63% 33% .
25	DD	276	61% 34% . .
26	BE	206	61% 31% 7% ..
26	DE	206	59% 32% 6% ..
27	BF	210	60% 29% 7% .
27	DF	210	55% 33% 8% .


























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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	



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Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	D9	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1614	-	-	-	X
54	MG	AA	1618	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1678	-	-	-	X
54	MG	AA	1692	-	-	-	X
54	MG	BA	3014	-	-	-	X
54	MG	BA	3097	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3146	-	-	-	X
54	MG	CA	1604	-	-	-	X
54	MG	CA	1633	-	-	-	X
54	MG	CA	1637	-	-	-	X
54	MG	CA	1652	-	-	-	X
54	MG	CA	1657	-	-	-	X
54	MG	CA	1660	-	-	-	X
54	MG	CA	1670	-	-	-	X
54	MG	CA	1692	-	-	-	X
54	MG	CE	201	-	-	-	X
54	MG	DA	3058	-	-	-	X
54	MG	DA	3081	-	-	-	X
54	MG	DA	3096	-	-	-	X
54	MG	DA	3115	-	-	-	X
54	MG	DA	3165	-	-	-	X
54	MG	DA	3239	-	-	-	X
54	MG	DA	3280	-	-	-	X
54	MG	DA	3290	-	-	-	X
54	MG	DB	204	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			
1	CA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	230	Total	C	N	O	S	0	0	0
			1787	1141	319	322	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	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
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	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
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	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
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			663	410	132	121	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			828	516	155	154	3	0	0
11	CK	114	Total	C	N	O	S		
			828	516	155	154	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			905	567	178	159	1	0	0
12	CL	122	Total	C	N	O	S		
			905	567	178	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S		
			804	497	164	142	1	0	0
13	CM	114	Total	C	N	O	S		
			804	497	164	142	1	0	0

- 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		
			478	303	99	72	4	0	0
14	CN	60	Total	C	N	O	S		
			478	303	99	72	4	0	0

- 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		
			724	453	143	126	2	0	0
15	CO	88	Total	C	N	O	S		
			724	453	143	126	2	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	87	Total	C	N	O	S	0	0	0
			665	410	142	111	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a protein called Probable sigma(54) modulation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AX	95	Total	C	N	O	S	0	0	0
			631	396	116	118	1			
22	CX	95	Total	C	N	O	S	0	0	0
			601	378	108	114	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	96	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	97	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	98	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	99	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	100	HIS	-	EXPRESSION TAG	UNP P0AFX0
AX	101	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	96	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	97	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	98	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	99	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	100	HIS	-	EXPRESSION TAG	UNP P0AFX0
CX	101	HIS	-	EXPRESSION TAG	UNP P0AFX0

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2837	Total	C	N	O	P	0	0	0
			61112	27197	11440	19639	2836			
23	DA	2814	Total	C	N	O	P	0	0	0
			60621	26978	11351	19479	2813			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	?	-	U	DELETION	GB AP008226.1
BA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

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Chain	Residue	Modelled	Actual	Comment	Reference
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
24	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	275	Total	C	N	O	S	0	0	0
			2135	1349	422	361	3			
25	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
26	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
28	DG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
29	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1037	666	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			953	608	168	176	1			

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
31	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
32	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
33	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
35	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			
36	DS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
38	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
40	DW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	201	Total	C	N	O	S	0	0	0
			1536	980	272	282	2			
43	DZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
45	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
46	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 50 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
51	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	660	Total	Mg	0	0
			660	660		
54	CA	162	Total	Mg	0	0
			162	162		
54	DQ	2	Total	Mg	0	0
			2	2		
54	DF	1	Total	Mg	0	0
			1	1		
54	B8	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BE	5	Total 5	Mg 5	0	0
54	B1	1	Total 1	Mg 1	0	0
54	BP	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	23	Total 23	Mg 23	0	0
54	BT	2	Total 2	Mg 2	0	0
54	D8	2	Total 2	Mg 2	0	0
54	B9	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	3	Total 3	Mg 3	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	135	Total 135	Mg 135	0	0
54	BQ	4	Total 4	Mg 4	0	0
54	CQ	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DD	2	Total 2	Mg 2	0	0
54	D0	2	Total 2	Mg 2	0	0
54	BG	1	Total 1	Mg 1	0	0
54	B3	1	Total 1	Mg 1	0	0
54	BR	1	Total 1	Mg 1	0	0
54	DA	598	Total 598	Mg 598	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DP	1	Total 1	Mg 1	0	0
54	BV	1	Total 1	Mg 1	0	0
54	DO	2	Total 2	Mg 2	0	0
54	DE	4	Total 4	Mg 4	0	0
54	AQ	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	1	Total 1	Mg 1	0	0
54	BS	1	Total 1	Mg 1	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	3	Total 3	Mg 3	0	0
54	B0	3	Total 3	Mg 3	0	0
54	CE	1	Total 1	Mg 1	0	0
54	BW	2	Total 2	Mg 2	0	0
54	AF	1	Total 1	Mg 1	0	0
54	DB	8	Total 8	Mg 8	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B5	1	Total 1	Zn 1	0	0
55	B4	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CD	1	Total 1	Zn 1	0	0
55	B9	1	Total 1	Zn 1	0	0
55	BY	1	Total 1	Zn 1	0	0
55	DY	1	Total 1	Zn 1	0	0
55	D5	1	Total 1	Zn 1	0	0
55	D4	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0
55	CN	1	Total 1	Zn 1	0	0
55	D6	1	Total 1	Zn 1	0	0
55	D9	1	Total 1	Zn 1	0	0
55	B6	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	268	Total 268	O 268	0	0
56	AE	1	Total 1	O 1	0	0
56	AL	1	Total 1	O 1	0	0
56	AO	1	Total 1	O 1	0	0
56	AP	1	Total 1	O 1	0	0
56	AT	1	Total 1	O 1	0	0
56	AX	1	Total 1	O 1	0	0
56	BA	1694	Total 1694	O 1694	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	57	Total 57	O 57	0	0
56	BD	20	Total 20	O 20	0	0
56	BE	11	Total 11	O 11	0	0
56	BF	6	Total 6	O 6	0	0
56	BH	1	Total 1	O 1	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	2	Total 2	O 2	0	0
56	BP	11	Total 11	O 11	0	0
56	BQ	5	Total 5	O 5	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	3	Total 3	O 3	0	0
56	BV	3	Total 3	O 3	0	0
56	BW	3	Total 3	O 3	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	4	Total 4	O 4	0	0
56	B0	8	Total 8	O 8	0	0
56	B1	2	Total 2	O 2	0	0
56	B3	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B6	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B7	5	Total 5	O 5	0	0
56	B8	10	Total 10	O 10	0	0
56	B9	1	Total 1	O 1	0	0
56	CA	265	Total 265	O 265	0	0
56	CC	1	Total 1	O 1	0	0
56	CD	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	1	Total 1	O 1	0	0
56	CP	1	Total 1	O 1	0	0
56	CQ	1	Total 1	O 1	0	0
56	CT	1	Total 1	O 1	0	0
56	CX	1	Total 1	O 1	0	0
56	DA	1174	Total 1174	O 1174	0	0
56	DB	17	Total 17	O 17	0	0
56	DD	8	Total 8	O 8	0	0
56	DE	11	Total 11	O 11	0	0
56	DF	7	Total 7	O 7	0	0
56	DN	1	Total 1	O 1	0	0
56	DO	5	Total 5	O 5	0	0

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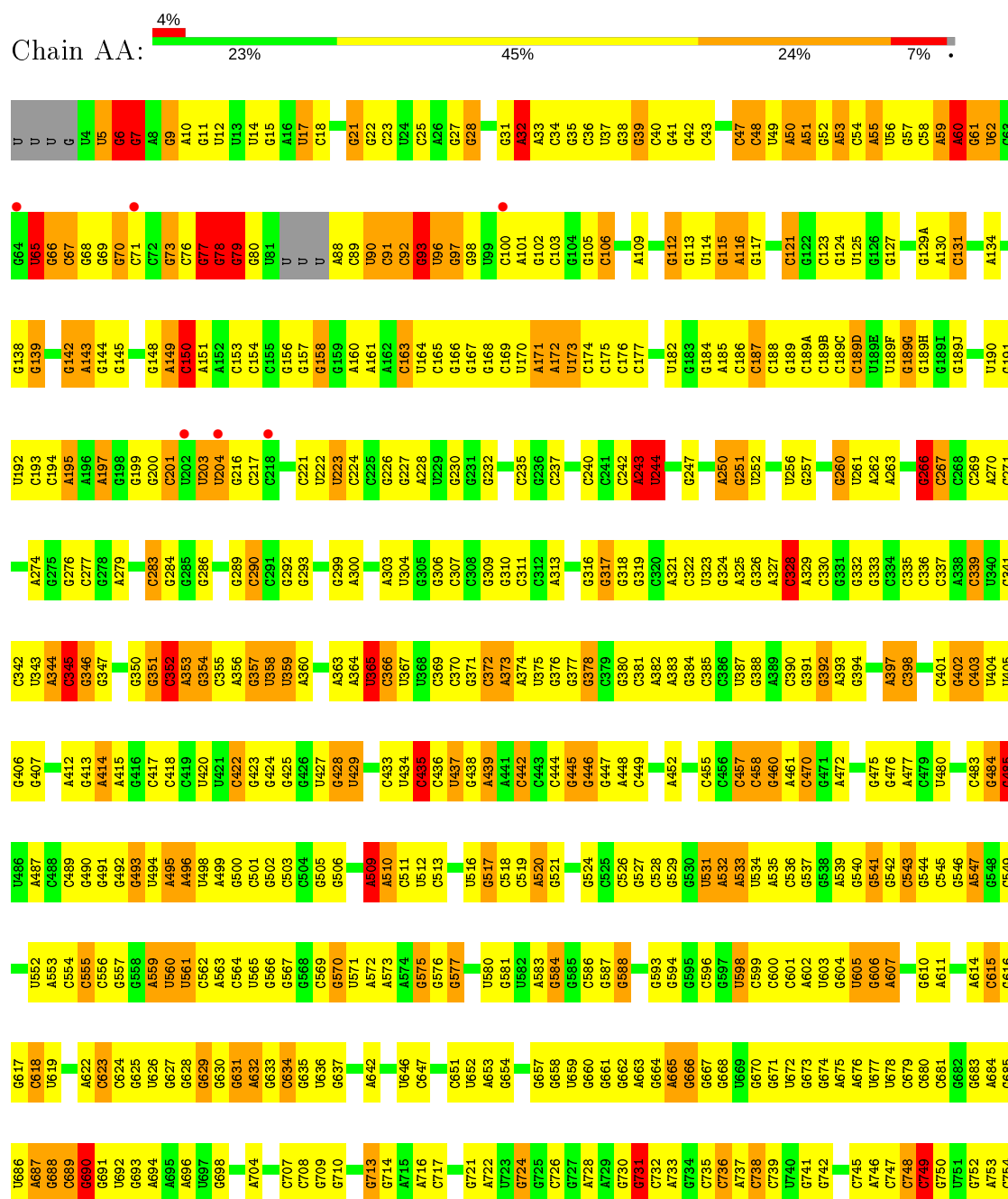
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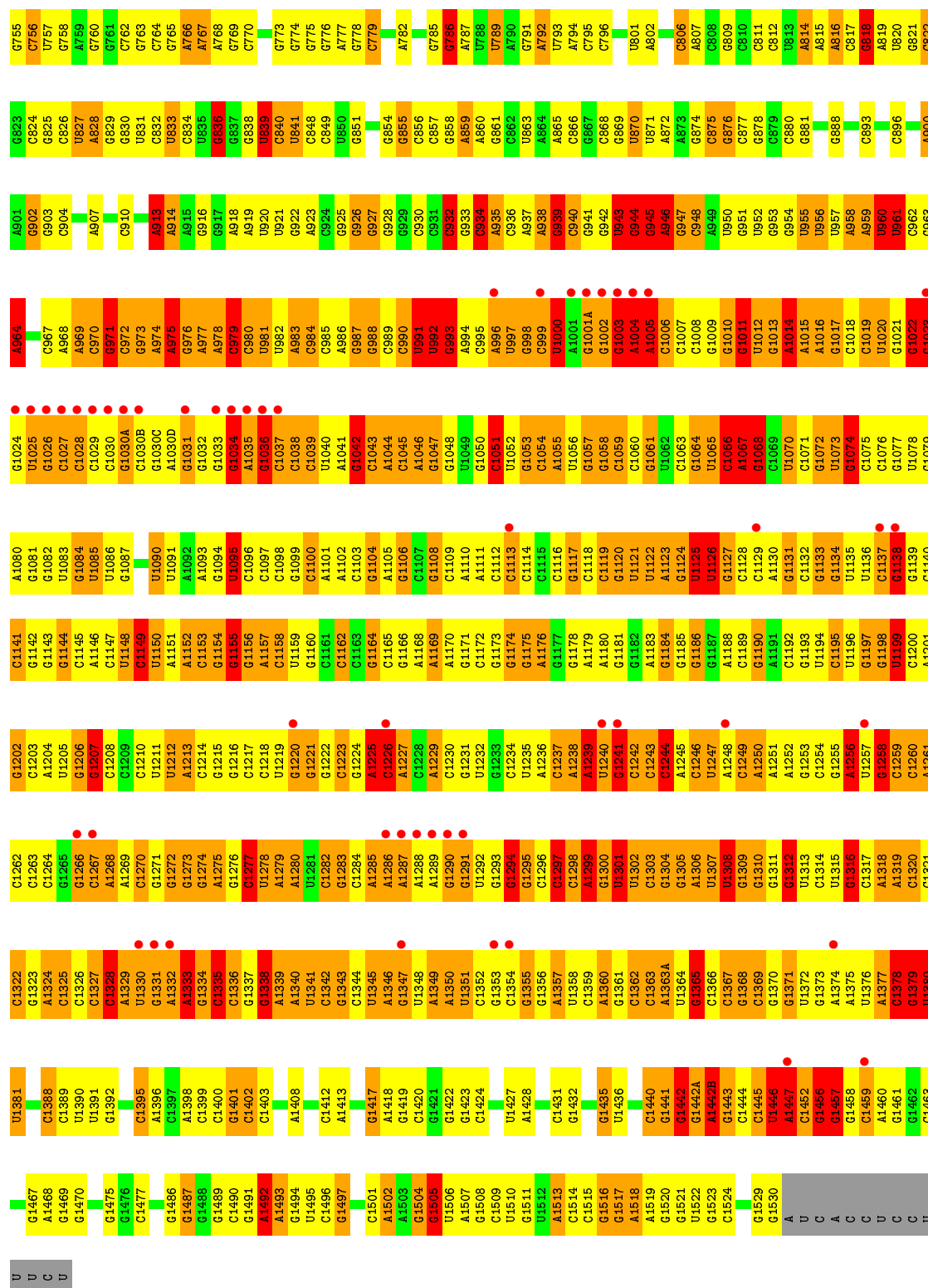
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			10	10		
56	DQ	3	Total	O	0	0
			3	3		
56	DR	2	Total	O	0	0
			2	2		
56	DT	2	Total	O	0	0
			2	2		
56	DU	5	Total	O	0	0
			5	5		
56	DV	2	Total	O	0	0
			2	2		
56	DW	2	Total	O	0	0
			2	2		
56	DX	1	Total	O	0	0
			1	1		
56	DY	2	Total	O	0	0
			2	2		
56	D0	1	Total	O	0	0
			1	1		
56	D1	5	Total	O	0	0
			5	5		
56	D3	1	Total	O	0	0
			1	1		
56	D4	1	Total	O	0	0
			1	1		
56	D7	3	Total	O	0	0
			3	3		
56	D8	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

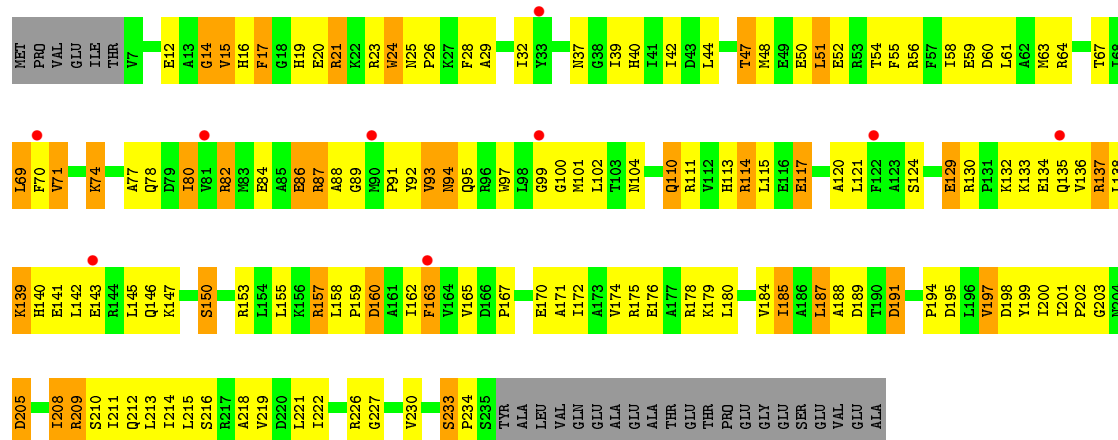
• Molecule 1: 16S Ribosomal RNA



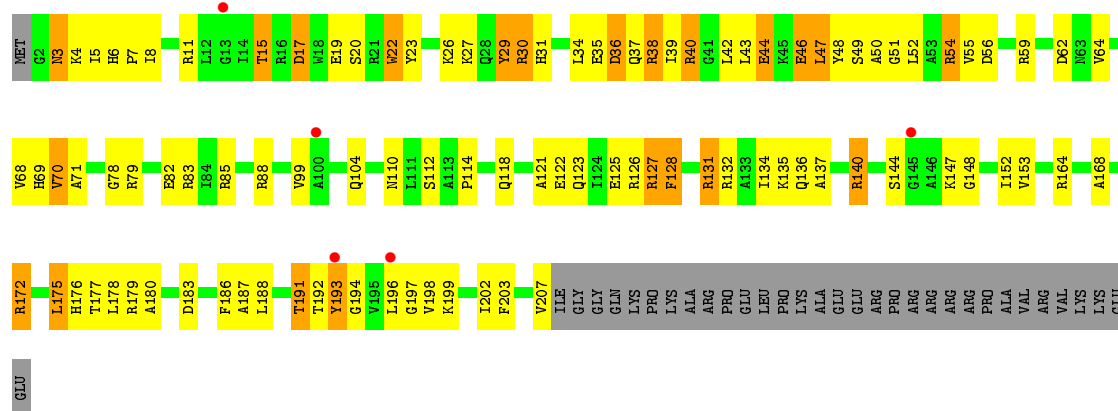


A994	C934	C956	A782	G710	U636	G594	G425	A360	C290	A197	A143	U
C995	A935	C957	C783	G713	G637	G505	G426	G361	C291	A201	G144	U
A996	C936	G958	C784	G714	G638	A509	U427	U365	G292	G202	G145	U
U997	A937	A859	G785	G715	A642	A510	U428	U366	G293	U202	G146	G
G998	A938	A860	G786	G716	A643	A511	U429	U367	U294	U203	G147	U4
C999	A939	G861	A787	G717	A644	C511	A430	U368	U295	U204	G148	U5
U1000	C940	A865	G791	G721	U646	U512	G433	U369	U296	G216	A149	G6
A1001	G941	C866	A792	G722	C647	C513	U434	C370	A297	C221	C150	G7
G1002	G942	C867	A793	U723	G650	C514	U435	G371	G298	U222	A151	A8
G1003	G943	C868	A794	G724	C651	U516	C436	G372	A300	U223	A152	G9
A1004	G944	G869	C795	G725	U652	G517	U437	A373	G309	G224	G157	A10
G1005	A945	A870	C796	C726	A653	C518	G438	A374	G310	C225	G157	G11
C1006	G947	U671	A802	A729	G657	C519	A439	U375	U304	G226	G157	U12
C1007	C948	A872	G803	G730	G658	A520	A441	G376	C307	G227	G158	G15
C1008	A949	A873	G804	G731	U659	G521	U442	G377	G308	G232	G159	A16
G1009	U950	G874	U804	G731	G660	G522	C443	G378	G309	G233	A161	U17
G1010	G951	C875	C805	G734	G661	C525	G444	C379	G310	C235	A162	U18
G1011	U952	G876	C806	C735	G662	G526	G446	G380	G316	G236	C163	G21
U1012	G953	C877	A807	C736	A663	G527	U447	C381	G317	C240	U164	G22
A1014	U955	C878	C808	G737	G664	C528	A448	A383	G318	C241	G166	C23
A1015	U956	C879	G809	A737	A665	G529	U449	G384	G319	G242	G167	A26
A1016	U957	G881	C810	C738	G666	G530	G450	C385	G320	A243	G168	G27
G1017	A958	C882	C811	C739	G667	U531	A451	C386	C321	U244	U170	G28
C1018	A959	C883	G812	U740	G668	A532	A452	U387	A322	A171	G171	G29
U1019	U960	U884	G813	G741	G669	A533	A453	G388	U323	A172	U99	A32
U1020	A961	A814	A815	G742	G671	U534	C454	A389	U324	U173	C100	A33
G1021	C962	G888	A816	C745	U672	A535	C455	C390	G325	C174	A101	C34
G1022	G963	C889	C817	A746	G673	C536	G456	G391	G326	C175	G102	G35
G1023	A964	C893	G818	C747	G674	G537	C457	G392	A327	C176	C103	C36
G1024	A965	C894	A819	C748	A675	G538	C458	A393	G328	C177	G104	U37
U1025	G966	C896	U820	C749	A676	A539	G460	U397	C329	U182	G105	G38
G1026	C967	A900	G821	U750	U677	G540	A461	A397	G330	G183	G106	G39
C1027	A968	A901	C822	U751	U678	G541	C470	C398	G331	G184	A109	G40
C1028	A969	G902	G823	G752	C679	G542	G471	C401	G332	A185	G113	G41
G1029	C970	G903	C826	G753	C681	G543	A472	G402	G333	C186	G114	G42
C1030	G971	G904	U827	G754	G682	C544	G475	C403	C334	C187	G115	U45
G1030A	C972	A909	A828	C755	G683	G545	G476	U404	C335	C188	A116	G46
C1030B	G973	C910	G829	U756	A684	A547	G486	U405	C336	G189	G117	C47
A1030C	A974	G830	G830	G757	G685	G548	U487	G406	C337	C189A	G120	U49
A1030D	A975	G831	U831	G758	U686	C549	U488	G407	C342	C189B	A120	A50
G1031	G976	A913	C832	A759	G687	G550	U489	A408	U343	C189C	C121	A51
G1032	A977	A914	C833	G760	A688	U551	U490	G409	C344	U189F	G122	G52
G1033	A978	A918	U833	G763	C689	C552	C489	A412	C345	G189G	C123	G53
G1034	C979	C834	U834	C764	A690	A553	G490	A413	G346	G189H	G124	A53
A1035	C980	U835	G835	G765	C691	C554	G491	G413	G347	G189I	U125	C54
G1036	U920	U920	G836	G766	U692	C555	G492	A414	G347	G189J	G126	A55
G1037	U982	U921	G837	A766	G693	C556	G493	A415	G350	U189K	G127	U56
C1038	A983	G922	G838	A767	A694	G557	U494	G416	C351	G189L	G128	G57
C1039	C984	U839	U839	A768	C695	G558	U495	C417	C352	U190	G129A	C58
U1040	C985	G925	C840	C770	U697	A559	A496	C418	A353	G191	A130	A59
A1041	A986	G926	U841	C770	A705	U560	U498	C419	G354	U192	G131	A60
G1042	G987	G927	C848	C771	A706	U561	U499	U420	C355	C193	C132	G61
C1043	G988	G928	C849	G774	U705	C562	G500	U421	A356	C194	U133	U62
G1044	C989	G929	U850	G775	A706	A563	G501	C422	G357	A195	G142	G64
C1045	C990	C930	G851	G776	A707	A564	C502	G423	U358	A196		
A1046	U991	C931	G854	G777	C707	U565	G502	G424	U359			
G1047	U992	C932	G854	A777	G708	U566	C503					
G1048	G993	G933	G855	G709	G709	G566						

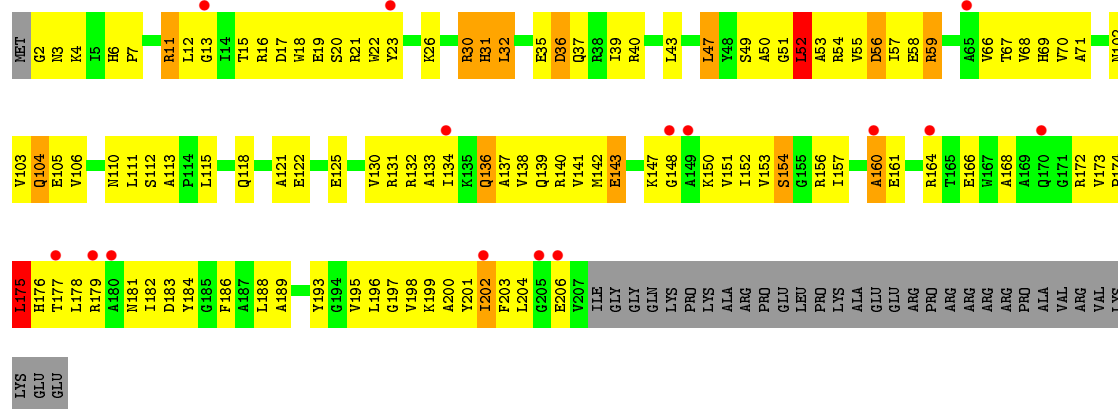




• Molecule 3: 30S Ribosomal Protein S3

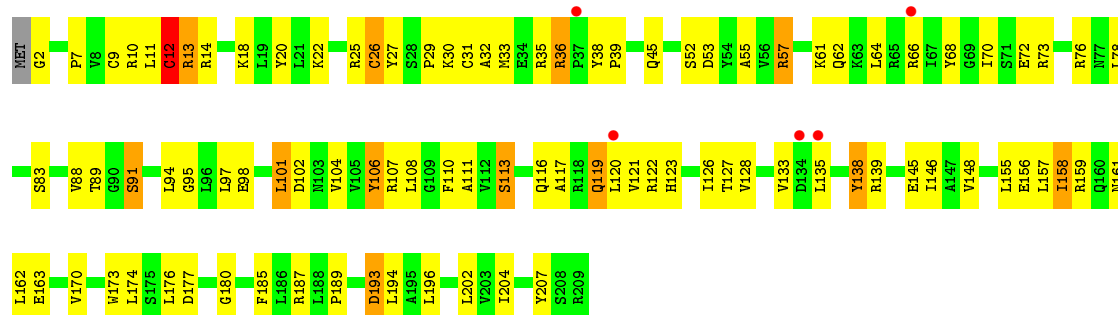


• Molecule 3: 30S Ribosomal Protein S3

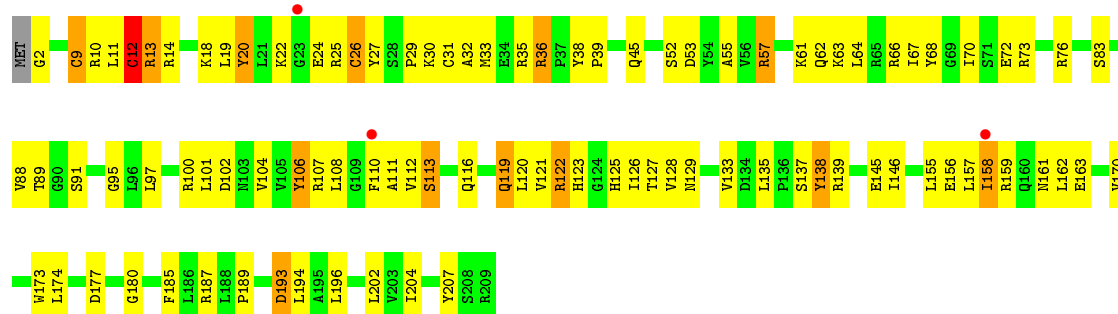


• Molecule 4: 30S Ribosomal Protein S4

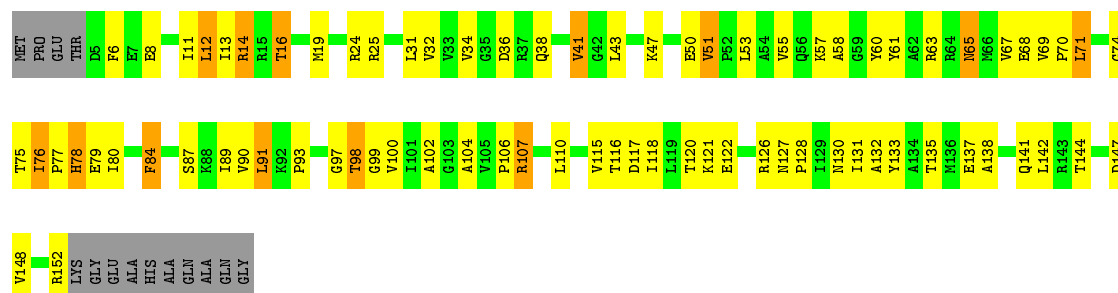




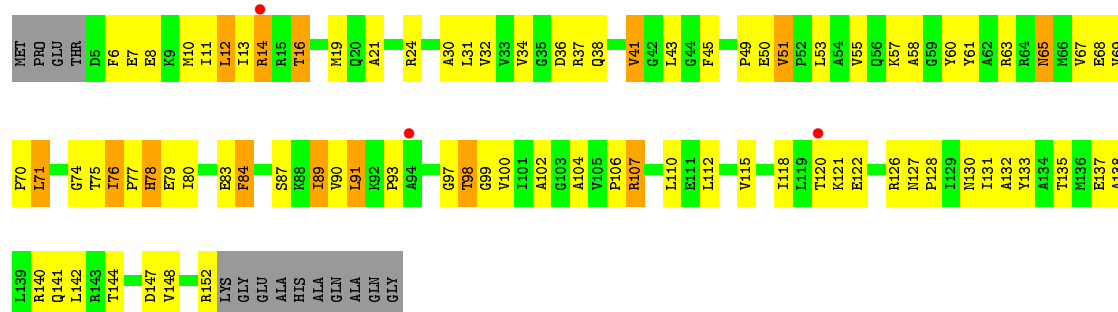
• Molecule 4: 30S Ribosomal Protein S4



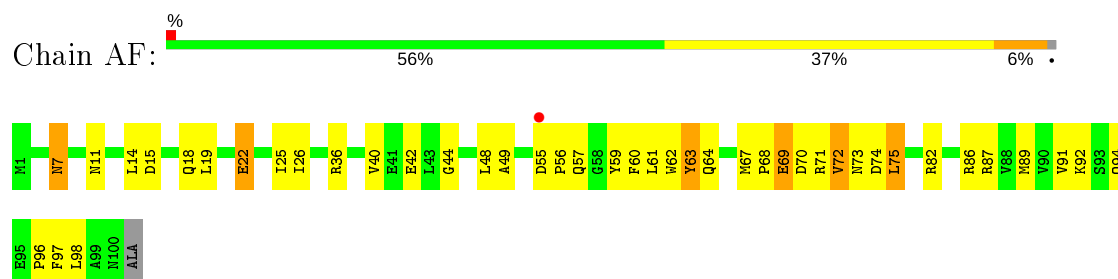
• Molecule 5: 30S Ribosomal Protein S5



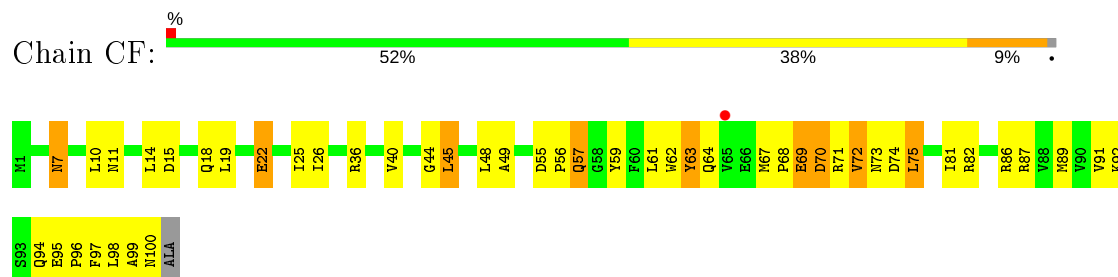
• Molecule 5: 30S Ribosomal Protein S5



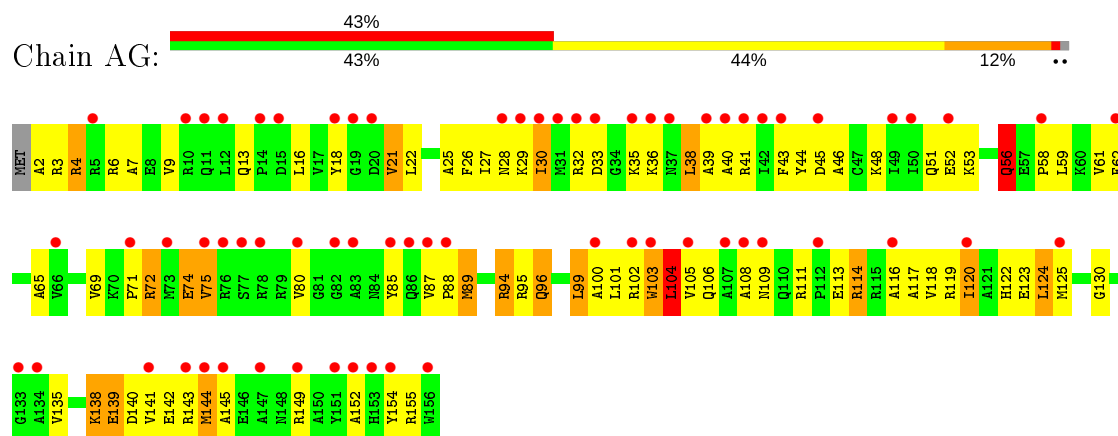
- Molecule 6: 30S Ribosomal Protein S6



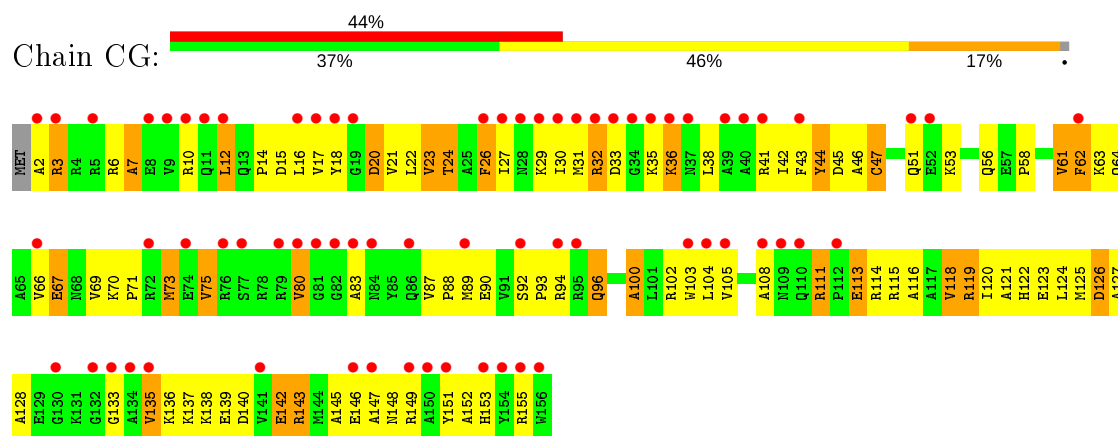
- Molecule 6: 30S Ribosomal Protein S6



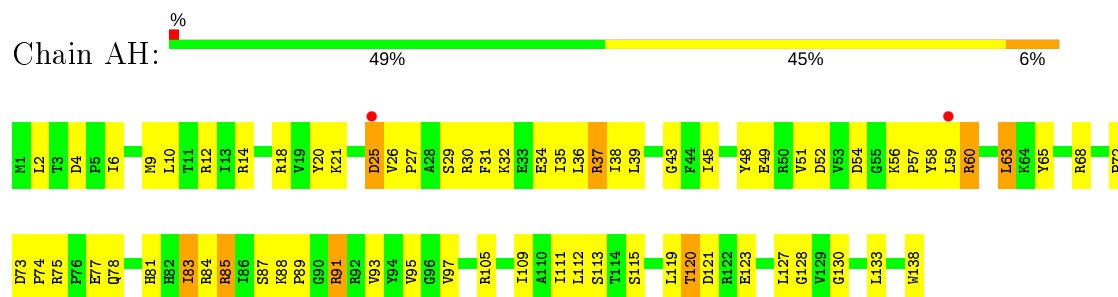
- Molecule 7: 30S Ribosomal Protein S7



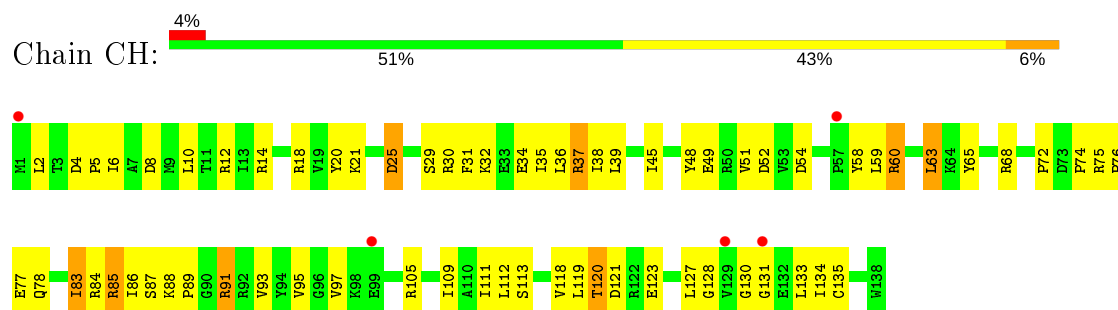
- Molecule 7: 30S Ribosomal Protein S7



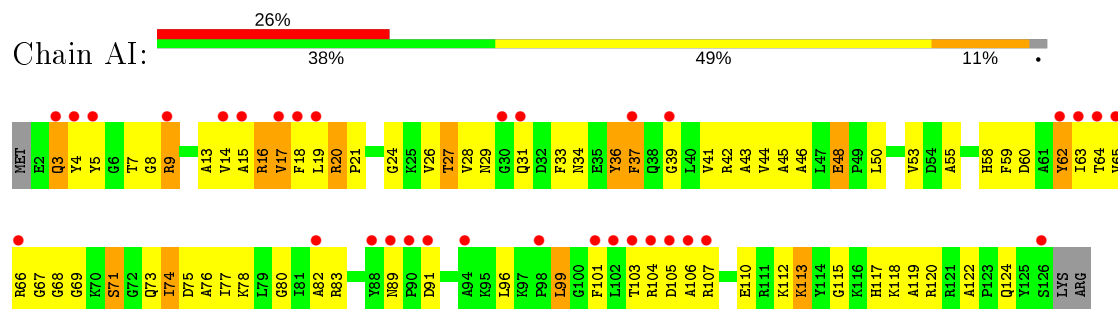
- Molecule 8: 30S Ribosomal Protein S8



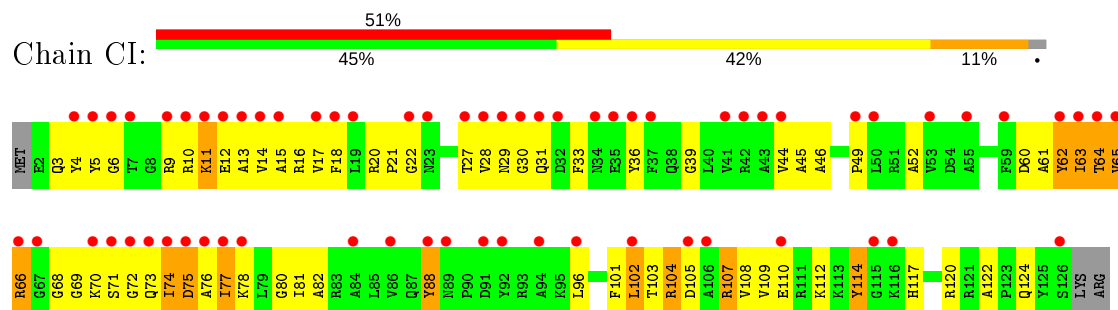
• Molecule 8: 30S Ribosomal Protein S8



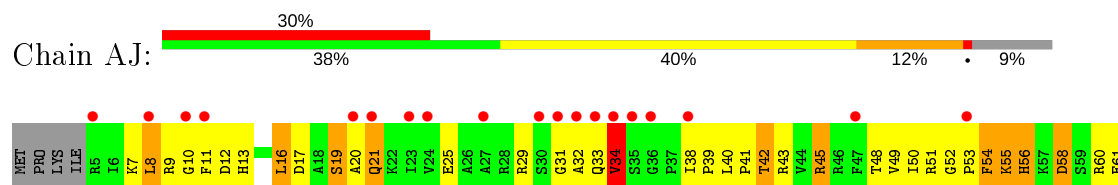
• Molecule 9: 30S Ribosomal Protein S9

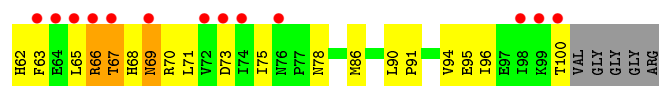


• Molecule 9: 30S Ribosomal Protein S9

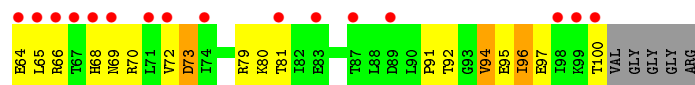
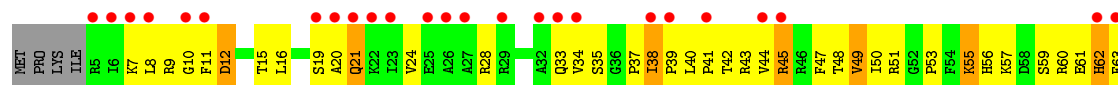


• Molecule 10: 30S Ribosomal Protein S10

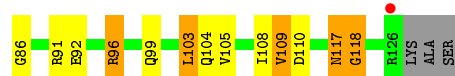
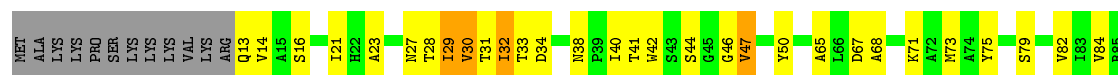




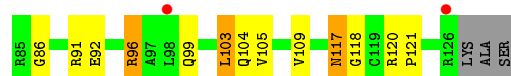
• Molecule 10: 30S Ribosomal Protein S10



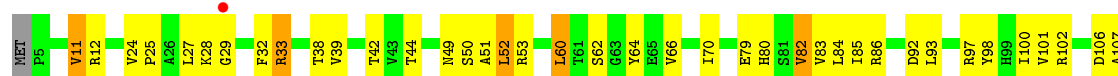
• Molecule 11: 30S Ribosomal Protein S11



• Molecule 11: 30S Ribosomal Protein S11

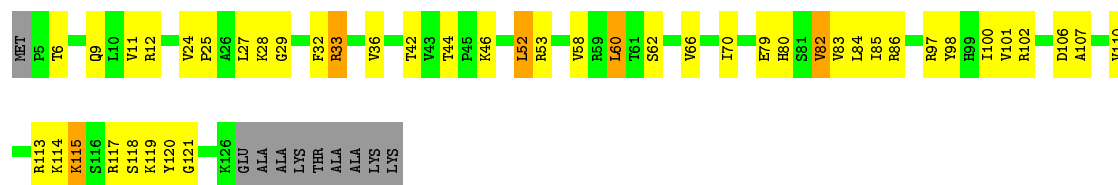


• Molecule 12: 30S Ribosomal Protein S12

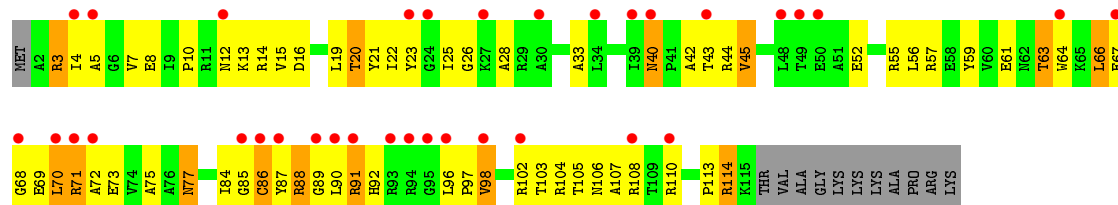


• Molecule 12: 30S Ribosomal Protein S12

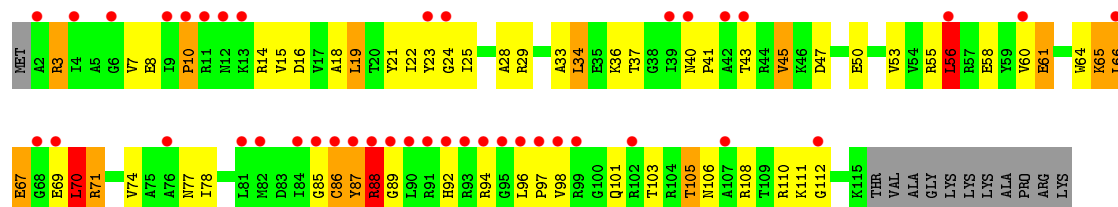
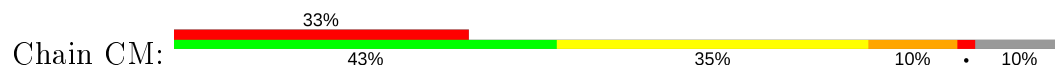




• Molecule 13: 30S Ribosomal Protein S13



• Molecule 13: 30S Ribosomal Protein S13



• Molecule 14: 30S Ribosomal Protein S14



• Molecule 14: 30S Ribosomal Protein S14



• Molecule 15: 30S Ribosomal Protein S15

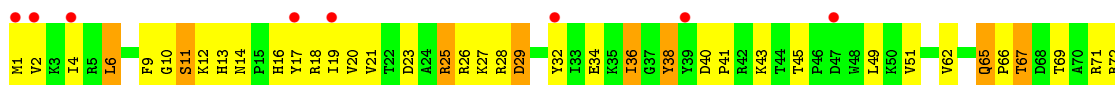
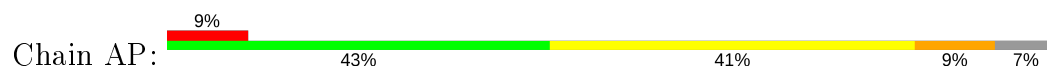




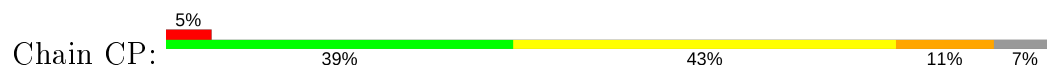
• Molecule 15: 30S Ribosomal Protein S15



• Molecule 16: 30S Ribosomal Protein S16



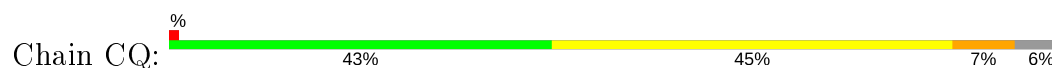
• Molecule 16: 30S Ribosomal Protein S16

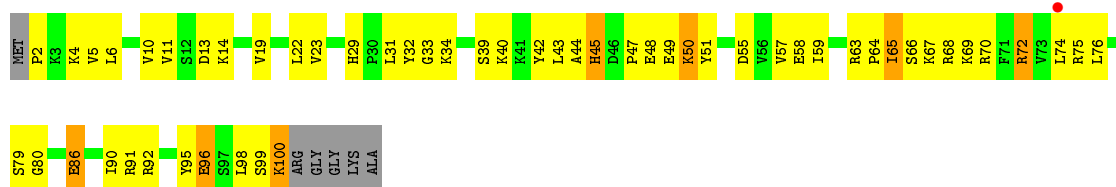


• Molecule 17: 30S Ribosomal Protein S17



• Molecule 17: 30S Ribosomal Protein S17





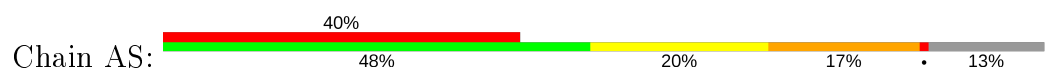
• Molecule 18: 30S Ribosomal Protein S18



• Molecule 18: 30S Ribosomal Protein S18



• Molecule 19: 30S Ribosomal Protein S19

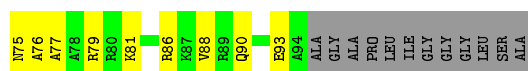


• Molecule 19: 30S Ribosomal Protein S19



• Molecule 20: 30S Ribosomal Protein S20





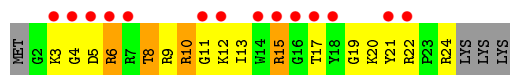
- Molecule 20: 30S Ribosomal Protein S20

Chain CT: 42% 42% 6% 8%



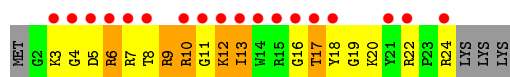
- Molecule 21: 30S Ribosomal Protein THX

Chain AU: 22% 52% 48% 15% 15%



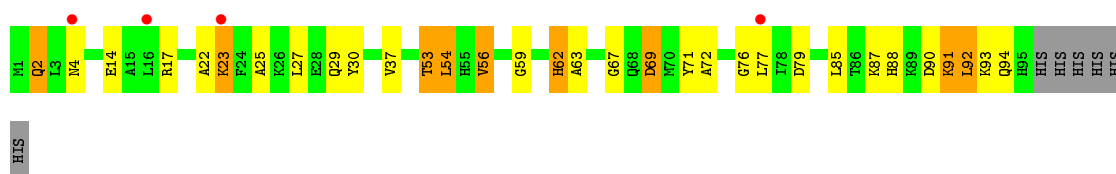
- Molecule 21: 30S Ribosomal Protein THX

Chain CU: 19% 67% 44% 22% 15%



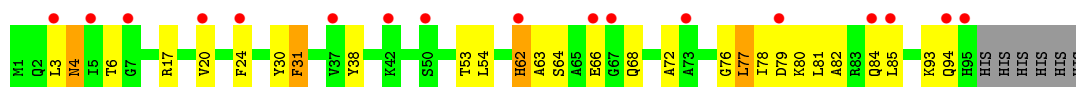
- Molecule 22: Probable sigma(54) modulation protein

Chain AX: 4% 62% 23% 9% 6%



- Molecule 22: Probable sigma(54) modulation protein

Chain CX: 17% 66% 24% 6%



- Molecule 23: 23S Ribosomal RNA

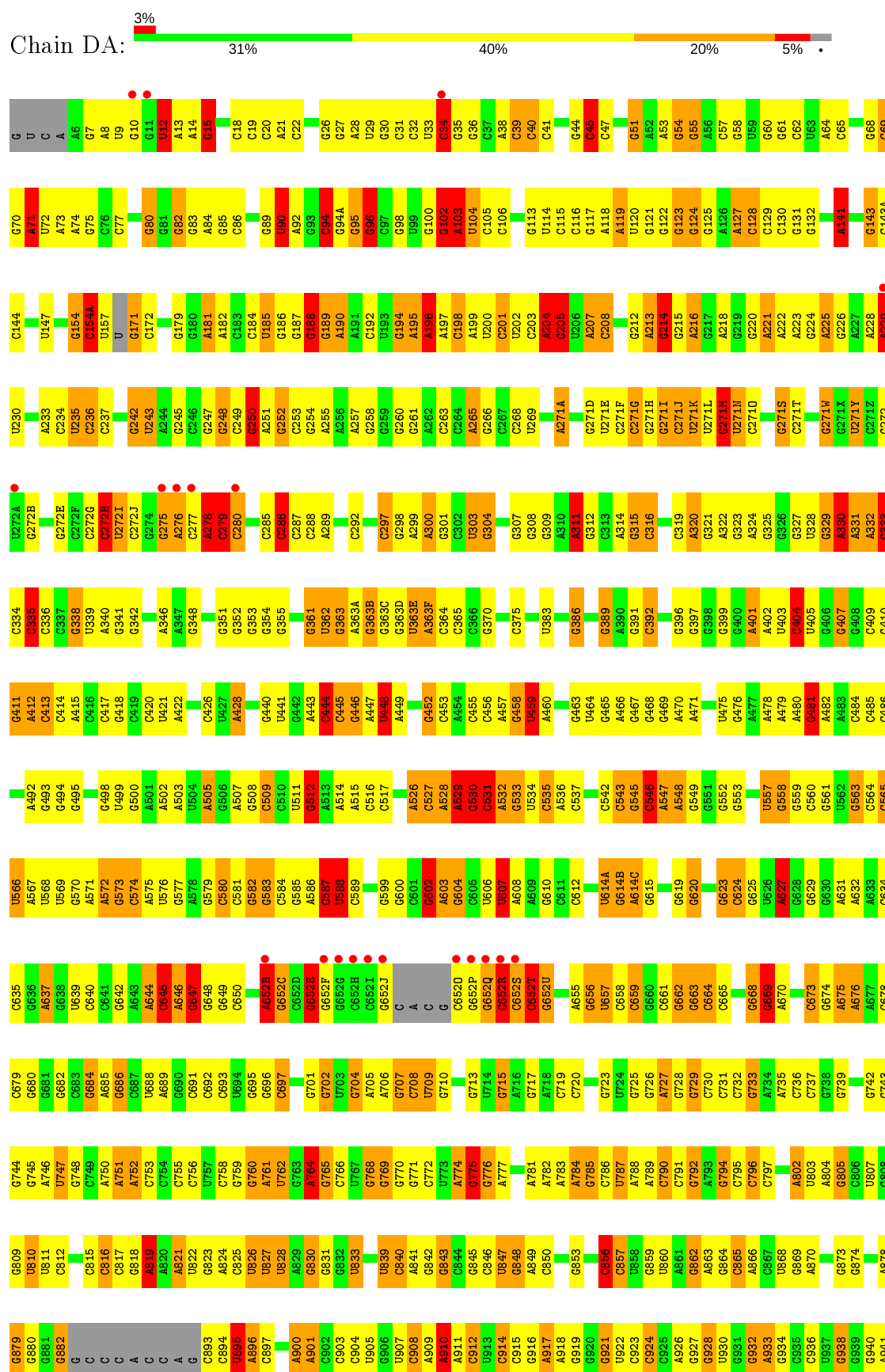
Chain BA: 2% 28% 41% 21% 6%

G934	G935	G936	U937	G938	G939	G940	A941	G942	U943	G944	A945	G946	G947	G948	G949	G950	G951	G952	A953	G954	G955	G956	G957	U958	A959	A960	C961	G962	U963	G966	G967	G968	A969	C970	G971	G972	A973	G974	G975	G975A	G976	G979	A980	G981	G982	A983	A984	G988	G989	G990	G991	G992	G993	G994	A995	A996																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U860	A861	G862	A863	G864	U868	G869	A870	A871	G872	G873	G874	A878	G879	G880	G881	G882	G883	G884	G885	G886	A887	G888	G889	A890	G891	G892	G893	C894	U895	G896	C897	A900	A901	G902	C903	C904	U907	G908	A909	A910	A911	C912	U913	C914	C915	G916	A917	G920	G921	U922	C923	C924	G928	G929	G930	G931	G932	G933	G934	A935	A936																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C796	C797	G798	G799	A800	G801	A802	U803	G804	G805	C806	U807	G808	G809	U810	U811	C812	C815	C816	C817	G818	A819	U820	A821	U822	G823	A824	C825	U826	U827	U828	A829	G830	G831	G832	U833	C834	U837	A838	A839	A840	C841	C844	G845	C846	U847	G848	G849	U850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	U907	C908	C909	C910	C911	C912	C913	C914	C915	C916	A917	G920	G921	U922	C923	C924	G928	G929	G930	G931	G932	G933	G934	A935	A936																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A735	C736	C737	G738	G739	G742	G743	A744	G745	A746	U747	G748	C749	G750	A751	A752	G753	C754	G755	C756	U757	C758	G759	G760	A761	U762	G763	A764	G765	U766	U767	G768	G769	G770	G771	G772	G773	A774	G775	C776	A777	G778	U779	G780	A781	A782	A783	A784	G785	G786	U787	A788	U789	C790	C791	G792	G793	A794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	U814A	G814B	A614C	G815	G820	G823																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G668	G669	C673	A674	A675	A676	A677	C678	C679	G682	G683	G684	A685	C686	G687	G688	G689	G690	C691	C692	C693	G696	C697	G698	U699	A700	G701	G702	G703	G704	G705	G706	G707	A708	G709	G710	G711	G712	G715	A716	G717	C718	G719	G723	G725	G726	A727	G728	G729	C730	C731	G732	G733	A734																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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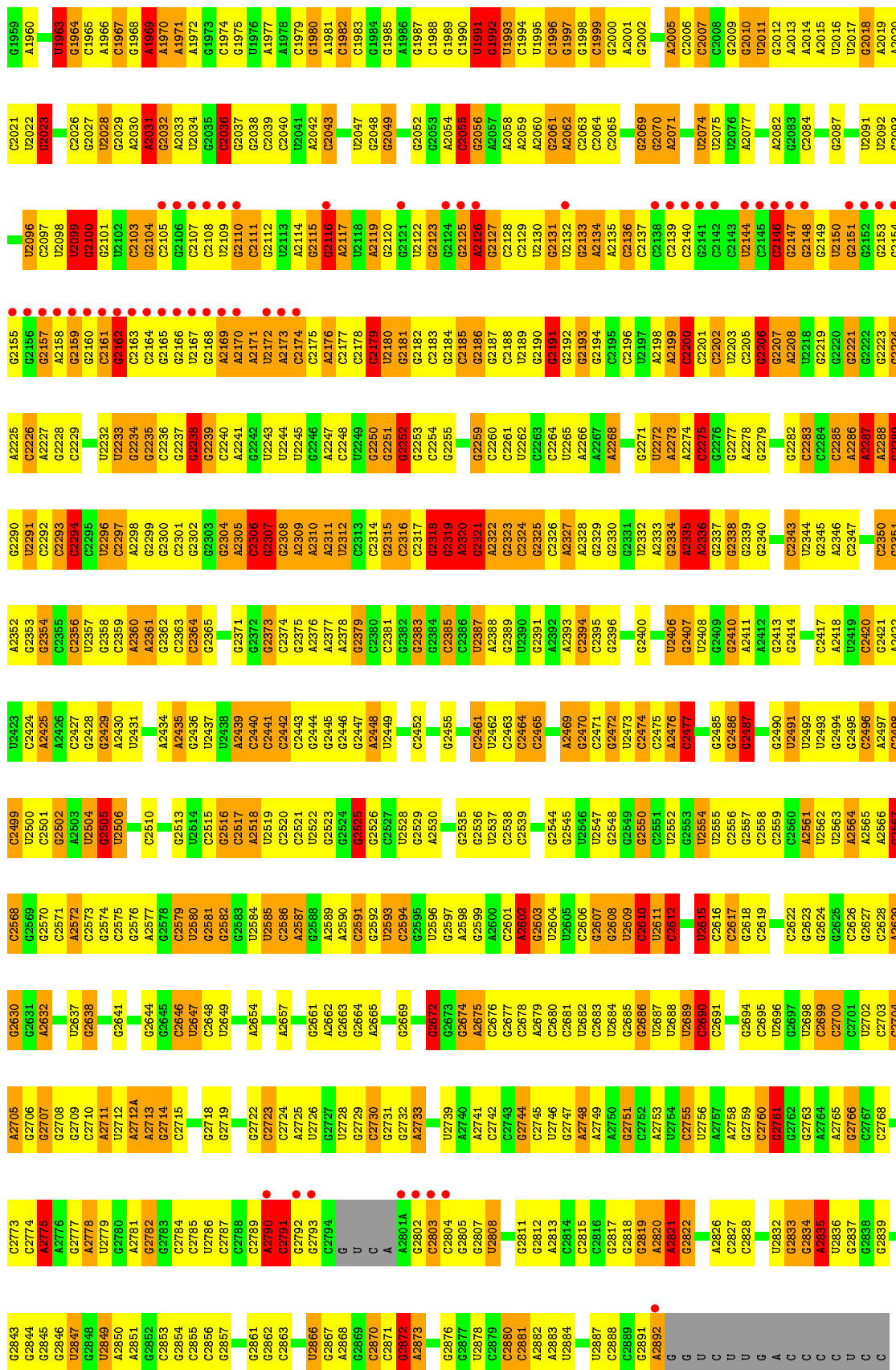


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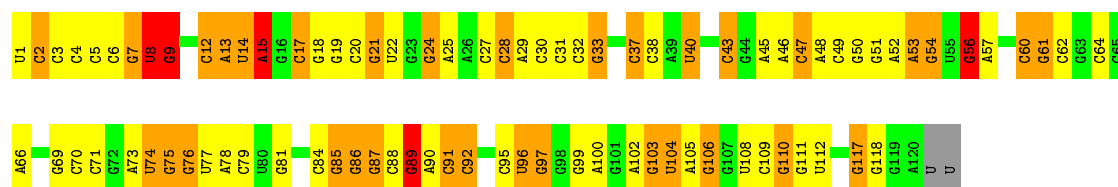






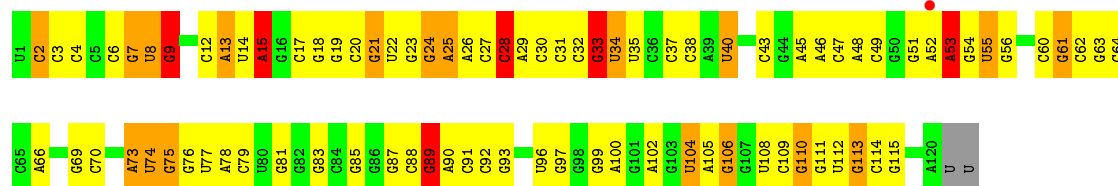
- Molecule 24: 5S Ribosomal RNA

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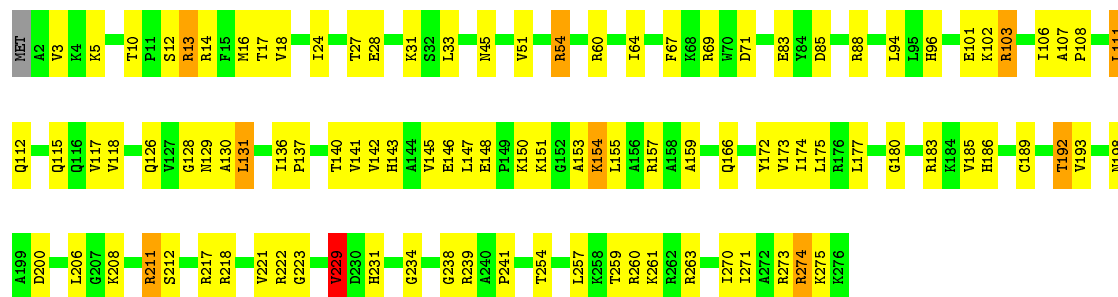
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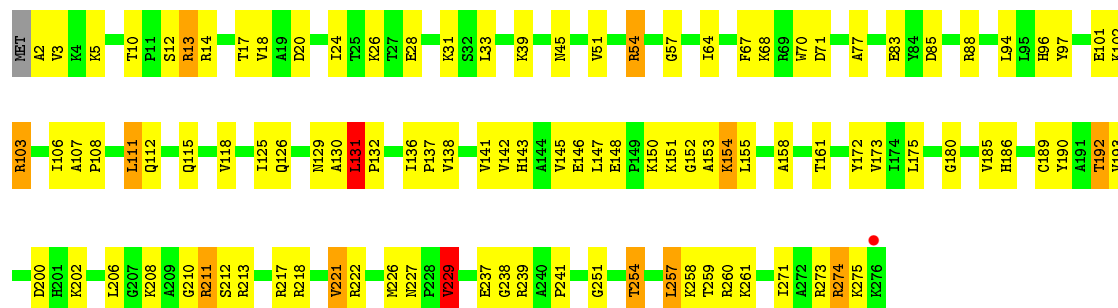
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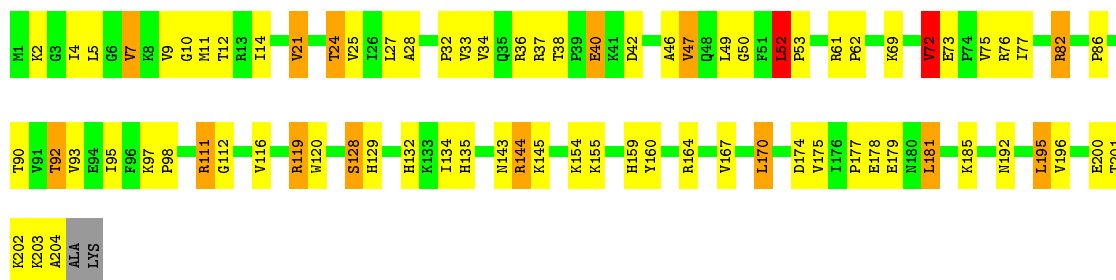
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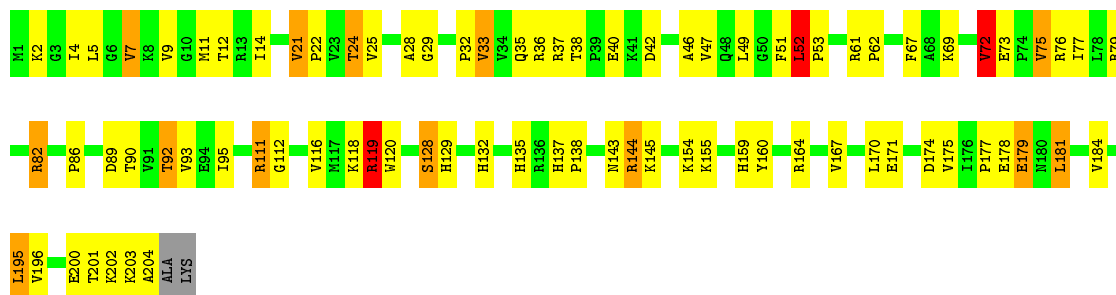
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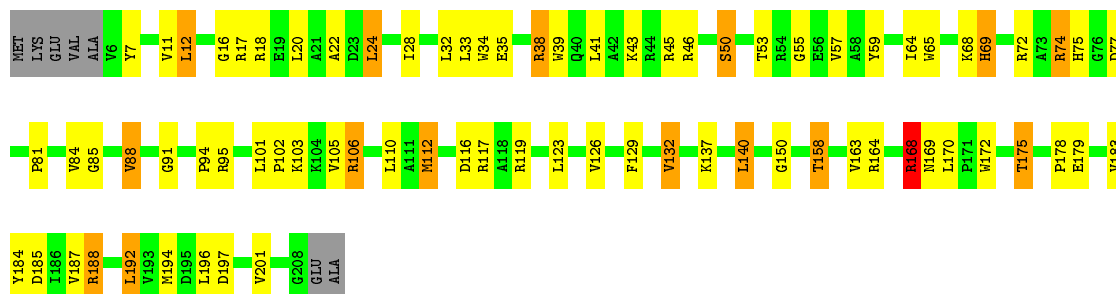
• Molecule 26: 50S Ribosomal Protein L3

Chain DE: 59% 32% 6% ..



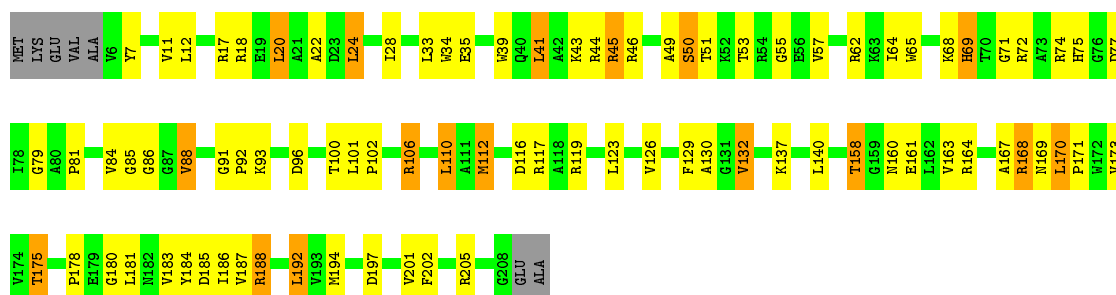
• Molecule 27: 50S Ribosomal Protein L4

Chain BF: 60% 29% 7% .

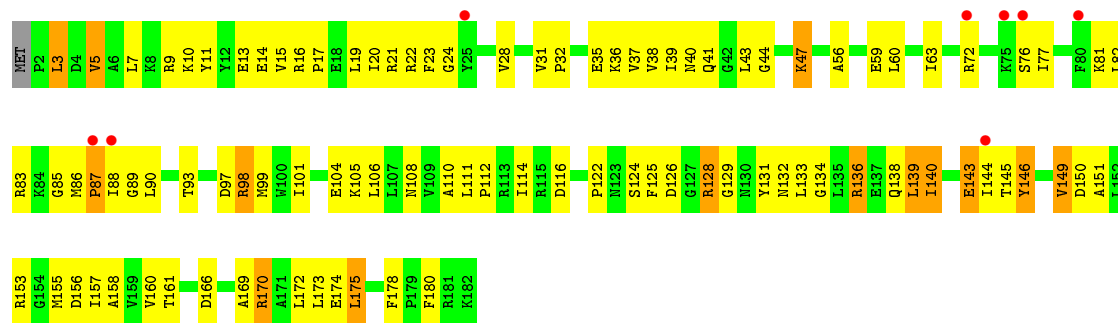


• Molecule 27: 50S Ribosomal Protein L4

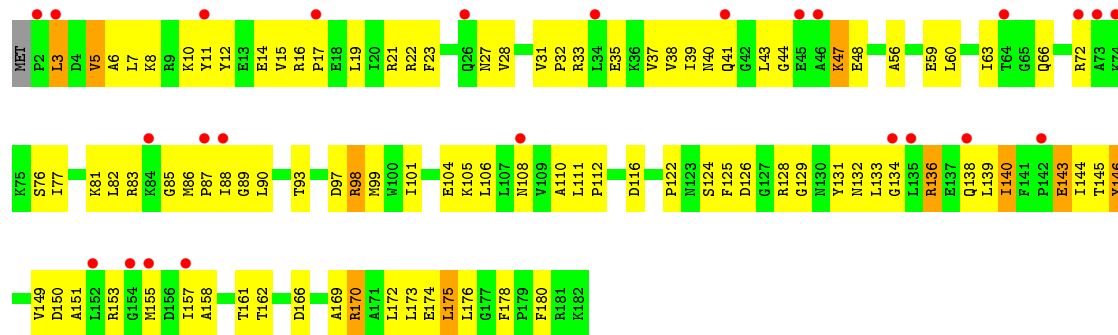
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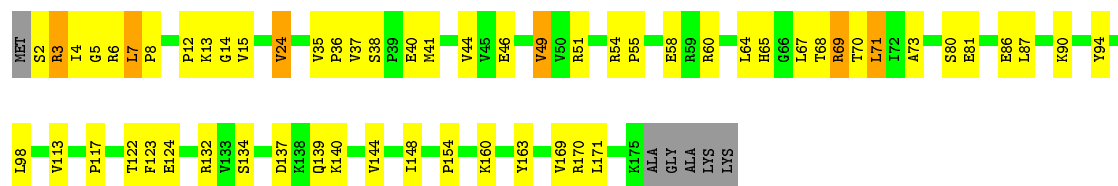
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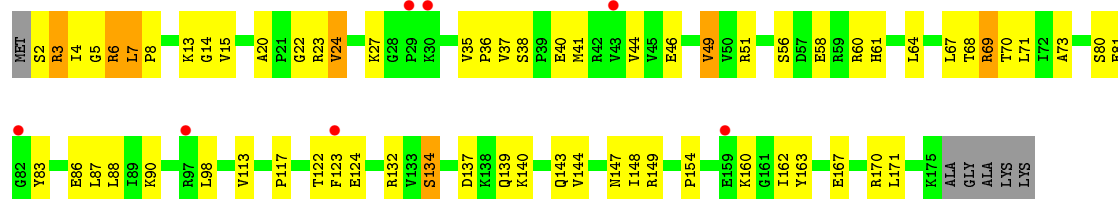
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• Molecule 29: 50S Ribosomal Protein L6

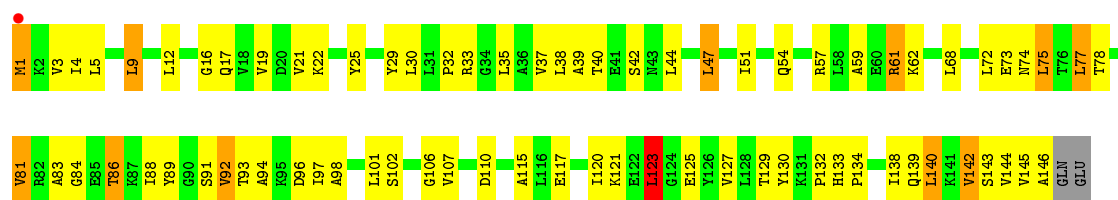


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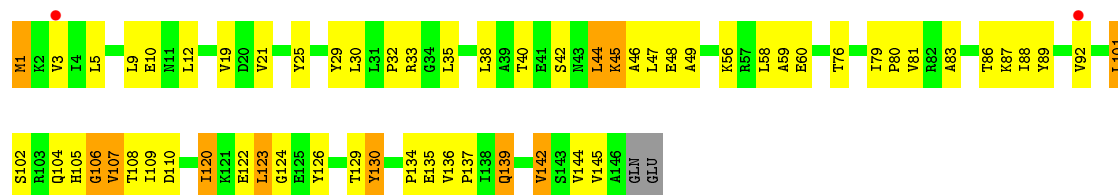


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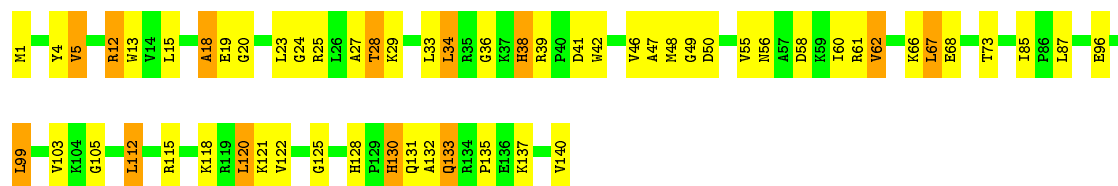




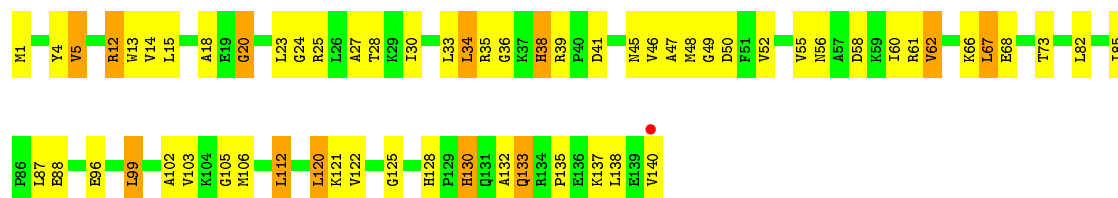
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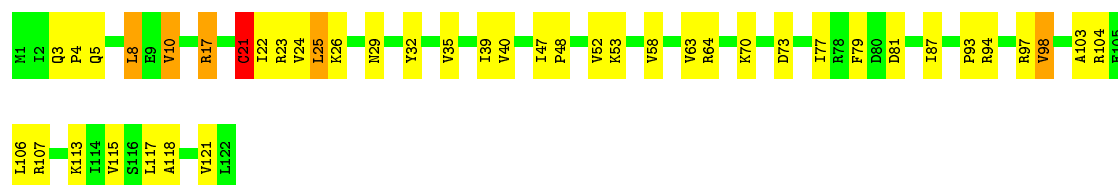
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• Molecule 31: 50S Ribosomal Protein L13

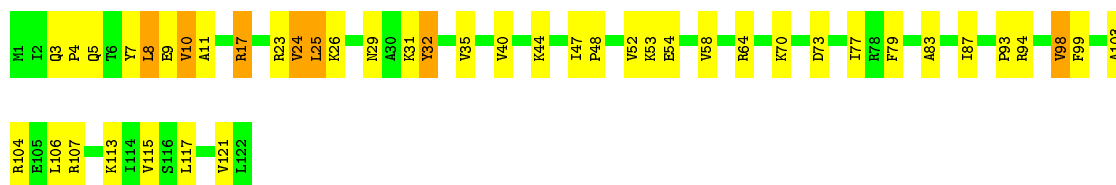


• Molecule 32: 50S Ribosomal Protein L14



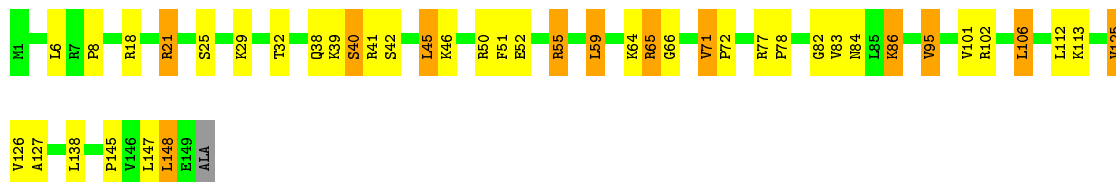
• Molecule 32: 50S Ribosomal Protein L14





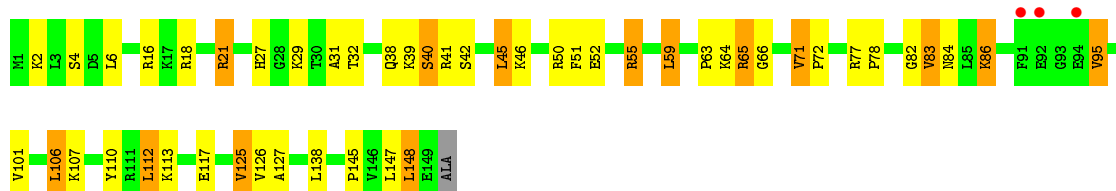
• Molecule 33: 50S Ribosomal Protein L15

Chain BP: 71% 21% 8% .



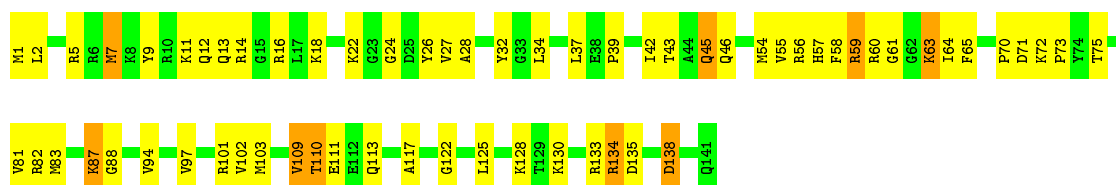
• Molecule 33: 50S Ribosomal Protein L15

Chain DP: 67% 23% 9% .



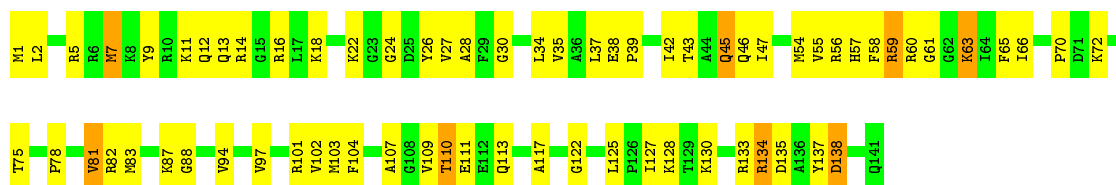
• Molecule 34: 50S Ribosomal Protein L16

Chain BQ: 55% 38% 6%



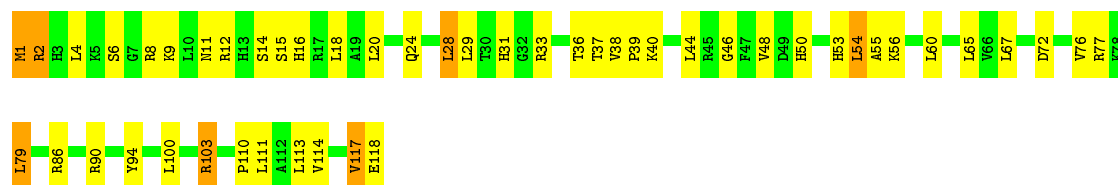
• Molecule 34: 50S Ribosomal Protein L16

Chain DQ: 51% 43% 6%



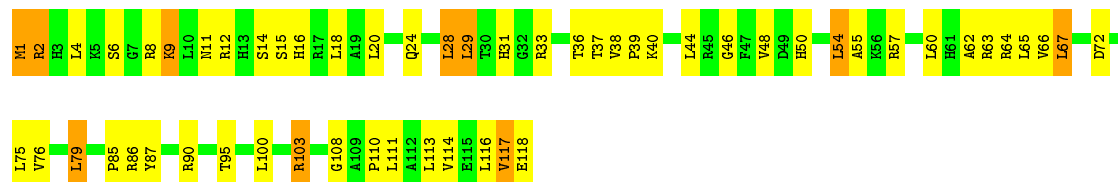
• Molecule 35: 50S Ribosomal Protein L17

Chain BR: 58% 36% 6%



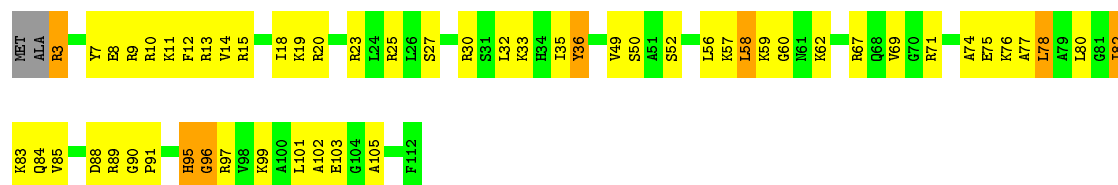
• Molecule 35: 50S Ribosomal Protein L17

Chain DR: 53% 39% 8%



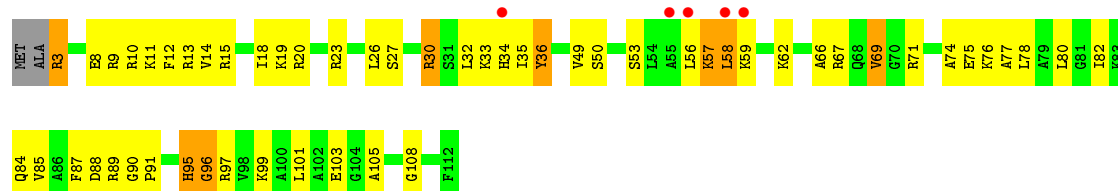
• Molecule 36: 50S Ribosomal Protein L18

Chain BS: 49% 43% 6%



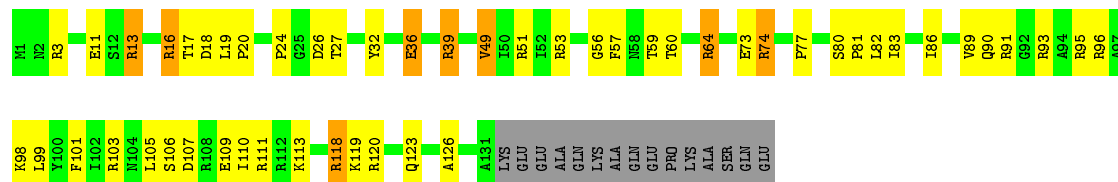
• Molecule 36: 50S Ribosomal Protein L18

Chain DS: 49% 42% 7%



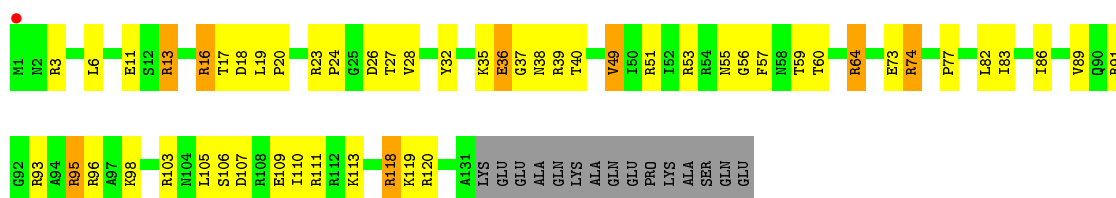
• Molecule 37: 50S Ribosomal Protein L19

Chain BT: 54% 30% 5% 10%



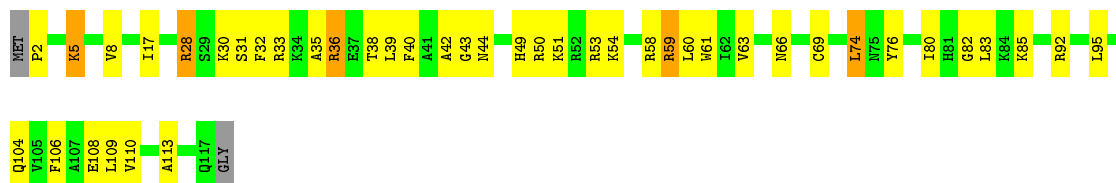
• Molecule 37: 50S Ribosomal Protein L19

Chain DT: 53% 31% 5% 10%



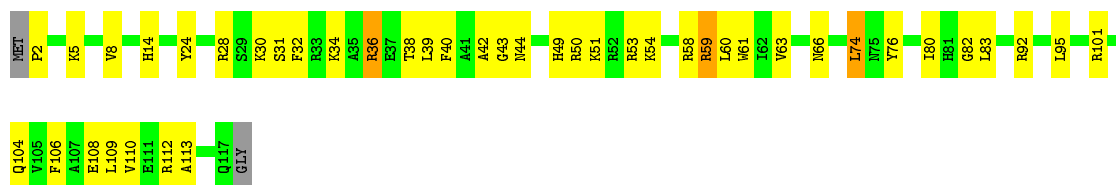
• Molecule 38: 50S Ribosomal Protein L20

Chain BU: 62% 32%



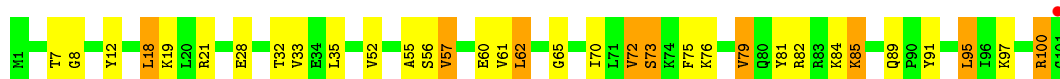
• Molecule 38: 50S Ribosomal Protein L20

Chain DU: 62% 34%



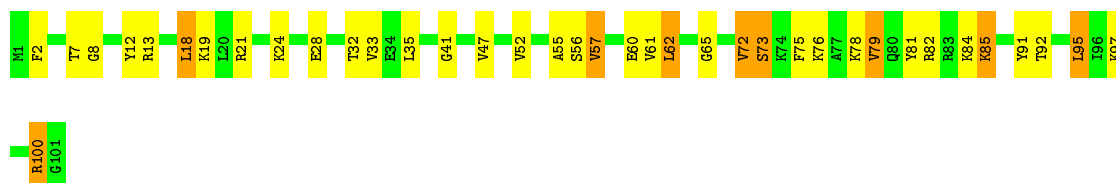
• Molecule 39: 50S Ribosomal Protein L21

Chain BV: 67% 24% 9%



• Molecule 39: 50S Ribosomal Protein L21

Chain DV: 62% 29% 9%



• Molecule 40: 50S Ribosomal Protein L22

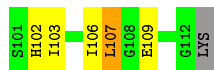
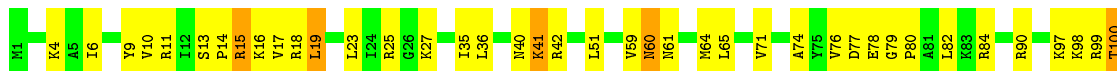
Chain BW: 68% 27%





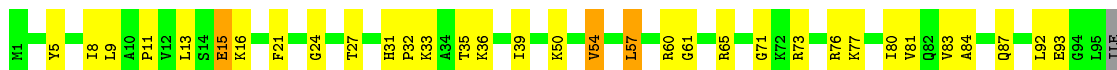
- Molecule 40: 50S Ribosomal Protein L22

Chain DW: 59% 35% 5%



- Molecule 41: 50S Ribosomal Protein L23

Chain BX: 65% 31% 4%



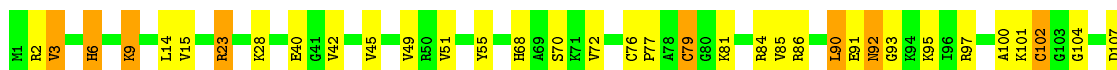
- Molecule 41: 50S Ribosomal Protein L23

Chain DX: 63% 34% 3%



- Molecule 42: 50S Ribosomal Protein L24

Chain BY: 65% 25% 7%



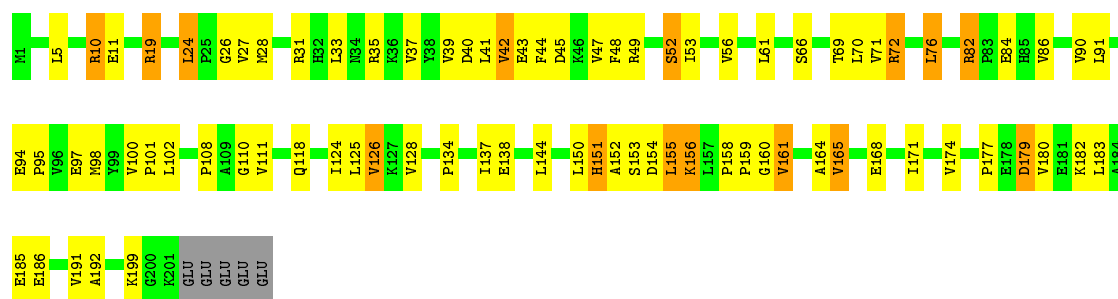
- Molecule 42: 50S Ribosomal Protein L24

Chain DY: 5% 64% 25% 8%

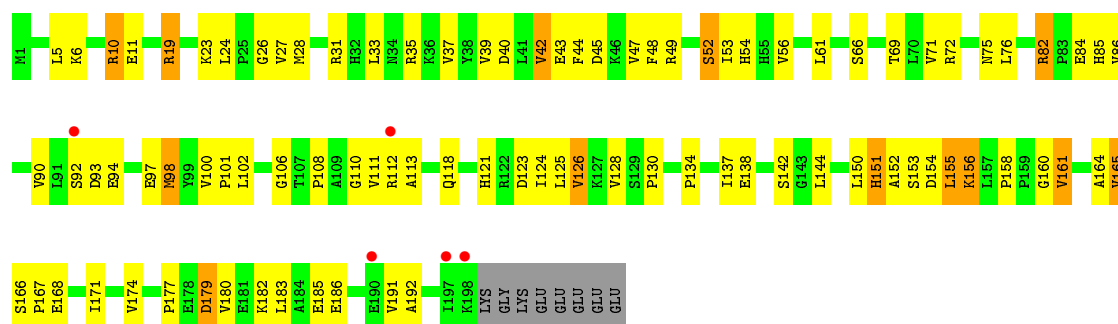


- Molecule 43: 50S Ribosomal Protein L25

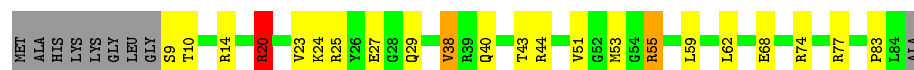
Chain BZ: 58% 33% 7%



• Molecule 43: 50S Ribosomal Protein L25



• Molecule 44: 50S Ribosomal Protein L27



• Molecule 44: 50S Ribosomal Protein L27



• Molecule 45: 50S Ribosomal Protein L28

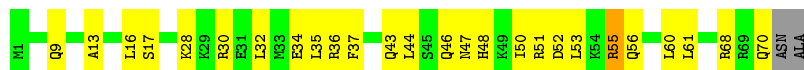


• Molecule 45: 50S Ribosomal Protein L28





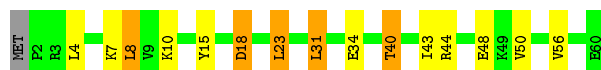
- Molecule 46: 50S Ribosomal Protein L29



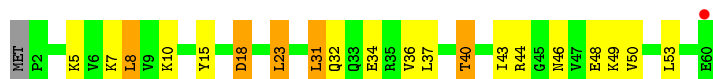
- Molecule 46: 50S Ribosomal Protein L29



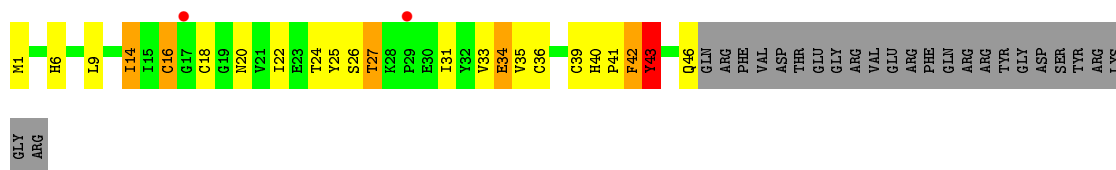
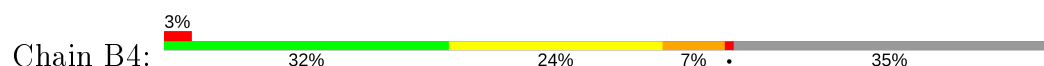
- Molecule 47: 50S Ribosomal Protein L30



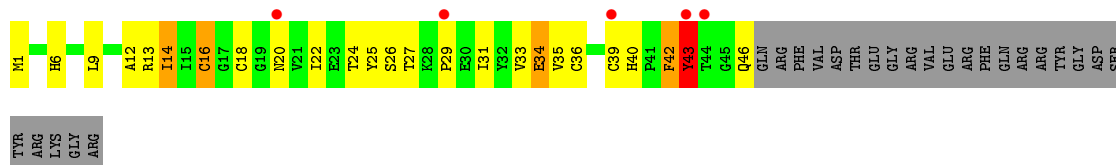
- Molecule 47: 50S Ribosomal Protein L30



- Molecule 48: 50S Ribosomal Protein L31



- Molecule 48: 50S Ribosomal Protein L31



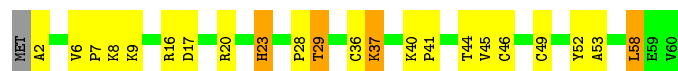
- Molecule 49: 50S Ribosomal Protein L32

Chain B5: 



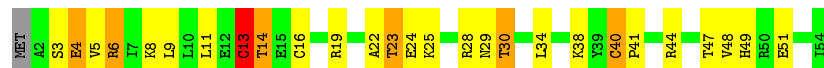
- Molecule 49: 50S Ribosomal Protein L32

Chain D5: 



- Molecule 50: 50S Ribosomal Protein L33

Chain B6: 



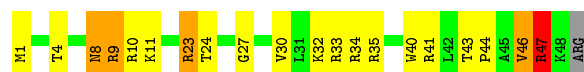
- Molecule 50: 50S Ribosomal Protein L33

Chain D6: 



- Molecule 51: 50S Ribosomal Protein L34

Chain B7: 



- Molecule 51: 50S Ribosomal Protein L34

Chain D7: 



- Molecule 52: 50S Ribosomal Protein L35

Chain B8: 



- Molecule 52: 50S Ribosomal Protein L35

Chain D8:

55%

35%

8%



• Molecule 53: 50S Ribosomal Protein L36

Chain B9:

62%

32%



• Molecule 53: 50S Ribosomal Protein L36

Chain D9:

3%

62%

32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.216 , 0.258 0.214 , 0.257	Depositor DCC
R_{free} test set	49829 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	286308	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.14	57/36123 (0.2%)	1.54	760/56379 (1.3%)
1	CA	1.11	53/36028 (0.1%)	1.55	750/56231 (1.3%)
2	AB	0.69	0/1822	0.79	1/2468 (0.0%)
2	CB	0.75	0/1809	0.79	1/2450 (0.0%)
3	AC	0.80	0/1474	0.88	0/2003
3	CC	0.78	0/1474	0.86	2/2003 (0.1%)
4	AD	0.68	2/1556 (0.1%)	0.87	3/2113 (0.1%)
4	CD	0.72	2/1556 (0.1%)	0.87	3/2113 (0.1%)
5	AE	0.61	0/1121	0.80	1/1517 (0.1%)
5	CE	0.63	0/1121	0.82	1/1517 (0.1%)
6	AF	0.59	0/790	0.73	0/1077
6	CF	0.62	0/790	0.73	0/1077
7	AG	1.04	0/1183	0.98	2/1599 (0.1%)
7	CG	0.96	0/1183	0.90	0/1599
8	AH	0.57	0/1065	0.73	0/1445
8	CH	0.58	0/1065	0.75	0/1445
9	AI	0.92	0/867	0.92	0/1180
9	CI	1.00	0/867	0.91	1/1180 (0.1%)
10	AJ	0.83	0/676	0.91	1/924 (0.1%)
10	CJ	0.90	0/676	0.97	0/924
11	AK	0.62	0/843	0.75	1/1144 (0.1%)
11	CK	0.61	0/843	0.75	1/1144 (0.1%)
12	AL	0.63	0/921	0.78	0/1247
12	CL	0.64	0/921	0.80	0/1247
13	AM	1.02	0/814	1.00	0/1107
13	CM	1.03	0/814	1.03	2/1107 (0.2%)
14	AN	0.76	0/487	0.90	0/649
14	CN	0.77	1/487 (0.2%)	0.87	1/649 (0.2%)
15	AO	0.62	0/735	0.84	0/981
15	CO	0.66	0/735	0.85	0/981
16	AP	0.63	0/667	0.82	0/905
16	CP	0.56	0/667	0.82	0/905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.66	0/836	0.84	0/1117
17	CQ	0.69	1/836 (0.1%)	0.85	0/1117
18	AR	0.59	0/519	0.76	1/699 (0.1%)
18	CR	0.63	0/519	0.76	1/699 (0.1%)
19	AS	0.96	0/574	0.87	0/781
19	CS	0.98	0/574	0.93	0/781
20	AT	0.63	0/666	0.79	0/880
20	CT	0.62	0/715	0.84	1/947 (0.1%)
21	AU	0.82	0/203	0.92	0/266
21	CU	0.91	0/203	0.97	0/266
22	AX	0.69	0/637	0.84	1/864 (0.1%)
22	CX	0.77	0/606	0.82	0/828
23	BA	1.58	572/68445 (0.8%)	1.72	2187/106848 (2.0%)
23	DA	1.21	155/67893 (0.2%)	1.65	1848/105980 (1.7%)
24	BB	1.13	6/2878 (0.2%)	1.53	60/4490 (1.3%)
24	DB	1.13	2/2878 (0.1%)	1.52	49/4490 (1.1%)
25	BD	0.90	1/2185 (0.0%)	0.91	4/2942 (0.1%)
25	DD	0.82	0/2186	0.91	2/2944 (0.1%)
26	BE	0.90	0/1588	0.92	0/2145
26	DE	0.78	0/1588	0.92	3/2145 (0.1%)
27	BF	0.91	0/1615	0.95	3/2188 (0.1%)
27	DF	0.74	0/1615	0.92	2/2188 (0.1%)
28	BG	0.61	0/1393	0.79	0/1892
28	DG	0.72	0/1393	0.81	0/1892
29	BH	0.72	0/1343	0.82	1/1820 (0.1%)
29	DH	0.66	0/1343	0.81	0/1820
30	BI	0.64	0/1052	0.87	1/1441 (0.1%)
30	DI	0.63	0/967	0.84	1/1334 (0.1%)
31	BN	0.87	0/1139	0.87	0/1538
31	DN	0.71	0/1139	0.89	1/1538 (0.1%)
32	BO	0.87	1/933 (0.1%)	0.88	1/1257 (0.1%)
32	DO	0.73	0/933	0.83	1/1257 (0.1%)
33	BP	0.84	0/1148	0.91	1/1529 (0.1%)
33	DP	0.73	0/1148	0.89	1/1529 (0.1%)
34	BQ	0.84	0/1143	0.87	1/1527 (0.1%)
34	DQ	0.74	0/1143	0.86	0/1527
35	BR	0.80	0/982	0.92	0/1312
35	DR	0.75	0/982	0.92	1/1312 (0.1%)
36	BS	0.67	0/875	0.88	1/1168 (0.1%)
36	DS	0.69	0/875	0.87	1/1168 (0.1%)
37	BT	0.83	0/1077	0.92	0/1444
37	DT	0.73	0/1077	0.90	0/1444
38	BU	1.00	1/977 (0.1%)	0.87	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	0.79	0/977	0.86	0/1301
39	BV	0.85	0/782	0.92	0/1049
39	DV	0.77	0/782	0.85	0/1049
40	BW	1.02	0/891	0.91	0/1197
40	DW	0.87	0/891	0.91	1/1197 (0.1%)
41	BX	0.91	0/756	0.88	2/1016 (0.2%)
41	DX	0.78	0/756	0.86	1/1016 (0.1%)
42	BY	0.80	1/798 (0.1%)	0.88	0/1073
42	DY	0.73	1/798 (0.1%)	0.89	0/1073
43	BZ	0.70	0/1569	0.82	1/2137 (0.0%)
43	DZ	0.72	0/1555	0.81	1/2118 (0.0%)
44	B0	0.85	0/602	0.92	1/804 (0.1%)
44	D0	0.78	0/602	0.92	0/804
45	B1	0.85	0/752	0.90	2/1003 (0.2%)
45	D1	0.80	0/752	0.89	1/1003 (0.1%)
46	B2	0.82	0/590	0.86	0/781
46	D2	0.79	0/590	0.86	0/781
47	B3	0.76	0/463	0.84	1/623 (0.2%)
47	D3	0.69	0/463	0.81	0/623
48	B4	0.68	0/358	0.84	1/487 (0.2%)
48	D4	0.85	0/358	0.83	1/487 (0.2%)
49	B5	0.93	1/469 (0.2%)	1.00	0/634
49	D5	0.86	1/469 (0.2%)	0.96	0/634
50	B6	0.93	2/456 (0.4%)	0.84	0/609
50	D6	0.75	0/456	0.87	2/609 (0.3%)
51	B7	1.03	1/426 (0.2%)	1.12	1/561 (0.2%)
51	D7	0.88	0/426	1.01	1/561 (0.2%)
52	B8	0.96	0/516	0.94	1/679 (0.1%)
52	D8	0.76	0/516	0.90	0/679
53	B9	0.79	0/300	0.95	0/395
53	D9	0.71	0/300	0.90	0/395
All	All	1.18	861/305420 (0.3%)	1.47	5724/457343 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
2	CB	0	4
3	AC	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	1
4	AD	0	1
4	CD	0	1
7	CG	0	2
9	AI	0	1
9	CI	0	1
10	AJ	0	2
10	CJ	0	2
13	AM	0	4
13	CM	0	2
14	AN	0	1
15	AO	0	1
15	CO	0	1
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
19	CS	0	1
20	AT	0	1
20	CT	0	1
23	BA	0	1
23	DA	0	1
26	BE	0	1
26	DE	0	1
27	DF	0	1
30	DI	0	1
34	BQ	0	1
34	DQ	0	1
36	BS	0	1
36	DS	0	1
41	BX	0	1
41	DX	0	1
43	BZ	0	3
43	DZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	1
48	D4	0	1
All	All	0	56

The worst 5 of 861 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1442(A)	G	N9-C4	17.19	1.51	1.38
1	AA	1442(A)	G	N9-C4	15.23	1.50	1.38
1	AA	1442(A)	G	C2-N3	15.04	1.44	1.32
1	CA	1442(A)	G	C2-N3	14.30	1.44	1.32
1	AA	1442(A)	G	N3-C4	13.24	1.44	1.35

The worst 5 of 5724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-26.14	115.53	128.60
23	DA	2296	U	N3-C4-O4	-25.95	101.23	119.40
1	AA	1442(A)	G	N3-C4-C5	-25.64	115.78	128.60
1	CA	1442(A)	G	N3-C4-N9	25.18	141.10	126.00
1	AA	1442(A)	G	N3-C4-N9	25.11	141.07	126.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	129	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	19	GLU	Peptide
3	AC	51	GLY	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32270	0	16286	1214	0
1	CA	32185	0	16244	1267	1
2	AB	1787	0	1752	122	0
2	CB	1775	0	1743	121	0
3	AC	1450	0	1314	92	0
3	CC	1450	0	1314	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1526	0	1415	71	0
4	CD	1526	0	1415	85	0
5	AE	1105	0	1130	56	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	31	0
6	CF	777	0	737	35	0
7	AG	1164	0	1106	87	0
7	CG	1164	0	1106	99	0
8	AH	1045	0	1033	48	0
8	CH	1045	0	1033	51	0
9	AI	852	0	742	83	0
9	CI	852	0	742	79	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	70	0
11	AK	828	0	822	29	0
11	CK	828	0	822	28	0
12	AL	905	0	916	41	0
12	CL	905	0	916	32	0
13	AM	804	0	752	58	0
13	CM	804	0	752	60	0
14	AN	478	0	497	33	0
14	CN	478	0	496	58	0
15	AO	724	0	749	34	0
15	CO	724	0	749	31	0
16	AP	651	0	638	31	0
16	CP	651	0	638	36	0
17	AQ	823	0	891	43	0
17	CQ	823	0	891	47	0
18	AR	514	0	530	25	0
18	CR	514	0	530	21	0
19	AS	560	0	466	46	0
19	CS	560	0	466	40	0
20	AT	665	0	731	34	0
20	CT	713	0	766	39	0
21	AU	199	0	208	31	0
21	CU	199	0	208	23	0
22	AX	631	0	540	20	0
22	CX	601	0	485	16	0
23	BA	61112	0	30809	1210	1
23	DA	60621	0	30566	1219	0
24	BB	2573	0	1306	56	0
24	DB	2573	0	1306	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BD	2135	0	2214	73	0
25	DD	2136	0	2218	79	0
26	BE	1555	0	1607	52	0
26	DE	1555	0	1607	56	0
27	BF	1580	0	1621	63	0
27	DF	1580	0	1621	63	0
28	BG	1368	0	1324	74	0
28	DG	1368	0	1324	86	0
29	BH	1317	0	1376	35	0
29	DH	1317	0	1376	36	0
30	BI	1037	0	1036	54	1
30	DI	953	0	858	38	0
31	BN	1112	0	1180	33	0
31	DN	1112	0	1180	44	0
32	BO	923	0	981	26	0
32	DO	923	0	981	28	0
33	BP	1131	0	1201	45	0
33	DP	1131	0	1201	55	0
34	BQ	1122	0	1179	46	0
34	DQ	1122	0	1179	49	0
35	BR	968	0	1033	32	0
35	DR	968	0	1033	36	0
36	BS	865	0	905	50	0
36	DS	865	0	905	50	0
37	BT	1063	0	1103	42	0
37	DT	1063	0	1103	43	0
38	BU	959	0	1019	34	0
38	DU	959	0	1019	35	0
39	BV	771	0	830	23	0
39	DV	771	0	830	25	0
40	BW	881	0	935	21	0
40	DW	881	0	935	31	0
41	BX	742	0	799	23	0
41	DX	742	0	799	26	0
42	BY	785	0	828	23	0
42	DY	785	0	828	23	0
43	BZ	1536	0	1518	52	0
43	DZ	1522	0	1511	65	0
44	B0	594	0	604	16	0
44	D0	594	0	604	17	0
45	B1	745	0	804	21	0
45	D1	745	0	804	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B2	588	0	643	16	0
46	D2	588	0	643	19	0
47	B3	458	0	503	8	0
47	D3	458	0	503	13	0
48	B4	349	0	336	23	0
48	D4	349	0	336	28	0
49	B5	455	0	472	13	0
49	D5	455	0	472	14	0
50	B6	449	0	462	18	0
50	D6	449	0	462	15	0
51	B7	418	0	467	14	0
51	D7	418	0	467	18	0
52	B8	509	0	565	18	0
52	D8	509	0	565	22	0
53	B9	297	0	316	9	0
53	D9	297	0	316	9	0
54	AA	135	0	0	0	0
54	AC	1	0	0	0	0
54	AD	1	0	0	0	0
54	AF	1	0	0	0	0
54	AQ	1	0	0	0	0
54	B0	3	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	1	0	0	0	0
54	B5	2	0	0	0	0
54	B8	2	0	0	0	0
54	B9	1	0	0	0	0
54	BA	660	0	0	0	0
54	BB	23	0	0	0	0
54	BD	3	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BG	1	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	4	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	2	0	0	0	0
54	BZ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	162	0	0	0	0
54	CE	1	0	0	0	0
54	CQ	1	0	0	0	0
54	D0	2	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	2	0	0	0	0
54	DA	598	0	0	0	0
54	DB	8	0	0	0	0
54	DD	2	0	0	0	0
54	DE	4	0	0	0	0
54	DF	1	0	0	0	0
54	DO	2	0	0	0	0
54	DP	1	0	0	0	0
54	DQ	2	0	0	0	0
54	DR	3	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	268	0	0	32	0
56	AE	1	0	0	0	0
56	AL	1	0	0	0	0
56	AO	1	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	AX	1	0	0	0	0
56	B0	8	0	0	0	0
56	B1	2	0	0	0	0
56	B3	1	0	0	0	0
56	B5	3	0	0	0	0
56	B6	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B7	5	0	0	0	0
56	B8	10	0	0	0	0
56	B9	1	0	0	1	0
56	BA	1694	0	0	169	0
56	BB	57	0	0	3	1
56	BD	20	0	0	3	0
56	BE	11	0	0	0	0
56	BF	6	0	0	1	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	2	0	0	0	0
56	BP	11	0	0	2	0
56	BQ	5	0	0	0	0
56	BR	6	0	0	1	0
56	BT	1	0	0	0	0
56	BU	3	0	0	0	0
56	BV	3	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	4	0	0	0	0
56	CA	265	0	0	25	0
56	CC	1	0	0	2	0
56	CD	1	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	1	0
56	CL	2	0	0	1	0
56	CN	1	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D1	5	0	0	0	0
56	D3	1	0	0	0	0
56	D4	1	0	0	0	0
56	D7	3	0	0	0	0
56	D8	1	0	0	0	0
56	DA	1174	0	0	171	0
56	DB	17	0	0	0	0
56	DD	8	0	0	2	0
56	DE	11	0	0	2	0
56	DF	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DN	1	0	0	0	0
56	DO	5	0	0	1	0
56	DP	10	0	0	1	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	1	0
56	DT	2	0	0	0	0
56	DU	5	0	0	0	0
56	DV	2	0	0	1	0
56	DW	2	0	0	0	0
56	DX	1	0	0	1	0
56	DY	2	0	0	0	0
All	All	286308	0	187082	8298	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8298 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1441:G:H2'	1:AA:1459:C:N4	1.20	1.46
1:AA:1459:C:C5	1:AA:1460:A:N6	1.79	1.44
1:AA:1441:G:C2'	1:AA:1459:C:N4	1.88	1.36
1:AA:1441:G:C2'	1:AA:1459:C:H41	1.44	1.29
1:CA:1441:G:H2'	1:CA:1459:C:N4	1.50	1.25

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BA:1594:G:OP1	56:BB:323:HOH:O[1_455]	2.18	0.02
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

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	228/256 (89%)	199 (87%)	28 (12%)	1 (0%)	34	69
2	CB	227/256 (89%)	197 (87%)	29 (13%)	1 (0%)	34	69
3	AC	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	29	64
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	CD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	AE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	22	57
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	42
7	CG	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	22	57
8	AH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
8	CH	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
9	AI	123/128 (96%)	112 (91%)	10 (8%)	1 (1%)	19	54
9	CI	123/128 (96%)	111 (90%)	11 (9%)	1 (1%)	19	54
10	AJ	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	4	22
10	CJ	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	7	30
11	AK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
11	CK	112/129 (87%)	106 (95%)	6 (5%)	0	100	100
12	AL	120/132 (91%)	110 (92%)	9 (8%)	1 (1%)	19	54
12	CL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	19	54
13	AM	112/126 (89%)	89 (80%)	21 (19%)	2 (2%)	8	34
13	CM	112/126 (89%)	87 (78%)	21 (19%)	4 (4%)	3	20
14	AN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	21
14	CN	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
15	CO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	6	28
16	AP	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	12	42
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
19	AS	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	12	42
19	CS	79/93 (85%)	65 (82%)	13 (16%)	1 (1%)	12	42
20	AT	85/106 (80%)	78 (92%)	7 (8%)	0	100	100
20	CT	95/106 (90%)	84 (88%)	8 (8%)	3 (3%)	4	22
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	AX	93/101 (92%)	79 (85%)	13 (14%)	1 (1%)	14	46
22	CX	93/101 (92%)	84 (90%)	9 (10%)	0	100	100
25	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	34	69
25	DD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	69
26	BE	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	49
26	DE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	15	49
27	BF	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
27	DF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	64
28	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	59
28	DG	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
29	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	59
29	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	59
30	BI	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	11	40
30	DI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	40
31	BN	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	6	29
31	DN	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	6	29
32	BO	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
32	DO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
33	BP	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
33	DP	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
34	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	57
35	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
35	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
36	BS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
36	DS	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
37	BT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	114 (100%)	0	0	100	100
38	DU	114/118 (97%)	114 (100%)	0	0	100	100
39	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	17	52
40	DW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	15	49
42	DY	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	15	49
43	BZ	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	15	49
43	DZ	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	15	49
44	B0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
44	D0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	46
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	46
46	B2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
46	D2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
47	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
47	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	B4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
48	D4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
50	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
51	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	29
51	D7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	29
52	B8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
52	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	11552/12330 (94%)	10628 (92%)	855 (7%)	69 (1%)	25	59

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	CT	100	ILE
12	AL	28	LYS
14	AN	15	LYS
16	AP	79	VAL
12	CL	28	LYS

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	178/220 (81%)	133 (75%)	45 (25%)	0	1
2	CB	177/220 (80%)	133 (75%)	44 (25%)	0	2
3	AC	114/188 (61%)	79 (69%)	35 (31%)	0	0
3	CC	114/188 (61%)	92 (81%)	22 (19%)	1	6
4	AD	141/181 (78%)	118 (84%)	23 (16%)	2	10
4	CD	141/181 (78%)	119 (84%)	22 (16%)	2	11
5	AE	108/123 (88%)	87 (81%)	21 (19%)	1	6
5	CE	108/123 (88%)	87 (81%)	21 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	76/90 (84%)	61 (80%)	15 (20%)	1	6
6	CF	76/90 (84%)	58 (76%)	18 (24%)	1	2
7	AG	103/127 (81%)	73 (71%)	30 (29%)	0	1
7	CG	103/127 (81%)	68 (66%)	35 (34%)	0	0
8	AH	103/119 (87%)	82 (80%)	21 (20%)	1	5
8	CH	103/119 (87%)	83 (81%)	20 (19%)	1	6
9	AI	62/99 (63%)	47 (76%)	15 (24%)	0	2
9	CI	62/99 (63%)	47 (76%)	15 (24%)	0	2
10	AJ	53/92 (58%)	38 (72%)	15 (28%)	0	1
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0	1
11	AK	81/99 (82%)	71 (88%)	10 (12%)	4	19
11	CK	81/99 (82%)	70 (86%)	11 (14%)	3	16
12	AL	91/109 (84%)	80 (88%)	11 (12%)	5	20
12	CL	91/109 (84%)	81 (89%)	10 (11%)	6	25
13	AM	64/101 (63%)	48 (75%)	16 (25%)	0	2
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	3
14	AN	46/50 (92%)	36 (78%)	10 (22%)	1	4
14	CN	46/50 (92%)	32 (70%)	14 (30%)	0	0
15	AO	77/80 (96%)	68 (88%)	9 (12%)	5	22
15	CO	77/80 (96%)	68 (88%)	9 (12%)	5	22
16	AP	63/74 (85%)	46 (73%)	17 (27%)	0	1
16	CP	63/74 (85%)	44 (70%)	19 (30%)	0	0
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	3	13
17	CQ	94/97 (97%)	81 (86%)	13 (14%)	3	16
18	AR	49/77 (64%)	44 (90%)	5 (10%)	7	27
18	CR	49/77 (64%)	44 (90%)	5 (10%)	7	27
19	AS	43/80 (54%)	26 (60%)	17 (40%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0	1
20	AT	64/82 (78%)	55 (86%)	9 (14%)	3	15
20	CT	65/82 (79%)	55 (85%)	10 (15%)	2	11
21	AU	18/22 (82%)	13 (72%)	5 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	18/22 (82%)	11 (61%)	7 (39%)	0	0
22	AX	45/87 (52%)	34 (76%)	11 (24%)	0	2
22	CX	38/87 (44%)	29 (76%)	9 (24%)	1	2
25	BD	215/218 (99%)	182 (85%)	33 (15%)	2	12
25	DD	215/218 (99%)	183 (85%)	32 (15%)	3	13
26	BE	163/166 (98%)	135 (83%)	28 (17%)	2	9
26	DE	163/166 (98%)	137 (84%)	26 (16%)	2	11
27	BF	159/166 (96%)	135 (85%)	24 (15%)	3	12
27	DF	159/166 (96%)	134 (84%)	25 (16%)	2	11
28	BG	128/156 (82%)	109 (85%)	19 (15%)	3	13
28	DG	128/156 (82%)	109 (85%)	19 (15%)	3	13
29	BH	141/148 (95%)	123 (87%)	18 (13%)	4	18
29	DH	141/148 (95%)	123 (87%)	18 (13%)	4	18
30	BI	98/124 (79%)	81 (83%)	17 (17%)	2	9
30	DI	74/124 (60%)	60 (81%)	14 (19%)	1	6
31	BN	117/119 (98%)	98 (84%)	19 (16%)	2	10
31	DN	117/119 (98%)	98 (84%)	19 (16%)	2	10
32	BO	98/100 (98%)	82 (84%)	16 (16%)	2	10
32	DO	98/100 (98%)	83 (85%)	15 (15%)	2	12
33	BP	114/116 (98%)	99 (87%)	15 (13%)	4	17
33	DP	114/116 (98%)	99 (87%)	15 (13%)	4	17
34	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
35	BR	101/101 (100%)	79 (78%)	22 (22%)	1	4
35	DR	101/101 (100%)	77 (76%)	24 (24%)	0	2
36	BS	84/88 (96%)	67 (80%)	17 (20%)	1	5
36	DS	84/88 (96%)	68 (81%)	16 (19%)	1	6
37	BT	110/127 (87%)	98 (89%)	12 (11%)	6	25
37	DT	110/127 (87%)	95 (86%)	15 (14%)	3	16
38	BU	93/94 (99%)	82 (88%)	11 (12%)	5	21
38	DU	93/94 (99%)	83 (89%)	10 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BV	80/82 (98%)	63 (79%)	17 (21%)	1	4
39	DV	80/82 (98%)	63 (79%)	17 (21%)	1	4
40	BW	89/92 (97%)	81 (91%)	8 (9%)	9	34
40	DW	89/92 (97%)	78 (88%)	11 (12%)	4	19
41	BX	75/78 (96%)	71 (95%)	4 (5%)	22	54
41	DX	75/78 (96%)	70 (93%)	5 (7%)	16	46
42	BY	80/91 (88%)	64 (80%)	16 (20%)	1	5
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	4
43	BZ	159/179 (89%)	137 (86%)	22 (14%)	3	16
43	DZ	159/179 (89%)	139 (87%)	20 (13%)	4	18
44	B0	59/67 (88%)	51 (86%)	8 (14%)	3	16
44	D0	59/67 (88%)	50 (85%)	9 (15%)	2	12
45	B1	78/83 (94%)	63 (81%)	15 (19%)	1	6
45	D1	78/83 (94%)	66 (85%)	12 (15%)	2	11
46	B2	65/67 (97%)	54 (83%)	11 (17%)	2	9
46	D2	65/67 (97%)	55 (85%)	10 (15%)	2	11
47	B3	49/52 (94%)	44 (90%)	5 (10%)	7	27
47	D3	49/52 (94%)	44 (90%)	5 (10%)	7	27
48	B4	39/63 (62%)	33 (85%)	6 (15%)	2	11
48	D4	39/63 (62%)	33 (85%)	6 (15%)	2	11
49	B5	50/52 (96%)	42 (84%)	8 (16%)	2	11
49	D5	50/52 (96%)	41 (82%)	9 (18%)	1	7
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	4
50	D6	50/52 (96%)	40 (80%)	10 (20%)	1	5
51	B7	41/42 (98%)	34 (83%)	7 (17%)	2	9
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2	9
52	B8	52/55 (94%)	42 (81%)	10 (19%)	1	6
52	D8	52/55 (94%)	42 (81%)	10 (19%)	1	6
53	B9	32/34 (94%)	28 (88%)	4 (12%)	4	18
53	D9	32/34 (94%)	28 (88%)	4 (12%)	4	18
All	All	8775/10240 (86%)	7244 (83%)	1531 (17%)	2	9

5 of 1531 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	74	ARG
4	CD	158	ILE
42	DY	6	HIS
46	B2	32	LEU
2	CB	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
38	BU	49	HIS
2	CB	140	HIS
33	DP	84	ASN
39	BV	80	GLN
46	B2	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1499/1522 (98%)	385 (25%)	33 (2%)
1	CA	1495/1522 (98%)	396 (26%)	34 (2%)
23	BA	2833/2913 (97%)	609 (21%)	60 (2%)
23	DA	2807/2913 (96%)	600 (21%)	56 (1%)
24	BB	119/122 (97%)	25 (21%)	0
24	DB	119/122 (97%)	26 (21%)	0
All	All	8872/9114 (97%)	2041 (23%)	183 (2%)

5 of 2041 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	32	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2126	A

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Mol	Chain	Res	Type
1	CA	495	A
23	DA	1819	A
23	BA	2318	G
23	BA	2802	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1662 ligands modelled in this entry, 1662 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1501/1522 (98%)	0.01	57 (3%) 40 20	47, 95, 155, 169	0
1	CA	1497/1522 (98%)	-0.01	63 (4%) 36 18	50, 96, 158, 171	0
2	AB	230/256 (89%)	-0.08	8 (3%) 44 23	87, 114, 134, 148	0
2	CB	229/256 (89%)	0.31	9 (3%) 39 20	92, 116, 136, 149	0
3	AC	206/239 (86%)	0.06	5 (2%) 59 37	85, 109, 127, 136	0
3	CC	206/239 (86%)	0.34	15 (7%) 15 6	94, 120, 143, 158	0
4	AD	208/209 (99%)	-0.05	5 (2%) 59 37	75, 94, 114, 125	0
4	CD	208/209 (99%)	0.03	3 (1%) 75 56	76, 93, 114, 124	0
5	AE	148/162 (91%)	-0.21	0 100 100	66, 86, 103, 125	0
5	CE	148/162 (91%)	-0.07	3 (2%) 65 44	69, 88, 104, 127	0
6	AF	100/101 (99%)	-0.31	1 (1%) 82 67	67, 82, 100, 116	0
6	CF	100/101 (99%)	-0.32	1 (1%) 82 67	70, 86, 103, 117	0
7	AG	155/156 (99%)	1.94	67 (43%) 0 0	113, 139, 153, 159	0
7	CG	155/156 (99%)	1.93	69 (44%) 0 0	122, 137, 149, 159	0
8	AH	138/138 (100%)	0.10	2 (1%) 75 56	71, 90, 100, 110	0
8	CH	138/138 (100%)	-0.04	5 (3%) 42 22	71, 92, 103, 113	0
9	AI	125/128 (97%)	1.16	33 (26%) 0 0	110, 137, 149, 154	0
9	CI	125/128 (97%)	2.58	65 (52%) 0 0	115, 139, 152, 163	0
10	AJ	96/105 (91%)	1.55	32 (33%) 0 0	92, 126, 141, 147	0
10	CJ	96/105 (91%)	1.93	41 (42%) 0 0	108, 134, 150, 160	0
11	AK	114/129 (88%)	-0.05	1 (0%) 84 69	60, 86, 108, 120	0
11	CK	114/129 (88%)	0.07	5 (4%) 34 17	63, 89, 107, 126	0
12	AL	122/132 (92%)	-0.12	1 (0%) 86 72	62, 77, 95, 112	0
12	CL	122/132 (92%)	-0.03	0 100 100	63, 77, 96, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	1.46	34 (29%) 0 0	112, 139, 150, 153	0
13	CM	114/126 (90%)	1.84	41 (35%) 0 0	116, 140, 151, 160	0
14	AN	60/61 (98%)	0.70	8 (13%) 3 1	93, 118, 131, 144	0
14	CN	60/61 (98%)	0.79	8 (13%) 3 1	103, 122, 134, 139	0
15	AO	88/89 (98%)	-0.12	0 100 100	63, 85, 103, 113	0
15	CO	88/89 (98%)	0.02	1 (1%) 80 64	63, 85, 105, 111	0
16	AP	82/88 (93%)	0.56	8 (9%) 7 2	76, 88, 110, 120	0
16	CP	82/88 (93%)	0.33	4 (4%) 29 14	73, 85, 105, 117	0
17	AQ	99/105 (94%)	-0.02	1 (1%) 82 67	68, 82, 102, 106	0
17	CQ	99/105 (94%)	0.08	1 (1%) 82 67	69, 83, 101, 108	0
18	AR	68/88 (77%)	-0.10	2 (2%) 51 28	71, 82, 105, 112	0
18	CR	68/88 (77%)	0.17	1 (1%) 73 54	75, 85, 105, 117	0
19	AS	81/93 (87%)	2.34	37 (45%) 0 0	113, 138, 147, 152	0
19	CS	81/93 (87%)	2.81	44 (54%) 0 0	114, 140, 150, 153	0
20	AT	87/106 (82%)	0.30	0 100 100	75, 88, 103, 111	0
20	CT	97/106 (91%)	0.06	0 100 100	72, 86, 105, 115	0
21	AU	23/27 (85%)	3.23	14 (60%) 0 0	128, 136, 145, 154	0
21	CU	23/27 (85%)	4.11	18 (78%) 0 0	129, 137, 148, 150	0
22	AX	95/101 (94%)	0.18	4 (4%) 36 18	69, 94, 115, 123	0
22	CX	95/101 (94%)	1.08	17 (17%) 1 0	88, 106, 129, 145	0
23	BA	2837/2913 (97%)	-0.26	49 (1%) 70 49	26, 47, 132, 176	0
23	DA	2814/2913 (96%)	-0.41	77 (2%) 54 31	28, 50, 133, 176	0
24	BB	120/122 (98%)	-0.37	0 100 100	43, 72, 93, 110	0
24	DB	120/122 (98%)	-0.14	1 (0%) 86 72	48, 81, 106, 117	0
25	BD	275/276 (99%)	-0.44	0 100 100	29, 45, 63, 113	0
25	DD	275/276 (99%)	-0.44	1 (0%) 92 84	30, 47, 66, 116	0
26	BE	204/206 (99%)	-0.40	0 100 100	28, 49, 72, 95	0
26	DE	204/206 (99%)	-0.42	0 100 100	29, 50, 76, 95	0
27	BF	203/210 (96%)	-0.40	0 100 100	29, 54, 88, 111	0
27	DF	203/210 (96%)	-0.35	0 100 100	31, 59, 90, 112	0
28	BG	181/182 (99%)	-0.03	8 (4%) 34 17	76, 110, 133, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	0.81	25 (13%) 2 1	86, 117, 138, 148	0
29	BH	174/180 (96%)	-0.30	0 100 100	54, 73, 94, 110	0
29	DH	174/180 (96%)	0.33	7 (4%) 38 19	65, 82, 101, 119	0
30	BI	146/148 (98%)	-0.38	1 (0%) 87 75	54, 81, 99, 115	0
30	DI	146/148 (98%)	-0.04	2 (1%) 75 56	56, 89, 108, 120	0
31	BN	140/140 (100%)	-0.38	0 100 100	38, 49, 78, 92	0
31	DN	140/140 (100%)	-0.29	1 (0%) 87 75	40, 54, 82, 96	0
32	BO	122/122 (100%)	-0.41	0 100 100	35, 50, 69, 77	0
32	DO	122/122 (100%)	-0.57	0 100 100	36, 52, 69, 77	0
33	BP	149/150 (99%)	-0.31	0 100 100	30, 58, 89, 105	0
33	DP	149/150 (99%)	-0.18	3 (2%) 65 44	31, 62, 92, 112	0
34	BQ	141/141 (100%)	-0.33	0 100 100	39, 54, 71, 83	0
34	DQ	141/141 (100%)	-0.36	0 100 100	41, 58, 77, 88	0
35	BR	118/118 (100%)	-0.32	0 100 100	34, 44, 58, 77	0
35	DR	118/118 (100%)	-0.32	0 100 100	36, 47, 62, 78	0
36	BS	110/112 (98%)	-0.11	0 100 100	50, 69, 89, 96	0
36	DS	110/112 (98%)	0.29	5 (4%) 33 16	55, 74, 94, 102	0
37	BT	131/146 (89%)	-0.44	0 100 100	43, 55, 92, 119	0
37	DT	131/146 (89%)	-0.36	1 (0%) 86 72	46, 57, 93, 128	0
38	BU	116/118 (98%)	-0.43	0 100 100	32, 44, 62, 71	0
38	DU	116/118 (98%)	-0.51	0 100 100	34, 48, 66, 73	0
39	BV	101/101 (100%)	-0.35	1 (0%) 82 67	29, 56, 79, 103	0
39	DV	101/101 (100%)	-0.23	0 100 100	32, 62, 85, 103	0
40	BW	112/113 (99%)	-0.42	0 100 100	33, 40, 62, 103	0
40	DW	112/113 (99%)	-0.49	0 100 100	35, 42, 67, 105	0
41	BX	95/96 (98%)	-0.28	0 100 100	38, 49, 72, 88	0
41	DX	95/96 (98%)	-0.31	1 (1%) 80 64	41, 52, 77, 90	0
42	BY	107/110 (97%)	-0.29	0 100 100	47, 61, 85, 108	0
42	DY	107/110 (97%)	0.16	6 (5%) 24 11	52, 65, 89, 113	0
43	BZ	201/206 (97%)	-0.42	0 100 100	53, 76, 99, 122	0
43	DZ	198/206 (96%)	0.02	5 (2%) 57 34	62, 81, 102, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	-0.31	0 100 100	39, 48, 64, 91	0
44	D0	76/85 (89%)	0.04	2 (2%) 56 33	43, 52, 66, 92	0
45	B1	97/98 (98%)	-0.23	0 100 100	36, 48, 82, 97	0
45	D1	97/98 (98%)	-0.18	2 (2%) 63 43	36, 51, 83, 98	0
46	B2	70/72 (97%)	-0.26	0 100 100	46, 60, 76, 107	0
46	D2	70/72 (97%)	-0.23	0 100 100	50, 64, 81, 103	0
47	B3	59/60 (98%)	-0.25	0 100 100	38, 49, 86, 97	0
47	D3	59/60 (98%)	0.14	1 (1%) 70 49	41, 53, 93, 102	0
48	B4	46/71 (64%)	-0.30	2 (4%) 35 17	101, 129, 144, 148	0
48	D4	46/71 (64%)	0.46	5 (10%) 5 2	113, 133, 144, 152	0
49	B5	59/60 (98%)	-0.54	0 100 100	30, 45, 66, 80	0
49	D5	59/60 (98%)	-0.54	0 100 100	32, 47, 68, 81	0
50	B6	53/54 (98%)	-0.56	0 100 100	42, 51, 70, 79	0
50	D6	53/54 (98%)	-0.26	2 (3%) 40 20	43, 54, 72, 82	0
51	B7	48/49 (97%)	-0.31	0 100 100	30, 34, 55, 80	0
51	D7	48/49 (97%)	-0.22	0 100 100	32, 35, 58, 84	0
52	B8	64/65 (98%)	-0.27	0 100 100	38, 43, 52, 70	0
52	D8	64/65 (98%)	-0.21	0 100 100	40, 45, 55, 70	0
53	B9	36/37 (97%)	0.24	0 100 100	44, 55, 62, 73	0
53	D9	36/37 (97%)	0.41	1 (2%) 53 30	47, 59, 68, 75	0
All	All	20641/21444 (96%)	-0.05	943 (4%) 32 16	26, 71, 144, 176	0

The worst 5 of 943 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	CU	11	GLY	11.7
19	CS	69	HIS	10.9
21	CU	12	LYS	10.2
19	CS	4	SER	10.1
19	AS	33	THR	9.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1669	1/1	0.15	0.17	103,103,103,103	0
54	MG	AA	1717	1/1	0.46	0.14	93,93,93,93	0
54	MG	CA	1755	1/1	0.50	0.12	129,129,129,129	0
54	MG	CA	1692	1/1	0.50	0.51	86,86,86,86	0
54	MG	CA	1660	1/1	0.51	0.41	70,70,70,70	0
54	MG	BA	3237	1/1	0.51	0.32	71,71,71,71	0
54	MG	BA	3232	1/1	0.53	0.18	64,64,64,64	0
54	MG	DA	3532	1/1	0.54	0.23	116,116,116,116	0
54	MG	AA	1705	1/1	0.55	0.39	97,97,97,97	0
54	MG	BA	3570	1/1	0.55	0.12	78,78,78,78	0
54	MG	BA	3654	1/1	0.57	0.15	126,126,126,126	0
55	ZN	D4	101	1/1	0.58	0.08	214,214,214,214	0
54	MG	BA	3512	1/1	0.59	0.28	109,109,109,109	0
54	MG	BA	3337	1/1	0.60	0.21	49,49,49,49	0
54	MG	DA	3202	1/1	0.61	0.33	66,66,66,66	0
54	MG	DA	3530	1/1	0.61	0.24	132,132,132,132	0
54	MG	DA	3410	1/1	0.61	0.12	86,86,86,86	0
54	MG	AA	1625	1/1	0.62	0.40	79,79,79,79	0
54	MG	CA	1633	1/1	0.64	0.56	77,77,77,77	0
54	MG	DA	3177	1/1	0.64	0.13	88,88,88,88	0
54	MG	BA	3240	1/1	0.65	0.28	71,71,71,71	0
54	MG	AA	1723	1/1	0.65	0.12	112,112,112,112	0
54	MG	DA	3164	1/1	0.66	0.38	56,56,56,56	0
54	MG	CA	1711	1/1	0.66	0.11	103,103,103,103	0
54	MG	BA	3367	1/1	0.67	0.20	71,71,71,71	0
54	MG	AA	1706	1/1	0.67	0.10	91,91,91,91	0
54	MG	AA	1603	1/1	0.67	0.36	79,79,79,79	0
54	MG	DA	3506	1/1	0.67	0.11	96,96,96,96	0
54	MG	BA	3239	1/1	0.67	0.15	67,67,67,67	0
54	MG	DA	3278	1/1	0.67	0.07	83,83,83,83	0
54	MG	BA	3097	1/1	0.68	0.54	47,47,47,47	0
54	MG	AA	1622	1/1	0.68	0.19	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1757	1/1	0.69	0.25	80,80,80,80	0
54	MG	AA	1614	1/1	0.69	0.50	56,56,56,56	0
54	MG	CE	201	1/1	0.69	0.56	77,77,77,77	0
54	MG	BA	3593	1/1	0.69	0.21	84,84,84,84	0
54	MG	DA	3165	1/1	0.69	0.41	60,60,60,60	0
54	MG	CA	1637	1/1	0.69	0.42	73,73,73,73	0
54	MG	BA	3600	1/1	0.69	0.07	81,81,81,81	0
54	MG	BA	3554	1/1	0.69	0.10	88,88,88,88	0
54	MG	AA	1651	1/1	0.70	0.31	60,60,60,60	0
54	MG	BA	3442	1/1	0.70	0.16	76,76,76,76	0
54	MG	BA	3146	1/1	0.70	0.60	65,65,65,65	0
54	MG	AA	1637	1/1	0.70	0.24	84,84,84,84	0
54	MG	DA	3081	1/1	0.70	0.58	58,58,58,58	0
54	MG	CA	1604	1/1	0.71	0.51	81,81,81,81	0
54	MG	DA	3401	1/1	0.71	0.29	108,108,108,108	0
54	MG	DA	3075	1/1	0.71	0.26	58,58,58,58	0
54	MG	BA	3340	1/1	0.71	0.14	79,79,79,79	0
54	MG	BA	3369	1/1	0.71	0.13	52,52,52,52	0
54	MG	DB	204	1/1	0.71	0.70	74,74,74,74	0
54	MG	BA	3642	1/1	0.72	0.15	139,139,139,139	0
54	MG	DA	3212	1/1	0.72	0.26	75,75,75,75	0
54	MG	CA	1684	1/1	0.72	0.33	91,91,91,91	0
54	MG	AA	1709	1/1	0.73	0.15	101,101,101,101	0
54	MG	CA	1747	1/1	0.73	0.11	95,95,95,95	0
54	MG	DA	3524	1/1	0.73	0.17	79,79,79,79	0
54	MG	AA	1659	1/1	0.73	0.86	70,70,70,70	0
54	MG	BA	3510	1/1	0.74	0.11	56,56,56,56	0
54	MG	BA	3532	1/1	0.74	0.23	79,79,79,79	0
54	MG	AA	1618	1/1	0.74	1.13	94,94,94,94	0
54	MG	AA	1619	1/1	0.74	0.26	86,86,86,86	0
54	MG	DA	3058	1/1	0.74	0.43	58,58,58,58	0
54	MG	DA	3290	1/1	0.74	0.48	58,58,58,58	0
54	MG	CA	1652	1/1	0.74	0.50	76,76,76,76	0
54	MG	AA	1678	1/1	0.74	0.52	74,74,74,74	0
54	MG	DA	3187	1/1	0.74	0.14	71,71,71,71	0
54	MG	BB	223	1/1	0.75	0.14	133,133,133,133	0
54	MG	CA	1640	1/1	0.75	0.23	82,82,82,82	0
54	MG	BA	3638	1/1	0.75	0.14	67,67,67,67	0
54	MG	AA	1607	1/1	0.76	0.19	78,78,78,78	0
54	MG	BA	3347	1/1	0.76	0.16	94,94,94,94	0
54	MG	DA	3331	1/1	0.76	0.13	71,71,71,71	0
54	MG	BA	3524	1/1	0.76	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3646	1/1	0.76	0.18	142,142,142,142	0
54	MG	DA	3541	1/1	0.76	0.12	130,130,130,130	0
54	MG	BA	3317	1/1	0.76	0.17	34,34,34,34	0
54	MG	DA	3342	1/1	0.76	0.18	38,38,38,38	0
54	MG	AA	1702	1/1	0.76	0.16	68,68,68,68	0
54	MG	BA	3038	1/1	0.76	0.26	76,76,76,76	0
54	MG	AA	1688	1/1	0.76	0.16	96,96,96,96	0
54	MG	BA	3261	1/1	0.77	0.36	34,34,34,34	0
54	MG	BA	3264	1/1	0.77	0.38	41,41,41,41	0
54	MG	BA	3368	1/1	0.77	0.21	53,53,53,53	0
54	MG	AA	1729	1/1	0.77	0.08	80,80,80,80	0
54	MG	DA	3280	1/1	0.77	0.44	58,58,58,58	0
54	MG	CA	1697	1/1	0.77	0.13	57,57,57,57	0
54	MG	BA	3113	1/1	0.77	0.09	60,60,60,60	0
54	MG	DA	3179	1/1	0.77	0.21	68,68,68,68	0
54	MG	BA	3338	1/1	0.77	0.15	62,62,62,62	0
54	MG	CA	1670	1/1	0.77	0.64	73,73,73,73	0
54	MG	BA	3133	1/1	0.78	0.27	53,53,53,53	0
54	MG	BA	3543	1/1	0.78	0.20	119,119,119,119	0
54	MG	DA	3096	1/1	0.78	0.53	59,59,59,59	0
54	MG	AA	1628	1/1	0.78	0.25	68,68,68,68	0
54	MG	DA	3115	1/1	0.78	0.42	59,59,59,59	0
54	MG	CA	1704	1/1	0.78	0.15	92,92,92,92	0
54	MG	DA	3284	1/1	0.79	0.22	55,55,55,55	0
54	MG	DA	3298	1/1	0.79	0.27	49,49,49,49	0
54	MG	DA	3196	1/1	0.79	0.39	58,58,58,58	0
54	MG	BA	3581	1/1	0.79	0.11	86,86,86,86	0
54	MG	AA	1719	1/1	0.79	0.16	144,144,144,144	0
54	MG	BA	3216	1/1	0.79	0.30	43,43,43,43	0
54	MG	BA	3109	1/1	0.79	0.41	62,62,62,62	0
54	MG	CA	1657	1/1	0.79	0.41	61,61,61,61	0
54	MG	DA	3239	1/1	0.79	0.55	58,58,58,58	0
54	MG	BV	201	1/1	0.79	0.22	67,67,67,67	0
54	MG	BA	3238	1/1	0.79	0.36	53,53,53,53	0
54	MG	BA	3236	1/1	0.79	0.23	66,66,66,66	0
54	MG	AA	1704	1/1	0.79	0.16	86,86,86,86	0
54	MG	DA	3172	1/1	0.79	0.29	64,64,64,64	0
54	MG	BA	3477	1/1	0.80	0.11	53,53,53,53	0
54	MG	CA	1706	1/1	0.80	0.10	103,103,103,103	0
54	MG	CA	1667	1/1	0.80	0.33	77,77,77,77	0
54	MG	DA	3466	1/1	0.80	0.15	68,68,68,68	0
54	MG	BA	3241	1/1	0.80	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1699	1/1	0.80	0.20	99,99,99,99	0
54	MG	BA	3287	1/1	0.80	0.42	44,44,44,44	0
54	MG	BA	3014	1/1	0.80	0.54	65,65,65,65	0
54	MG	CA	1707	1/1	0.80	0.19	94,94,94,94	0
54	MG	CA	1705	1/1	0.80	0.14	96,96,96,96	0
54	MG	CA	1720	1/1	0.80	0.14	89,89,89,89	0
54	MG	BA	3547	1/1	0.80	0.24	105,105,105,105	0
54	MG	BA	3102	1/1	0.80	0.34	44,44,44,44	0
54	MG	AA	1690	1/1	0.80	0.09	72,72,72,72	0
54	MG	BA	3616	1/1	0.80	0.28	131,131,131,131	0
54	MG	AA	1692	1/1	0.80	0.57	144,144,144,144	0
54	MG	BA	3582	1/1	0.80	0.23	79,79,79,79	0
54	MG	AA	1697	1/1	0.80	0.20	106,106,106,106	0
54	MG	DA	3478	1/1	0.81	0.17	87,87,87,87	0
54	MG	DA	3525	1/1	0.81	0.16	106,106,106,106	0
54	MG	DA	3591	1/1	0.81	0.11	66,66,66,66	0
54	MG	BA	3394	1/1	0.81	0.15	50,50,50,50	0
54	MG	CA	1753	1/1	0.81	0.14	86,86,86,86	0
54	MG	AA	1671	1/1	0.81	0.34	67,67,67,67	0
54	MG	DA	3134	1/1	0.81	0.28	62,62,62,62	0
54	MG	DA	3361	1/1	0.81	0.10	30,30,30,30	0
54	MG	BA	3544	1/1	0.81	0.15	46,46,46,46	0
54	MG	BA	3627	1/1	0.81	0.10	50,50,50,50	0
54	MG	BA	3648	1/1	0.81	0.11	91,91,91,91	0
54	MG	CA	1686	1/1	0.81	0.21	61,61,61,61	0
54	MG	DA	3055	1/1	0.81	0.32	56,56,56,56	0
54	MG	BA	3234	1/1	0.81	0.14	69,69,69,69	0
54	MG	BA	3403	1/1	0.81	0.15	67,67,67,67	0
54	MG	DA	3110	1/1	0.81	0.31	53,53,53,53	0
54	MG	AA	1731	1/1	0.81	0.17	119,119,119,119	0
54	MG	AA	1646	1/1	0.81	0.22	59,59,59,59	0
54	MG	BA	3358	1/1	0.81	0.12	55,55,55,55	0
54	MG	DA	3149	1/1	0.81	0.37	53,53,53,53	0
54	MG	DA	3424	1/1	0.81	0.10	52,52,52,52	0
54	MG	CA	1714	1/1	0.81	0.15	87,87,87,87	0
54	MG	CA	1608	1/1	0.81	0.53	93,93,93,93	0
54	MG	BA	3074	1/1	0.81	0.44	53,53,53,53	0
54	MG	BA	3269	1/1	0.81	0.48	35,35,35,35	0
54	MG	BA	3645	1/1	0.81	0.09	102,102,102,102	0
54	MG	BE	305	1/1	0.82	0.16	60,60,60,60	0
54	MG	CA	1626	1/1	0.82	0.39	62,62,62,62	0
54	MG	DA	3198	1/1	0.82	0.78	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3016	1/1	0.82	0.23	47,47,47,47	0
54	MG	DA	3476	1/1	0.82	0.13	66,66,66,66	0
54	MG	DA	3297	1/1	0.82	0.22	78,78,78,78	0
54	MG	DA	3180	1/1	0.82	0.24	49,49,49,49	0
54	MG	BA	3343	1/1	0.82	0.09	73,73,73,73	0
54	MG	DA	3220	1/1	0.82	0.24	51,51,51,51	0
54	MG	BA	3504	1/1	0.82	0.14	65,65,65,65	0
54	MG	CA	1702	1/1	0.82	0.12	64,64,64,64	0
54	MG	CA	1756	1/1	0.82	0.19	80,80,80,80	0
54	MG	BA	3062	1/1	0.82	0.34	45,45,45,45	0
54	MG	BA	3577	1/1	0.82	0.13	77,77,77,77	0
54	MG	BA	3562	1/1	0.82	0.13	59,59,59,59	0
54	MG	CA	1681	1/1	0.82	0.40	82,82,82,82	0
54	MG	DA	3246	1/1	0.82	0.38	68,68,68,68	0
54	MG	CA	1717	1/1	0.82	0.14	110,110,110,110	0
54	MG	DA	3268	1/1	0.82	0.59	54,54,54,54	0
54	MG	AA	1629	1/1	0.82	0.29	44,44,44,44	0
54	MG	AA	1661	1/1	0.82	0.26	55,55,55,55	0
54	MG	DA	3590	1/1	0.82	0.23	82,82,82,82	0
54	MG	BA	3149	1/1	0.83	0.28	57,57,57,57	0
54	MG	DA	3063	1/1	0.83	0.32	60,60,60,60	0
54	MG	DA	3309	1/1	0.83	0.40	28,28,28,28	0
54	MG	BA	3637	1/1	0.83	0.18	108,108,108,108	0
54	MG	DA	3557	1/1	0.83	0.16	103,103,103,103	0
54	MG	CA	1603	1/1	0.83	0.30	56,56,56,56	0
54	MG	DA	3167	1/1	0.83	0.21	51,51,51,51	0
54	MG	DA	3247	1/1	0.83	0.32	67,67,67,67	0
54	MG	DA	3569	1/1	0.83	0.12	104,104,104,104	0
54	MG	DA	3438	1/1	0.83	0.17	90,90,90,90	0
54	MG	DA	3451	1/1	0.83	0.14	103,103,103,103	0
54	MG	BA	3164	1/1	0.83	0.35	50,50,50,50	0
54	MG	BA	3304	1/1	0.83	0.35	54,54,54,54	0
54	MG	AA	1686	1/1	0.83	0.11	68,68,68,68	0
54	MG	DA	3282	1/1	0.83	0.14	64,64,64,64	0
54	MG	BA	3141	1/1	0.83	0.30	36,36,36,36	0
54	MG	DA	3170	1/1	0.83	0.13	56,56,56,56	0
54	MG	CA	1618	1/1	0.83	0.39	64,64,64,64	0
54	MG	BA	3399	1/1	0.83	0.13	43,43,43,43	0
54	MG	CA	1664	1/1	0.83	0.08	80,80,80,80	0
54	MG	BA	3649	1/1	0.83	0.22	125,125,125,125	0
54	MG	BA	3567	1/1	0.83	0.10	54,54,54,54	0
54	MG	DA	3515	1/1	0.83	0.28	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3370	1/1	0.83	0.23	41,41,41,41	0
54	MG	BA	3090	1/1	0.83	0.12	62,62,62,62	0
54	MG	BA	3061	1/1	0.83	0.47	54,54,54,54	0
54	MG	BS	201	1/1	0.83	0.55	49,49,49,49	0
54	MG	DA	3371	1/1	0.83	0.26	43,43,43,43	0
54	MG	DA	3189	1/1	0.83	0.18	84,84,84,84	0
54	MG	BA	3531	1/1	0.83	0.09	89,89,89,89	0
54	MG	DA	3122	1/1	0.84	0.20	49,49,49,49	0
54	MG	DA	3587	1/1	0.84	0.24	95,95,95,95	0
54	MG	AA	1635	1/1	0.84	0.15	61,61,61,61	0
54	MG	DA	3207	1/1	0.84	0.28	54,54,54,54	0
54	MG	BA	3077	1/1	0.84	0.27	42,42,42,42	0
54	MG	BA	3225	1/1	0.84	0.18	44,44,44,44	0
54	MG	AA	1636	1/1	0.84	0.27	79,79,79,79	0
54	MG	DA	3523	1/1	0.84	0.07	74,74,74,74	0
54	MG	DA	3193	1/1	0.84	0.58	40,40,40,40	0
54	MG	DA	3197	1/1	0.84	0.33	49,49,49,49	0
54	MG	DA	3065	1/1	0.84	0.14	53,53,53,53	0
54	MG	BA	3139	1/1	0.84	0.27	46,46,46,46	0
54	MG	CA	1683	1/1	0.84	0.21	100,100,100,100	0
54	MG	BA	3288	1/1	0.84	0.21	66,66,66,66	0
54	MG	DA	3195	1/1	0.84	0.24	48,48,48,48	0
54	MG	DA	3398	1/1	0.84	0.26	88,88,88,88	0
54	MG	BA	3018	1/1	0.84	0.59	40,40,40,40	0
54	MG	BA	3462	1/1	0.84	0.09	43,43,43,43	0
54	MG	BB	206	1/1	0.84	0.20	57,57,57,57	0
54	MG	AD	302	1/1	0.84	0.29	77,77,77,77	0
54	MG	DA	3548	1/1	0.84	0.12	89,89,89,89	0
54	MG	DA	3271	1/1	0.84	0.38	57,57,57,57	0
54	MG	DA	3497	1/1	0.84	0.26	83,83,83,83	0
54	MG	BA	3534	1/1	0.84	0.19	25,25,25,25	0
54	MG	BP	201	1/1	0.84	0.13	45,45,45,45	0
54	MG	DA	3257	1/1	0.84	0.32	56,56,56,56	0
54	MG	BA	3068	1/1	0.84	0.40	50,50,50,50	0
54	MG	DA	3016	1/1	0.84	0.21	62,62,62,62	0
54	MG	DA	3358	1/1	0.84	0.12	39,39,39,39	0
54	MG	AA	1712	1/1	0.85	0.34	86,86,86,86	0
54	MG	DA	3454	1/1	0.85	0.08	64,64,64,64	0
54	MG	DA	3258	1/1	0.85	0.45	52,52,52,52	0
54	MG	CA	1661	1/1	0.85	0.63	67,67,67,67	0
54	MG	DA	3353	1/1	0.85	0.20	61,61,61,61	0
54	MG	BA	3455	1/1	0.85	0.23	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3123	1/1	0.85	0.27	43,43,43,43	0
54	MG	BA	3424	1/1	0.85	0.21	72,72,72,72	0
54	MG	DA	3289	1/1	0.85	0.58	54,54,54,54	0
54	MG	D8	102	1/1	0.85	0.28	45,45,45,45	0
54	MG	BA	3142	1/1	0.85	0.26	42,42,42,42	0
54	MG	DA	3130	1/1	0.85	0.33	47,47,47,47	0
54	MG	BA	3366	1/1	0.85	0.15	83,83,83,83	0
54	MG	BA	3658	1/1	0.85	0.14	114,114,114,114	0
54	MG	DA	3024	1/1	0.85	0.35	47,47,47,47	0
54	MG	DA	3209	1/1	0.85	0.25	51,51,51,51	0
54	MG	BA	3114	1/1	0.85	0.32	63,63,63,63	0
54	MG	BA	3486	1/1	0.85	0.17	75,75,75,75	0
54	MG	BA	3385	1/1	0.85	0.15	63,63,63,63	0
54	MG	CA	1632	1/1	0.85	0.27	69,69,69,69	0
54	MG	DA	3528	1/1	0.85	0.17	124,124,124,124	0
54	MG	BG	201	1/1	0.85	0.21	60,60,60,60	0
54	MG	DA	3559	1/1	0.85	0.07	79,79,79,79	0
54	MG	BA	3329	1/1	0.85	0.19	74,74,74,74	0
54	MG	BA	3100	1/1	0.85	0.20	42,42,42,42	0
54	MG	AA	1676	1/1	0.85	0.29	59,59,59,59	0
54	MG	D5	101	1/1	0.85	0.34	52,52,52,52	0
54	MG	BA	3215	1/1	0.85	0.22	50,50,50,50	0
54	MG	DA	3397	1/1	0.85	0.19	34,34,34,34	0
54	MG	DA	3185	1/1	0.85	0.16	57,57,57,57	0
54	MG	DA	3028	1/1	0.85	0.31	67,67,67,67	0
54	MG	DA	3526	1/1	0.85	0.12	98,98,98,98	0
54	MG	DA	3262	1/1	0.85	0.33	53,53,53,53	0
54	MG	CA	1645	1/1	0.85	0.93	60,60,60,60	0
54	MG	DA	3488	1/1	0.85	0.17	58,58,58,58	0
54	MG	DA	3434	1/1	0.85	0.14	60,60,60,60	0
54	MG	CA	1677	1/1	0.85	0.15	64,64,64,64	0
54	MG	BA	3388	1/1	0.85	0.10	47,47,47,47	0
54	MG	DA	3025	1/1	0.85	0.27	49,49,49,49	0
54	MG	AA	1663	1/1	0.85	0.52	64,64,64,64	0
54	MG	DA	3567	1/1	0.85	0.24	46,46,46,46	0
54	MG	BA	3075	1/1	0.85	0.19	46,46,46,46	0
54	MG	DA	3222	1/1	0.85	0.22	68,68,68,68	0
54	MG	BQ	204	1/1	0.85	0.10	43,43,43,43	0
55	ZN	AN	101	1/1	0.85	0.12	117,117,117,117	0
54	MG	BA	3104	1/1	0.85	0.23	63,63,63,63	0
54	MG	BA	3339	1/1	0.85	0.11	70,70,70,70	0
54	MG	CA	1649	1/1	0.86	0.41	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3587	1/1	0.86	0.14	60,60,60,60	0
54	MG	DA	3059	1/1	0.86	0.22	45,45,45,45	0
54	MG	BB	204	1/1	0.86	0.21	52,52,52,52	0
54	MG	BA	3107	1/1	0.86	0.20	60,60,60,60	0
54	MG	DA	3324	1/1	0.86	0.13	51,51,51,51	0
54	MG	DA	3153	1/1	0.86	0.42	58,58,58,58	0
54	MG	BB	207	1/1	0.86	0.20	52,52,52,52	0
54	MG	CA	1621	1/1	0.86	0.56	64,64,64,64	0
54	MG	AA	1606	1/1	0.86	0.19	79,79,79,79	0
54	MG	AA	1654	1/1	0.86	0.52	59,59,59,59	0
54	MG	DA	3537	1/1	0.86	0.09	63,63,63,63	0
54	MG	CA	1738	1/1	0.86	0.08	112,112,112,112	0
54	MG	CA	1635	1/1	0.86	0.10	60,60,60,60	0
54	MG	DA	3312	1/1	0.86	0.52	29,29,29,29	0
54	MG	AA	1718	1/1	0.86	0.05	96,96,96,96	0
54	MG	BA	3437	1/1	0.86	0.11	49,49,49,49	0
54	MG	BA	3043	1/1	0.86	0.12	39,39,39,39	0
54	MG	DA	3368	1/1	0.86	0.16	52,52,52,52	0
54	MG	AA	1647	1/1	0.86	0.23	55,55,55,55	0
54	MG	CA	1679	1/1	0.86	0.50	59,59,59,59	0
54	MG	AA	1674	1/1	0.86	0.32	63,63,63,63	0
54	MG	DA	3436	1/1	0.86	0.14	81,81,81,81	0
54	MG	BA	3279	1/1	0.86	0.49	27,27,27,27	0
54	MG	BA	3557	1/1	0.86	0.15	78,78,78,78	0
54	MG	DA	3452	1/1	0.86	0.10	90,90,90,90	0
54	MG	DA	3223	1/1	0.86	0.18	54,54,54,54	0
54	MG	DA	3465	1/1	0.86	0.08	75,75,75,75	0
54	MG	DA	3308	1/1	0.86	0.31	33,33,33,33	0
54	MG	BA	3414	1/1	0.86	0.13	29,29,29,29	0
54	MG	DR	203	1/1	0.86	0.51	51,51,51,51	0
54	MG	BA	3408	1/1	0.86	0.22	50,50,50,50	0
54	MG	DA	3521	1/1	0.86	0.12	86,86,86,86	0
54	MG	CA	1627	1/1	0.86	0.37	55,55,55,55	0
54	MG	CA	1606	1/1	0.86	0.23	59,59,59,59	0
55	ZN	B4	101	1/1	0.86	0.07	199,199,199,199	0
54	MG	DA	3277	1/1	0.86	0.17	77,77,77,77	0
54	MG	BA	3128	1/1	0.86	0.18	49,49,49,49	0
54	MG	AA	1707	1/1	0.86	0.17	102,102,102,102	0
54	MG	BA	3503	1/1	0.86	0.10	64,64,64,64	0
54	MG	DA	3328	1/1	0.86	0.40	57,57,57,57	0
54	MG	BA	3609	1/1	0.86	0.10	75,75,75,75	0
54	MG	BQ	201	1/1	0.86	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3433	1/1	0.86	0.12	47,47,47,47	0
54	MG	DA	3442	1/1	0.86	0.13	82,82,82,82	0
54	MG	BA	3037	1/1	0.86	0.20	75,75,75,75	0
54	MG	AA	1627	1/1	0.86	0.33	59,59,59,59	0
54	MG	DA	3245	1/1	0.87	0.27	57,57,57,57	0
54	MG	BA	3448	1/1	0.87	0.14	38,38,38,38	0
54	MG	BA	3143	1/1	0.87	0.21	30,30,30,30	0
54	MG	BA	3203	1/1	0.87	0.50	55,55,55,55	0
54	MG	AA	1620	1/1	0.87	0.17	65,65,65,65	0
54	MG	BA	3514	1/1	0.87	0.12	61,61,61,61	0
54	MG	DA	3221	1/1	0.87	0.47	51,51,51,51	0
54	MG	DA	3522	1/1	0.87	0.23	61,61,61,61	0
54	MG	BA	3427	1/1	0.87	0.14	89,89,89,89	0
54	MG	AA	1684	1/1	0.87	0.82	60,60,60,60	0
54	MG	AA	1734	1/1	0.87	0.11	96,96,96,96	0
54	MG	DA	3417	1/1	0.87	0.16	31,31,31,31	0
54	MG	BA	3411	1/1	0.87	0.08	63,63,63,63	0
54	MG	BA	3185	1/1	0.87	0.51	51,51,51,51	0
54	MG	CA	1651	1/1	0.87	0.35	46,46,46,46	0
54	MG	BA	3048	1/1	0.87	0.18	68,68,68,68	0
54	MG	BA	3579	1/1	0.87	0.09	100,100,100,100	0
54	MG	DA	3188	1/1	0.87	0.11	69,69,69,69	0
54	MG	DA	3364	1/1	0.87	0.13	32,32,32,32	0
54	MG	BA	3580	1/1	0.87	0.15	49,49,49,49	0
54	MG	AA	1681	1/1	0.87	0.24	50,50,50,50	0
54	MG	AA	1609	1/1	0.87	0.27	51,51,51,51	0
54	MG	BB	209	1/1	0.87	0.11	60,60,60,60	0
54	MG	DA	3391	1/1	0.87	0.09	37,37,37,37	0
54	MG	CA	1732	1/1	0.87	0.12	110,110,110,110	0
54	MG	DA	3276	1/1	0.87	0.85	60,60,60,60	0
54	MG	BA	3029	1/1	0.87	0.18	32,32,32,32	0
54	MG	DA	3563	1/1	0.87	0.15	70,70,70,70	0
54	MG	BA	3553	1/1	0.87	0.11	89,89,89,89	0
54	MG	DA	3589	1/1	0.87	0.12	75,75,75,75	0
54	MG	BA	3120	1/1	0.87	0.13	51,51,51,51	0
54	MG	DA	3001	1/1	0.87	0.31	48,48,48,48	0
54	MG	DA	3176	1/1	0.87	0.43	70,70,70,70	0
54	MG	CA	1758	1/1	0.87	0.22	84,84,84,84	0
54	MG	DA	3402	1/1	0.87	0.13	44,44,44,44	0
54	MG	BA	3523	1/1	0.87	0.11	110,110,110,110	0
54	MG	BF	302	1/1	0.87	0.24	42,42,42,42	0
54	MG	BA	3459	1/1	0.87	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3139	1/1	0.87	0.50	59,59,59,59	0
54	MG	BA	3194	1/1	0.87	0.20	63,63,63,63	0
54	MG	BA	3333	1/1	0.87	0.19	40,40,40,40	0
54	MG	BA	3084	1/1	0.87	0.11	59,59,59,59	0
54	MG	BA	3552	1/1	0.87	0.23	82,82,82,82	0
54	MG	BA	3470	1/1	0.88	0.27	60,60,60,60	0
54	MG	CA	1698	1/1	0.88	0.10	47,47,47,47	0
54	MG	CA	1674	1/1	0.88	0.10	74,74,74,74	0
54	MG	BA	3335	1/1	0.88	0.11	66,66,66,66	0
54	MG	AA	1612	1/1	0.88	0.31	86,86,86,86	0
54	MG	DA	3370	1/1	0.88	0.10	32,32,32,32	0
54	MG	CA	1708	1/1	0.88	0.07	80,80,80,80	0
54	MG	BA	3035	1/1	0.88	0.19	45,45,45,45	0
54	MG	DA	3457	1/1	0.88	0.08	64,64,64,64	0
54	MG	BA	3569	1/1	0.88	0.08	69,69,69,69	0
54	MG	DE	301	1/1	0.88	0.22	41,41,41,41	0
54	MG	DA	3215	1/1	0.88	0.09	49,49,49,49	0
54	MG	DA	3435	1/1	0.88	0.44	57,57,57,57	0
54	MG	DA	3125	1/1	0.88	0.30	50,50,50,50	0
54	MG	CA	1676	1/1	0.88	0.24	73,73,73,73	0
54	MG	BA	3065	1/1	0.88	0.24	41,41,41,41	0
54	MG	DA	3147	1/1	0.88	0.42	54,54,54,54	0
54	MG	DA	3325	1/1	0.88	0.19	38,38,38,38	0
54	MG	AA	1658	1/1	0.88	0.51	57,57,57,57	0
54	MG	DA	3049	1/1	0.88	0.19	49,49,49,49	0
54	MG	CA	1762	1/1	0.88	0.07	156,156,156,156	0
54	MG	DA	3029	1/1	0.88	0.30	40,40,40,40	0
54	MG	CA	1612	1/1	0.88	0.14	65,65,65,65	0
54	MG	BA	3655	1/1	0.88	0.18	104,104,104,104	0
54	MG	BA	3301	1/1	0.88	0.66	75,75,75,75	0
54	MG	DA	3383	1/1	0.88	0.10	54,54,54,54	0
54	MG	DA	3087	1/1	0.88	0.09	54,54,54,54	0
54	MG	DA	3003	1/1	0.88	0.22	46,46,46,46	0
54	MG	DA	3235	1/1	0.88	0.38	54,54,54,54	0
54	MG	BA	3659	1/1	0.88	0.07	81,81,81,81	0
54	MG	CA	1751	1/1	0.88	0.26	61,61,61,61	0
54	MG	AA	1638	1/1	0.88	0.13	53,53,53,53	0
54	MG	BA	3119	1/1	0.88	0.34	42,42,42,42	0
54	MG	AA	1642	1/1	0.88	0.81	54,54,54,54	0
54	MG	BA	3461	1/1	0.88	0.17	79,79,79,79	0
54	MG	CA	1616	1/1	0.88	0.26	58,58,58,58	0
54	MG	BB	213	1/1	0.88	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3621	1/1	0.88	0.30	52,52,52,52	0
54	MG	DA	3191	1/1	0.88	0.19	51,51,51,51	0
54	MG	BA	3214	1/1	0.88	0.22	52,52,52,52	0
54	MG	BA	3217	1/1	0.88	0.23	41,41,41,41	0
54	MG	BA	3598	1/1	0.88	0.11	65,65,65,65	0
54	MG	BA	3572	1/1	0.88	0.17	63,63,63,63	0
54	MG	BA	3159	1/1	0.88	0.22	46,46,46,46	0
54	MG	DA	3281	1/1	0.88	0.20	42,42,42,42	0
54	MG	DA	3319	1/1	0.88	0.32	57,57,57,57	0
54	MG	DA	3237	1/1	0.88	0.29	62,62,62,62	0
54	MG	BA	3397	1/1	0.88	0.17	86,86,86,86	0
54	MG	BB	216	1/1	0.88	0.10	82,82,82,82	0
54	MG	DA	3318	1/1	0.88	0.14	58,58,58,58	0
54	MG	AA	1616	1/1	0.88	0.14	92,92,92,92	0
54	MG	CA	1617	1/1	0.88	0.13	87,87,87,87	0
54	MG	BA	3153	1/1	0.88	0.38	51,51,51,51	0
54	MG	DA	3255	1/1	0.88	0.20	58,58,58,58	0
54	MG	DA	3487	1/1	0.88	0.17	48,48,48,48	0
54	MG	DA	3012	1/1	0.88	0.19	30,30,30,30	0
54	MG	AA	1604	1/1	0.88	0.15	73,73,73,73	0
54	MG	DA	3254	1/1	0.88	0.19	64,64,64,64	0
54	MG	BA	3219	1/1	0.88	0.15	46,46,46,46	0
54	MG	DA	3201	1/1	0.88	0.30	49,49,49,49	0
54	MG	CA	1665	1/1	0.88	0.23	84,84,84,84	0
54	MG	CA	1642	1/1	0.88	0.17	87,87,87,87	0
54	MG	BA	3021	1/1	0.88	0.20	44,44,44,44	0
54	MG	CA	1693	1/1	0.88	0.86	59,59,59,59	0
54	MG	BA	3303	1/1	0.88	0.11	64,64,64,64	0
54	MG	DA	3583	1/1	0.88	0.10	65,65,65,65	0
54	MG	DE	303	1/1	0.89	0.12	45,45,45,45	0
54	MG	CA	1731	1/1	0.89	0.12	74,74,74,74	0
54	MG	DA	3092	1/1	0.89	0.32	41,41,41,41	0
54	MG	CA	1648	1/1	0.89	0.40	60,60,60,60	0
54	MG	CA	1639	1/1	0.89	0.26	76,76,76,76	0
54	MG	BA	3060	1/1	0.89	0.14	54,54,54,54	0
54	MG	BA	3002	1/1	0.89	0.34	51,51,51,51	0
54	MG	CA	1739	1/1	0.89	0.12	87,87,87,87	0
54	MG	CA	1631	1/1	0.89	0.45	48,48,48,48	0
54	MG	BA	3300	1/1	0.89	0.42	48,48,48,48	0
54	MG	AF	201	1/1	0.89	0.20	62,62,62,62	0
54	MG	DA	3413	1/1	0.89	0.12	56,56,56,56	0
54	MG	BA	3056	1/1	0.89	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3285	1/1	0.89	0.57	38,38,38,38	0
54	MG	BA	3297	1/1	0.89	0.26	46,46,46,46	0
54	MG	DA	3211	1/1	0.89	0.22	48,48,48,48	0
54	MG	DA	3287	1/1	0.89	0.27	57,57,57,57	0
54	MG	DA	3227	1/1	0.89	0.28	52,52,52,52	0
54	MG	DA	3464	1/1	0.89	0.10	89,89,89,89	0
54	MG	BA	3015	1/1	0.89	0.18	48,48,48,48	0
54	MG	DA	3141	1/1	0.89	0.52	60,60,60,60	0
54	MG	AA	1682	1/1	0.89	0.13	76,76,76,76	0
54	MG	DA	3384	1/1	0.89	0.08	45,45,45,45	0
54	MG	DA	3508	1/1	0.89	0.10	60,60,60,60	0
54	MG	CA	1701	1/1	0.89	0.08	72,72,72,72	0
54	MG	BA	3026	1/1	0.89	0.19	52,52,52,52	0
54	MG	DA	3109	1/1	0.89	0.17	59,59,59,59	0
54	MG	CA	1620	1/1	0.89	0.12	58,58,58,58	0
54	MG	BA	3179	1/1	0.89	0.27	37,37,37,37	0
54	MG	DA	3458	1/1	0.89	0.05	62,62,62,62	0
54	MG	BA	3243	1/1	0.89	0.30	42,42,42,42	0
54	MG	CA	1607	1/1	0.89	0.20	50,50,50,50	0
54	MG	DA	3412	1/1	0.89	0.09	58,58,58,58	0
54	MG	CA	1694	1/1	0.89	0.17	62,62,62,62	0
54	MG	BT	202	1/1	0.89	0.27	52,52,52,52	0
54	MG	DA	3416	1/1	0.89	0.13	66,66,66,66	0
54	MG	DA	3380	1/1	0.89	0.10	42,42,42,42	0
54	MG	DA	3596	1/1	0.89	0.19	125,125,125,125	0
54	MG	DA	3492	1/1	0.89	0.07	56,56,56,56	0
54	MG	BA	3221	1/1	0.89	0.34	57,57,57,57	0
54	MG	DA	3231	1/1	0.89	0.29	36,36,36,36	0
54	MG	BA	3342	1/1	0.89	0.15	32,32,32,32	0
54	MG	DA	3163	1/1	0.89	0.39	30,30,30,30	0
54	MG	BA	3539	1/1	0.89	0.08	47,47,47,47	0
54	MG	CA	1638	1/1	0.89	0.26	52,52,52,52	0
54	MG	AA	1708	1/1	0.89	0.29	91,91,91,91	0
54	MG	BA	3131	1/1	0.89	0.81	62,62,62,62	0
54	MG	BA	3085	1/1	0.89	0.49	52,52,52,52	0
54	MG	CA	1646	1/1	0.89	0.38	59,59,59,59	0
54	MG	DA	3017	1/1	0.89	0.20	50,50,50,50	0
54	MG	CA	1625	1/1	0.89	0.36	63,63,63,63	0
54	MG	AA	1649	1/1	0.89	0.30	43,43,43,43	0
54	MG	BA	3471	1/1	0.89	0.18	27,27,27,27	0
54	MG	CA	1672	1/1	0.89	0.20	66,66,66,66	0
54	MG	BA	3030	1/1	0.89	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3576	1/1	0.89	0.09	48,48,48,48	0
54	MG	DA	3070	1/1	0.89	0.36	57,57,57,57	0
54	MG	AA	1621	1/1	0.89	0.29	62,62,62,62	0
54	MG	BA	3117	1/1	0.89	0.27	39,39,39,39	0
54	MG	DA	3387	1/1	0.89	0.11	60,60,60,60	0
54	MG	BA	3054	1/1	0.89	0.17	34,34,34,34	0
54	MG	BA	3205	1/1	0.89	0.12	54,54,54,54	0
54	MG	DA	3322	1/1	0.89	0.38	49,49,49,49	0
54	MG	DA	3145	1/1	0.89	0.23	61,61,61,61	0
54	MG	DA	3273	1/1	0.89	0.33	50,50,50,50	0
54	MG	AA	1716	1/1	0.89	0.08	116,116,116,116	0
54	MG	DA	3447	1/1	0.89	0.27	74,74,74,74	0
54	MG	DA	3517	1/1	0.89	0.24	66,66,66,66	0
54	MG	BA	3407	1/1	0.89	0.17	47,47,47,47	0
54	MG	DA	3512	1/1	0.89	0.13	42,42,42,42	0
54	MG	AQ	201	1/1	0.89	0.25	58,58,58,58	0
54	MG	CA	1713	1/1	0.89	0.14	73,73,73,73	0
54	MG	DA	3089	1/1	0.89	0.11	52,52,52,52	0
54	MG	DA	3251	1/1	0.89	0.18	40,40,40,40	0
54	MG	DA	3073	1/1	0.89	0.51	68,68,68,68	0
54	MG	DA	3119	1/1	0.89	0.33	48,48,48,48	0
54	MG	DA	3146	1/1	0.89	0.17	44,44,44,44	0
54	MG	B0	101	1/1	0.89	0.18	39,39,39,39	0
54	MG	BA	3353	1/1	0.89	0.21	91,91,91,91	0
54	MG	BA	3013	1/1	0.89	0.25	49,49,49,49	0
54	MG	DA	3090	1/1	0.89	0.11	53,53,53,53	0
54	MG	DQ	202	1/1	0.89	0.17	33,33,33,33	0
54	MG	DA	3582	1/1	0.89	0.24	63,63,63,63	0
54	MG	DA	3132	1/1	0.89	0.43	49,49,49,49	0
54	MG	DA	3260	1/1	0.89	0.20	41,41,41,41	0
54	MG	DA	3437	1/1	0.89	0.16	85,85,85,85	0
54	MG	DA	3275	1/1	0.89	0.35	47,47,47,47	0
54	MG	DA	3152	1/1	0.89	0.44	61,61,61,61	0
54	MG	BA	3008	1/1	0.89	0.23	28,28,28,28	0
54	MG	BA	3292	1/1	0.89	0.32	70,70,70,70	0
54	MG	DA	3504	1/1	0.89	0.07	63,63,63,63	0
54	MG	AA	1655	1/1	0.90	0.46	43,43,43,43	0
54	MG	CA	1716	1/1	0.90	0.16	102,102,102,102	0
54	MG	BA	3152	1/1	0.90	0.37	54,54,54,54	0
54	MG	BA	3586	1/1	0.90	0.10	63,63,63,63	0
54	MG	BA	3346	1/1	0.90	0.12	52,52,52,52	0
54	MG	AA	1644	1/1	0.90	0.33	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1613	1/1	0.90	0.34	66,66,66,66	0
54	MG	BA	3421	1/1	0.90	0.07	68,68,68,68	0
54	MG	BA	3080	1/1	0.90	0.23	39,39,39,39	0
54	MG	DA	3086	1/1	0.90	0.21	48,48,48,48	0
54	MG	CA	1680	1/1	0.90	0.23	78,78,78,78	0
54	MG	BA	3393	1/1	0.90	0.19	37,37,37,37	0
54	MG	DA	3238	1/1	0.90	0.44	56,56,56,56	0
54	MG	BB	215	1/1	0.90	0.17	65,65,65,65	0
54	MG	BB	211	1/1	0.90	0.21	47,47,47,47	0
54	MG	DA	3148	1/1	0.90	0.16	48,48,48,48	0
54	MG	DA	3020	1/1	0.90	0.18	56,56,56,56	0
54	MG	CA	1668	1/1	0.90	0.54	87,87,87,87	0
54	MG	BA	3007	1/1	0.90	0.30	28,28,28,28	0
54	MG	DA	3593	1/1	0.90	0.15	83,83,83,83	0
54	MG	BA	3073	1/1	0.90	0.42	52,52,52,52	0
54	MG	BA	3086	1/1	0.90	0.95	57,57,57,57	0
54	MG	AA	1683	1/1	0.90	0.66	58,58,58,58	0
54	MG	DA	3218	1/1	0.90	0.65	62,62,62,62	0
54	MG	DA	3027	1/1	0.90	0.35	56,56,56,56	0
54	MG	DA	3128	1/1	0.90	0.24	45,45,45,45	0
54	MG	BA	3456	1/1	0.90	0.22	32,32,32,32	0
54	MG	DA	3346	1/1	0.90	0.12	35,35,35,35	0
54	MG	DA	3213	1/1	0.90	0.33	48,48,48,48	0
54	MG	DA	3261	1/1	0.90	0.31	44,44,44,44	0
54	MG	BA	3094	1/1	0.90	0.21	54,54,54,54	0
54	MG	DA	3174	1/1	0.90	0.19	51,51,51,51	0
54	MG	AA	1689	1/1	0.90	0.06	99,99,99,99	0
54	MG	DA	3248	1/1	0.90	0.18	42,42,42,42	0
54	MG	BA	3231	1/1	0.90	0.11	47,47,47,47	0
54	MG	DA	3098	1/1	0.90	0.19	37,37,37,37	0
54	MG	BA	3594	1/1	0.90	0.05	86,86,86,86	0
54	MG	DA	3597	1/1	0.90	0.11	93,93,93,93	0
54	MG	DA	3486	1/1	0.90	0.21	64,64,64,64	0
54	MG	BA	3212	1/1	0.90	0.21	68,68,68,68	0
54	MG	DA	3456	1/1	0.90	0.08	42,42,42,42	0
54	MG	BA	3218	1/1	0.90	0.15	55,55,55,55	0
54	MG	DA	3495	1/1	0.90	0.06	83,83,83,83	0
54	MG	DA	3214	1/1	0.90	0.24	37,37,37,37	0
54	MG	DA	3030	1/1	0.90	0.29	55,55,55,55	0
54	MG	CA	1729	1/1	0.90	0.17	81,81,81,81	0
54	MG	DA	3230	1/1	0.90	0.20	45,45,45,45	0
54	MG	CA	1629	1/1	0.90	0.20	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1656	1/1	0.90	0.31	86,86,86,86	0
54	MG	DA	3270	1/1	0.90	0.17	64,64,64,64	0
54	MG	DA	3274	1/1	0.90	0.41	61,61,61,61	0
54	MG	DA	3094	1/1	0.90	0.16	56,56,56,56	0
54	MG	BA	3222	1/1	0.90	0.49	60,60,60,60	0
54	MG	DA	3229	1/1	0.90	0.30	44,44,44,44	0
54	MG	BA	3010	1/1	0.90	0.22	39,39,39,39	0
54	MG	DA	3459	1/1	0.90	0.07	53,53,53,53	0
54	MG	DA	3321	1/1	0.90	0.43	51,51,51,51	0
54	MG	BB	208	1/1	0.90	0.23	43,43,43,43	0
54	MG	AA	1730	1/1	0.90	0.10	51,51,51,51	0
54	MG	DA	3479	1/1	0.90	0.16	62,62,62,62	0
54	MG	DA	3252	1/1	0.90	0.53	59,59,59,59	0
54	MG	BA	3323	1/1	0.90	0.17	23,23,23,23	0
54	MG	AA	1675	1/1	0.90	0.23	76,76,76,76	0
54	MG	BA	3045	1/1	0.90	0.22	45,45,45,45	0
54	MG	CA	1636	1/1	0.90	0.36	59,59,59,59	0
54	MG	BA	3590	1/1	0.90	0.31	31,31,31,31	0
54	MG	BA	3144	1/1	0.90	0.25	46,46,46,46	0
54	MG	BA	3229	1/1	0.90	0.22	41,41,41,41	0
54	MG	DA	3326	1/1	0.90	0.21	46,46,46,46	0
54	MG	BA	3210	1/1	0.90	0.20	40,40,40,40	0
54	MG	BA	3298	1/1	0.90	0.54	54,54,54,54	0
54	MG	DA	3408	1/1	0.90	0.15	51,51,51,51	0
54	MG	BD	302	1/1	0.90	0.21	28,28,28,28	0
54	MG	BA	3076	1/1	0.90	0.22	44,44,44,44	0
54	MG	DA	3421	1/1	0.90	0.10	93,93,93,93	0
54	MG	BA	3267	1/1	0.90	0.33	36,36,36,36	0
54	MG	CA	1695	1/1	0.90	0.35	50,50,50,50	0
54	MG	DA	3111	1/1	0.90	0.17	50,50,50,50	0
54	MG	AA	1624	1/1	0.90	0.38	70,70,70,70	0
54	MG	BA	3482	1/1	0.90	0.19	27,27,27,27	0
54	MG	DA	3354	1/1	0.90	0.09	49,49,49,49	0
54	MG	DA	3372	1/1	0.90	0.15	41,41,41,41	0
54	MG	DA	3470	1/1	0.90	0.10	47,47,47,47	0
54	MG	AA	1670	1/1	0.90	0.32	53,53,53,53	0
54	MG	DF	301	1/1	0.90	0.30	50,50,50,50	0
54	MG	BB	210	1/1	0.90	0.15	60,60,60,60	0
54	MG	BA	3175	1/1	0.90	0.14	43,43,43,43	0
54	MG	CA	1746	1/1	0.90	0.11	97,97,97,97	0
54	MG	DO	202	1/1	0.90	0.17	39,39,39,39	0
54	MG	BA	3046	1/1	0.90	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3400	1/1	0.90	0.17	66,66,66,66	0
54	MG	BA	3592	1/1	0.90	0.13	47,47,47,47	0
54	MG	AA	1640	1/1	0.90	0.20	58,58,58,58	0
54	MG	DA	3500	1/1	0.90	0.12	74,74,74,74	0
54	MG	BA	3332	1/1	0.90	0.09	50,50,50,50	0
54	MG	CA	1609	1/1	0.90	0.24	70,70,70,70	0
54	MG	BA	3525	1/1	0.90	0.14	35,35,35,35	0
54	MG	BA	3439	1/1	0.90	0.16	59,59,59,59	0
54	MG	DA	3543	1/1	0.90	0.09	53,53,53,53	0
54	MG	BA	3589	1/1	0.90	0.17	94,94,94,94	0
54	MG	DA	3295	1/1	0.90	0.25	59,59,59,59	0
54	MG	BA	3025	1/1	0.91	0.23	48,48,48,48	0
54	MG	BA	3425	1/1	0.91	0.15	53,53,53,53	0
54	MG	DA	3136	1/1	0.91	0.34	62,62,62,62	0
54	MG	BA	3468	1/1	0.91	0.18	24,24,24,24	0
54	MG	DA	3151	1/1	0.91	0.11	43,43,43,43	0
54	MG	BA	3154	1/1	0.91	0.37	50,50,50,50	0
54	MG	CA	1745	1/1	0.91	0.34	116,116,116,116	0
54	MG	BA	3011	1/1	0.91	0.29	26,26,26,26	0
54	MG	BE	301	1/1	0.91	0.43	34,34,34,34	0
54	MG	BB	218	1/1	0.91	0.09	45,45,45,45	0
54	MG	DA	3360	1/1	0.91	0.20	37,37,37,37	0
54	MG	DA	3267	1/1	0.91	0.27	54,54,54,54	0
54	MG	BA	3091	1/1	0.91	0.35	40,40,40,40	0
54	MG	BA	3550	1/1	0.91	0.06	87,87,87,87	0
54	MG	DD	301	1/1	0.91	0.22	47,47,47,47	0
54	MG	BA	3546	1/1	0.91	0.18	73,73,73,73	0
54	MG	AA	1634	1/1	0.91	0.10	56,56,56,56	0
54	MG	BA	3563	1/1	0.91	0.09	70,70,70,70	0
54	MG	BA	3363	1/1	0.91	0.14	64,64,64,64	0
54	MG	BA	3108	1/1	0.91	0.24	51,51,51,51	0
54	MG	AA	1611	1/1	0.91	0.28	83,83,83,83	0
54	MG	BA	3377	1/1	0.91	0.22	32,32,32,32	0
54	MG	BA	3396	1/1	0.91	0.16	29,29,29,29	0
54	MG	BA	3578	1/1	0.91	0.10	44,44,44,44	0
54	MG	BA	3230	1/1	0.91	0.19	30,30,30,30	0
54	MG	BA	3452	1/1	0.91	0.13	64,64,64,64	0
54	MG	AA	1713	1/1	0.91	0.10	91,91,91,91	0
54	MG	BA	3017	1/1	0.91	0.13	31,31,31,31	0
54	MG	BA	3566	1/1	0.91	0.14	44,44,44,44	0
54	MG	CA	1650	1/1	0.91	0.20	60,60,60,60	0
54	MG	BA	3177	1/1	0.91	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	219	1/1	0.91	0.06	105,105,105,105	0
54	MG	CA	1750	1/1	0.91	0.12	78,78,78,78	0
54	MG	DA	3008	1/1	0.91	0.44	58,58,58,58	0
54	MG	BA	3438	1/1	0.91	0.20	65,65,65,65	0
54	MG	DA	3166	1/1	0.91	0.30	45,45,45,45	0
54	MG	DA	3542	1/1	0.91	0.07	83,83,83,83	0
54	MG	BA	3262	1/1	0.91	0.37	27,27,27,27	0
54	MG	BA	3515	1/1	0.91	0.16	72,72,72,72	0
54	MG	DA	3066	1/1	0.91	0.20	62,62,62,62	0
54	MG	BA	3626	1/1	0.91	0.09	64,64,64,64	0
54	MG	DA	3123	1/1	0.91	0.23	53,53,53,53	0
54	MG	DA	3288	1/1	0.91	0.25	39,39,39,39	0
54	MG	DA	3499	1/1	0.91	0.14	67,67,67,67	0
54	MG	BA	3571	1/1	0.91	0.17	44,44,44,44	0
54	MG	DA	3169	1/1	0.91	0.16	45,45,45,45	0
54	MG	CA	1754	1/1	0.91	0.05	74,74,74,74	0
54	MG	CA	1602	1/1	0.91	0.39	62,62,62,62	0
54	MG	DA	3431	1/1	0.91	0.10	59,59,59,59	0
54	MG	BA	3024	1/1	0.91	0.40	41,41,41,41	0
54	MG	BA	3101	1/1	0.91	0.11	37,37,37,37	0
54	MG	BA	3418	1/1	0.91	0.12	49,49,49,49	0
54	MG	BA	3612	1/1	0.91	0.07	59,59,59,59	0
54	MG	DA	3033	1/1	0.91	0.16	66,66,66,66	0
54	MG	BA	3469	1/1	0.91	0.15	40,40,40,40	0
54	MG	AA	1656	1/1	0.91	0.57	59,59,59,59	0
54	MG	BA	3650	1/1	0.91	0.17	88,88,88,88	0
54	MG	BA	3305	1/1	0.91	0.26	69,69,69,69	0
54	MG	AA	1617	1/1	0.91	0.17	45,45,45,45	0
54	MG	BA	3254	1/1	0.91	0.35	25,25,25,25	0
54	MG	CA	1718	1/1	0.91	0.15	83,83,83,83	0
54	MG	DP	201	1/1	0.91	0.18	54,54,54,54	0
54	MG	CA	1615	1/1	0.91	0.12	65,65,65,65	0
54	MG	DA	3419	1/1	0.91	0.11	44,44,44,44	0
54	MG	BA	3003	1/1	0.91	0.31	74,74,74,74	0
54	MG	AA	1727	1/1	0.91	0.10	61,61,61,61	0
54	MG	DA	3509	1/1	0.91	0.19	37,37,37,37	0
54	MG	CA	1700	1/1	0.91	0.09	70,70,70,70	0
54	MG	BA	3001	1/1	0.91	0.21	43,43,43,43	0
54	MG	BA	3183	1/1	0.91	0.33	29,29,29,29	0
54	MG	BA	3601	1/1	0.91	0.15	76,76,76,76	0
54	MG	BA	3507	1/1	0.91	0.28	41,41,41,41	0
54	MG	BA	3039	1/1	0.91	0.20	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3012	1/1	0.91	0.34	27,27,27,27	0
54	MG	BB	212	1/1	0.91	0.27	60,60,60,60	0
54	MG	AA	1645	1/1	0.91	0.26	60,60,60,60	0
54	MG	BA	3585	1/1	0.91	0.10	52,52,52,52	0
54	MG	BA	3055	1/1	0.91	0.20	53,53,53,53	0
54	MG	DA	3127	1/1	0.91	0.25	56,56,56,56	0
54	MG	DA	3366	1/1	0.91	0.19	31,31,31,31	0
54	MG	DA	3236	1/1	0.92	0.30	47,47,47,47	0
54	MG	BB	205	1/1	0.92	0.38	45,45,45,45	0
54	MG	AA	1679	1/1	0.92	0.22	44,44,44,44	0
54	MG	DA	3409	1/1	0.92	0.09	73,73,73,73	0
54	MG	DA	3244	1/1	0.92	0.52	33,33,33,33	0
54	MG	BA	3022	1/1	0.92	0.27	46,46,46,46	0
54	MG	BA	3150	1/1	0.92	0.12	42,42,42,42	0
54	MG	DA	3060	1/1	0.92	0.34	41,41,41,41	0
54	MG	AA	1677	1/1	0.92	0.32	62,62,62,62	0
54	MG	DA	3144	1/1	0.92	0.46	42,42,42,42	0
54	MG	DA	3200	1/1	0.92	0.24	34,34,34,34	0
54	MG	DA	3352	1/1	0.92	0.11	33,33,33,33	0
54	MG	CQ	201	1/1	0.92	0.35	62,62,62,62	0
54	MG	DA	3544	1/1	0.92	0.06	72,72,72,72	0
54	MG	BA	3656	1/1	0.92	0.16	68,68,68,68	0
54	MG	BA	3390	1/1	0.92	0.08	62,62,62,62	0
54	MG	BA	3584	1/1	0.92	0.11	42,42,42,42	0
54	MG	BA	3171	1/1	0.92	0.32	31,31,31,31	0
54	MG	CA	1759	1/1	0.92	0.22	69,69,69,69	0
54	MG	DA	3513	1/1	0.92	0.14	34,34,34,34	0
54	MG	BA	3422	1/1	0.92	0.17	76,76,76,76	0
54	MG	BA	3067	1/1	0.92	0.18	43,43,43,43	0
54	MG	DA	3382	1/1	0.92	0.23	53,53,53,53	0
54	MG	BA	3137	1/1	0.92	0.22	38,38,38,38	0
54	MG	BA	3290	1/1	0.92	0.17	63,63,63,63	0
54	MG	DR	202	1/1	0.92	0.37	34,34,34,34	0
54	MG	DB	202	1/1	0.92	0.21	50,50,50,50	0
54	MG	BA	3564	1/1	0.92	0.11	59,59,59,59	0
54	MG	DA	3175	1/1	0.92	0.36	44,44,44,44	0
54	MG	DA	3162	1/1	0.92	0.35	35,35,35,35	0
54	MG	DA	3306	1/1	0.92	0.35	29,29,29,29	0
54	MG	DA	3427	1/1	0.92	0.06	59,59,59,59	0
54	MG	AA	1613	1/1	0.92	0.19	65,65,65,65	0
54	MG	BA	3233	1/1	0.92	0.44	41,41,41,41	0
54	MG	BA	3318	1/1	0.92	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3022	1/1	0.92	0.16	34,34,34,34	0
54	MG	B5	103	1/1	0.92	0.08	57,57,57,57	0
54	MG	BA	3191	1/1	0.92	0.27	40,40,40,40	0
54	MG	DA	3445	1/1	0.92	0.17	42,42,42,42	0
54	MG	DA	3048	1/1	0.92	0.25	40,40,40,40	0
54	MG	DA	3411	1/1	0.92	0.11	49,49,49,49	0
54	MG	BA	3641	1/1	0.92	0.22	72,72,72,72	0
54	MG	BA	3405	1/1	0.92	0.15	61,61,61,61	0
54	MG	AA	1664	1/1	0.92	0.14	57,57,57,57	0
54	MG	BA	3331	1/1	0.92	0.15	48,48,48,48	0
54	MG	DA	3332	1/1	0.92	0.23	53,53,53,53	0
54	MG	BA	3096	1/1	0.92	0.43	47,47,47,47	0
54	MG	BA	3458	1/1	0.92	0.17	35,35,35,35	0
54	MG	DA	3116	1/1	0.92	0.20	43,43,43,43	0
54	MG	BA	3124	1/1	0.92	0.19	33,33,33,33	0
54	MG	DA	3103	1/1	0.92	0.17	54,54,54,54	0
54	MG	DA	3225	1/1	0.92	0.50	51,51,51,51	0
54	MG	DA	3142	1/1	0.92	0.21	37,37,37,37	0
54	MG	DA	3432	1/1	0.92	0.10	70,70,70,70	0
54	MG	BA	3083	1/1	0.92	0.18	43,43,43,43	0
54	MG	BA	3103	1/1	0.92	0.20	29,29,29,29	0
54	MG	DA	3545	1/1	0.92	0.08	82,82,82,82	0
54	MG	BA	3431	1/1	0.92	0.08	71,71,71,71	0
54	MG	BA	3400	1/1	0.92	0.21	47,47,47,47	0
54	MG	BA	3526	1/1	0.92	0.13	22,22,22,22	0
54	MG	BT	201	1/1	0.92	0.15	53,53,53,53	0
54	MG	BA	3516	1/1	0.92	0.25	63,63,63,63	0
54	MG	DA	3460	1/1	0.92	0.19	65,65,65,65	0
54	MG	DA	3031	1/1	0.92	0.23	53,53,53,53	0
54	MG	AA	1660	1/1	0.92	0.51	80,80,80,80	0
54	MG	BA	3019	1/1	0.92	0.18	34,34,34,34	0
54	MG	BA	3496	1/1	0.92	0.17	39,39,39,39	0
54	MG	CA	1673	1/1	0.92	0.60	57,57,57,57	0
54	MG	CA	1605	1/1	0.92	0.34	67,67,67,67	0
54	MG	BB	202	1/1	0.92	0.12	43,43,43,43	0
54	MG	BA	3306	1/1	0.92	0.18	55,55,55,55	0
54	MG	DA	3378	1/1	0.92	0.15	33,33,33,33	0
54	MG	DA	3129	1/1	0.92	0.13	61,61,61,61	0
54	MG	BA	3356	1/1	0.92	0.17	29,29,29,29	0
54	MG	BA	3330	1/1	0.92	0.13	34,34,34,34	0
54	MG	AA	1633	1/1	0.92	0.28	62,62,62,62	0
54	MG	DA	3556	1/1	0.92	0.06	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3305	1/1	0.92	0.22	35,35,35,35	0
54	MG	DA	3266	1/1	0.92	0.32	47,47,47,47	0
54	MG	DA	3343	1/1	0.92	0.06	37,37,37,37	0
54	MG	BA	3162	1/1	0.92	0.35	42,42,42,42	0
54	MG	DA	3489	1/1	0.92	0.14	79,79,79,79	0
54	MG	DA	3538	1/1	0.92	0.14	87,87,87,87	0
54	MG	BA	3132	1/1	0.92	0.12	33,33,33,33	0
54	MG	DA	3444	1/1	0.92	0.14	41,41,41,41	0
54	MG	CA	1634	1/1	0.92	0.18	64,64,64,64	0
54	MG	DA	3120	1/1	0.92	0.26	43,43,43,43	0
54	MG	BA	3196	1/1	0.92	0.17	46,46,46,46	0
54	MG	BA	3197	1/1	0.92	0.35	41,41,41,41	0
54	MG	BA	3040	1/1	0.92	0.34	30,30,30,30	0
54	MG	DA	3481	1/1	0.92	0.44	61,61,61,61	0
54	MG	AA	1632	1/1	0.92	0.22	71,71,71,71	0
54	MG	BA	3020	1/1	0.92	0.09	82,82,82,82	0
54	MG	DA	3100	1/1	0.92	0.22	38,38,38,38	0
54	MG	BA	3308	1/1	0.92	0.17	52,52,52,52	0
54	MG	DA	3093	1/1	0.92	0.27	56,56,56,56	0
54	MG	DA	3228	1/1	0.92	0.48	40,40,40,40	0
54	MG	BA	3138	1/1	0.92	0.35	42,42,42,42	0
54	MG	BA	3193	1/1	0.92	0.67	35,35,35,35	0
55	ZN	BY	201	1/1	0.92	0.11	69,69,69,69	0
54	MG	BA	3134	1/1	0.92	0.43	41,41,41,41	0
54	MG	BA	3536	1/1	0.92	0.08	68,68,68,68	0
54	MG	BA	3410	1/1	0.92	0.08	77,77,77,77	0
54	MG	DA	3074	1/1	0.92	0.19	54,54,54,54	0
54	MG	DA	3329	1/1	0.92	0.13	41,41,41,41	0
54	MG	DA	3469	1/1	0.93	0.07	56,56,56,56	0
54	MG	DA	3002	1/1	0.93	0.12	69,69,69,69	0
54	MG	CA	1737	1/1	0.93	0.13	89,89,89,89	0
54	MG	BA	3115	1/1	0.93	0.12	45,45,45,45	0
54	MG	BA	3548	1/1	0.93	0.13	29,29,29,29	0
54	MG	DA	3550	1/1	0.93	0.13	58,58,58,58	0
54	MG	BA	3559	1/1	0.93	0.07	71,71,71,71	0
54	MG	DA	3040	1/1	0.93	0.26	48,48,48,48	0
54	MG	BQ	202	1/1	0.93	0.21	34,34,34,34	0
54	MG	BA	3436	1/1	0.93	0.13	70,70,70,70	0
54	MG	DA	3316	1/1	0.93	0.73	69,69,69,69	0
54	MG	BA	3373	1/1	0.93	0.08	44,44,44,44	0
54	MG	BA	3258	1/1	0.93	0.37	55,55,55,55	0
54	MG	BA	3359	1/1	0.93	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3259	1/1	0.93	0.19	43,43,43,43	0
54	MG	BA	3538	1/1	0.93	0.11	66,66,66,66	0
54	MG	DA	3407	1/1	0.93	0.06	70,70,70,70	0
54	MG	DA	3536	1/1	0.93	0.16	51,51,51,51	0
54	MG	BA	3252	1/1	0.93	0.32	36,36,36,36	0
54	MG	BA	3565	1/1	0.93	0.07	68,68,68,68	0
54	MG	DA	3314	1/1	0.93	0.39	43,43,43,43	0
54	MG	DA	3061	1/1	0.93	0.17	32,32,32,32	0
54	MG	BA	3176	1/1	0.93	0.16	60,60,60,60	0
54	MG	DA	3505	1/1	0.93	0.13	91,91,91,91	0
54	MG	BA	3519	1/1	0.93	0.05	64,64,64,64	0
54	MG	DA	3256	1/1	0.93	0.24	52,52,52,52	0
54	MG	BA	3009	1/1	0.93	0.29	45,45,45,45	0
54	MG	DA	3117	1/1	0.93	0.17	47,47,47,47	0
54	MG	DA	3137	1/1	0.93	0.11	38,38,38,38	0
54	MG	AA	1714	1/1	0.93	0.25	57,57,57,57	0
54	MG	BA	3417	1/1	0.93	0.08	48,48,48,48	0
54	MG	BA	3257	1/1	0.93	0.41	23,23,23,23	0
54	MG	CA	1740	1/1	0.93	0.40	68,68,68,68	0
54	MG	BE	302	1/1	0.93	0.20	41,41,41,41	0
54	MG	DA	3588	1/1	0.93	0.18	34,34,34,34	0
54	MG	DA	3171	1/1	0.93	0.17	61,61,61,61	0
54	MG	CA	1643	1/1	0.93	0.22	70,70,70,70	0
54	MG	DA	3461	1/1	0.93	0.14	41,41,41,41	0
54	MG	DA	3555	1/1	0.93	0.14	56,56,56,56	0
54	MG	AA	1623	1/1	0.93	0.17	74,74,74,74	0
54	MG	BA	3450	1/1	0.93	0.10	38,38,38,38	0
54	MG	DA	3586	1/1	0.93	0.14	49,49,49,49	0
55	ZN	CD	301	1/1	0.93	0.26	71,71,71,71	0
54	MG	DA	3133	1/1	0.93	0.38	36,36,36,36	0
54	MG	DA	3296	1/1	0.93	0.09	67,67,67,67	0
54	MG	DA	3333	1/1	0.93	0.15	37,37,37,37	0
54	MG	DA	3085	1/1	0.93	0.21	43,43,43,43	0
54	MG	DA	3199	1/1	0.93	0.18	44,44,44,44	0
54	MG	DA	3571	1/1	0.93	0.14	55,55,55,55	0
54	MG	BA	3095	1/1	0.93	0.19	48,48,48,48	0
54	MG	BA	3492	1/1	0.93	0.21	27,27,27,27	0
54	MG	AA	1605	1/1	0.93	0.17	66,66,66,66	0
54	MG	DA	3077	1/1	0.93	0.17	49,49,49,49	0
54	MG	DA	3565	1/1	0.93	0.20	34,34,34,34	0
54	MG	DA	3283	1/1	0.93	0.18	61,61,61,61	0
54	MG	BA	3005	1/1	0.93	0.28	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3250	1/1	0.93	0.40	26,26,26,26	0
54	MG	BA	3295	1/1	0.93	0.58	54,54,54,54	0
54	MG	DA	3186	1/1	0.93	0.13	54,54,54,54	0
54	MG	DA	3194	1/1	0.93	0.23	37,37,37,37	0
54	MG	BA	3181	1/1	0.93	0.20	38,38,38,38	0
54	MG	CA	1611	1/1	0.93	0.22	43,43,43,43	0
54	MG	DA	3375	1/1	0.93	0.14	31,31,31,31	0
54	MG	DA	3042	1/1	0.93	0.23	33,33,33,33	0
54	MG	CA	1628	1/1	0.93	0.09	75,75,75,75	0
54	MG	DA	3091	1/1	0.93	0.17	55,55,55,55	0
54	MG	AA	1643	1/1	0.93	0.59	47,47,47,47	0
54	MG	DA	3443	1/1	0.93	0.11	75,75,75,75	0
54	MG	BA	3660	1/1	0.93	0.13	104,104,104,104	0
54	MG	BA	3522	1/1	0.93	0.11	74,74,74,74	0
54	MG	BA	3111	1/1	0.93	0.20	56,56,56,56	0
54	MG	DA	3021	1/1	0.93	0.13	51,51,51,51	0
54	MG	DA	3113	1/1	0.93	0.41	59,59,59,59	0
54	MG	BA	3050	1/1	0.93	0.22	35,35,35,35	0
54	MG	BA	3348	1/1	0.93	0.08	59,59,59,59	0
54	MG	DA	3264	1/1	0.93	0.45	61,61,61,61	0
54	MG	DA	3019	1/1	0.93	0.16	40,40,40,40	0
54	MG	BD	301	1/1	0.93	0.46	49,49,49,49	0
54	MG	AA	1657	1/1	0.93	0.39	58,58,58,58	0
54	MG	BA	3474	1/1	0.93	0.08	37,37,37,37	0
54	MG	CA	1655	1/1	0.93	0.22	98,98,98,98	0
54	MG	BA	3105	1/1	0.93	0.36	28,28,28,28	0
54	MG	BA	3041	1/1	0.93	0.26	40,40,40,40	0
54	MG	BA	3583	1/1	0.93	0.15	34,34,34,34	0
54	MG	BA	3201	1/1	0.93	0.33	31,31,31,31	0
54	MG	BA	3072	1/1	0.93	0.10	59,59,59,59	0
54	MG	DA	3272	1/1	0.93	0.39	30,30,30,30	0
54	MG	BA	3053	1/1	0.93	0.44	57,57,57,57	0
54	MG	BA	3433	1/1	0.93	0.09	55,55,55,55	0
54	MG	BA	3161	1/1	0.93	0.18	40,40,40,40	0
54	MG	BA	3147	1/1	0.93	0.11	55,55,55,55	0
54	MG	CA	1658	1/1	0.93	0.34	58,58,58,58	0
54	MG	CA	1663	1/1	0.93	0.33	64,64,64,64	0
54	MG	BA	3444	1/1	0.93	0.11	53,53,53,53	0
54	MG	DA	3204	1/1	0.93	0.44	43,43,43,43	0
54	MG	AA	1601	1/1	0.93	0.28	55,55,55,55	0
54	MG	BA	3204	1/1	0.93	0.13	38,38,38,38	0
54	MG	BA	3398	1/1	0.93	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3192	1/1	0.93	0.17	50,50,50,50	0
54	MG	DA	3340	1/1	0.93	0.12	45,45,45,45	0
54	MG	BA	3291	1/1	0.93	0.13	39,39,39,39	0
54	MG	BA	3432	1/1	0.93	0.04	67,67,67,67	0
54	MG	BA	3027	1/1	0.93	0.15	38,38,38,38	0
54	MG	DA	3263	1/1	0.93	0.20	40,40,40,40	0
54	MG	DA	3595	1/1	0.93	0.12	58,58,58,58	0
54	MG	DA	3046	1/1	0.93	0.19	42,42,42,42	0
54	MG	BA	3170	1/1	0.93	0.22	29,29,29,29	0
54	MG	DA	3004	1/1	0.93	0.07	88,88,88,88	0
54	MG	BA	3479	1/1	0.93	0.18	32,32,32,32	0
54	MG	BA	3311	1/1	0.93	0.17	24,24,24,24	0
54	MG	BA	3180	1/1	0.93	0.28	41,41,41,41	0
54	MG	CA	1662	1/1	0.93	0.39	75,75,75,75	0
54	MG	BA	3280	1/1	0.93	0.30	46,46,46,46	0
54	MG	BA	3574	1/1	0.93	0.31	33,33,33,33	0
54	MG	CA	1610	1/1	0.93	0.29	60,60,60,60	0
54	MG	BA	3622	1/1	0.93	0.11	45,45,45,45	0
54	MG	CA	1712	1/1	0.93	0.29	87,87,87,87	0
54	MG	DA	3558	1/1	0.93	0.15	36,36,36,36	0
54	MG	DA	3015	1/1	0.93	0.13	38,38,38,38	0
54	MG	BA	3256	1/1	0.93	0.34	23,23,23,23	0
54	MG	DA	3450	1/1	0.93	0.10	67,67,67,67	0
54	MG	BA	3355	1/1	0.93	0.14	29,29,29,29	0
54	MG	DA	3592	1/1	0.93	0.06	83,83,83,83	0
54	MG	BA	3404	1/1	0.93	0.10	45,45,45,45	0
54	MG	DA	3503	1/1	0.93	0.24	34,34,34,34	0
54	MG	BA	3063	1/1	0.93	0.12	54,54,54,54	0
54	MG	BA	3478	1/1	0.93	0.16	41,41,41,41	0
54	MG	DA	3339	1/1	0.93	0.07	44,44,44,44	0
54	MG	DA	3095	1/1	0.93	0.24	53,53,53,53	0
54	MG	BA	3374	1/1	0.93	0.08	34,34,34,34	0
54	MG	BA	3542	1/1	0.94	0.11	83,83,83,83	0
54	MG	DA	3293	1/1	0.94	0.25	33,33,33,33	0
54	MG	CA	1671	1/1	0.94	0.42	49,49,49,49	0
54	MG	DR	201	1/1	0.94	0.31	40,40,40,40	0
54	MG	BA	3428	1/1	0.94	0.09	56,56,56,56	0
54	MG	DA	3159	1/1	0.94	0.20	45,45,45,45	0
54	MG	BA	3643	1/1	0.94	0.11	59,59,59,59	0
54	MG	DA	3344	1/1	0.94	0.09	30,30,30,30	0
54	MG	BA	3165	1/1	0.94	0.28	51,51,51,51	0
54	MG	DA	3226	1/1	0.94	0.49	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3064	1/1	0.94	0.36	48,48,48,48	0
54	MG	DQ	201	1/1	0.94	0.15	40,40,40,40	0
54	MG	BA	3607	1/1	0.94	0.17	99,99,99,99	0
54	MG	AA	1673	1/1	0.94	0.59	60,60,60,60	0
54	MG	DA	3414	1/1	0.94	0.17	51,51,51,51	0
54	MG	BA	3169	1/1	0.94	0.23	31,31,31,31	0
54	MG	BA	3623	1/1	0.94	0.12	73,73,73,73	0
54	MG	DA	3072	1/1	0.94	0.49	50,50,50,50	0
54	MG	BA	3336	1/1	0.94	0.12	45,45,45,45	0
54	MG	BA	3122	1/1	0.94	0.31	49,49,49,49	0
54	MG	DA	3568	1/1	0.94	0.11	78,78,78,78	0
54	MG	CA	1630	1/1	0.94	0.62	72,72,72,72	0
54	MG	DA	3292	1/1	0.94	0.27	33,33,33,33	0
54	MG	BA	3446	1/1	0.94	0.15	30,30,30,30	0
54	MG	BA	3615	1/1	0.94	0.12	52,52,52,52	0
54	MG	BA	3207	1/1	0.94	0.13	33,33,33,33	0
54	MG	CA	1752	1/1	0.94	0.13	71,71,71,71	0
54	MG	BA	3268	1/1	0.94	0.37	27,27,27,27	0
54	MG	BA	3220	1/1	0.94	0.27	31,31,31,31	0
54	MG	BA	3004	1/1	0.94	0.08	76,76,76,76	0
54	MG	AA	1666	1/1	0.94	0.13	74,74,74,74	0
54	MG	AA	1722	1/1	0.94	0.18	66,66,66,66	0
54	MG	DA	3477	1/1	0.94	0.15	53,53,53,53	0
54	MG	BA	3129	1/1	0.94	0.37	37,37,37,37	0
54	MG	CA	1675	1/1	0.94	0.59	61,61,61,61	0
54	MG	DA	3250	1/1	0.94	0.17	49,49,49,49	0
54	MG	DA	3484	1/1	0.94	0.07	64,64,64,64	0
54	MG	BA	3088	1/1	0.94	0.19	33,33,33,33	0
54	MG	CA	1703	1/1	0.94	0.18	56,56,56,56	0
54	MG	BA	3379	1/1	0.94	0.09	22,22,22,22	0
54	MG	CA	1614	1/1	0.94	0.43	85,85,85,85	0
54	MG	DA	3491	1/1	0.94	0.19	44,44,44,44	0
54	MG	DA	3317	1/1	0.94	0.23	47,47,47,47	0
54	MG	DA	3216	1/1	0.94	0.15	51,51,51,51	0
54	MG	DA	3356	1/1	0.94	0.16	60,60,60,60	0
54	MG	BA	3081	1/1	0.94	0.35	42,42,42,42	0
54	MG	BA	3495	1/1	0.94	0.13	35,35,35,35	0
54	MG	AC	301	1/1	0.94	0.14	57,57,57,57	0
54	MG	BA	3413	1/1	0.94	0.12	57,57,57,57	0
54	MG	BA	3235	1/1	0.94	0.20	50,50,50,50	0
54	MG	BA	3031	1/1	0.94	0.17	44,44,44,44	0
54	MG	DA	3462	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3482	1/1	0.94	0.19	56,56,56,56	0
54	MG	CA	1622	1/1	0.94	0.28	47,47,47,47	0
54	MG	DA	3579	1/1	0.94	0.08	57,57,57,57	0
54	MG	DA	3099	1/1	0.94	0.23	36,36,36,36	0
54	MG	BA	3473	1/1	0.94	0.23	30,30,30,30	0
54	MG	BA	3653	1/1	0.94	0.15	104,104,104,104	0
54	MG	BA	3382	1/1	0.94	0.19	100,100,100,100	0
54	MG	BA	3535	1/1	0.94	0.11	55,55,55,55	0
54	MG	B3	101	1/1	0.94	0.35	51,51,51,51	0
54	MG	DA	3265	1/1	0.94	0.32	44,44,44,44	0
54	MG	AA	1732	1/1	0.94	0.10	94,94,94,94	0
54	MG	CA	1682	1/1	0.94	0.13	58,58,58,58	0
54	MG	D8	101	1/1	0.94	0.15	48,48,48,48	0
54	MG	DA	3357	1/1	0.94	0.19	36,36,36,36	0
54	MG	CA	1735	1/1	0.94	0.27	69,69,69,69	0
54	MG	DA	3035	1/1	0.94	0.17	60,60,60,60	0
54	MG	AA	1733	1/1	0.94	0.07	78,78,78,78	0
54	MG	AA	1735	1/1	0.94	0.17	110,110,110,110	0
54	MG	BA	3172	1/1	0.94	0.38	47,47,47,47	0
54	MG	CA	1653	1/1	0.94	0.80	57,57,57,57	0
54	MG	DA	3584	1/1	0.94	0.30	48,48,48,48	0
54	MG	DA	3561	1/1	0.94	0.19	71,71,71,71	0
54	MG	BA	3383	1/1	0.94	0.13	70,70,70,70	0
54	MG	BA	3273	1/1	0.94	0.40	37,37,37,37	0
54	MG	DA	3294	1/1	0.94	0.15	42,42,42,42	0
54	MG	DA	3510	1/1	0.94	0.10	74,74,74,74	0
54	MG	B0	103	1/1	0.94	0.12	89,89,89,89	0
54	MG	DA	3011	1/1	0.94	0.26	42,42,42,42	0
54	MG	AA	1626	1/1	0.94	0.42	71,71,71,71	0
54	MG	BA	3349	1/1	0.94	0.10	36,36,36,36	0
54	MG	CA	1666	1/1	0.94	0.37	64,64,64,64	0
54	MG	DA	3044	1/1	0.94	0.19	46,46,46,46	0
54	MG	DA	3184	1/1	0.94	0.15	46,46,46,46	0
54	MG	BA	3449	1/1	0.94	0.29	29,29,29,29	0
54	MG	BA	3481	1/1	0.94	0.16	25,25,25,25	0
54	MG	DA	3224	1/1	0.94	0.37	32,32,32,32	0
54	MG	BA	3182	1/1	0.94	0.41	37,37,37,37	0
54	MG	AA	1668	1/1	0.94	0.57	62,62,62,62	0
54	MG	BB	221	1/1	0.94	0.06	50,50,50,50	0
54	MG	DA	3047	1/1	0.94	0.15	38,38,38,38	0
54	MG	CA	1669	1/1	0.94	0.30	76,76,76,76	0
54	MG	BA	3249	1/1	0.94	0.35	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3539	1/1	0.94	0.09	67,67,67,67	0
54	MG	BA	3387	1/1	0.94	0.06	63,63,63,63	0
54	MG	BZ	301	1/1	0.94	0.17	55,55,55,55	0
54	MG	BA	3490	1/1	0.94	0.10	28,28,28,28	0
54	MG	CA	1710	1/1	0.94	0.09	48,48,48,48	0
54	MG	BA	3281	1/1	0.94	0.25	24,24,24,24	0
54	MG	BA	3272	1/1	0.94	0.37	31,31,31,31	0
54	MG	DA	3468	1/1	0.94	0.07	53,53,53,53	0
54	MG	DE	302	1/1	0.94	0.35	21,21,21,21	0
54	MG	CA	1685	1/1	0.94	0.34	71,71,71,71	0
54	MG	BA	3435	1/1	0.94	0.15	48,48,48,48	0
54	MG	BA	3528	1/1	0.94	0.17	39,39,39,39	0
54	MG	DA	3057	1/1	0.94	0.15	35,35,35,35	0
54	MG	DA	3069	1/1	0.94	0.39	42,42,42,42	0
54	MG	DA	3540	1/1	0.94	0.10	53,53,53,53	0
54	MG	BA	3520	1/1	0.94	0.14	95,95,95,95	0
54	MG	DA	3190	1/1	0.94	0.09	59,59,59,59	0
54	MG	BA	3155	1/1	0.94	0.19	41,41,41,41	0
54	MG	BA	3613	1/1	0.94	0.07	65,65,65,65	0
54	MG	AA	1615	1/1	0.94	0.36	54,54,54,54	0
54	MG	DA	3473	1/1	0.94	0.20	38,38,38,38	0
54	MG	BA	3354	1/1	0.94	0.09	37,37,37,37	0
54	MG	DA	3126	1/1	0.94	0.59	63,63,63,63	0
54	MG	B8	102	1/1	0.94	0.10	61,61,61,61	0
54	MG	BA	3136	1/1	0.94	0.36	45,45,45,45	0
54	MG	BA	3110	1/1	0.94	0.20	66,66,66,66	0
54	MG	BA	3406	1/1	0.94	0.06	66,66,66,66	0
54	MG	BA	3426	1/1	0.94	0.08	37,37,37,37	0
54	MG	BA	3401	1/1	0.94	0.14	58,58,58,58	0
54	MG	DA	3304	1/1	0.94	0.42	29,29,29,29	0
54	MG	DA	3182	1/1	0.94	0.31	46,46,46,46	0
54	MG	BA	3341	1/1	0.94	0.05	44,44,44,44	0
54	MG	BA	3195	1/1	0.94	0.22	60,60,60,60	0
54	MG	DA	3514	1/1	0.94	0.19	42,42,42,42	0
54	MG	BA	3098	1/1	0.94	0.24	40,40,40,40	0
54	MG	BA	3488	1/1	0.94	0.17	24,24,24,24	0
54	MG	BA	3224	1/1	0.94	0.28	50,50,50,50	0
54	MG	DA	3291	1/1	0.94	0.33	53,53,53,53	0
54	MG	DA	3551	1/1	0.94	0.20	62,62,62,62	0
54	MG	BA	3555	1/1	0.94	0.12	47,47,47,47	0
54	MG	DA	3527	1/1	0.94	0.15	91,91,91,91	0
54	MG	DA	3173	1/1	0.94	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3494	1/1	0.94	0.14	37,37,37,37	0
54	MG	DA	3426	1/1	0.94	0.07	81,81,81,81	0
54	MG	BA	3189	1/1	0.94	0.32	41,41,41,41	0
54	MG	AA	1662	1/1	0.94	0.12	58,58,58,58	0
54	MG	AA	1694	1/1	0.94	0.08	80,80,80,80	0
54	MG	BA	3242	1/1	0.94	0.20	38,38,38,38	0
54	MG	BA	3036	1/1	0.94	0.12	36,36,36,36	0
54	MG	DA	3155	1/1	0.95	0.37	64,64,64,64	0
54	MG	BA	3389	1/1	0.95	0.18	46,46,46,46	0
54	MG	DO	201	1/1	0.95	0.09	120,120,120,120	0
54	MG	BA	3632	1/1	0.95	0.05	54,54,54,54	0
54	MG	DA	3051	1/1	0.95	0.14	38,38,38,38	0
54	MG	DA	3233	1/1	0.95	0.14	38,38,38,38	0
54	MG	BA	3049	1/1	0.95	0.37	53,53,53,53	0
54	MG	BA	3125	1/1	0.95	0.31	45,45,45,45	0
54	MG	DA	3300	1/1	0.95	0.14	41,41,41,41	0
54	MG	BA	3460	1/1	0.95	0.30	61,61,61,61	0
54	MG	DA	3381	1/1	0.95	0.05	42,42,42,42	0
54	MG	DA	3140	1/1	0.95	0.32	64,64,64,64	0
54	MG	BA	3364	1/1	0.95	0.07	81,81,81,81	0
54	MG	BA	3652	1/1	0.95	0.06	97,97,97,97	0
54	MG	BA	3174	1/1	0.95	0.18	32,32,32,32	0
54	MG	BA	3244	1/1	0.95	0.14	30,30,30,30	0
54	MG	BA	3202	1/1	0.95	0.16	48,48,48,48	0
54	MG	DA	3026	1/1	0.95	0.08	39,39,39,39	0
54	MG	DA	3379	1/1	0.95	0.12	59,59,59,59	0
54	MG	BA	3071	1/1	0.95	0.17	34,34,34,34	0
54	MG	B2	101	1/1	0.95	0.17	45,45,45,45	0
54	MG	BA	3208	1/1	0.95	0.28	38,38,38,38	0
54	MG	DA	3301	1/1	0.95	0.46	50,50,50,50	0
54	MG	AA	1700	1/1	0.95	0.09	42,42,42,42	0
54	MG	DA	3108	1/1	0.95	0.11	42,42,42,42	0
54	MG	DB	203	1/1	0.95	0.39	58,58,58,58	0
54	MG	BA	3657	1/1	0.95	0.45	65,65,65,65	0
54	MG	DA	3455	1/1	0.95	0.05	68,68,68,68	0
54	MG	DA	3546	1/1	0.95	0.11	64,64,64,64	0
54	MG	BA	3093	1/1	0.95	0.19	42,42,42,42	0
54	MG	CA	1699	1/1	0.95	0.16	83,83,83,83	0
54	MG	DA	3007	1/1	0.95	0.14	48,48,48,48	0
54	MG	BA	3639	1/1	0.95	0.20	65,65,65,65	0
54	MG	BA	3633	1/1	0.95	0.12	43,43,43,43	0
54	MG	D0	101	1/1	0.95	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3253	1/1	0.95	0.44	19,19,19,19	0
54	MG	AA	1631	1/1	0.95	0.16	41,41,41,41	0
54	MG	BA	3521	1/1	0.95	0.09	40,40,40,40	0
54	MG	DA	3313	1/1	0.95	0.35	29,29,29,29	0
54	MG	DA	3056	1/1	0.95	0.18	43,43,43,43	0
54	MG	BA	3344	1/1	0.95	0.31	61,61,61,61	0
54	MG	BA	3441	1/1	0.95	0.08	56,56,56,56	0
54	MG	B1	101	1/1	0.95	0.18	45,45,45,45	0
54	MG	BA	3476	1/1	0.95	0.18	49,49,49,49	0
54	MG	BA	3286	1/1	0.95	0.46	52,52,52,52	0
55	ZN	D9	101	1/1	0.95	0.06	65,65,65,65	0
54	MG	DA	3249	1/1	0.95	0.29	49,49,49,49	0
54	MG	BA	3245	1/1	0.95	0.34	23,23,23,23	0
54	MG	BA	3251	1/1	0.95	0.25	27,27,27,27	0
54	MG	BA	3052	1/1	0.95	0.17	52,52,52,52	0
54	MG	BA	3617	1/1	0.95	0.07	94,94,94,94	0
54	MG	DA	3560	1/1	0.95	0.14	57,57,57,57	0
54	MG	BA	3378	1/1	0.95	0.16	25,25,25,25	0
54	MG	DA	3131	1/1	0.95	0.32	56,56,56,56	0
54	MG	DA	3118	1/1	0.95	0.24	43,43,43,43	0
54	MG	DA	3406	1/1	0.95	0.07	58,58,58,58	0
54	MG	BA	3228	1/1	0.95	0.40	37,37,37,37	0
54	MG	DA	3485	1/1	0.95	0.26	58,58,58,58	0
54	MG	BA	3033	1/1	0.95	0.10	36,36,36,36	0
54	MG	AA	1687	1/1	0.95	0.18	62,62,62,62	0
54	MG	AA	1667	1/1	0.95	0.19	38,38,38,38	0
54	MG	DA	3547	1/1	0.95	0.17	29,29,29,29	0
54	MG	DA	3598	1/1	0.95	0.11	76,76,76,76	0
54	MG	DA	3441	1/1	0.95	0.26	48,48,48,48	0
54	MG	DA	3104	1/1	0.95	0.22	34,34,34,34	0
54	MG	DA	3553	1/1	0.95	0.08	54,54,54,54	0
54	MG	DA	3520	1/1	0.95	0.13	56,56,56,56	0
54	MG	DA	3045	1/1	0.95	0.12	38,38,38,38	0
54	MG	DA	3299	1/1	0.95	0.42	65,65,65,65	0
54	MG	BB	222	1/1	0.95	0.18	80,80,80,80	0
54	MG	CA	1742	1/1	0.95	0.07	113,113,113,113	0
54	MG	DA	3320	1/1	0.95	0.14	38,38,38,38	0
54	MG	DA	3574	1/1	0.95	0.07	41,41,41,41	0
54	MG	BA	3384	1/1	0.95	0.15	88,88,88,88	0
54	MG	BA	3079	1/1	0.95	0.20	50,50,50,50	0
54	MG	DA	3210	1/1	0.95	0.26	53,53,53,53	0
54	MG	DA	3178	1/1	0.95	0.33	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3529	1/1	0.95	0.07	65,65,65,65	0
54	MG	BF	301	1/1	0.95	0.21	33,33,33,33	0
54	MG	BA	3070	1/1	0.95	0.20	37,37,37,37	0
54	MG	DA	3084	1/1	0.95	0.24	37,37,37,37	0
54	MG	DA	3013	1/1	0.95	0.12	37,37,37,37	0
54	MG	BA	3028	1/1	0.95	0.15	22,22,22,22	0
54	MG	DA	3511	1/1	0.95	0.09	49,49,49,49	0
54	MG	DA	3564	1/1	0.95	0.10	61,61,61,61	0
54	MG	BA	3560	1/1	0.95	0.08	74,74,74,74	0
54	MG	DA	3156	1/1	0.95	0.20	35,35,35,35	0
54	MG	BA	3457	1/1	0.95	0.19	27,27,27,27	0
54	MG	BA	3314	1/1	0.95	0.17	37,37,37,37	0
54	MG	DA	3219	1/1	0.95	0.16	38,38,38,38	0
54	MG	DA	3071	1/1	0.95	0.19	44,44,44,44	0
54	MG	DA	3269	1/1	0.95	0.29	47,47,47,47	0
54	MG	DA	3154	1/1	0.95	0.33	26,26,26,26	0
54	MG	BA	3608	1/1	0.95	0.26	71,71,71,71	0
54	MG	BA	3166	1/1	0.95	0.29	36,36,36,36	0
54	MG	AA	1639	1/1	0.95	0.45	67,67,67,67	0
54	MG	DA	3311	1/1	0.95	0.35	26,26,26,26	0
54	MG	BB	217	1/1	0.95	0.11	67,67,67,67	0
54	MG	DA	3472	1/1	0.95	0.33	50,50,50,50	0
54	MG	BA	3533	1/1	0.95	0.14	61,61,61,61	0
54	MG	DA	3053	1/1	0.95	0.14	40,40,40,40	0
54	MG	BA	3651	1/1	0.95	0.21	87,87,87,87	0
54	MG	DA	3429	1/1	0.95	0.07	56,56,56,56	0
54	MG	DA	3349	1/1	0.95	0.15	35,35,35,35	0
54	MG	CA	1725	1/1	0.95	0.17	65,65,65,65	0
54	MG	DA	3135	1/1	0.95	0.32	47,47,47,47	0
54	MG	BA	3351	1/1	0.95	0.08	60,60,60,60	0
54	MG	DA	3067	1/1	0.95	0.23	49,49,49,49	0
54	MG	DA	3161	1/1	0.95	0.34	39,39,39,39	0
54	MG	BA	3409	1/1	0.95	0.07	68,68,68,68	0
54	MG	BA	3157	1/1	0.95	0.30	48,48,48,48	0
54	MG	BA	3429	1/1	0.95	0.21	47,47,47,47	0
54	MG	DA	3054	1/1	0.95	0.12	46,46,46,46	0
54	MG	CA	1696	1/1	0.95	0.43	61,61,61,61	0
54	MG	BA	3453	1/1	0.95	0.08	46,46,46,46	0
54	MG	CA	1619	1/1	0.95	0.15	50,50,50,50	0
54	MG	CA	1715	1/1	0.95	0.05	103,103,103,103	0
54	MG	BQ	203	1/1	0.95	0.12	73,73,73,73	0
54	MG	CA	1734	1/1	0.95	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3392	1/1	0.95	0.13	110,110,110,110	0
54	MG	AA	1695	1/1	0.95	0.11	74,74,74,74	0
54	MG	BA	3209	1/1	0.95	0.21	56,56,56,56	0
54	MG	BA	3265	1/1	0.95	0.39	29,29,29,29	0
54	MG	BA	3058	1/1	0.95	0.14	32,32,32,32	0
54	MG	BA	3255	1/1	0.95	0.31	25,25,25,25	0
54	MG	BA	3513	1/1	0.95	0.09	86,86,86,86	0
54	MG	DA	3359	1/1	0.95	0.10	33,33,33,33	0
54	MG	DA	3241	1/1	0.95	0.27	35,35,35,35	0
54	MG	BA	3588	1/1	0.95	0.12	64,64,64,64	0
54	MG	BA	3610	1/1	0.95	0.08	63,63,63,63	0
54	MG	BA	3116	1/1	0.95	0.17	53,53,53,53	0
54	MG	DA	3393	1/1	0.95	0.14	41,41,41,41	0
54	MG	DA	3531	1/1	0.95	0.18	91,91,91,91	0
54	MG	DA	3552	1/1	0.95	0.39	35,35,35,35	0
54	MG	DA	3439	1/1	0.95	0.07	57,57,57,57	0
54	MG	BA	3618	1/1	0.95	0.08	52,52,52,52	0
54	MG	BA	3246	1/1	0.95	0.47	20,20,20,20	0
54	MG	DA	3430	1/1	0.95	0.12	30,30,30,30	0
54	MG	BA	3275	1/1	0.95	0.29	26,26,26,26	0
54	MG	BW	202	1/1	0.95	0.12	33,33,33,33	0
54	MG	BA	3517	1/1	0.95	0.11	26,26,26,26	0
54	MG	DA	3010	1/1	0.95	0.18	42,42,42,42	0
54	MG	CA	1691	1/1	0.95	0.42	51,51,51,51	0
54	MG	BB	201	1/1	0.95	0.12	57,57,57,57	0
54	MG	AA	1725	1/1	0.95	0.20	56,56,56,56	0
54	MG	BA	3597	1/1	0.96	0.24	84,84,84,84	0
54	MG	BA	3508	1/1	0.96	0.14	29,29,29,29	0
54	MG	B0	102	1/1	0.96	0.17	54,54,54,54	0
54	MG	DA	3327	1/1	0.96	0.49	52,52,52,52	0
54	MG	DA	3534	1/1	0.96	0.14	28,28,28,28	0
54	MG	BA	3211	1/1	0.96	0.10	26,26,26,26	0
54	MG	BA	3135	1/1	0.96	0.41	45,45,45,45	0
54	MG	DA	3018	1/1	0.96	0.20	54,54,54,54	0
54	MG	BA	3467	1/1	0.96	0.24	30,30,30,30	0
54	MG	DA	3158	1/1	0.96	0.29	46,46,46,46	0
54	MG	BA	3324	1/1	0.96	0.10	42,42,42,42	0
54	MG	DB	207	1/1	0.96	0.24	57,57,57,57	0
54	MG	DD	302	1/1	0.96	0.41	38,38,38,38	0
54	MG	BA	3160	1/1	0.96	0.35	39,39,39,39	0
54	MG	DA	3323	1/1	0.96	0.13	40,40,40,40	0
54	MG	DA	3157	1/1	0.96	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3082	1/1	0.96	0.42	36,36,36,36	0
54	MG	DB	208	1/1	0.96	0.10	104,104,104,104	0
54	MG	DA	3039	1/1	0.96	0.20	28,28,28,28	0
54	MG	BA	3620	1/1	0.96	0.05	68,68,68,68	0
54	MG	BA	3412	1/1	0.96	0.17	78,78,78,78	0
54	MG	DA	3347	1/1	0.96	0.17	35,35,35,35	0
54	MG	CA	1641	1/1	0.96	0.09	52,52,52,52	0
54	MG	BA	3640	1/1	0.96	0.14	116,116,116,116	0
54	MG	DA	3150	1/1	0.96	0.33	42,42,42,42	0
54	MG	CA	1678	1/1	0.96	0.24	55,55,55,55	0
54	MG	AA	1648	1/1	0.96	0.43	44,44,44,44	0
54	MG	DA	3453	1/1	0.96	0.07	79,79,79,79	0
54	MG	AA	1691	1/1	0.96	0.12	43,43,43,43	0
54	MG	DA	3043	1/1	0.96	0.10	54,54,54,54	0
54	MG	DA	3037	1/1	0.96	0.12	43,43,43,43	0
54	MG	BA	3130	1/1	0.96	0.24	43,43,43,43	0
54	MG	BA	3629	1/1	0.96	0.09	24,24,24,24	0
54	MG	BA	3223	1/1	0.96	0.51	60,60,60,60	0
55	ZN	AD	301	1/1	0.96	0.28	74,74,74,74	0
54	MG	BA	3263	1/1	0.96	0.38	36,36,36,36	0
54	MG	BA	3386	1/1	0.96	0.09	40,40,40,40	0
54	MG	CA	1654	1/1	0.96	0.13	65,65,65,65	0
54	MG	CA	1690	1/1	0.96	0.25	64,64,64,64	0
54	MG	BA	3371	1/1	0.96	0.11	33,33,33,33	0
54	MG	DA	3367	1/1	0.96	0.24	30,30,30,30	0
54	MG	CA	1709	1/1	0.96	0.14	63,63,63,63	0
54	MG	DA	3386	1/1	0.96	0.08	39,39,39,39	0
54	MG	BA	3042	1/1	0.96	0.27	40,40,40,40	0
54	MG	CA	1730	1/1	0.96	0.10	62,62,62,62	0
54	MG	BA	3112	1/1	0.96	0.19	55,55,55,55	0
54	MG	DA	3448	1/1	0.96	0.10	42,42,42,42	0
54	MG	DA	3475	1/1	0.96	0.11	30,30,30,30	0
54	MG	BA	3106	1/1	0.96	0.21	52,52,52,52	0
54	MG	DA	3369	1/1	0.96	0.07	50,50,50,50	0
54	MG	BA	3168	1/1	0.96	0.26	28,28,28,28	0
54	MG	DA	3168	1/1	0.96	0.20	42,42,42,42	0
54	MG	DA	3390	1/1	0.96	0.07	47,47,47,47	0
54	MG	DA	3501	1/1	0.96	0.08	58,58,58,58	0
54	MG	BA	3628	1/1	0.96	0.15	35,35,35,35	0
54	MG	DA	3009	1/1	0.96	0.27	46,46,46,46	0
54	MG	AA	1701	1/1	0.96	0.12	48,48,48,48	0
54	MG	DA	3208	1/1	0.96	0.39	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3405	1/1	0.96	0.16	32,32,32,32	0
54	MG	DA	3106	1/1	0.96	0.40	37,37,37,37	0
54	MG	CA	1723	1/1	0.96	0.13	55,55,55,55	0
54	MG	DA	3493	1/1	0.96	0.04	63,63,63,63	0
54	MG	BA	3625	1/1	0.96	0.06	53,53,53,53	0
54	MG	CA	1601	1/1	0.96	0.21	45,45,45,45	0
54	MG	BA	3069	1/1	0.96	0.36	42,42,42,42	0
54	MG	DA	3315	1/1	0.96	0.11	31,31,31,31	0
54	MG	BA	3199	1/1	0.96	0.14	41,41,41,41	0
54	MG	DA	3396	1/1	0.96	0.17	52,52,52,52	0
54	MG	CA	1689	1/1	0.96	0.38	61,61,61,61	0
54	MG	AA	1728	1/1	0.96	0.12	53,53,53,53	0
54	MG	BA	3415	1/1	0.96	0.08	33,33,33,33	0
54	MG	BA	3247	1/1	0.96	0.46	26,26,26,26	0
54	MG	AA	1711	1/1	0.96	0.24	46,46,46,46	0
54	MG	DA	3575	1/1	0.96	0.21	35,35,35,35	0
54	MG	BA	3276	1/1	0.96	0.24	23,23,23,23	0
54	MG	BA	3313	1/1	0.96	0.08	37,37,37,37	0
54	MG	BA	3126	1/1	0.96	0.22	41,41,41,41	0
54	MG	DA	3581	1/1	0.96	0.09	52,52,52,52	0
54	MG	B9	102	1/1	0.96	0.12	28,28,28,28	0
54	MG	DA	3535	1/1	0.96	0.15	64,64,64,64	0
54	MG	DA	3079	1/1	0.96	0.18	47,47,47,47	0
54	MG	DA	3348	1/1	0.96	0.15	41,41,41,41	0
54	MG	BA	3278	1/1	0.96	0.38	30,30,30,30	0
54	MG	DA	3080	1/1	0.96	0.16	44,44,44,44	0
54	MG	BA	3381	1/1	0.96	0.06	66,66,66,66	0
54	MG	BD	303	1/1	0.96	0.18	35,35,35,35	0
54	MG	BA	3541	1/1	0.96	0.09	42,42,42,42	0
54	MG	DA	3302	1/1	0.96	0.51	21,21,21,21	0
54	MG	DA	3023	1/1	0.96	0.06	43,43,43,43	0
54	MG	DA	3498	1/1	0.96	0.10	28,28,28,28	0
54	MG	BA	3440	1/1	0.96	0.07	46,46,46,46	0
54	MG	BA	3140	1/1	0.96	0.56	36,36,36,36	0
54	MG	BA	3296	1/1	0.96	0.22	43,43,43,43	0
54	MG	AA	1665	1/1	0.96	0.10	51,51,51,51	0
54	MG	DA	3206	1/1	0.96	0.60	52,52,52,52	0
54	MG	BA	3556	1/1	0.96	0.20	57,57,57,57	0
54	MG	BR	201	1/1	0.96	0.17	29,29,29,29	0
54	MG	BA	3604	1/1	0.96	0.07	50,50,50,50	0
54	MG	BA	3167	1/1	0.96	0.45	31,31,31,31	0
54	MG	DA	3362	1/1	0.96	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3385	1/1	0.96	0.09	49,49,49,49	0
54	MG	BA	3127	1/1	0.96	0.28	38,38,38,38	0
54	MG	DA	3076	1/1	0.96	0.15	42,42,42,42	0
54	MG	DA	3006	1/1	0.96	0.29	38,38,38,38	0
54	MG	BA	3391	1/1	0.96	0.11	39,39,39,39	0
54	MG	DA	3036	1/1	0.96	0.29	44,44,44,44	0
54	MG	BA	3647	1/1	0.96	0.15	70,70,70,70	0
54	MG	BA	3078	1/1	0.96	0.27	30,30,30,30	0
54	MG	DA	3205	1/1	0.96	0.28	47,47,47,47	0
54	MG	BA	3376	1/1	0.96	0.11	26,26,26,26	0
54	MG	AA	1685	1/1	0.96	0.10	71,71,71,71	0
54	MG	CA	1624	1/1	0.96	0.54	63,63,63,63	0
54	MG	DA	3041	1/1	0.96	0.51	36,36,36,36	0
54	MG	BA	3545	1/1	0.96	0.07	43,43,43,43	0
54	MG	DA	3392	1/1	0.96	0.14	35,35,35,35	0
54	MG	BA	3395	1/1	0.96	0.10	60,60,60,60	0
54	MG	DA	3307	1/1	0.96	0.22	35,35,35,35	0
54	MG	BA	3325	1/1	0.96	0.11	40,40,40,40	0
54	MG	DA	3351	1/1	0.96	0.12	40,40,40,40	0
54	MG	DA	3440	1/1	0.96	0.28	42,42,42,42	0
54	MG	BA	3226	1/1	0.96	0.22	50,50,50,50	0
54	MG	BA	3192	1/1	0.96	0.10	51,51,51,51	0
54	MG	BA	3518	1/1	0.96	0.10	50,50,50,50	0
54	MG	AA	1610	1/1	0.96	0.41	56,56,56,56	0
54	MG	CA	1687	1/1	0.96	0.22	62,62,62,62	0
54	MG	BA	3148	1/1	0.96	0.23	47,47,47,47	0
54	MG	DA	3395	1/1	0.96	0.11	39,39,39,39	0
54	MG	BA	3362	1/1	0.96	0.10	43,43,43,43	0
54	MG	DA	3160	1/1	0.96	0.10	42,42,42,42	0
55	ZN	DY	201	1/1	0.96	0.05	94,94,94,94	0
54	MG	BA	3487	1/1	0.96	0.15	20,20,20,20	0
54	MG	DA	3253	1/1	0.96	0.09	50,50,50,50	0
54	MG	DA	3389	1/1	0.96	0.07	51,51,51,51	0
54	MG	BB	203	1/1	0.96	0.23	70,70,70,70	0
54	MG	BA	3059	1/1	0.96	0.12	48,48,48,48	0
54	MG	DA	3232	1/1	0.96	0.32	57,57,57,57	0
54	MG	BA	3561	1/1	0.96	0.09	54,54,54,54	0
54	MG	BA	3145	1/1	0.96	0.20	44,44,44,44	0
54	MG	DA	3183	1/1	0.96	0.45	26,26,26,26	0
54	MG	BA	3619	1/1	0.96	0.13	64,64,64,64	0
54	MG	AA	1693	1/1	0.96	0.11	51,51,51,51	0
54	MG	DA	3310	1/1	0.96	0.37	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3445	1/1	0.96	0.17	31,31,31,31	0
54	MG	DA	3303	1/1	0.96	0.48	34,34,34,34	0
54	MG	BA	3530	1/1	0.96	0.14	56,56,56,56	0
54	MG	BA	3509	1/1	0.96	0.15	50,50,50,50	0
54	MG	DE	304	1/1	0.96	0.21	42,42,42,42	0
54	MG	BA	3605	1/1	0.96	0.07	55,55,55,55	0
54	MG	BA	3321	1/1	0.96	0.06	32,32,32,32	0
54	MG	AA	1672	1/1	0.96	0.41	46,46,46,46	0
54	MG	BA	3494	1/1	0.97	0.13	34,34,34,34	0
54	MG	BA	3057	1/1	0.97	0.24	51,51,51,51	0
54	MG	BA	3505	1/1	0.97	0.21	41,41,41,41	0
54	MG	CA	1727	1/1	0.97	0.17	46,46,46,46	0
54	MG	BA	3602	1/1	0.97	0.05	56,56,56,56	0
54	MG	BA	3485	1/1	0.97	0.10	32,32,32,32	0
54	MG	DA	3052	1/1	0.97	0.37	52,52,52,52	0
54	MG	DA	3285	1/1	0.97	0.04	64,64,64,64	0
54	MG	BA	3289	1/1	0.97	0.34	34,34,34,34	0
54	MG	CA	1743	1/1	0.97	0.08	61,61,61,61	0
54	MG	BB	220	1/1	0.97	0.18	60,60,60,60	0
54	MG	DA	3365	1/1	0.97	0.08	40,40,40,40	0
54	MG	BA	3434	1/1	0.97	0.11	62,62,62,62	0
54	MG	DA	3474	1/1	0.97	0.10	30,30,30,30	0
54	MG	BE	303	1/1	0.97	0.13	26,26,26,26	0
54	MG	DA	3243	1/1	0.97	0.22	28,28,28,28	0
54	MG	DA	3467	1/1	0.97	0.11	43,43,43,43	0
54	MG	BA	3352	1/1	0.97	0.14	81,81,81,81	0
54	MG	BA	3184	1/1	0.97	0.21	40,40,40,40	0
54	MG	BA	3624	1/1	0.97	0.11	36,36,36,36	0
54	MG	BA	3023	1/1	0.97	0.14	52,52,52,52	0
54	MG	DA	3088	1/1	0.97	0.39	55,55,55,55	0
54	MG	BA	3551	1/1	0.97	0.11	82,82,82,82	0
54	MG	BA	3299	1/1	0.97	0.28	66,66,66,66	0
54	MG	BA	3248	1/1	0.97	0.41	27,27,27,27	0
54	MG	CA	1726	1/1	0.97	0.19	52,52,52,52	0
54	MG	DA	3143	1/1	0.97	0.20	60,60,60,60	0
54	MG	CA	1647	1/1	0.97	0.15	86,86,86,86	0
54	MG	DA	3337	1/1	0.97	0.28	30,30,30,30	0
54	MG	DA	3422	1/1	0.97	0.18	43,43,43,43	0
54	MG	BA	3089	1/1	0.97	0.32	41,41,41,41	0
54	MG	CA	1728	1/1	0.97	0.16	60,60,60,60	0
54	MG	DA	3578	1/1	0.97	0.22	29,29,29,29	0
54	MG	AA	1726	1/1	0.97	0.14	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3271	1/1	0.97	0.14	30,30,30,30	0
54	MG	BA	3006	1/1	0.97	0.19	25,25,25,25	0
54	MG	DA	3562	1/1	0.97	0.14	58,58,58,58	0
54	MG	AA	1724	1/1	0.97	0.27	74,74,74,74	0
54	MG	BA	3260	1/1	0.97	0.39	30,30,30,30	0
54	MG	BA	3316	1/1	0.97	0.13	45,45,45,45	0
54	MG	BA	3178	1/1	0.97	0.29	43,43,43,43	0
54	MG	CA	1644	1/1	0.97	0.26	53,53,53,53	0
54	MG	BA	3365	1/1	0.97	0.07	69,69,69,69	0
54	MG	DA	3496	1/1	0.97	0.20	66,66,66,66	0
54	MG	BA	3156	1/1	0.97	0.27	39,39,39,39	0
54	MG	BA	3360	1/1	0.97	0.22	35,35,35,35	0
54	MG	DA	3373	1/1	0.97	0.27	32,32,32,32	0
54	MG	CA	1760	1/1	0.97	0.09	87,87,87,87	0
54	MG	DA	3518	1/1	0.97	0.09	69,69,69,69	0
54	MG	CA	1721	1/1	0.97	0.21	64,64,64,64	0
54	MG	BA	3163	1/1	0.97	0.28	23,23,23,23	0
54	MG	BA	3484	1/1	0.97	0.18	27,27,27,27	0
54	MG	DA	3490	1/1	0.97	0.12	33,33,33,33	0
54	MG	AA	1721	1/1	0.97	0.06	62,62,62,62	0
54	MG	BA	3274	1/1	0.97	0.29	26,26,26,26	0
54	MG	CA	1724	1/1	0.97	0.11	49,49,49,49	0
54	MG	DA	3415	1/1	0.97	0.11	43,43,43,43	0
54	MG	DA	3102	1/1	0.97	0.47	40,40,40,40	0
54	MG	DA	3234	1/1	0.97	0.18	41,41,41,41	0
54	MG	BA	3540	1/1	0.97	0.13	35,35,35,35	0
54	MG	BA	3310	1/1	0.97	0.35	23,23,23,23	0
54	MG	CA	1623	1/1	0.97	0.39	43,43,43,43	0
54	MG	DA	3471	1/1	0.97	0.19	31,31,31,31	0
54	MG	DA	3529	1/1	0.97	0.09	56,56,56,56	0
54	MG	DA	3062	1/1	0.97	0.36	49,49,49,49	0
54	MG	DA	3388	1/1	0.97	0.14	43,43,43,43	0
54	MG	CA	1688	1/1	0.97	0.35	54,54,54,54	0
54	MG	AA	1710	1/1	0.97	0.07	79,79,79,79	0
54	MG	BA	3326	1/1	0.97	0.11	49,49,49,49	0
54	MG	BB	214	1/1	0.97	0.12	40,40,40,40	0
54	MG	BA	3573	1/1	0.97	0.21	23,23,23,23	0
54	MG	BA	3293	1/1	0.97	0.18	48,48,48,48	0
54	MG	DA	3181	1/1	0.97	0.28	49,49,49,49	0
54	MG	BA	3284	1/1	0.97	0.37	24,24,24,24	0
54	MG	BA	3334	1/1	0.97	0.09	51,51,51,51	0
54	MG	DB	206	1/1	0.97	0.26	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3279	1/1	0.97	0.12	44,44,44,44	0
54	MG	BA	3614	1/1	0.97	0.04	66,66,66,66	0
54	MG	DA	3533	1/1	0.97	0.10	89,89,89,89	0
54	MG	BA	3511	1/1	0.97	0.15	32,32,32,32	0
54	MG	DA	3446	1/1	0.97	0.24	42,42,42,42	0
54	MG	DA	3341	1/1	0.97	0.14	43,43,43,43	0
54	MG	BA	3047	1/1	0.97	0.30	35,35,35,35	0
54	MG	DA	3420	1/1	0.97	0.22	37,37,37,37	0
54	MG	CA	1659	1/1	0.97	0.20	48,48,48,48	0
54	MG	AA	1630	1/1	0.97	0.26	39,39,39,39	0
54	MG	BA	3576	1/1	0.97	0.19	21,21,21,21	0
54	MG	BA	3599	1/1	0.97	0.17	30,30,30,30	0
54	MG	DA	3034	1/1	0.97	0.10	32,32,32,32	0
54	MG	BA	3064	1/1	0.97	0.24	34,34,34,34	0
54	MG	BA	3282	1/1	0.97	0.33	27,27,27,27	0
54	MG	DA	3138	1/1	0.97	0.31	41,41,41,41	0
54	MG	CA	1749	1/1	0.97	0.23	61,61,61,61	0
54	MG	B5	102	1/1	0.97	0.10	52,52,52,52	0
54	MG	DA	3121	1/1	0.97	0.13	34,34,34,34	0
54	MG	BA	3315	1/1	0.97	0.15	31,31,31,31	0
54	MG	BA	3493	1/1	0.97	0.20	40,40,40,40	0
54	MG	BA	3118	1/1	0.97	0.22	44,44,44,44	0
54	MG	DA	3114	1/1	0.97	0.39	30,30,30,30	0
54	MG	AA	1608	1/1	0.97	0.33	67,67,67,67	0
54	MG	DB	205	1/1	0.97	0.16	55,55,55,55	0
54	MG	DA	3083	1/1	0.97	0.22	37,37,37,37	0
54	MG	BA	3596	1/1	0.97	0.07	48,48,48,48	0
54	MG	BA	3464	1/1	0.97	0.11	39,39,39,39	0
54	MG	BA	3595	1/1	0.97	0.29	27,27,27,27	0
54	MG	AA	1602	1/1	0.97	0.29	89,89,89,89	0
54	MG	BA	3480	1/1	0.97	0.13	31,31,31,31	0
54	MG	BA	3489	1/1	0.97	0.15	23,23,23,23	0
54	MG	DA	3097	1/1	0.97	0.26	23,23,23,23	0
54	MG	BA	3206	1/1	0.97	0.26	49,49,49,49	0
54	MG	BA	3472	1/1	0.97	0.27	26,26,26,26	0
54	MG	AA	1720	1/1	0.97	0.07	68,68,68,68	0
54	MG	BA	3227	1/1	0.97	0.14	32,32,32,32	0
54	MG	BA	3451	1/1	0.97	0.21	28,28,28,28	0
54	MG	BA	3294	1/1	0.97	0.18	39,39,39,39	0
54	MG	BA	3611	1/1	0.97	0.08	44,44,44,44	0
54	MG	DA	3124	1/1	0.97	0.37	37,37,37,37	0
54	MG	CA	1733	1/1	0.97	0.14	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3014	1/1	0.97	0.19	31,31,31,31	0
54	MG	BA	3092	1/1	0.97	0.40	26,26,26,26	0
54	MG	BA	3568	1/1	0.97	0.12	39,39,39,39	0
55	ZN	CN	101	1/1	0.97	0.08	107,107,107,107	0
54	MG	BA	3606	1/1	0.97	0.10	34,34,34,34	0
54	MG	DA	3107	1/1	0.97	0.08	54,54,54,54	0
54	MG	DA	3335	1/1	0.97	0.10	36,36,36,36	0
54	MG	DA	3399	1/1	0.97	0.10	51,51,51,51	0
54	MG	DA	3573	1/1	0.97	0.24	31,31,31,31	0
54	MG	AA	1652	1/1	0.97	0.25	49,49,49,49	0
54	MG	BA	3499	1/1	0.97	0.12	60,60,60,60	0
54	MG	DA	3005	1/1	0.97	0.23	77,77,77,77	0
54	MG	DA	3418	1/1	0.97	0.15	31,31,31,31	0
54	MG	BA	3051	1/1	0.97	0.17	48,48,48,48	0
54	MG	DA	3078	1/1	0.97	0.17	48,48,48,48	0
54	MG	BA	3322	1/1	0.97	0.08	37,37,37,37	0
54	MG	CA	1744	1/1	0.97	0.06	83,83,83,83	0
54	MG	BA	3187	1/1	0.97	0.59	42,42,42,42	0
54	MG	BA	3491	1/1	0.97	0.10	28,28,28,28	0
54	MG	BA	3420	1/1	0.97	0.19	61,61,61,61	0
54	MG	BA	3283	1/1	0.97	0.45	21,21,21,21	0
54	MG	D0	102	1/1	0.97	0.16	72,72,72,72	0
54	MG	DA	3376	1/1	0.97	0.14	30,30,30,30	0
54	MG	BA	3497	1/1	0.97	0.26	61,61,61,61	0
54	MG	CA	1741	1/1	0.97	0.31	79,79,79,79	0
54	MG	BA	3302	1/1	0.97	0.13	47,47,47,47	0
54	MG	CA	1748	1/1	0.97	0.06	58,58,58,58	0
54	MG	BA	3259	1/1	0.97	0.34	27,27,27,27	0
54	MG	BA	3066	1/1	0.97	0.35	39,39,39,39	0
54	MG	BA	3636	1/1	0.97	0.06	28,28,28,28	0
54	MG	BA	3307	1/1	0.97	0.11	44,44,44,44	0
54	MG	AA	1696	1/1	0.97	0.16	66,66,66,66	0
54	MG	DA	3338	1/1	0.97	0.21	42,42,42,42	0
54	MG	AA	1715	1/1	0.97	0.10	61,61,61,61	0
54	MG	BA	3644	1/1	0.97	0.08	88,88,88,88	0
54	MG	BA	3213	1/1	0.98	0.10	43,43,43,43	0
54	MG	BA	3500	1/1	0.98	0.17	44,44,44,44	0
54	MG	AA	1703	1/1	0.98	0.05	66,66,66,66	0
54	MG	DA	3404	1/1	0.98	0.14	36,36,36,36	0
54	MG	DA	3050	1/1	0.98	0.27	34,34,34,34	0
54	MG	BA	3198	1/1	0.98	0.12	44,44,44,44	0
54	MG	DA	3240	1/1	0.98	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3394	1/1	0.98	0.06	47,47,47,47	0
54	MG	DA	3502	1/1	0.98	0.11	37,37,37,37	0
54	MG	BA	3186	1/1	0.98	0.35	26,26,26,26	0
54	MG	CA	1761	1/1	0.98	0.18	65,65,65,65	0
54	MG	DA	3105	1/1	0.98	0.09	46,46,46,46	0
54	MG	BA	3537	1/1	0.98	0.17	31,31,31,31	0
54	MG	BA	3099	1/1	0.98	0.16	46,46,46,46	0
54	MG	AA	1641	1/1	0.98	0.17	42,42,42,42	0
54	MG	BA	3200	1/1	0.98	0.18	31,31,31,31	0
54	MG	BA	3465	1/1	0.98	0.15	44,44,44,44	0
54	MG	DA	3572	1/1	0.98	0.10	71,71,71,71	0
54	MG	DA	3345	1/1	0.98	0.31	54,54,54,54	0
54	MG	BA	3158	1/1	0.98	0.09	40,40,40,40	0
54	MG	DA	3463	1/1	0.98	0.09	69,69,69,69	0
54	MG	BA	3121	1/1	0.98	0.33	36,36,36,36	0
54	MG	BA	3312	1/1	0.98	0.10	51,51,51,51	0
54	MG	BA	3430	1/1	0.98	0.06	49,49,49,49	0
54	MG	DA	3101	1/1	0.98	0.19	39,39,39,39	0
54	MG	BA	3402	1/1	0.98	0.06	54,54,54,54	0
54	MG	DA	3374	1/1	0.98	0.20	37,37,37,37	0
54	MG	DA	3203	1/1	0.98	0.41	33,33,33,33	0
54	MG	BW	201	1/1	0.98	0.12	32,32,32,32	0
54	MG	BA	3447	1/1	0.98	0.14	29,29,29,29	0
54	MG	BA	3603	1/1	0.98	0.08	40,40,40,40	0
54	MG	BA	3380	1/1	0.98	0.14	26,26,26,26	0
54	MG	BA	3151	1/1	0.98	0.35	33,33,33,33	0
54	MG	DA	3112	1/1	0.98	0.24	51,51,51,51	0
54	MG	DA	3242	1/1	0.98	0.56	34,34,34,34	0
54	MG	BA	3375	1/1	0.98	0.16	34,34,34,34	0
54	MG	DA	3068	1/1	0.98	0.12	33,33,33,33	0
54	MG	BA	3345	1/1	0.98	0.10	71,71,71,71	0
54	MG	BA	3087	1/1	0.98	0.20	46,46,46,46	0
54	MG	BA	3309	1/1	0.98	0.10	31,31,31,31	0
54	MG	BA	3372	1/1	0.98	0.07	49,49,49,49	0
54	MG	DA	3507	1/1	0.98	0.13	80,80,80,80	0
54	MG	D1	101	1/1	0.98	0.22	38,38,38,38	0
54	MG	DA	3334	1/1	0.98	0.12	52,52,52,52	0
55	ZN	D6	101	1/1	0.98	0.07	63,63,63,63	0
54	MG	BA	3635	1/1	0.98	0.08	23,23,23,23	0
54	MG	DA	3423	1/1	0.98	0.16	32,32,32,32	0
54	MG	DA	3350	1/1	0.98	0.11	47,47,47,47	0
54	MG	DA	3428	1/1	0.98	0.05	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1650	1/1	0.98	0.55	53,53,53,53	0
54	MG	BA	3266	1/1	0.98	0.47	22,22,22,22	0
54	MG	BA	3361	1/1	0.98	0.04	59,59,59,59	0
54	MG	DA	3363	1/1	0.98	0.18	26,26,26,26	0
54	MG	DA	3286	1/1	0.98	0.20	33,33,33,33	0
54	MG	CA	1736	1/1	0.98	0.18	70,70,70,70	0
54	MG	BA	3443	1/1	0.98	0.21	47,47,47,47	0
54	MG	CA	1722	1/1	0.98	0.08	71,71,71,71	0
54	MG	BA	3558	1/1	0.98	0.19	28,28,28,28	0
54	MG	DA	3480	1/1	0.98	0.18	52,52,52,52	0
54	MG	DA	3516	1/1	0.98	0.20	32,32,32,32	0
54	MG	BA	3466	1/1	0.98	0.16	39,39,39,39	0
54	MG	DA	3483	1/1	0.98	0.26	59,59,59,59	0
54	MG	DA	3577	1/1	0.98	0.09	57,57,57,57	0
54	MG	BA	3173	1/1	0.98	0.39	32,32,32,32	0
54	MG	DA	3570	1/1	0.98	0.18	28,28,28,28	0
54	MG	BA	3527	1/1	0.98	0.18	29,29,29,29	0
54	MG	DA	3519	1/1	0.98	0.07	52,52,52,52	0
54	MG	DA	3425	1/1	0.98	0.07	47,47,47,47	0
54	MG	DA	3449	1/1	0.98	0.20	42,42,42,42	0
54	MG	BA	3419	1/1	0.98	0.40	21,21,21,21	0
54	MG	BA	3549	1/1	0.98	0.04	55,55,55,55	0
54	MG	DA	3330	1/1	0.98	0.13	37,37,37,37	0
54	MG	DA	3554	1/1	0.98	0.09	47,47,47,47	0
54	MG	CA	1719	1/1	0.98	0.07	54,54,54,54	0
54	MG	BA	3630	1/1	0.98	0.08	34,34,34,34	0
54	MG	BA	3277	1/1	0.98	0.37	22,22,22,22	0
54	MG	AA	1653	1/1	0.98	0.08	49,49,49,49	0
54	MG	BA	3328	1/1	0.98	0.21	30,30,30,30	0
54	MG	DA	3549	1/1	0.98	0.20	45,45,45,45	0
54	MG	BA	3032	1/1	0.98	0.09	40,40,40,40	0
54	MG	AA	1698	1/1	0.98	0.15	69,69,69,69	0
54	MG	DA	3566	1/1	0.98	0.13	54,54,54,54	0
54	MG	BA	3502	1/1	0.98	0.24	34,34,34,34	0
55	ZN	D5	102	1/1	0.98	0.08	69,69,69,69	0
54	MG	BA	3475	1/1	0.98	0.14	39,39,39,39	0
54	MG	BA	3483	1/1	0.98	0.13	28,28,28,28	0
54	MG	DA	3580	1/1	0.98	0.17	52,52,52,52	0
54	MG	BA	3498	1/1	0.98	0.08	32,32,32,32	0
54	MG	BA	3575	1/1	0.98	0.08	41,41,41,41	0
54	MG	DB	201	1/1	0.98	0.14	43,43,43,43	0
54	MG	BA	3320	1/1	0.98	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3032	1/1	0.98	0.21	49,49,49,49	0
54	MG	BA	3454	1/1	0.98	0.12	25,25,25,25	0
54	MG	AA	1680	1/1	0.98	0.25	72,72,72,72	0
54	MG	DA	3377	1/1	0.99	0.07	33,33,33,33	0
54	MG	B8	101	1/1	0.99	0.21	51,51,51,51	0
54	MG	BA	3188	1/1	0.99	0.27	39,39,39,39	0
54	MG	BA	3034	1/1	0.99	0.10	41,41,41,41	0
54	MG	BA	3044	1/1	0.99	0.08	33,33,33,33	0
54	MG	BA	3631	1/1	0.99	0.16	26,26,26,26	0
54	MG	BA	3463	1/1	0.99	0.09	28,28,28,28	0
54	MG	BA	3634	1/1	0.99	0.11	53,53,53,53	0
54	MG	DA	3038	1/1	0.99	0.08	37,37,37,37	0
54	MG	BA	3506	1/1	0.99	0.11	30,30,30,30	0
54	MG	BA	3270	1/1	0.99	0.45	25,25,25,25	0
54	MG	BA	3190	1/1	0.99	0.17	27,27,27,27	0
54	MG	DA	3217	1/1	0.99	0.49	32,32,32,32	0
55	ZN	B5	101	1/1	0.99	0.09	45,45,45,45	0
55	ZN	B6	101	1/1	0.99	0.11	48,48,48,48	0
54	MG	BA	3591	1/1	0.99	0.10	34,34,34,34	0
54	MG	DA	3336	1/1	0.99	0.17	41,41,41,41	0
54	MG	BA	3350	1/1	0.99	0.09	40,40,40,40	0
54	MG	BA	3357	1/1	0.99	0.16	25,25,25,25	0
54	MG	BA	3416	1/1	0.99	0.08	25,25,25,25	0
54	MG	BA	3082	1/1	0.99	0.12	36,36,36,36	0
54	MG	DA	3355	1/1	0.99	0.13	49,49,49,49	0
54	MG	DA	3585	1/1	0.99	0.13	33,33,33,33	0
54	MG	BA	3319	1/1	0.99	0.12	54,54,54,54	0
54	MG	DA	3403	1/1	0.99	0.07	34,34,34,34	0
54	MG	DA	3594	1/1	0.99	0.18	58,58,58,58	0
54	MG	BA	3327	1/1	0.99	0.18	23,23,23,23	0
54	MG	BA	3423	1/1	0.99	0.17	33,33,33,33	0
55	ZN	B9	101	1/1	0.99	0.08	50,50,50,50	0
54	MG	BA	3501	1/1	0.99	0.10	29,29,29,29	0
54	MG	BE	304	1/1	1.00	0.19	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.