



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2024 – 12:41 am BST

PDB ID : 8OJ3
Title : Crystal structure of the Candida albicans 80S ribosome in complex with geneticin G418 (rotated state)
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-23
Resolution : 3.50 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

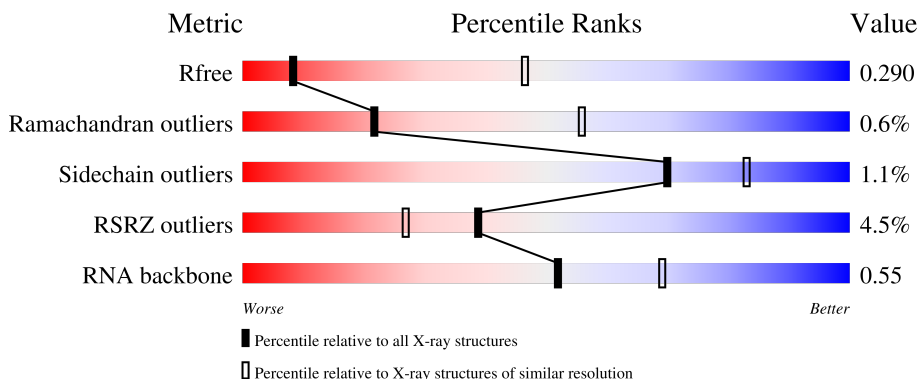
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	164625	1094 (3.56-3.44)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)
RNA backbone	3690	1089 (4.00-3.00)

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 of 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	1	3359	 2% 76% 18% . .
1	AS	3359	 3% 75% 16% . 8%
2	3	121	 2% 93% 7%
2	AT	121	 % 93% 7%
3	4	158	 3% 84% 15% .

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Mol	Chain	Length	Quality of chain
3	AU	158	4% 82% 16%
4	AW	254	8% 98%
4	j	254	5% 98%
5	AX	389	7% 98%
5	k	389	4% 99%
6	AY	363	12% 98%
6	l	363	7% 98%
7	AZ	298	9% 97%
7	m	298	6% 98%
8	BA	176	7% 87% 13%
8	n	176	3% 89% 11%
9	BB	241	8% 93% 6%
9	o	241	5% 94% 5%
10	BC	262	3% 85% 11%
10	p	262	2% 89% 10%
11	BD	191	5% 99%
11	q	191	% 99%
12	r	219	3% 94% 5%
13	BF	174	3% 97%
13	s	174	6% 97%
14	BG	202	3% 95%
14	t	202	3% 98%
15	BH	131	2% 99%
15	u	131	6% 97%
16	BI	204	15% 100%

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Mol	Chain	Length	Quality of chain
16	v	204	16% 99%
17	BJ	200	7% 100%
17	w	200	4% 99%
18	BK	185	3% 93% 6%
18	x	185	4% 91% 9%
19	BL	186	9% 99% ..
19	y	186	8% 99% .
20	BM	190	6% 92% 6%
20	z	190	6% 92% 6%
21	0	172	2% 98% ..
21	BN	172	98% ..
22	2	160	6% 99% .
22	BO	160	10% 99% ..
23	5	124	77% 19%
23	BP	124	70% 10% 20%
24	6	137	4% 95% ..
24	BQ	137	3% 95% ..
25	7	155	74% 24%
25	BR	155	3% 68% 30%
26	8	142	8% 84% 15%
26	BS	142	2% 82% 16%
27	9	127	2% 98% ..
27	BT	127	6% 98% ..
28	AA	136	% 99% .
28	BU	136	% 96% ..

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Mol	Chain	Length	Quality of chain
29	AB	149	8% 99% ..
29	BV	149	5% 99% ..
30	AC	63	14% 87% 5% 8%
30	BW	63	13% 95% 5%
31	AD	106	91% . 8%
31	BX	106	88% . 11%
32	AE	112	4% 96% ..
32	BY	112	7% 96% ..
33	AF	131	11% 95% 5%
33	BZ	131	6% 93% 7%
34	AG	107	7% 98% ..
34	CA	107	% 98% ..
35	AH	122	17% 90% . 8%
35	CB	122	16% 89% . 10%
36	AI	120	5% 96% .
36	CC	120	6% 94% ..
37	AJ	99	% 97% ..
37	CD	99	2% 94% . .
38	AK	90	6% 96% .
38	CE	90	7% 96% .
39	AL	78	% 99% .
39	CF	78	3% 91% 8% .
40	AM	51	6% 98% .
40	CG	51	10% 98% .
41	AN	52	10% 96% .

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Mol	Chain	Length	Quality of chain
41	CH	52	13% 94%
42	AO	25	16% 96%
42	CI	25	16% 96%
43	AP	106	2% 96%
43	CJ	106	6% 95%
44	AQ	92	5% 99%
44	CK	92	% 99%
45	CL	267	2% 40% 55%
45	i	267	2% 30% 10% 60%
46	B	1787	4% 70% 24%
46	CM	1787	2% 69% 25%
47	C	261	3% 79% 20%
47	CN	261	3% 79% 20%
48	CO	256	2% 78% 5% 17%
48	D	256	2% 84% 16%
49	CP	249	3% 87% 13%
49	E	249	7% 87% 13%
50	CQ	251	4% 86% 11%
50	F	251	6% 88% 11%
51	CR	262	6% 99%
51	G	262	10% 98%
52	CS	225	5% 86% 5% 9%
52	H	225	8% 92% 8%
53	CT	236	4% 99%
53	I	236	10% 94% 6%

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Mol	Chain	Length	Quality of chain
54	CU	186	2% 90% 6%
54	J	186	6% 97% ..
55	CV	206	8% 99% .
55	K	206	7% 98% .
56	CW	189	5% 94% 6%
56	L	189	12% 94% 6%
57	CX	118	80% 20%
57	M	118	2% 81% 17%
58	CY	155	90% 9%
58	N	155	6% 91% 7%
59	CZ	143	74% 8% 17%
59	O	143	3% 73% 8% 19%
60	DA	151	3% 99% ..
60	P	151	7% 98% .
61	DB	132	2% 92% 8%
61	Q	132	6% 95% ..
62	DC	142	2% 85% 6% 8%
62	R	142	4% 89% 8%
63	DD	142	11% 96% ..
63	S	142	8% 96% ..
64	DE	137	4% 91% 9%
64	T	137	3% 88% 9%
65	DF	145	% 94% ..
65	U	145	2% 97% ..
66	DG	145	3% 97% .

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Mol	Chain	Length	Quality of chain
66	V	145	97%
67	DH	119	79%
67	W	119	83%
68	DI	87	100%
68	X	87	100%
69	DJ	130	98%
69	Y	130	99%
70	DK	145	98%
70	Z	145	98%
71	DL	135	98%
71	a	135	99%
72	DM	105	68%
72	b	105	69%
73	DN	119	82%
73	c	119	80%
74	DO	82	99%
74	d	82	99%
75	DP	67	91%
75	e	67	88%
76	DQ	56	91%
76	f	56	89%
77	DR	63	89%
77	g	63	95%
78	DS	193	28%
78	h	193	34%

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Mol	Chain	Length	Quality of chain
79	AR	317	
79	DT	317	
80	BE	220	
81	P0	312	
82	12	165	

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
84	MG	1	3508	-	-	-	X
84	MG	1	3731	-	-	-	X
84	MG	1	3870	-	-	-	X
84	MG	AS	3422	-	-	-	X
84	MG	AS	3641	-	-	-	X
84	MG	AS	3654	-	-	-	X
84	MG	CL	301	-	-	-	X

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 400037 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3218	Total 68791	C 30731	N 12364	O 22478	P 3218	0	0	0
1	AS	3101	Total 66291	C 29614	N 11913	O 21663	P 3101	0	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	Total 2579	C 1153	N 463	O 842	P 121	0	0	0
2	AT	121	Total 2579	C 1153	N 463	O 842	P 121	0	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	156	Total 3313	C 1482	N 581	O 1094	P 156	0	0	0
3	AU	158	Total 3353	C 1500	N 585	O 1110	P 158	0	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	249	Total 1888	C 1180	N 376	O 330	S 2	0	0	0
4	AW	249	Total 1888	C 1180	N 376	O 330	S 2	0	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			
5	AX	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			

- Molecule 6 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	359	Total	C	N	O	S	0	0	0
			2734	1720	524	487	3			
6	AY	359	Total	C	N	O	S	0	0	0
			2734	1720	524	487	3			

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	294	Total	C	N	O	S	0	0	0
			2409	1534	419	455	1			
7	AZ	292	Total	C	N	O	S	0	0	0
			2394	1526	416	450	2			

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	157	Total	C	N	O	S	0	0	0
			1242	796	226	219	1			
8	BA	153	Total	C	N	O		0	0	0
			1210	777	221	212				

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	229	Total	C	N	O	S	0	0	0
			1843	1182	338	322	1			
9	BB	226	Total	C	N	O	S	0	0	0
			1816	1165	333	317	1			

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	236	Total	C	N	O	S	0	0	0
			1825	1168	324	330	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BC	233	Total	C	N	O	S	0	0	0
			1805	1156	321	325	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	q	190	Total	C	N	O	S	0	0	0
			1519	958	276	281	4			
11	BD	190	Total	C	N	O	S	0	0	0
			1519	958	276	281	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	r	207	Total	C	N	O	S	0	0	0
			1681	1064	321	290	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	s	171	Total	C	N	O	S	0	0	0
			1371	857	260	250	4			
13	BF	171	Total	C	N	O	S	0	0	0
			1371	857	260	250	4			

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	t	200	Total	C	N	O	0	0	0
			1610	1009	318	283			
14	BG	200	Total	C	N	O	0	0	0
			1610	1009	318	283			

- Molecule 15 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	u	128	Total	C	N	O	S	0	0	0
			1015	651	190	173	1			
15	BH	130	Total	C	N	O	S	0	0	0
			1029	660	193	175	1			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	v	203	Total 1713	C 1075	N 356	O 280	S 2	0	0	0
16	BI	203	Total 1713	C 1075	N 356	O 280	S 2	0	0	0

- Molecule 17 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	w	199	Total 1590	C 1025	N 294	O 269	S 2	0	0	0
17	BJ	199	Total 1590	C 1025	N 294	O 269	S 2	0	0	0

- Molecule 18 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	x	169	Total 1352	C 835	N 273	O 244	0	0	0
18	BK	174	Total 1396	C 862	N 282	O 252	0	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	y	185	Total 1458	C 916	N 297	O 245	0	0	0
19	BL	185	Total 1458	C 916	N 297	O 245	0	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	z	179	Total 1457	C 901	N 310	O 243	S 3	0	0	0
20	BM	179	Total 1457	C 901	N 310	O 243	S 3	0	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	0	170	Total 1423	C 921	N 258	O 241	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	BN	170	1423	921	258	241	3	0	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	2	159	1262	798	241	221	2	0	0	0
22	BO	159	1262	798	241	221	2	0	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22-B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				
23	5	100	803	518	135	150		0	0	0
23	BP	99	794	512	133	149		0	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	6	131	977	615	183	171	8	0	0	0
24	BQ	131	977	615	183	171	8	0	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	7	118	945	591	192	161	1	0	0	0
25	BR	109	877	549	178	149	1	0	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	8	120	965	616	173	175	1	0	0	0
26	BS	119	960	613	172	174	1	0	0	0

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O	0	0	0
			989	618	190	181			
27	BT	126	Total	C	N	O	0	0	0
			989	618	190	181			

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AA	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			
28	BU	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AB	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			
29	BV	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	AC	58	Total	C	N	O	0	0	0
			464	290	100	74			
30	BW	60	Total	C	N	O	0	0	0
			482	301	103	78			

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	98	Total	C	N	O	S	0	0	0
			747	479	124	142	2			
31	BX	94	Total	C	N	O	S	0	0	0
			715	460	119	134	2			

- Molecule 32 is a protein called 60S ribosomal protein L31-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	108	Total	C	N	O	S	0	0	0
			881	556	166	157	2			
32	BY	108	Total	C	N	O	S	0	0	0
			881	556	166	157	2			

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AF	124	Total	C	N	O	S	0	0	0
			1000	638	194	167	1			
33	BZ	122	Total	C	N	O	S	0	0	0
			991	633	192	165	1			

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AG	106	Total	C	N	O	S	0	0	0
			847	543	161	142	1			
34	CA	106	Total	C	N	O	S	0	0	0
			847	543	161	142	1			

- Molecule 35 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	112	Total	C	N	O	S	0	0	0
			887	547	182	154	4			
35	CB	110	Total	C	N	O	S	0	0	0
			869	536	179	150	4			

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	AI	115	Total	C	N	O	0	0	0
			963	611	190	162			
36	CC	117	Total	C	N	O	0	0	0
			974	618	192	164			

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	CD	95	736	459	148	128	1	0	0	0

- Molecule 38 is a protein called 60S ribosomal protein L37-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	AK	86	677	413	148	110	6	0	0	0
38	CE	86	677	413	148	110	6	0	0	0

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	AL	77	617	393	115	109	0	0	0
39	CF	77	617	393	115	109	0	0	0

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	AM	50	438	275	97	66	0	0	0
40	CG	50	438	275	97	66	0	0	0

- Molecule 41 is a protein called 60S ribosomal protein L40-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	AN	50	402	249	83	65	5	0	0	0
41	CH	50	403	249	84	65	5	0	0	0

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	AO	25	236	144	63	28	1	0	0	0
42	CI	24	227	138	61	27	1	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	AP	103	Total 828	C 521	N 165	O 137	S 5	0	0	0
43	CJ	103	Total 828	C 521	N 165	O 137	S 5	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	AQ	91	Total 698	C 430	N 140	O 124	S 4	0	0	0
44	CK	91	Total 698	C 430	N 140	O 124	S 4	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein CAALFM_C304810CA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	i	106	Total 805	C 483	N 147	O 175	0	0	0
45	CL	120	Total 919	C 554	N 165	O 200	0	0	0

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
46	B	1708	Total 36410	C 16276	N 6460	O 11966	P 1708	0	0	0
46	CM	1728	Total 36839	C 16468	N 6538	O 12105	P 1728	0	0	0

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	C	208	Total 1627	C 1041	N 284	O 297	S 5	0	0	0
47	CN	208	Total 1627	C 1041	N 284	O 297	S 5	0	0	0

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	D	214	Total 1724	C 1094	N 313	O 313	S 4	0	0	0
48	CO	213	Total 1717	C 1089	N 312	O 312	S 4	0	0	0

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	E	217	Total 1629	C 1039	N 289	O 296	S 5	0	0	0
49	CP	217	Total 1629	C 1039	N 289	O 296	S 5	0	0	0

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	F	223	Total 1707	C 1087	N 311	O 305	S 4	0	0	0
50	CQ	223	Total 1707	C 1087	N 311	O 305	S 4	0	0	0

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	G	258	Total 2042	C 1299	N 383	O 355	S 5	0	0	0
51	CR	260	Total 2055	C 1306	N 386	O 358	S 5	0	0	0

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	H	206	Total 1614	C 1008	N 301	O 301	S 4	0	0	0
52	CS	205	Total 1606	C 1002	N 300	O 300	S 4	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	I	223	Total 1798	C 1119	N 348	O 325	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	CT	236	Total	C	N	O	S	0	0	0
			1904	1184	369	345	6			

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
54	J	182	Total	C	N	O	0	0	0
			1466	939	264	263			
54	CU	179	Total	C	N	O	0	0	0
			1449	929	261	259			

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	K	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			
55	CV	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			

- Molecule 56 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	L	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			
56	CW	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	M	98	Total	C	N	O	S	0	0	0
			817	531	135	150	1			
57	CX	94	Total	C	N	O	S	0	0	0
			791	515	131	144	1			

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	N	144	Total	C	N	O	S	0	0	0
			1150	734	215	198	3			
58	CY	141	Total	C	N	O	S	0	0	0
			1129	722	212	192	3			

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	O	116	Total 885	C 550	N 158	O 172	S 5	0	0	0
59	CZ	119	Total 913	C 566	N 163	O 179	S 5	0	0	0

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	P	148	Total 1175	C 749	N 217	O 208	S 1	0	0	0
60	DA	150	Total 1187	C 757	N 219	O 210	S 1	0	0	0

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	Q	127	Total 942	C 579	N 186	O 174	S 3	0	0	0
61	DB	122	Total 905	C 555	N 180	O 167	S 3	0	0	0

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
62	R	131	Total 1034	C 658	N 190	O 179	S 7	0	0	0
62	DC	130	Total 1029	C 655	N 189	O 178	S 7	0	0	0

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
63	S	139	Total 1085	C 697	N 197	O 190	S 1	0	0	0
63	DD	139	Total 1085	C 697	N 197	O 190	S 1	0	0	0

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	T	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			
64	DE	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	U	144	Total	C	N	O	S	0	0	0
			1187	744	233	207	3			
65	DF	141	Total	C	N	O	S	0	0	0
			1161	727	227	204	3			

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	V	141	Total	C	N	O	S	0	0	0
			1100	689	210	200	1			
66	DG	141	Total	C	N	O	S	0	0	0
			1100	689	210	200	1			

- Molecule 67 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	W	102	Total	C	N	O	S	0	0	0
			808	509	150	147	2			
67	DH	97	Total	C	N	O	S	0	0	0
			763	481	140	140	2			

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	X	87	Total	C	N	O	S	0	0	0
			676	415	126	133	2			
68	DI	87	Total	C	N	O	S	0	0	0
			676	415	126	133	2			

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	Y	129	Total	C	N	O	S	0	0	0
			1032	655	191	183	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	DJ	129	1032	655	191	183	3	0	0	0

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
70	Z	143	1110	701	219	188	2	0	0	0
70	DK	143	1110	701	219	188	2	0	0	0

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
71	a	134	1086	677	218	191	0	0	0
71	DL	132	1072	670	216	186	0	0	0

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
72	b	72	578	369	103	106	0	0	0
72	DM	71	570	365	102	103	0	0	0

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
73	c	97	770	477	161	126	6	0	0	0
73	DN	98	779	482	163	128	6	0	0	0

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
74	d	81	614	383	110	114	7	0	0	0
74	DO	81	614	383	110	114	7	0	0	0

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	e	60	Total	C	N	O	S	0	0	0
			468	287	93	86	2			
75	DP	61	Total	C	N	O	S	0	0	0
			476	293	94	87	2			

- Molecule 76 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	f	55	Total	C	N	O	S	0	0	0
			454	281	94	75	4			
76	DQ	54	Total	C	N	O	S	0	0	0
			449	278	93	74	4			

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	g	60	Total	C	N	O	S	0	0	0
			474	297	96	79	2			
77	DR	59	Total	C	N	O	S	0	0	0
			470	295	95	78	2			

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	h	70	Total	C	N	O	S	0	0	0
			574	362	113	93	6			
78	DS	68	Total	C	N	O	S	0	0	0
			555	350	108	91	6			

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	AR	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			
79	DT	307	Total	C	N	O	S	0	0	0
			2362	1498	403	456	5			

- Molecule 80 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	BE	205	Total 1662	C 1052	N 318	O 285	S 7	0	0	0

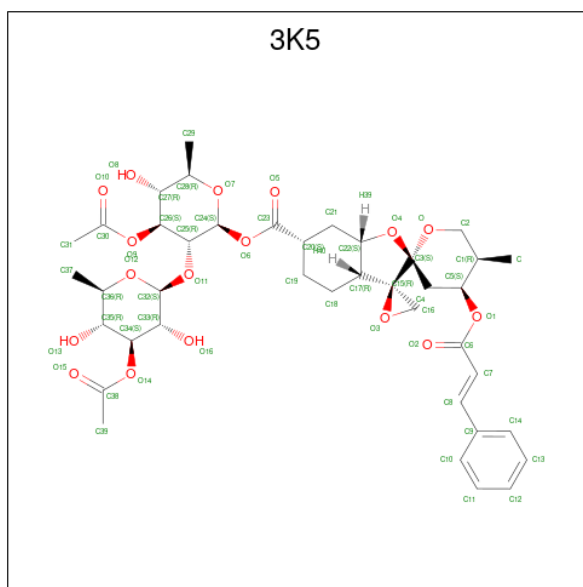
- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	P0	107	Total 845	C 542	N 150	O 150	S 3	0	0	0

- Molecule 82 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	12	63	Total 480	C 297	N 85	O 96	S 2	0	0	0

- Molecule 83 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-
 {[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-
 {[(2E)-3-phenylprop-2-enoyl]oxy}decahy
 drodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose
 (three-letter code: 3K5) (formula: C₄₀H₅₂O₁₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
83	1	1	Total 57	C 40	O 17	0	0
83	AS	1	Total 57	C 40	O 17	0	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	469	Total Mg 469 469	0	0
84	3	7	Total Mg 7 7	0	0
84	4	1	Total Mg 1 1	0	0
84	j	1	Total Mg 1 1	0	0
84	k	3	Total Mg 3 3	0	0
84	m	1	Total Mg 1 1	0	0
84	o	4	Total Mg 4 4	0	0
84	r	1	Total Mg 1 1	0	0
84	u	1	Total Mg 1 1	0	0
84	v	2	Total Mg 2 2	0	0
84	w	1	Total Mg 1 1	0	0
84	x	1	Total Mg 1 1	0	0
84	y	3	Total Mg 3 3	0	0
84	0	4	Total Mg 4 4	0	0
84	2	1	Total Mg 1 1	0	0
84	6	1	Total Mg 1 1	0	0
84	AB	2	Total Mg 2 2	0	0
84	AC	1	Total Mg 1 1	0	0
84	AD	1	Total Mg 1 1	0	0
84	AJ	1	Total Mg 1 1	0	0
84	AP	2	Total Mg 2 2	0	0
84	B	99	Total Mg 99 99	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	C	1	Total Mg 1 1	0	0
84	D	1	Total Mg 1 1	0	0
84	E	1	Total Mg 1 1	0	0
84	F	1	Total Mg 1 1	0	0
84	G	1	Total Mg 1 1	0	0
84	K	1	Total Mg 1 1	0	0
84	L	1	Total Mg 1 1	0	0
84	Q	2	Total Mg 2 2	0	0
84	R	4	Total Mg 4 4	0	0
84	T	1	Total Mg 1 1	0	0
84	Y	2	Total Mg 2 2	0	0
84	a	1	Total Mg 1 1	0	0
84	AS	389	Total Mg 389 389	0	0
84	AT	5	Total Mg 5 5	0	0
84	AU	5	Total Mg 5 5	0	0
84	AW	1	Total Mg 1 1	0	0
84	AX	3	Total Mg 3 3	0	0
84	AY	2	Total Mg 2 2	0	0
84	AZ	1	Total Mg 1 1	0	0
84	BB	2	Total Mg 2 2	0	0
84	BC	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	BE	1	Total Mg 1 1	0	0
84	BI	1	Total Mg 1 1	0	0
84	BK	1	Total Mg 1 1	0	0
84	BL	2	Total Mg 2 2	0	0
84	BO	1	Total Mg 1 1	0	0
84	BQ	1	Total Mg 1 1	0	0
84	BZ	1	Total Mg 1 1	0	0
84	CA	1	Total Mg 1 1	0	0
84	CB	1	Total Mg 1 1	0	0
84	CG	1	Total Mg 1 1	0	0
84	CL	2	Total Mg 2 2	0	0
84	CM	78	Total Mg 78 78	0	0
84	CW	1	Total Mg 1 1	0	0
84	DA	1	Total Mg 1 1	0	0
84	DG	1	Total Mg 1 1	0	0
84	DH	1	Total Mg 1 1	0	0
84	DK	2	Total Mg 2 2	0	0
84	P0	1	Total Mg 1 1	0	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

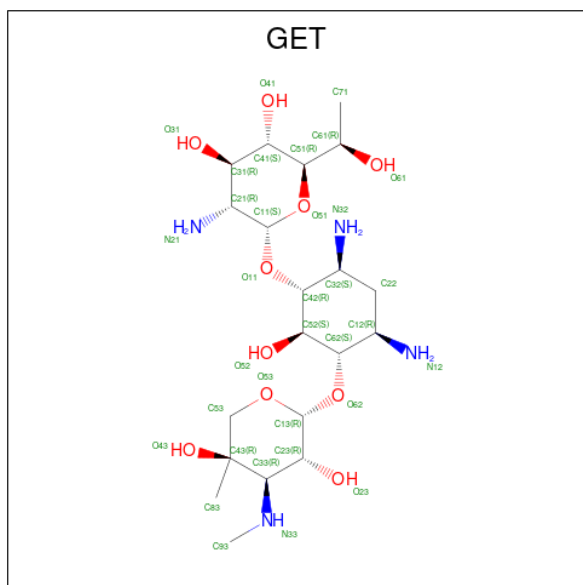
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	AH	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	AK	1	Total Zn 1 1	0	0
85	AN	1	Total Zn 1 1	0	0
85	AP	1	Total Zn 1 1	0	0
85	AQ	1	Total Zn 1 1	0	0
85	c	1	Total Zn 1 1	0	0
85	d	1	Total Zn 1 1	0	0
85	f	1	Total Zn 1 1	0	0
85	h	1	Total Zn 1 1	0	0
85	CB	1	Total Zn 1 1	0	0
85	CE	1	Total Zn 1 1	0	0
85	CH	1	Total Zn 1 1	0	0
85	CJ	1	Total Zn 1 1	0	0
85	CK	1	Total Zn 1 1	0	0
85	DN	1	Total Zn 1 1	0	0
85	DQ	1	Total Zn 1 1	0	0
85	DS	1	Total Zn 1 1	0	0

- Molecule 86 is GENETICIN (three-letter code: GET) (formula: C₂₀H₄₀N₄O₁₀) (labeled as "Ligand of Interest" by depositor).

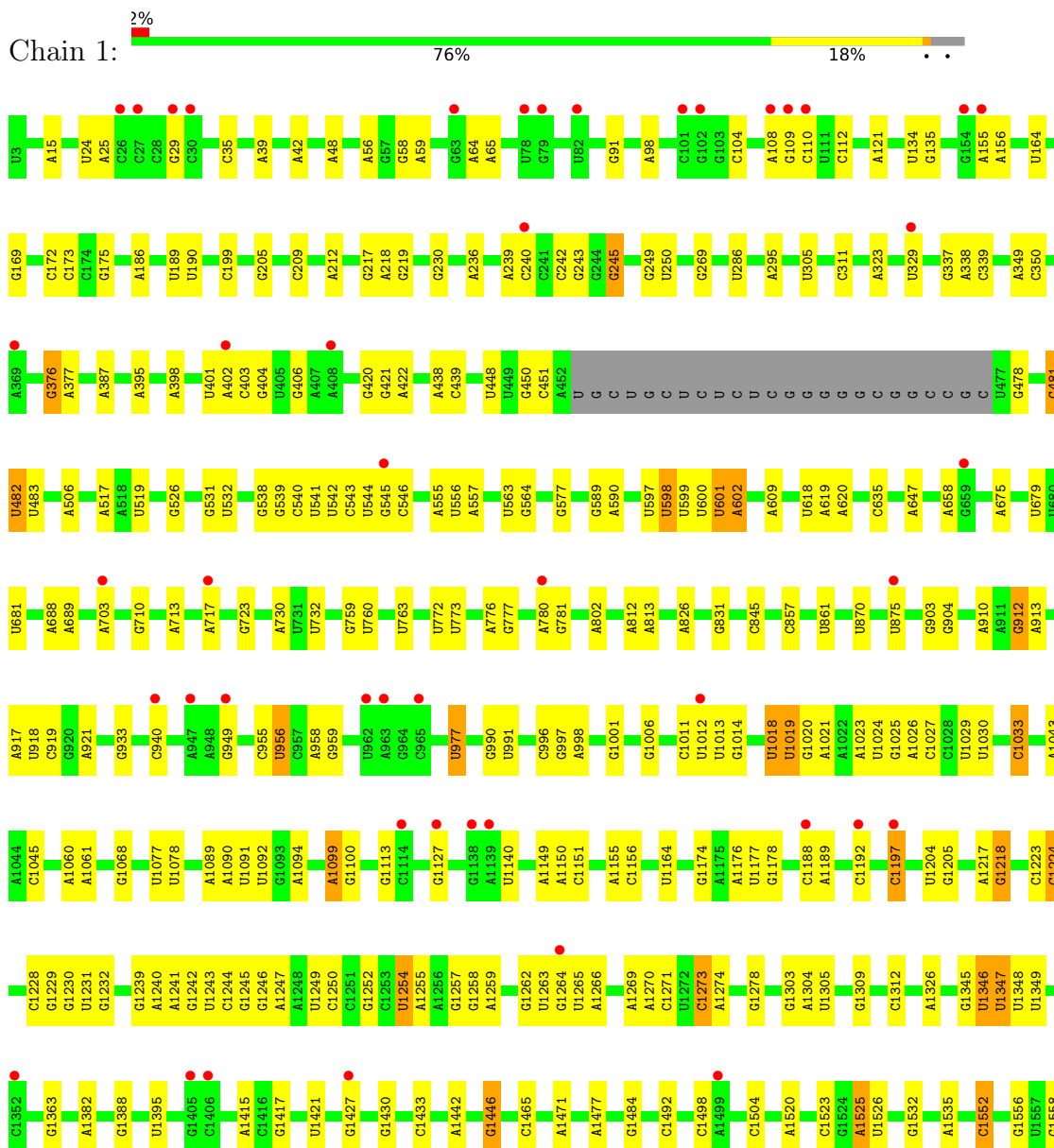


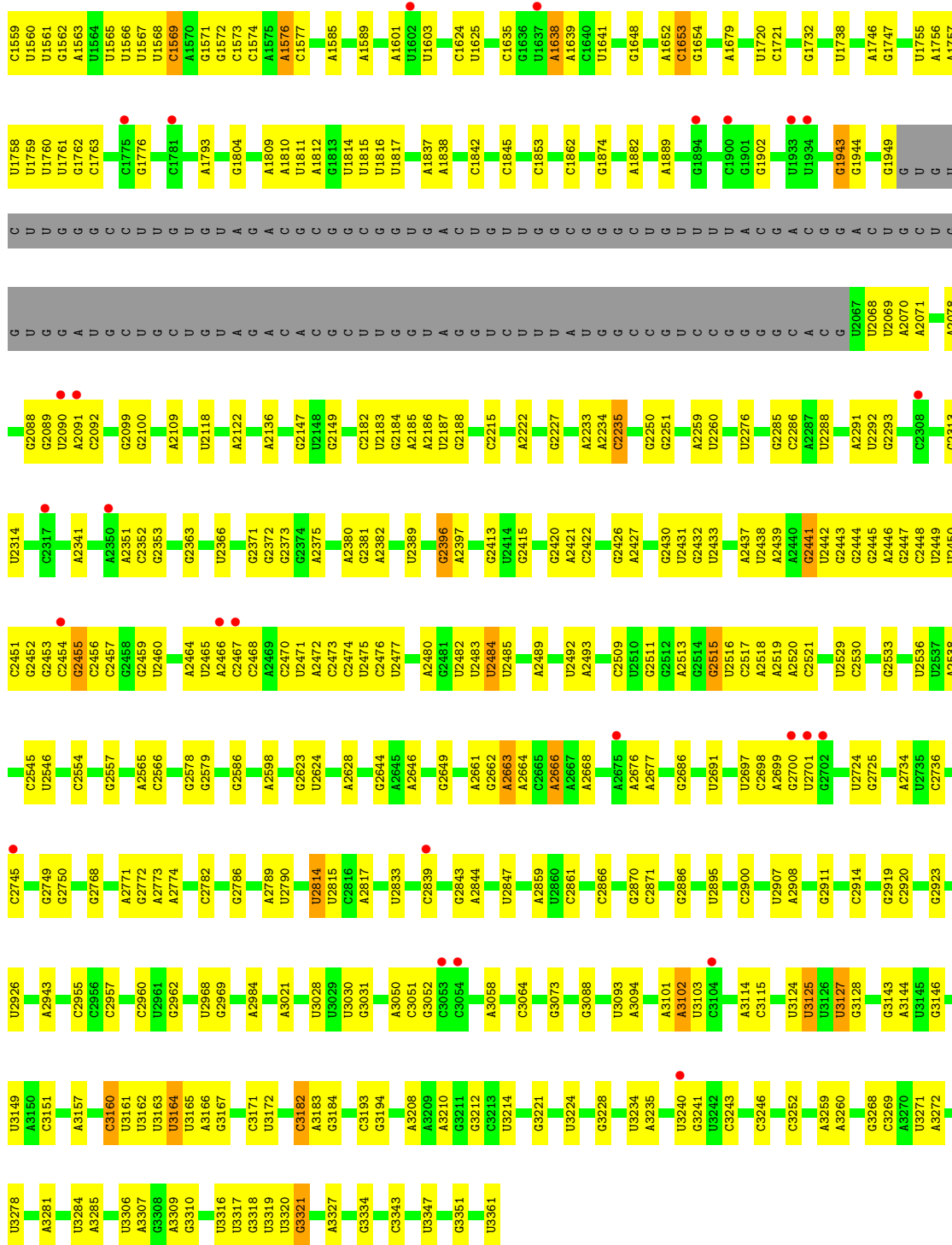
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
86	B	1	34	20	4	10	0	0
86	CM	1	34	20	4	10	0	0

3 Residue-property plots [i](#)

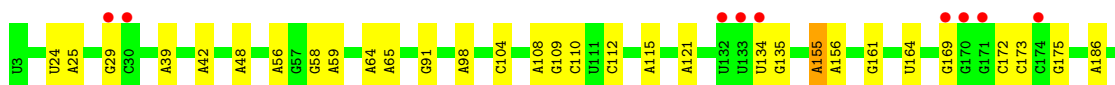
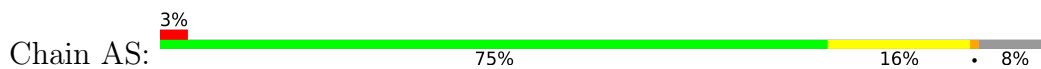
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

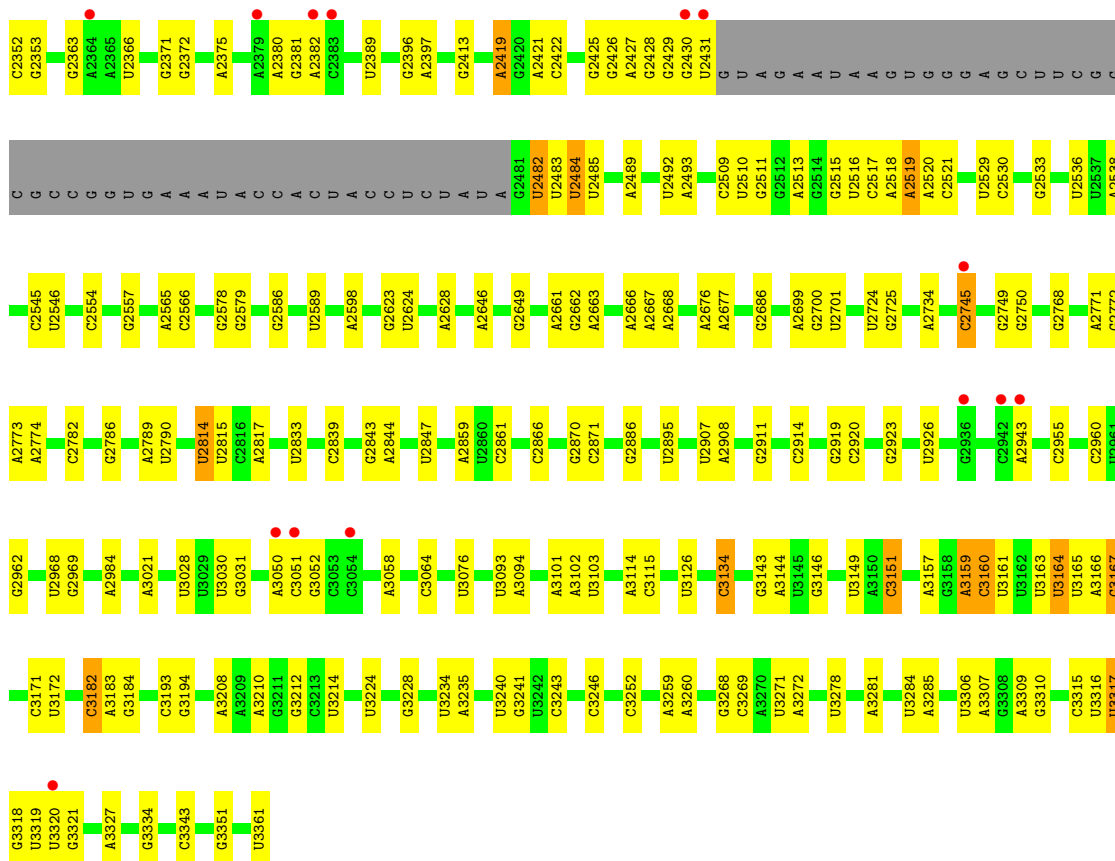
- Molecule 1: 25S ribosomal RNA



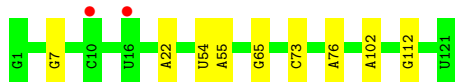


• Molecule 1: 25S ribosomal RNA

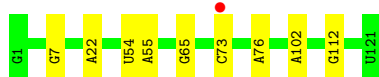




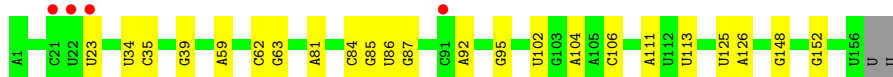
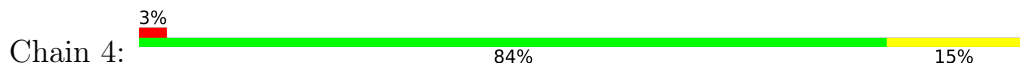
• Molecule 2: 5S ribosomal RNA



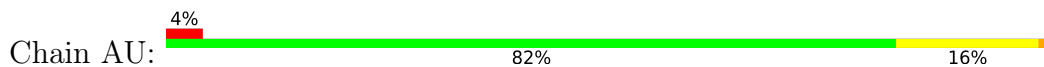
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA

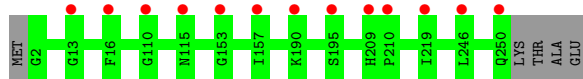


• Molecule 3: 5.8S ribosomal RNA

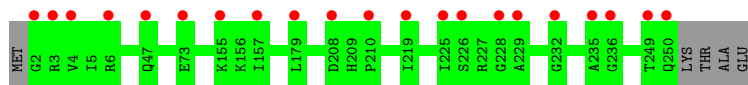




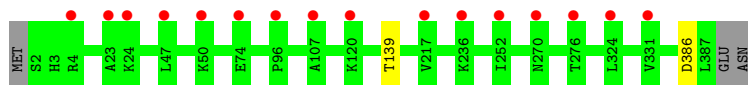
- Molecule 4: 60S ribosomal protein L2-B



- Molecule 4: 60S ribosomal protein L2-B



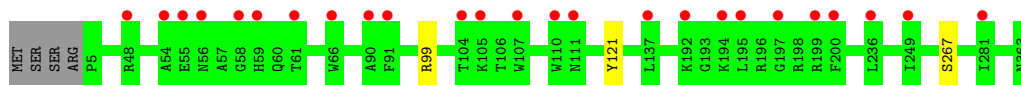
- Molecule 5: 60S ribosomal protein L3



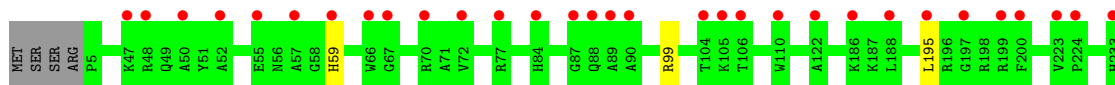
- Molecule 5: 60S ribosomal protein L3



- Molecule 6: 60S ribosomal protein L4-B



- Molecule 6: 60S ribosomal protein L4-B

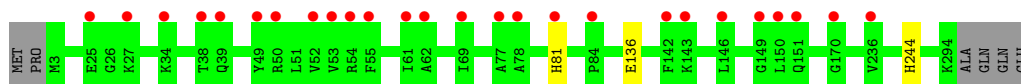




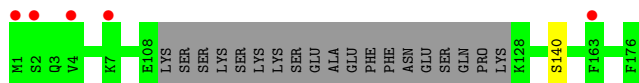
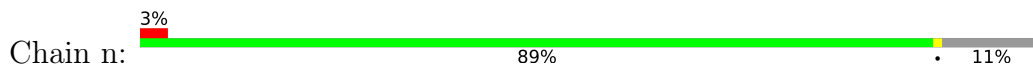
- Molecule 7: Uncharacterized protein CaJ7.0206



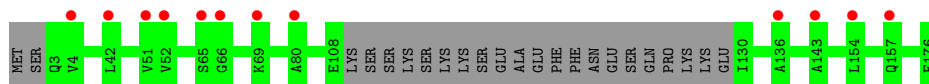
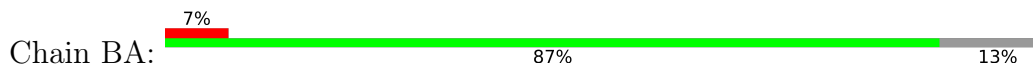
- Molecule 7: Uncharacterized protein CaJ7.0206



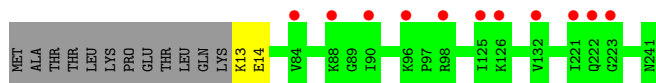
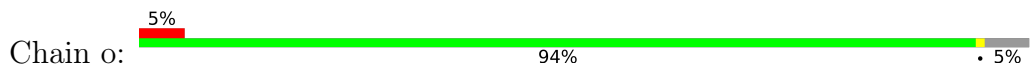
- Molecule 8: 60S ribosomal protein L6



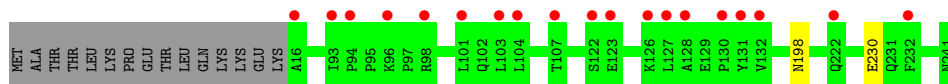
- Molecule 8: 60S ribosomal protein L6



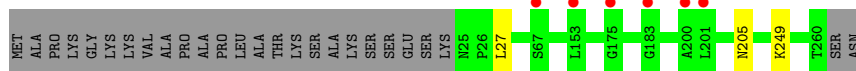
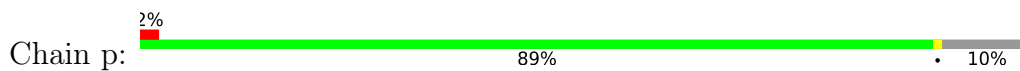
- Molecule 9: 60S ribosomal protein L7-A



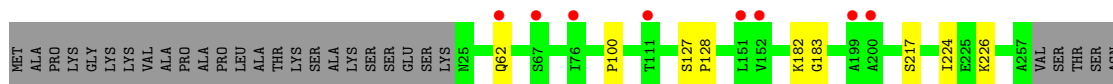
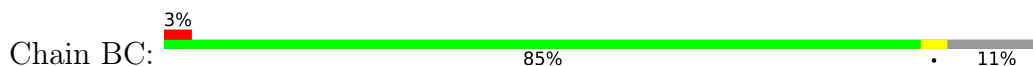
- Molecule 9: 60S ribosomal protein L7-A



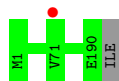
- Molecule 10: 60S ribosomal protein L8



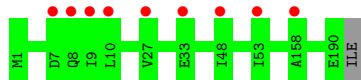
- Molecule 10: 60S ribosomal protein L8



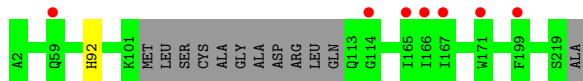
- Molecule 11: 60S ribosomal protein L9-B



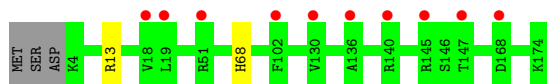
- Molecule 11: 60S ribosomal protein L9-B



- Molecule 12: 60S ribosomal protein L10



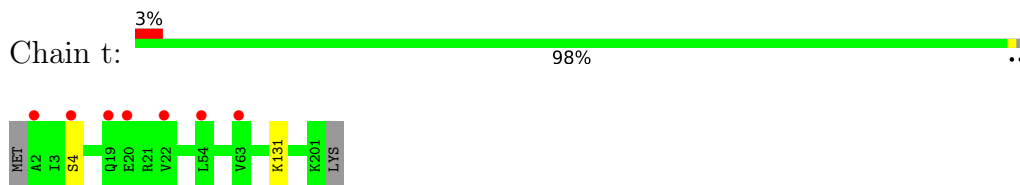
- Molecule 13: 60S ribosomal protein L11-B



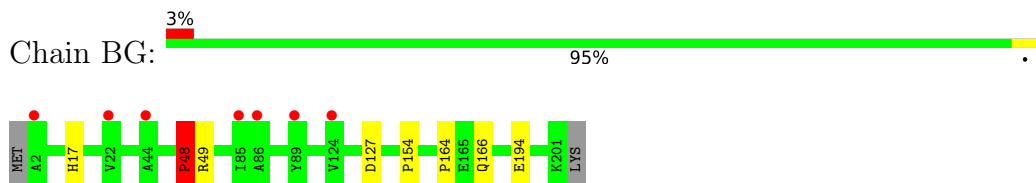
- Molecule 13: 60S ribosomal protein L11-B



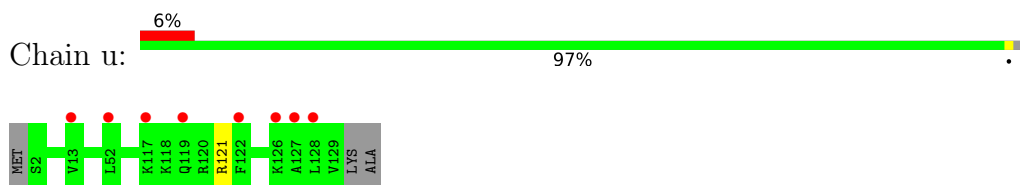
- Molecule 14: 60S ribosomal protein L13



- Molecule 14: 60S ribosomal protein L13



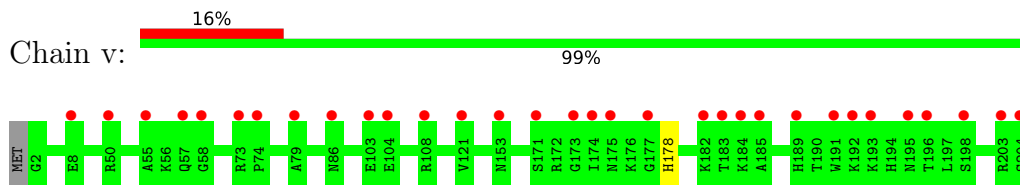
- Molecule 15: 60S ribosomal protein L14-B



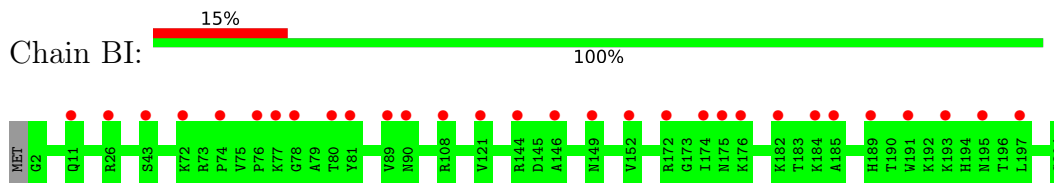
- Molecule 15: 60S ribosomal protein L14-B



- Molecule 16: 60S ribosomal protein L15-A

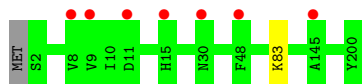


- Molecule 16: 60S ribosomal protein L15-A

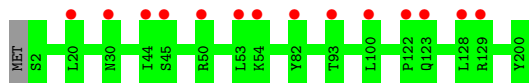


- Molecule 17: Ribosomal protein L13

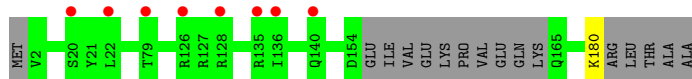
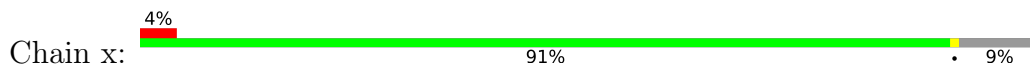




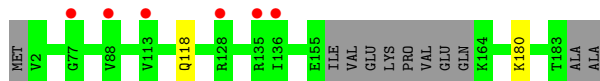
- Molecule 17: Ribosomal protein L13



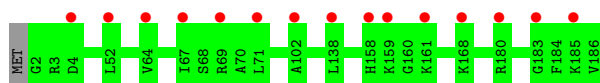
- Molecule 18: Ribosomal protein L22



- Molecule 18: Ribosomal protein L22



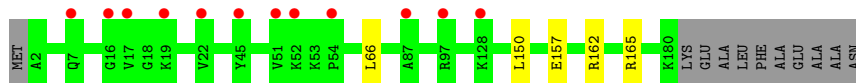
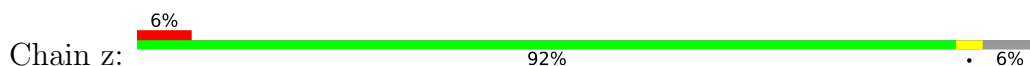
- Molecule 19: 60S ribosomal protein L18-A



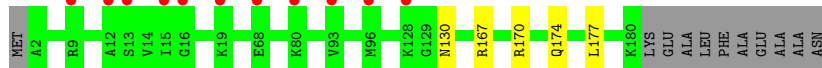
- Molecule 19: 60S ribosomal protein L18-A



- Molecule 20: 60S ribosomal protein L19-A



- Molecule 20: 60S ribosomal protein L19-A



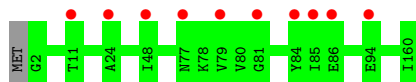
- Molecule 21: 60S ribosomal protein L20



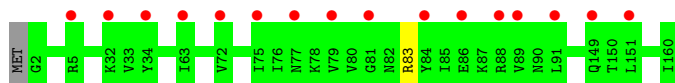
- Molecule 21: 60S ribosomal protein L20



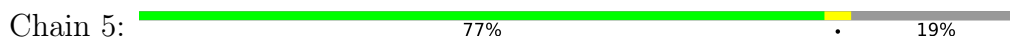
- Molecule 22: 60S ribosomal protein L21-A



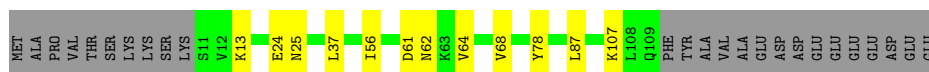
- Molecule 22: 60S ribosomal protein L21-A



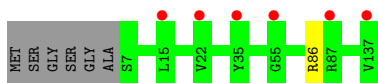
- Molecule 23: 60S ribosomal protein L22-B



- Molecule 23: 60S ribosomal protein L22-B



- Molecule 24: 60S ribosomal protein L23-A



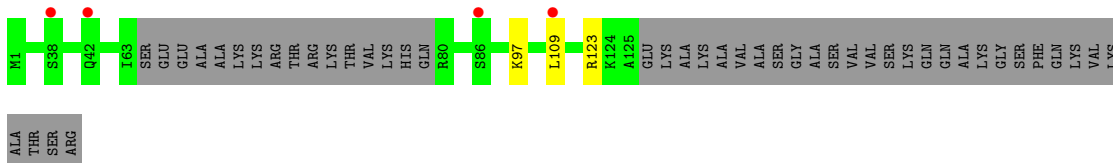
- Molecule 24: 60S ribosomal protein L23-A



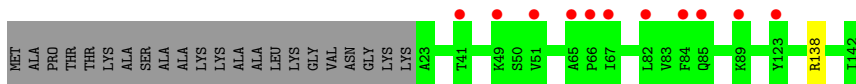
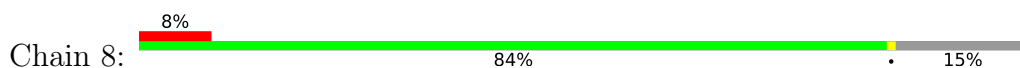
- Molecule 25: 60S ribosomal protein L24-A



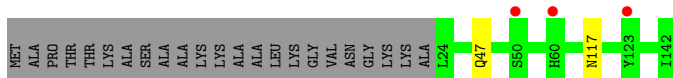
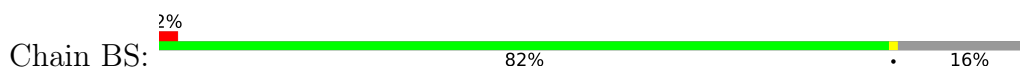
- Molecule 25: 60S ribosomal protein L24-A



- Molecule 26: 60S ribosomal protein L25

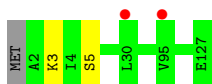


- Molecule 26: 60S ribosomal protein L25

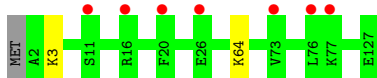


- Molecule 27: Ribosomal protein L24

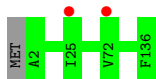




- Molecule 27: Ribosomal protein L24



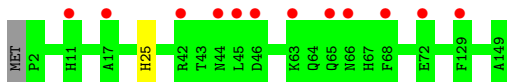
- Molecule 28: 60S ribosomal protein L27



- Molecule 28: 60S ribosomal protein L27



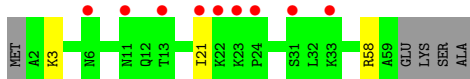
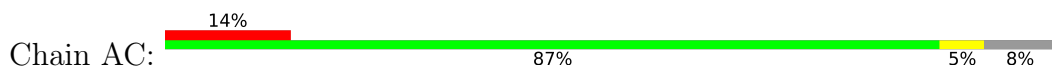
- Molecule 29: 60S ribosomal protein L28



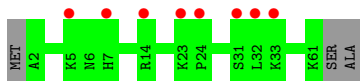
- Molecule 29: 60S ribosomal protein L28



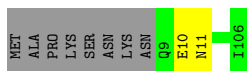
- Molecule 30: 60S ribosomal protein L29



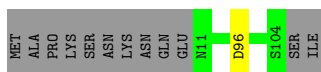
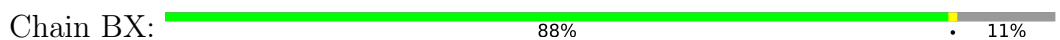
- Molecule 30: 60S ribosomal protein L29



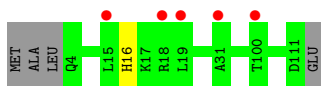
- Molecule 31: 60S ribosomal protein L30



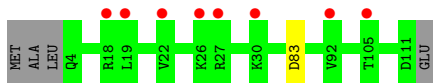
- Molecule 31: 60S ribosomal protein L30



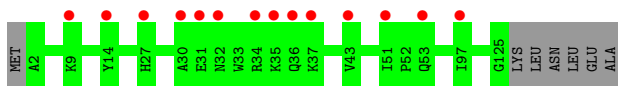
- Molecule 32: 60S ribosomal protein L31-B



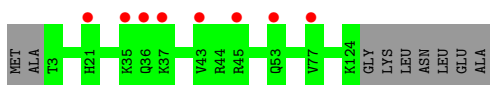
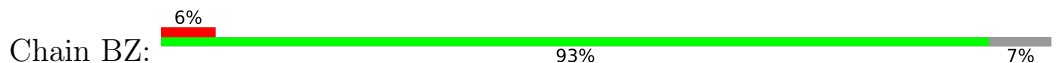
- Molecule 32: 60S ribosomal protein L31-B



- Molecule 33: 60S ribosomal protein L32



- Molecule 33: 60S ribosomal protein L32



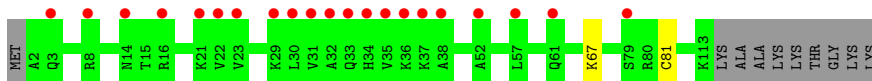
- Molecule 34: 60S ribosomal protein L33-A



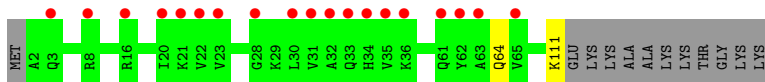
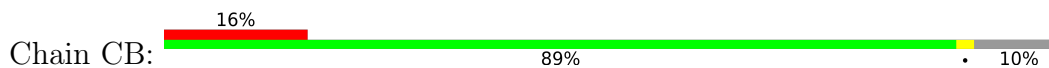
- Molecule 34: 60S ribosomal protein L33-A



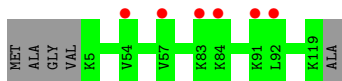
- Molecule 35: 60S ribosomal protein L34-B



- Molecule 35: 60S ribosomal protein L34-B



- Molecule 36: Ribosomal protein L29



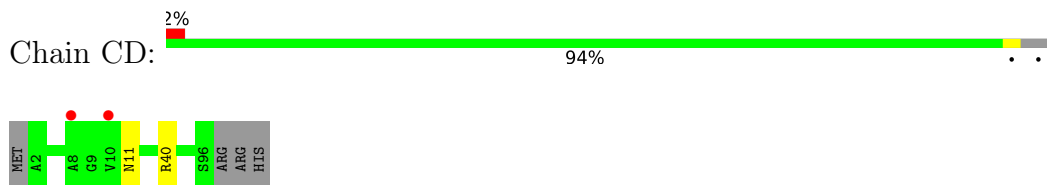
- Molecule 36: Ribosomal protein L29



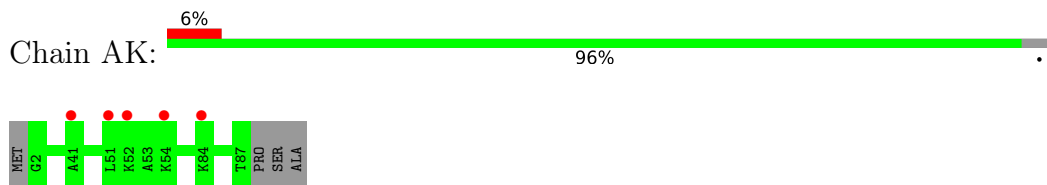
- Molecule 37: 60S ribosomal protein L36



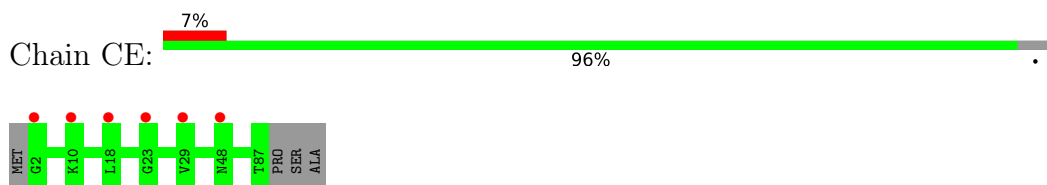
- Molecule 37: 60S ribosomal protein L36



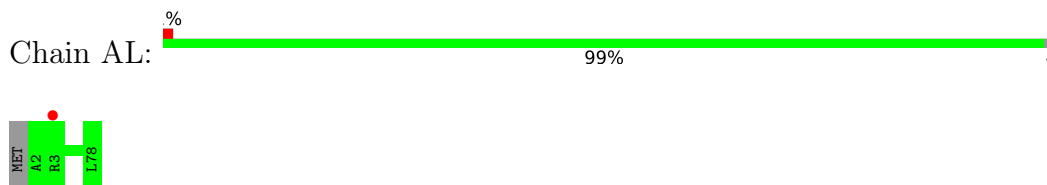
- Molecule 38: 60S ribosomal protein L37-B



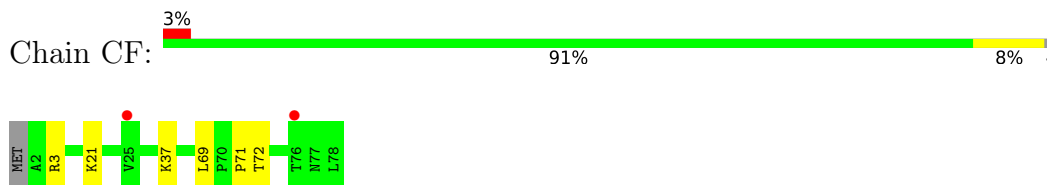
- Molecule 38: 60S ribosomal protein L37-B



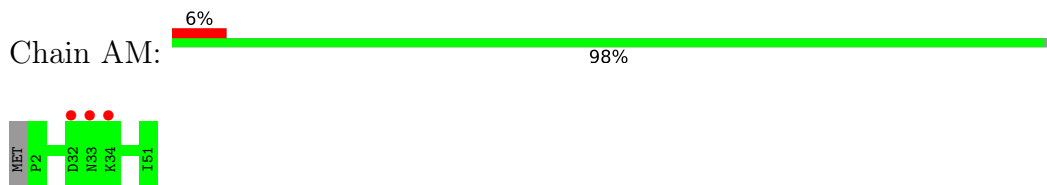
- Molecule 39: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L38

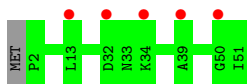


- Molecule 40: 60S ribosomal protein L39

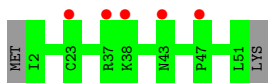


- Molecule 40: 60S ribosomal protein L39

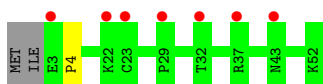




- Molecule 41: 60S ribosomal protein L40-B



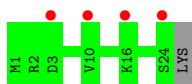
- Molecule 41: 60S ribosomal protein L40-B



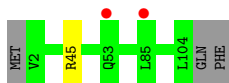
- Molecule 42: 60S ribosomal protein L41



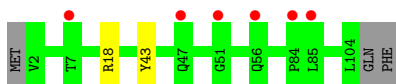
- Molecule 42: 60S ribosomal protein L41



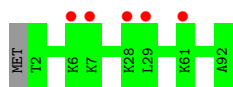
- Molecule 43: 60S ribosomal protein L42-B



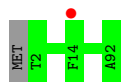
- Molecule 43: 60S ribosomal protein L42-B



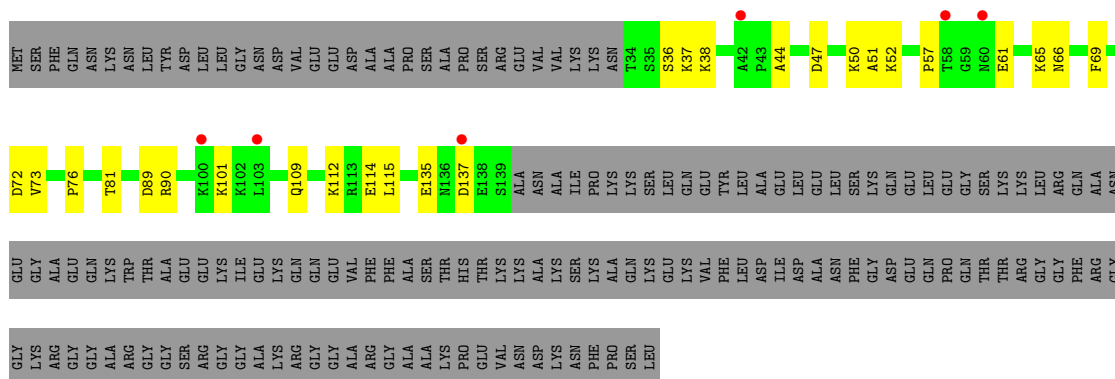
- Molecule 44: 60S ribosomal protein L43-A



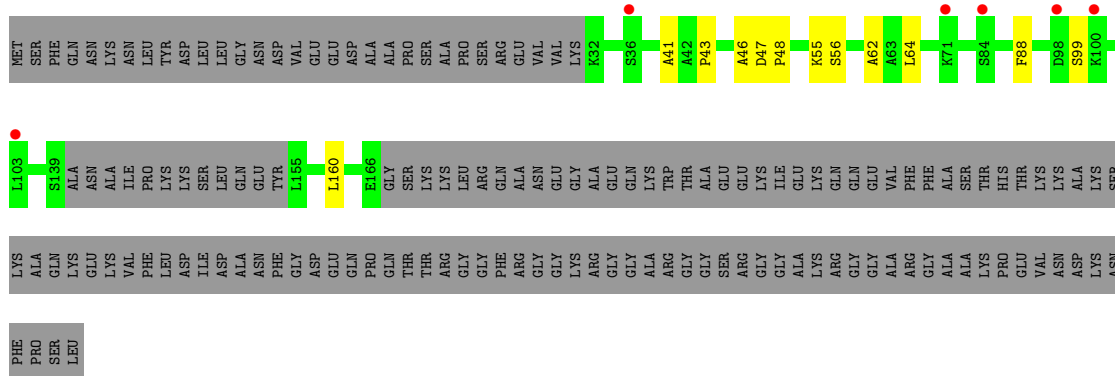
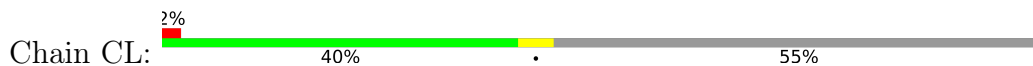
• Molecule 44: 60S ribosomal protein L43-A



• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

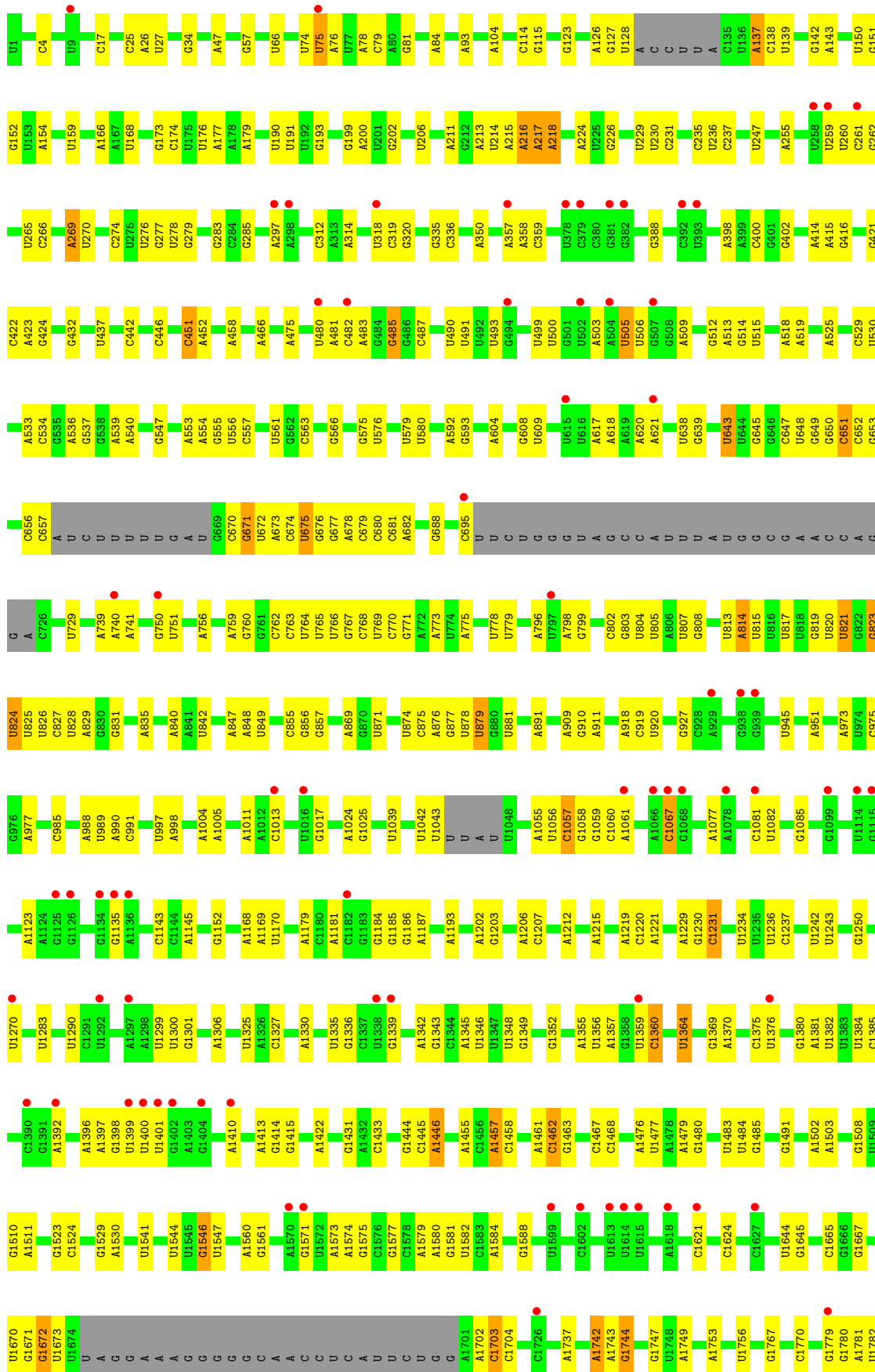


• Molecule 45: 60S ribosomal protein CAALFM_C304810CA



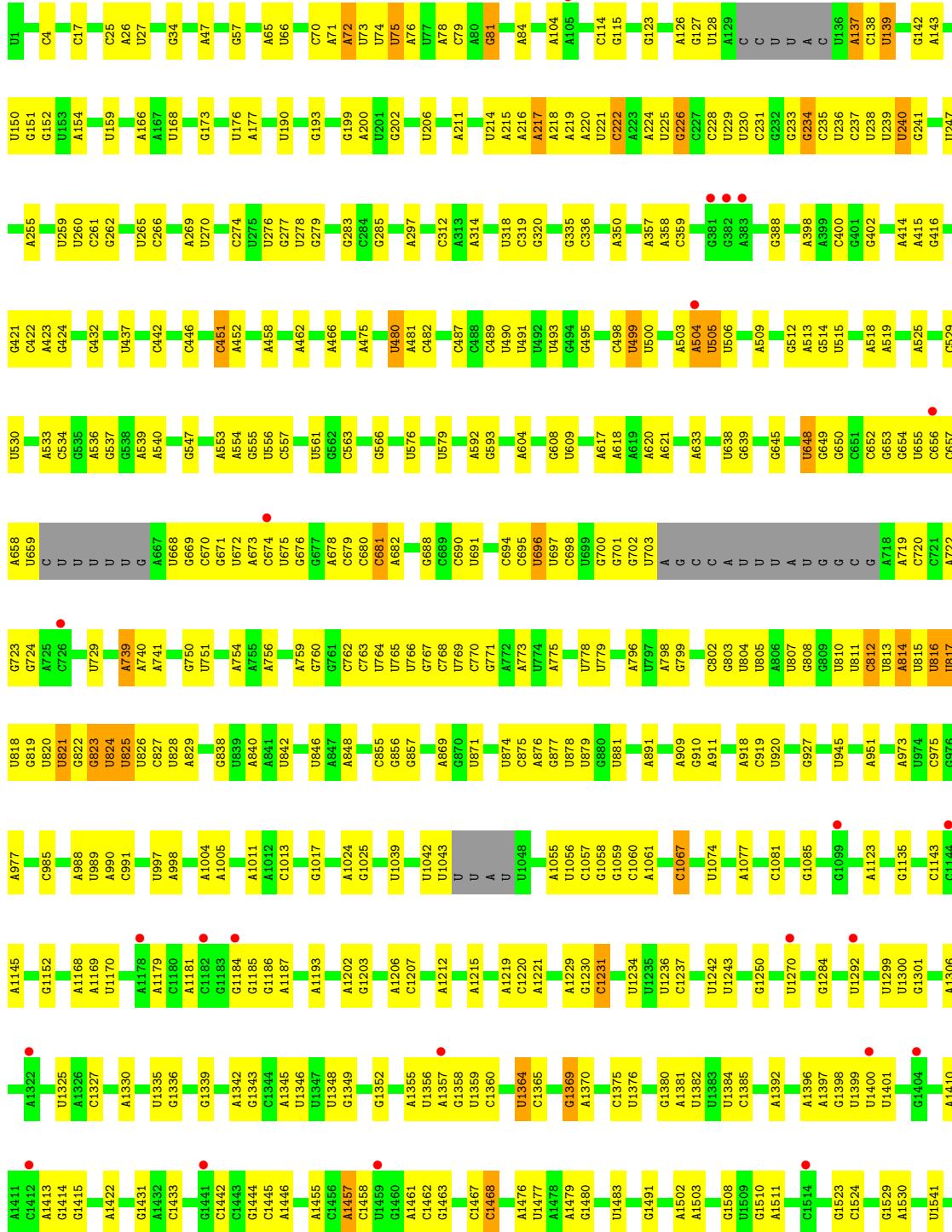
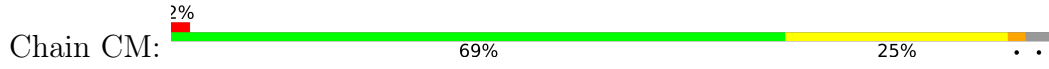
• Molecule 46: 18S ribosomal RNA

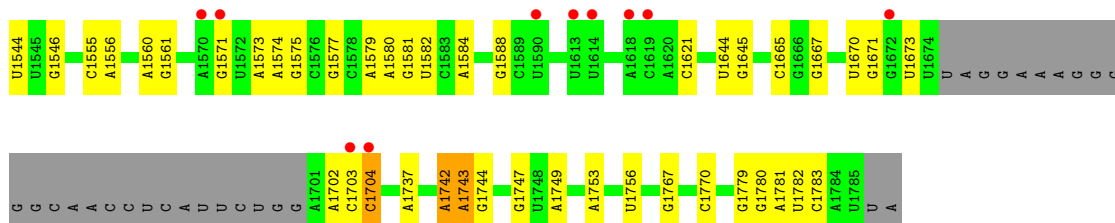




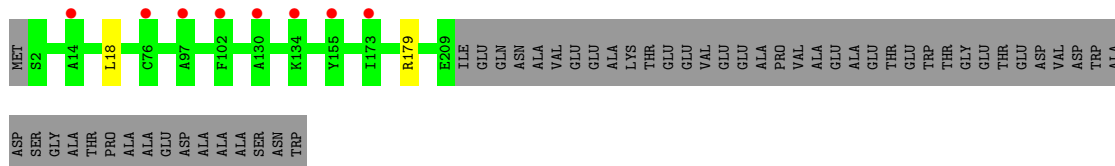
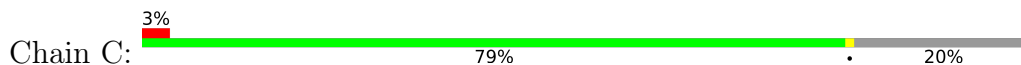
C1783
A1784
U1785
U
A

• Molecule 46: 18S ribosomal RNA

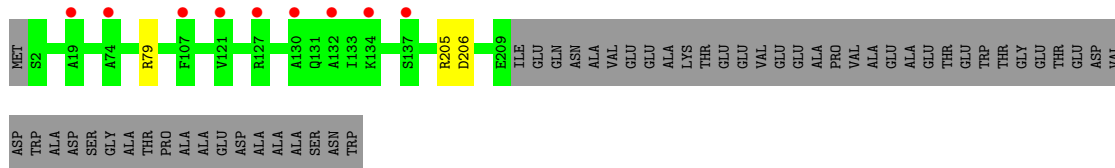
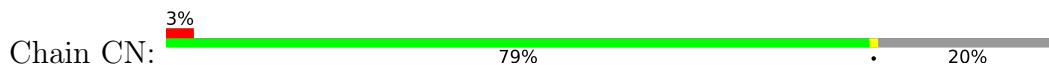




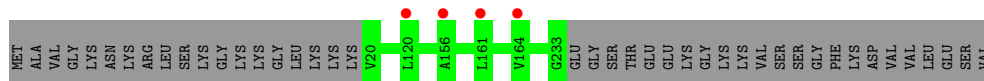
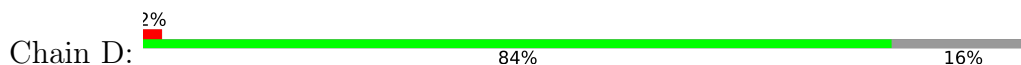
• Molecule 47: 40S ribosomal protein S0



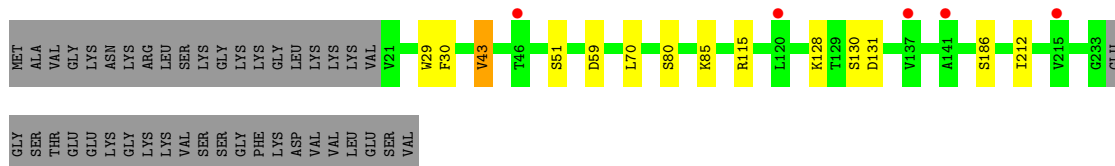
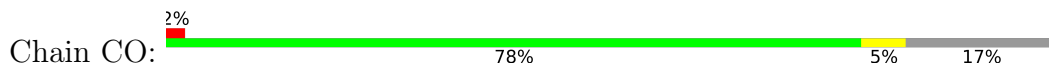
• Molecule 47: 40S ribosomal protein S0



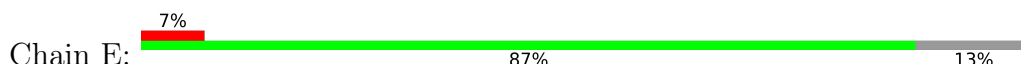
• Molecule 48: 40S ribosomal protein S1

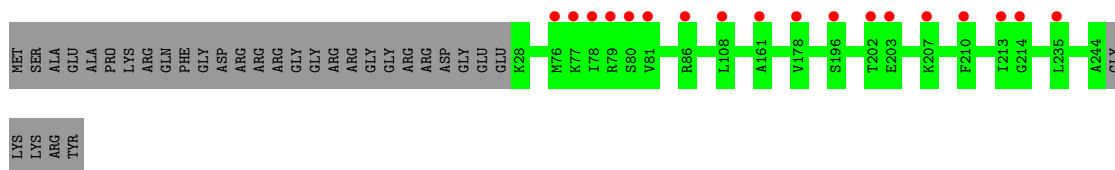


• Molecule 48: 40S ribosomal protein S1

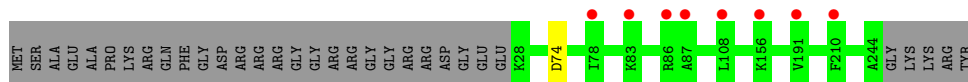
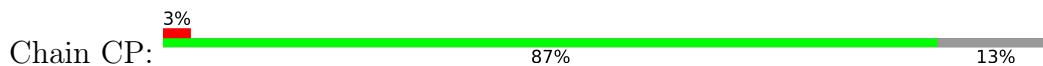


• Molecule 49: Ribosomal protein S5

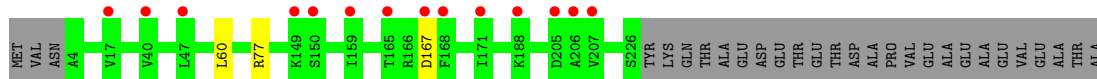
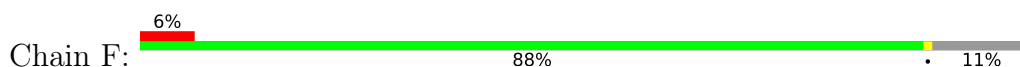




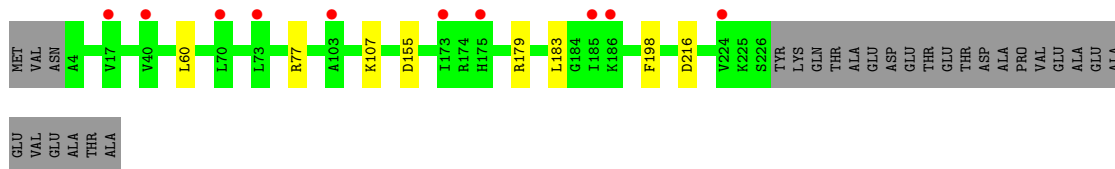
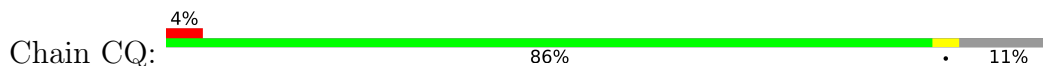
- Molecule 49: Ribosomal protein S5



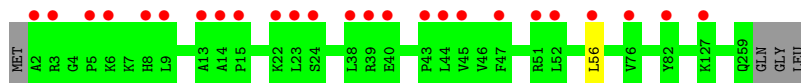
- Molecule 50: Ribosomal protein S3



- Molecule 50: Ribosomal protein S3



- Molecule 51: 40S ribosomal protein S4

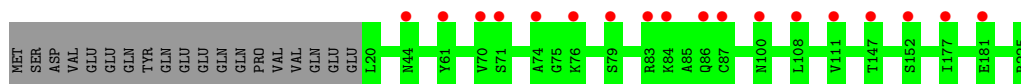


- Molecule 51: 40S ribosomal protein S4

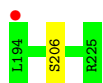
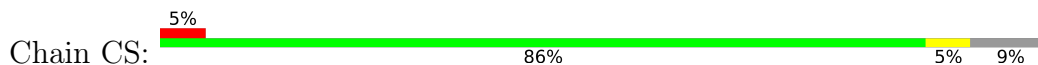


- Molecule 52: Ribosomal protein S7

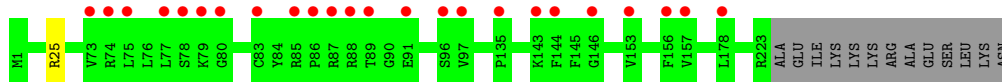
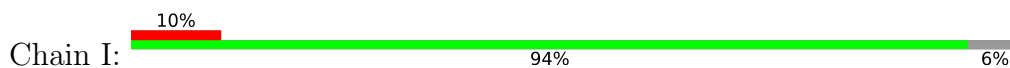




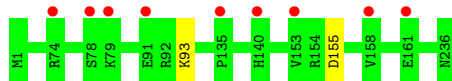
- Molecule 52: Ribosomal protein S7



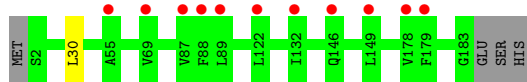
- Molecule 53: 40S ribosomal protein S6



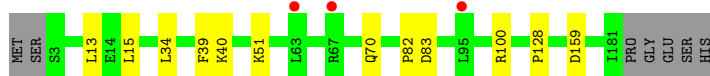
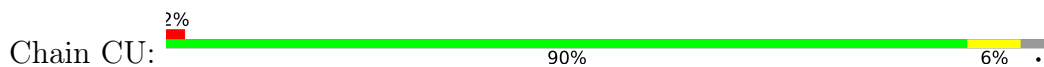
- Molecule 53: 40S ribosomal protein S6



- Molecule 54: 40S ribosomal protein S7

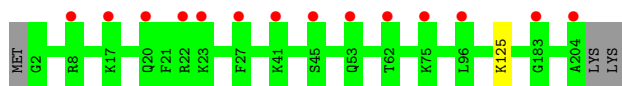


- Molecule 54: 40S ribosomal protein S7

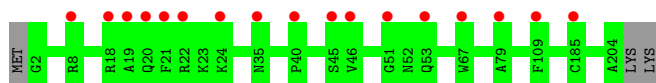


- Molecule 55: 40S ribosomal protein S8

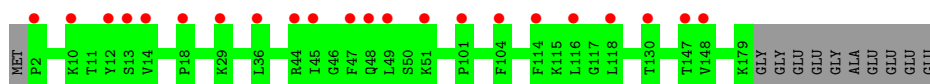
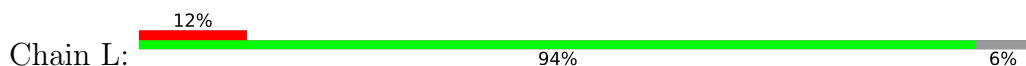




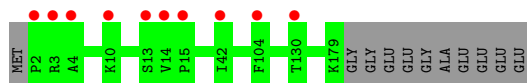
- Molecule 55: 40S ribosomal protein S8



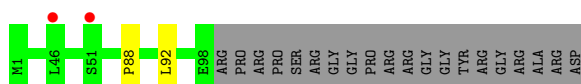
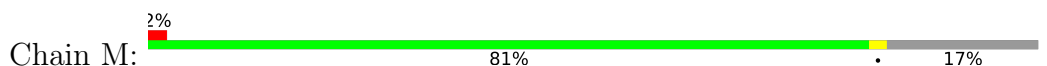
- Molecule 56: Ribosomal protein S4



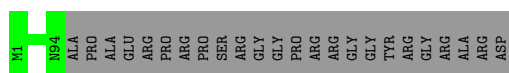
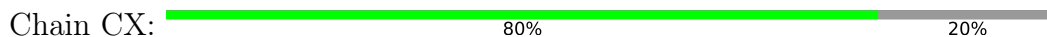
- Molecule 56: Ribosomal protein S4



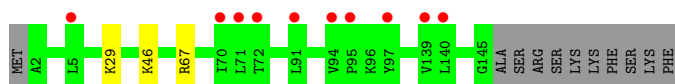
- Molecule 57: 40S ribosomal protein S10-A



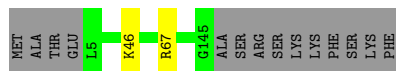
- Molecule 57: 40S ribosomal protein S10-A



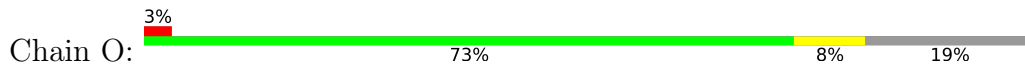
- Molecule 58: 40S ribosomal protein S11A



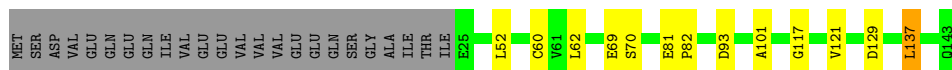
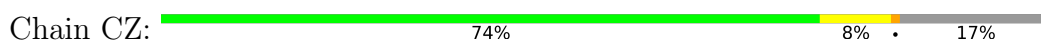
- Molecule 58: 40S ribosomal protein S11A



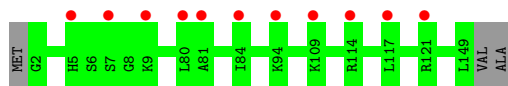
• Molecule 59: 40S ribosomal protein S12



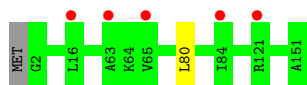
• Molecule 59: 40S ribosomal protein S12



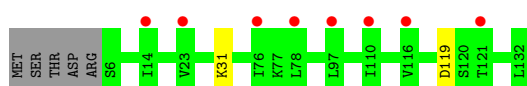
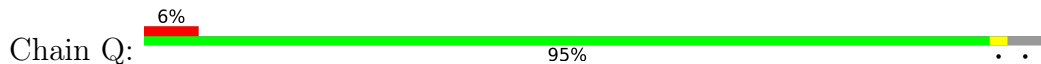
• Molecule 60: 40S ribosomal protein S13



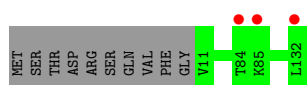
• Molecule 60: 40S ribosomal protein S13



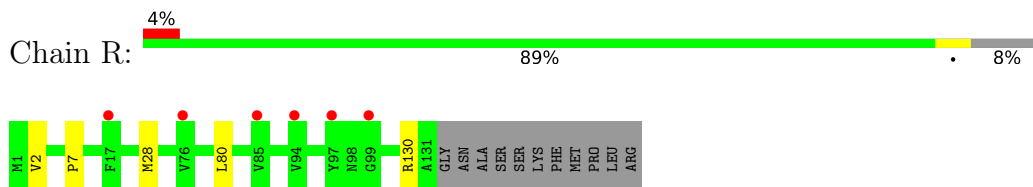
• Molecule 61: 40S ribosomal protein S14-A



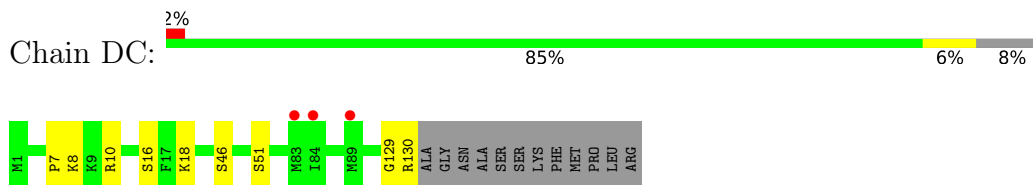
• Molecule 61: 40S ribosomal protein S14-A



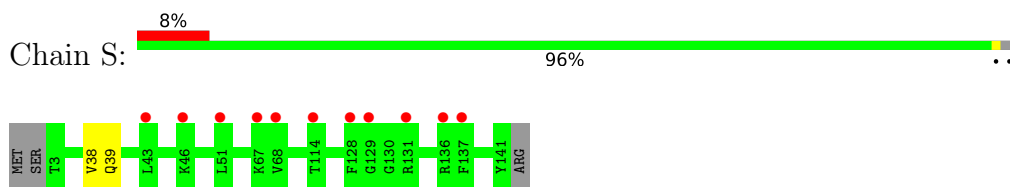
- Molecule 62: 40S ribosomal protein S15



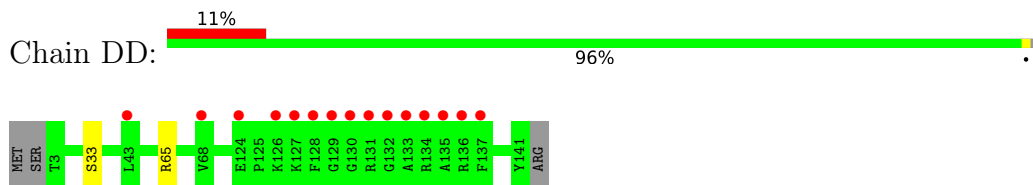
- Molecule 62: 40S ribosomal protein S15



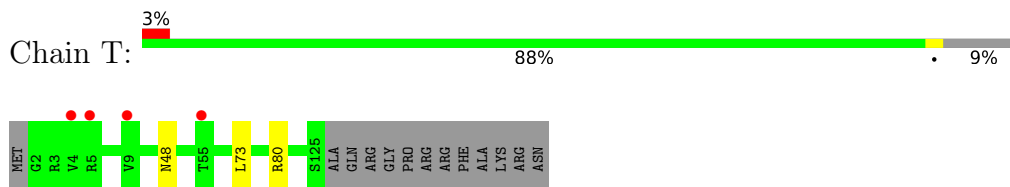
- Molecule 63: 40S ribosomal protein S16



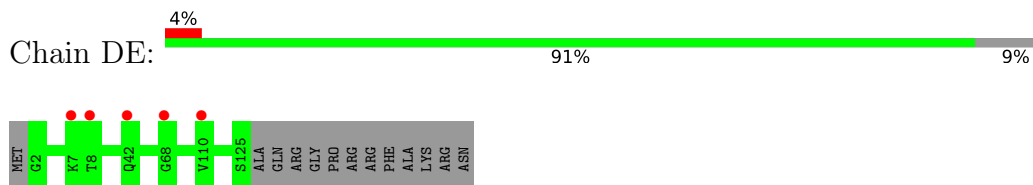
- Molecule 63: 40S ribosomal protein S16



- Molecule 64: 40S ribosomal protein S17-B



- Molecule 64: 40S ribosomal protein S17-B



- Molecule 65: 40S ribosomal protein S18-B

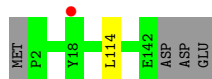




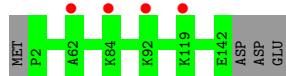
- Molecule 65: 40S ribosomal protein S18-B



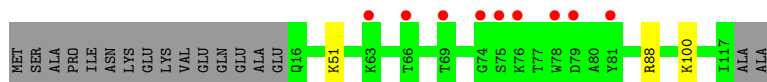
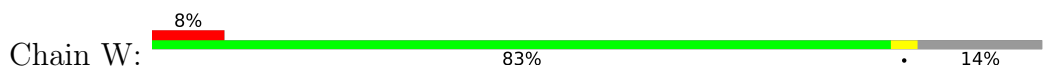
- Molecule 66: 40S ribosomal protein S19-A



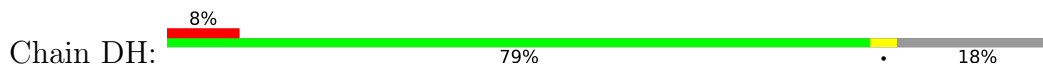
- Molecule 66: 40S ribosomal protein S19-A



- Molecule 67: Ribosomal protein S10



- Molecule 67: Ribosomal protein S10



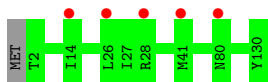
- Molecule 68: 40S ribosomal protein S21



- Molecule 68: 40S ribosomal protein S21



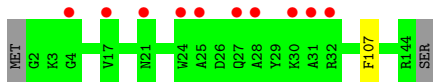
- Molecule 69: 40S ribosomal protein S22-A



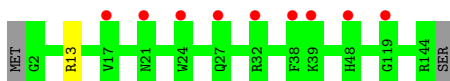
- Molecule 69: 40S ribosomal protein S22-A



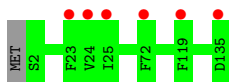
- Molecule 70: Ribosomal protein S23 (S12)



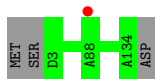
- Molecule 70: Ribosomal protein S23 (S12)



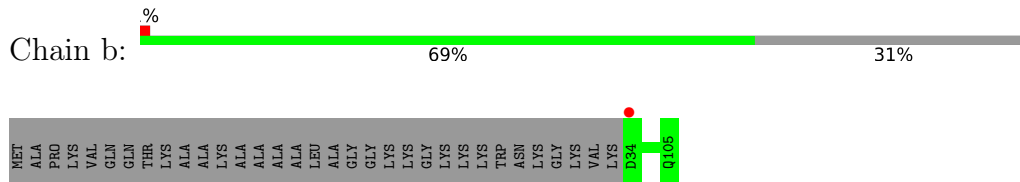
- Molecule 71: 40S ribosomal protein S24



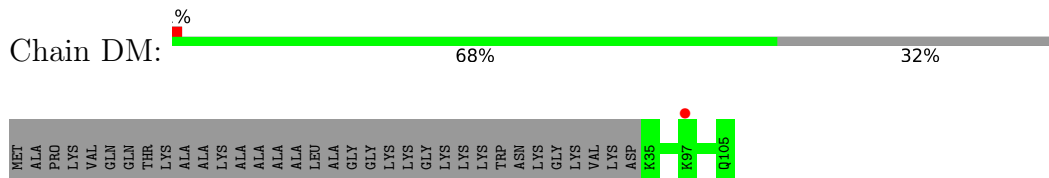
- Molecule 71: 40S ribosomal protein S24



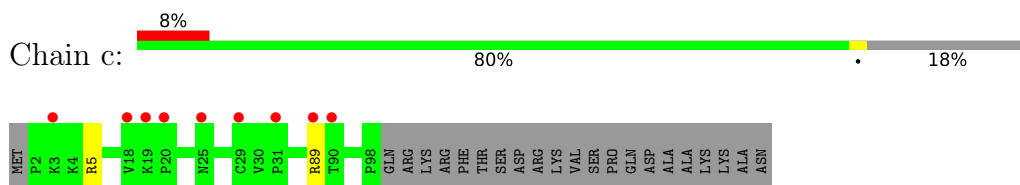
- Molecule 72: 40S ribosomal protein S25



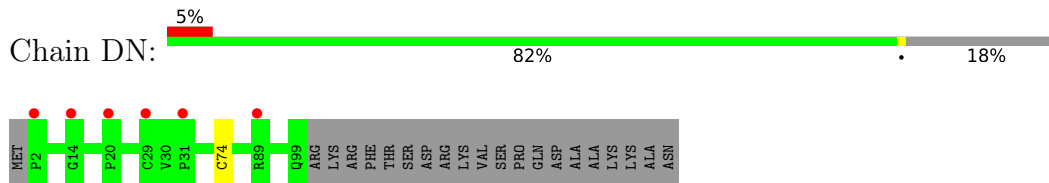
- Molecule 72: 40S ribosomal protein S25



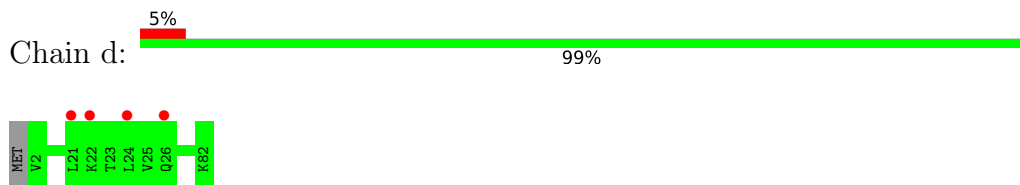
- Molecule 73: 40S ribosomal protein S26



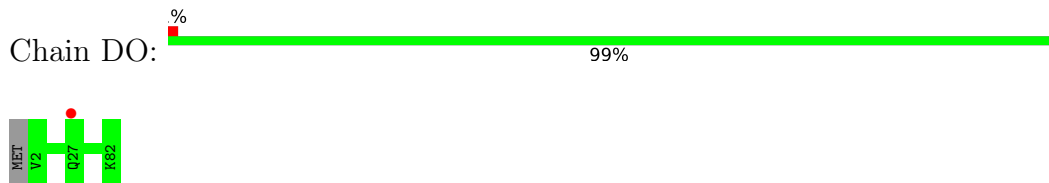
- Molecule 73: 40S ribosomal protein S26



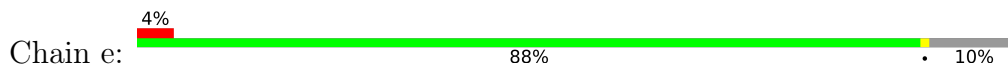
- Molecule 74: 40S ribosomal protein S27

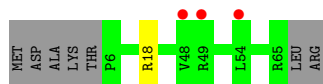


- Molecule 74: 40S ribosomal protein S27

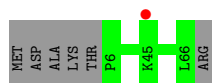
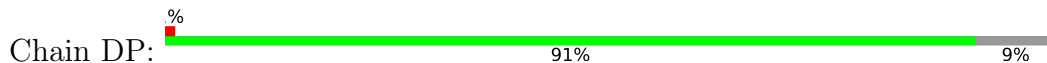


- Molecule 75: 40S ribosomal protein S28-B

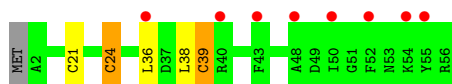
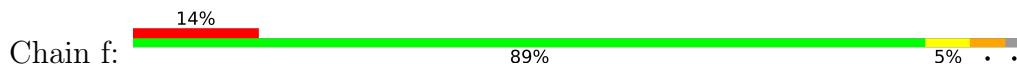




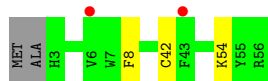
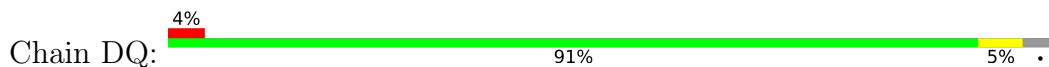
• Molecule 75: 40S ribosomal protein S28-B



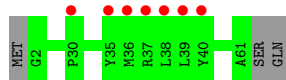
• Molecule 76: 40S ribosomal protein S29A



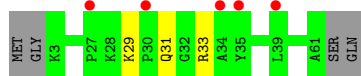
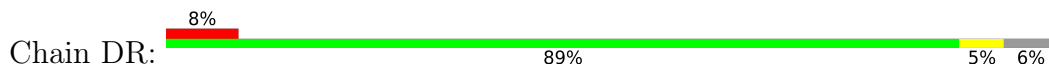
• Molecule 76: 40S ribosomal protein S29A



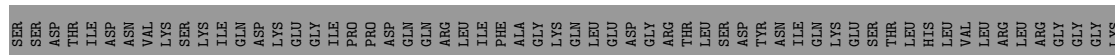
• Molecule 77: 40S ribosomal protein S30



• Molecule 77: 40S ribosomal protein S30



• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein



LEU ASP
 THR THR
 ASP ASP
 LEU LEU
 LEU LEU
 SER SER
 HIS HIS
 PHE PHE
 VAL VAL
 SER SER
 ALA ALA
 ALA ALA
 ASN ASN
 THR THR
 THR THR
 ILE ILE
 ALA ALA
 SER SER
 ILE ILE
 ALA ALA
 LEU LEU
 ALA ALA
 ALA ALA
 GLY GLY
 TYR TYR
 PRO PRO
 THR THR
 LEU LEU
 PRO PRO
 SER SER
 VAL VAL
 HIS HIS
 ASP ASP
 ILE ILE
 ILE ILE
 ASN ASN
 SER SER
 TYR TYR
 LYS LYS
 ASP ASP
 ASN ASN
 VAL VAL
 MET MET
 PHE PHE
 GLY GLY
 LEU LEU
 VAL VAL
 PHE PHE
 ASP ASP

ALA VAL
 LYS ASP
 ARG ARG
 LEU LEU
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 ASN ASN
 PRO PRO
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 THR THR
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 ILE ILE
 ASN ASN
 SER SER
 TYR TYR
 LYS LYS
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 ASN ASN
 VAL VAL
 MET MET
 PHE PHE
 GLY GLY
 LEU LEU
 VAL VAL
 PHE PHE
 ASP ASP

● Molecule 82: 60S ribosomal protein L12-A



MET PRO
 PRO PRO
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 PHE PHE
 GLN GLN
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 PRO PRO
 ARG ARG
 ASN ASN
 VAL VAL
 THR THR
 LYS LYS
 PHE PHE
 LEU LEU
 TYR TYR
 LEU LEU
 ARG ARG
 SER SER
 ALA ALA
 ALA ALA
 ASN ASN
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 ALA ALA
 LEU LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	300.29Å 294.06Å 442.55Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	266.82 – 3.50 266.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (266.82-3.50) 86.6 (266.82-3.50)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.249 , 0.293 0.251 , 0.290	Depositor DCC
R_{free} test set	1526 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	400037	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GET, 3K5, MG, ZN

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	1	0.34	0/76993	0.97	129/120031 (0.1%)
1	AS	0.33	0/74190	0.97	118/115649 (0.1%)
2	3	0.29	0/2884	0.83	0/4492
2	AT	0.31	0/2884	0.87	0/4492
3	4	0.27	0/3702	0.86	1/5764 (0.0%)
3	AU	0.31	0/3746	0.93	7/5832 (0.1%)
4	AW	0.28	0/1922	0.59	0/2581
4	j	0.27	0/1922	0.61	0/2581
5	AX	0.29	0/3145	0.64	4/4231 (0.1%)
5	k	0.29	0/3145	0.60	0/4231
6	AY	0.27	0/2782	0.57	0/3754
6	l	0.28	0/2782	0.59	0/3754
7	AZ	0.28	0/2447	0.56	0/3294
7	m	0.28	0/2462	0.57	0/3315
8	BA	0.29	0/1231	0.59	0/1662
8	n	0.30	0/1263	0.60	0/1703
9	BB	0.28	0/1849	0.55	0/2485
9	o	0.30	0/1876	0.56	0/2519
10	BC	0.47	0/1835	0.83	1/2472 (0.0%)
10	p	0.32	0/1855	0.63	1/2500 (0.0%)
11	BD	0.26	0/1537	0.56	0/2067
11	q	0.30	0/1537	0.63	0/2067
12	r	0.29	0/1716	0.59	0/2304
13	BF	0.28	0/1390	0.61	0/1861
13	s	0.28	0/1390	0.61	0/1861
14	BG	0.48	0/1637	0.85	1/2195 (0.0%)
14	t	0.32	0/1637	0.68	1/2195 (0.0%)
15	BH	0.27	0/1044	0.57	0/1407
15	u	0.30	0/1030	0.59	0/1389
16	BI	0.27	0/1753	0.63	0/2347
16	v	0.27	0/1753	0.63	0/2347
17	BJ	0.29	0/1620	0.57	0/2167

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	w	0.28	0/1620	0.59	0/2167
18	BK	0.27	0/1419	0.61	0/1906
18	x	0.30	0/1375	0.64	0/1848
19	BL	0.27	0/1482	0.61	0/1985
19	y	0.28	0/1482	0.62	0/1985
20	BM	0.34	0/1475	0.71	1/1961 (0.1%)
20	z	0.39	0/1475	0.71	4/1961 (0.2%)
21	0	0.27	0/1457	0.59	0/1962
21	BN	0.27	0/1457	0.56	0/1962
22	2	0.27	0/1285	0.57	0/1723
22	BO	0.37	0/1285	0.69	0/1723
23	5	0.30	0/816	0.60	0/1099
23	BP	0.50	0/807	0.91	4/1088 (0.4%)
24	6	0.28	0/993	0.61	0/1339
24	BQ	0.29	0/993	0.61	0/1339
25	7	0.31	0/958	0.60	0/1267
25	BR	0.31	0/889	0.63	1/1175 (0.1%)
26	8	0.28	0/981	0.59	0/1326
26	BS	0.49	0/976	0.91	0/1319
27	9	0.32	0/999	0.63	0/1334
27	BT	0.27	0/999	0.58	0/1334
28	AA	0.28	0/1112	0.52	0/1488
28	BU	0.50	0/1112	0.89	1/1488 (0.1%)
29	AB	0.27	0/1199	0.57	0/1607
29	BV	0.29	0/1199	0.58	0/1607
30	AC	0.26	0/474	0.67	0/630
30	BW	0.27	0/492	0.54	0/653
31	AD	0.30	0/756	0.55	0/1018
31	BX	0.27	0/724	0.52	0/975
32	AE	0.27	0/894	0.61	0/1201
32	BY	0.25	0/894	0.59	0/1201
33	AF	0.27	0/1021	0.59	0/1368
33	BZ	0.28	0/1012	0.61	0/1356
34	AG	0.29	0/866	0.59	0/1165
34	CA	0.29	0/866	0.56	0/1165
35	AH	0.28	0/896	0.61	0/1195
35	CB	0.31	0/878	0.69	1/1172 (0.1%)
36	AI	0.27	0/974	0.59	0/1297
36	CC	0.50	0/985	0.89	0/1312
37	AJ	0.27	0/763	0.60	0/1012
37	CD	0.47	0/741	0.91	0/984
38	AK	0.27	0/690	0.66	0/916
38	CE	0.27	0/690	0.65	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	AL	0.27	0/623	0.56	0/831
39	CF	0.45	0/623	0.84	1/831 (0.1%)
40	AM	0.27	0/447	0.64	0/594
40	CG	0.27	0/447	0.64	0/594
41	AN	0.25	0/408	0.59	0/542
41	CH	0.30	0/409	0.62	0/542
42	AO	0.29	0/237	0.74	0/304
42	CI	0.29	0/228	0.74	0/293
43	AP	0.28	0/840	0.60	0/1110
43	CJ	0.28	0/840	0.63	1/1110 (0.1%)
44	AQ	0.29	0/705	0.65	0/940
44	CK	0.26	0/705	0.62	0/940
45	CL	0.52	0/929	0.90	0/1240
45	i	0.48	0/816	0.99	3/1091 (0.3%)
46	B	0.34	0/40724	1.00	96/63452 (0.2%)
46	CM	0.36	0/41205	1.03	126/64202 (0.2%)
47	C	0.27	0/1666	0.54	0/2273
47	CN	0.27	0/1666	0.55	0/2273
48	CO	0.55	0/1743	0.99	3/2344 (0.1%)
48	D	0.26	0/1750	0.60	0/2354
49	CP	0.27	0/1657	0.56	0/2248
49	E	0.27	0/1657	0.54	0/2248
50	CQ	0.28	0/1731	0.66	3/2324 (0.1%)
50	F	0.30	0/1731	0.67	1/2324 (0.0%)
51	CR	0.27	0/2096	0.58	0/2822
51	G	0.28	0/2083	0.59	1/2805 (0.0%)
52	CS	0.57	0/1623	0.97	3/2188 (0.1%)
52	H	0.26	0/1631	0.57	0/2199
53	CT	0.29	0/1929	0.67	0/2571
53	I	0.27	0/1823	0.59	0/2434
54	CU	0.49	0/1472	0.96	3/1979 (0.2%)
54	J	0.26	0/1490	0.58	0/2004
55	CV	0.30	0/1606	0.63	0/2150
55	K	0.29	0/1606	0.61	0/2150
56	CW	0.26	0/1478	0.59	0/1978
56	L	0.27	0/1478	0.59	0/1978
57	CX	0.29	0/809	0.61	0/1092
57	M	0.31	0/836	0.67	0/1130
58	CY	0.30	0/1154	0.61	0/1553
58	N	0.27	0/1175	0.59	0/1582
59	CZ	0.53	0/921	1.03	4/1240 (0.3%)
59	O	0.32	0/892	0.76	1/1203 (0.1%)
60	DA	0.25	0/1210	0.55	0/1631

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	P	0.27	0/1198	0.55	0/1614
61	DB	0.27	0/915	0.65	0/1228
61	Q	0.28	0/953	0.64	0/1279
62	DC	0.50	0/1049	0.96	1/1409 (0.1%)
62	R	0.33	0/1054	0.69	1/1416 (0.1%)
63	DD	0.27	0/1103	0.58	0/1478
63	S	0.28	0/1103	0.56	0/1478
64	DE	0.29	0/1009	0.66	0/1354
64	T	0.26	0/1009	0.64	1/1354 (0.1%)
65	DF	0.27	0/1178	0.62	0/1579
65	U	0.29	0/1205	0.66	1/1615 (0.1%)
66	DG	0.27	0/1120	0.58	0/1508
66	V	0.28	0/1120	0.61	1/1508 (0.1%)
67	DH	0.27	0/772	0.63	1/1045 (0.1%)
67	W	0.27	0/818	0.60	0/1106
68	DI	0.30	0/683	0.63	0/918
68	X	0.28	0/683	0.60	0/918
69	DJ	0.27	0/1049	0.57	0/1412
69	Y	0.27	0/1049	0.57	0/1412
70	DK	0.28	0/1128	0.63	0/1505
70	Z	0.29	0/1128	0.66	0/1505
71	DL	0.28	0/1086	0.62	0/1447
71	a	0.27	0/1100	0.59	0/1466
72	DM	0.33	0/577	0.60	0/778
72	b	0.26	0/585	0.56	0/789
73	DN	0.25	0/791	0.63	0/1060
73	c	0.27	0/782	0.64	0/1048
74	DO	0.27	0/624	0.61	0/843
74	d	0.27	0/624	0.56	0/843
75	DP	0.29	0/478	0.74	0/640
75	e	0.27	0/470	0.70	0/629
76	DQ	0.37	0/461	0.63	0/613
76	f	0.39	0/466	0.77	3/620 (0.5%)
77	DR	0.37	0/478	0.72	0/637
77	g	0.34	0/482	0.66	0/642
78	DS	0.51	0/564	1.08	0/749
78	h	0.29	0/585	0.73	1/778 (0.1%)
79	AR	0.26	0/2451	0.57	0/3337
79	DT	0.56	0/2414	1.05	6/3286 (0.2%)
80	BE	0.29	0/1696	0.60	0/2276
81	P0	0.37	0/857	0.71	0/1148
82	12	0.40	0/486	0.67	1/653 (0.2%)
All	All	0.33	0/427902	0.87	538/627694 (0.1%)

There are no bond length outliers.

All (538) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3127	U	O4'-C1'-N1	13.98	119.38	108.20
46	B	676	G	O4'-C1'-N9	12.71	118.37	108.20
79	DT	40	LYS	CD-CE-NZ	12.13	139.60	111.70
46	CM	679	C	O5'-P-OP2	-12.11	94.81	105.70
1	AS	1576	A	O4'-C1'-N9	11.40	117.32	108.20
3	AU	102	U	P-O3'-C3'	-11.20	106.26	119.70
46	B	835	A	O5'-P-OP1	11.09	124.01	110.70
1	AS	2419	A	C8-N9-C4	-10.75	101.50	105.80
1	1	1576	A	O4'-C1'-N9	10.70	116.76	108.20
1	AS	524	G	P-O3'-C3'	-10.68	106.89	119.70
46	CM	72	A	P-O3'-C3'	-10.64	106.94	119.70
52	CS	25	LEU	CA-CB-CG	10.41	139.24	115.30
1	AS	523	G	P-O3'-C3'	-10.37	107.25	119.70
46	CM	75	U	P-O3'-C3'	-10.22	107.44	119.70
1	1	1254	U	O5'-P-OP1	-10.17	96.54	105.70
1	1	598	U	O4'-C1'-N1	9.81	116.05	108.20
1	1	1653	C	P-O3'-C3'	-9.78	107.96	119.70
46	B	824	U	O4'-C1'-N1	-9.73	100.42	108.20
1	AS	1576	A	C4-N9-C1'	9.72	143.80	126.30
46	CM	218	A	C8-N9-C4	-9.72	101.91	105.80
1	1	602	A	P-O3'-C3'	-9.67	108.10	119.70
3	AU	105	A	P-O3'-C3'	-9.47	108.34	119.70
46	CM	71	A	P-O3'-C3'	-9.37	108.46	119.70
1	1	1652	A	P-O3'-C3'	-9.29	108.56	119.70
1	1	3125	U	P-O3'-C3'	-9.15	108.72	119.70
1	1	1576	A	C4-N9-C1'	9.10	142.68	126.30
46	B	1742	A	O4'-C1'-N9	8.88	115.31	108.20
1	AS	478	G	C8-N9-C1'	-8.81	115.54	127.00
46	CM	1743	A	C8-N9-C4	-8.73	102.31	105.80
46	CM	226	G	C6-C5-N7	-8.72	125.17	130.40
1	1	1019	U	O4'-C1'-N1	8.72	115.18	108.20
46	B	451	C	N1-C2-O2	8.70	124.12	118.90
1	AS	646	C	P-O3'-C3'	-8.62	109.35	119.70
1	1	1218	G	O4'-C1'-N9	8.59	115.07	108.20
3	AU	104	A	P-O3'-C3'	-8.54	109.45	119.70
46	B	485	G	C4-N9-C1'	8.45	137.48	126.50
1	1	2814	U	C2-N1-C1'	8.38	127.76	117.70
1	AS	1576	A	C8-N9-C1'	-8.36	112.65	127.70
46	CM	482	C	O4'-C1'-N1	8.34	114.87	108.20
1	1	597	U	C5-C6-N1	-8.32	118.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CM	233	G	C6-C5-N7	-8.31	125.41	130.40
1	1	3124	U	P-O3'-C3'	-8.29	109.75	119.70
46	CM	451	C	N1-C2-O2	8.27	123.86	118.90
1	AS	1576	A	N7-C8-N9	8.19	117.89	113.80
1	1	1576	A	C8-N9-C1'	-8.17	113.00	127.70
1	AS	2814	U	C2-N1-C1'	8.11	127.43	117.70
46	CM	222	C	C5-C6-N1	8.11	125.05	121.00
1	1	401	U	O4'-C1'-N1	8.10	114.68	108.20
46	B	485	G	C6-C5-N7	-7.96	125.63	130.40
3	AU	103	G	P-O3'-C3'	-7.95	110.16	119.70
46	CM	812	C	P-O3'-C3'	-7.90	110.22	119.70
1	1	1217	A	N1-C2-N3	7.89	133.24	129.30
46	CM	825	U	N3-C2-O2	-7.86	116.70	122.20
1	1	481	G	O4'-C1'-N9	7.81	114.45	108.20
50	F	60	LEU	CA-CB-CG	7.80	133.24	115.30
46	CM	1743	A	N7-C8-N9	7.78	117.69	113.80
46	B	451	C	C2-N1-C1'	7.76	127.34	118.80
1	AS	977	U	C2-N1-C1'	7.67	126.90	117.70
46	B	217	A	O4'-C1'-N9	7.66	114.33	108.20
46	CM	1742	A	N9-C4-C5	7.66	108.86	105.80
46	CM	1242	U	N3-C2-O2	-7.65	116.85	122.20
1	1	598	U	N3-C2-O2	-7.60	116.88	122.20
46	CM	608	G	C4-N9-C1'	7.56	136.32	126.50
5	AX	142	LYS	CB-CA-C	-7.54	95.33	110.40
46	CM	451	C	C2-N1-C1'	7.53	127.08	118.80
1	AS	478	G	C4-N9-C1'	7.42	136.14	126.50
46	CM	1375	C	C2-N1-C1'	7.41	126.95	118.80
1	AS	1349	U	C2-N1-C1'	7.40	126.58	117.70
46	B	656	C	C2-N1-C1'	7.39	126.93	118.80
46	B	485	G	C8-N9-C1'	-7.35	117.44	127.00
1	1	482	U	O4'-C1'-N1	7.35	114.08	108.20
1	1	977	U	C2-N1-C1'	7.33	126.50	117.70
46	CM	233	G	N1-C6-O6	7.33	124.30	119.90
1	1	597	U	N3-C4-O4	-7.31	114.28	119.40
46	CM	226	G	N1-C6-O6	7.31	124.28	119.90
1	AS	645	A	P-O3'-C3'	-7.27	110.97	119.70
1	1	245	G	C8-N9-C1'	-7.27	117.55	127.00
20	z	157	GLU	CB-CA-C	-7.22	95.95	110.40
1	AS	3126	U	C2-N1-C1'	7.21	126.35	117.70
1	AS	2419	A	N9-C4-C5	7.20	108.68	105.80
1	AS	3160	C	C2-N1-C1'	7.18	126.70	118.80
5	AX	140	ASP	CB-CG-OD1	-7.18	111.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	485	G	N3-C4-N9	7.16	130.29	126.00
14	t	131	LYS	CD-CE-NZ	-7.15	95.26	111.70
1	1	245	G	N9-C4-C5	-7.15	102.54	105.40
46	CM	811	U	P-O3'-C3'	-7.12	111.16	119.70
46	B	651	C	C5-C6-N1	7.07	124.53	121.00
1	AS	3182	C	C2-N1-C1'	7.07	126.58	118.80
3	AU	155	G	O4'-C1'-N9	7.06	113.85	108.20
46	B	1375	C	C2-N1-C1'	7.06	126.57	118.80
46	CM	810	U	P-O3'-C3'	-7.04	111.25	119.70
1	1	597	U	C2-N1-C1'	-7.01	109.28	117.70
1	1	3321	G	O5'-P-OP1	-7.00	99.40	105.70
46	B	656	C	N1-C2-O2	6.98	123.09	118.90
1	AS	3160	C	C6-N1-C1'	-6.97	112.43	120.80
46	CM	823	G	O4'-C1'-N9	-6.96	102.63	108.20
46	B	651	C	C6-N1-C2	-6.96	117.52	120.30
1	AS	918	U	C2-N1-C1'	6.96	126.05	117.70
1	1	1019	U	C6-N1-C2	-6.94	116.84	121.00
46	B	1744	G	P-O3'-C3'	-6.91	111.41	119.70
46	CM	838	G	O5'-P-OP1	-6.90	99.49	105.70
1	1	918	U	C2-N1-C1'	6.89	125.97	117.70
46	CM	217	A	O4'-C1'-N9	6.89	113.71	108.20
1	1	2215	C	N3-C2-O2	-6.87	117.09	121.90
1	AS	2484	U	C2-N1-C1'	6.86	125.94	117.70
1	1	1025	G	C5'-C4'-C3'	-6.84	105.06	116.00
14	BG	48	PRO	N-CA-CB	-6.83	95.09	102.60
46	CM	821	U	C5-C6-N1	6.82	126.11	122.70
46	CM	481	A	O4'-C1'-N9	6.82	113.66	108.20
46	B	835	A	OP1-P-OP2	-6.82	109.37	119.60
54	CU	34	LEU	CB-CG-CD2	-6.77	99.49	111.00
46	CM	1242	U	N1-C2-O2	6.77	127.54	122.80
46	CM	226	G	C4-C5-N7	6.76	113.50	110.80
1	1	401	U	C2-N1-C1'	6.73	125.78	117.70
1	1	3321	G	O5'-P-OP2	6.72	118.77	110.70
1	1	3182	C	C2-N1-C1'	6.71	126.18	118.80
46	CM	233	G	C4-C5-N7	6.71	113.48	110.80
46	CM	991	C	O4'-C1'-N1	6.68	113.55	108.20
1	AS	478	G	O5'-P-OP1	-6.66	99.70	105.70
62	DC	8	LYS	CD-CE-NZ	-6.66	96.38	111.70
46	CM	822	G	O4'-C1'-N9	6.65	113.52	108.20
1	1	1019	U	C5-C6-N1	6.64	126.02	122.70
46	CM	218	A	C5'-C4'-O4'	-6.64	101.13	109.10
1	1	1576	A	N7-C8-N9	6.62	117.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	i	38	LYS	CD-CE-NZ	6.61	126.90	111.70
46	B	451	C	N3-C2-O2	-6.61	117.28	121.90
79	DT	129	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	AS	155	A	O5'-P-OP2	-6.60	99.76	105.70
46	B	1444	G	N3-C4-N9	6.59	129.96	126.00
1	AS	451	C	C2-N1-C1'	6.55	126.01	118.80
46	CM	1242	U	C5-C6-N1	6.55	125.97	122.70
1	1	599	U	O4'-C1'-N1	-6.53	102.97	108.20
1	1	3271	U	O4'-C1'-N1	6.53	113.42	108.20
46	CM	1242	U	C6-N1-C2	-6.50	117.10	121.00
46	CM	81	G	C6-C5-N7	-6.48	126.51	130.40
46	CM	817	U	O4'-C1'-N1	6.48	113.38	108.20
1	AS	3167	G	N9-C4-C5	-6.48	102.81	105.40
46	CM	504	A	O4'-C1'-N9	-6.48	103.02	108.20
1	AS	1562	G	C4-N9-C1'	6.46	134.90	126.50
46	CM	754	A	C8-N9-C4	-6.45	103.22	105.80
39	CF	69	LEU	CA-CB-CG	6.44	130.12	115.30
1	1	1254	U	O5'-P-OP2	6.42	118.40	110.70
1	1	3243	C	N1-C2-O2	6.42	122.75	118.90
52	CS	25	LEU	CB-CA-C	6.42	122.39	110.20
67	DH	25	LEU	CA-CB-CG	6.42	130.05	115.30
46	B	1375	C	N1-C2-O2	6.41	122.75	118.90
46	B	1703	C	OP1-P-O3'	6.39	119.26	105.20
1	AS	620	A	N1-C6-N6	6.39	122.43	118.60
1	AS	1492	C	C2-N1-C1'	6.38	125.82	118.80
46	B	269	A	OP1-P-O3'	6.38	119.24	105.20
46	B	991	C	O4'-C1'-N1	6.36	113.29	108.20
46	CM	657	C	C6-N1-C2	-6.36	117.76	120.30
46	B	1067	C	C2-N1-C1'	6.35	125.79	118.80
46	CM	816	U	C5-C4-O4	6.35	129.71	125.90
1	1	2663	A	P-O3'-C3'	6.35	127.32	119.70
1	1	1346	U	P-O3'-C3'	6.35	127.32	119.70
46	CM	451	C	N3-C2-O2	-6.35	117.45	121.90
10	p	249	LYS	CB-CG-CD	6.34	128.10	111.60
46	B	481	A	O4'-C1'-N9	6.34	113.27	108.20
1	AS	3160	C	N1-C2-O2	6.33	122.70	118.90
1	AS	3167	G	N3-C4-N9	6.33	129.80	126.00
1	1	597	U	C2-N3-C4	-6.33	123.20	127.00
1	1	3243	C	N3-C2-O2	-6.32	117.47	121.90
1	1	1738	U	C5-C6-N1	6.32	125.86	122.70
1	AS	486	C	C2-N1-C1'	6.32	125.75	118.80
46	CM	1242	U	C2-N1-C1'	6.31	125.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CM	656	C	C6-N1-C2	-6.31	117.78	120.30
1	1	1492	C	C2-N1-C1'	6.30	125.73	118.80
1	AS	1576	A	C6-C5-N7	-6.30	127.89	132.30
46	CM	656	C	C2-N1-C1'	6.29	125.72	118.80
1	1	2814	U	C6-N1-C1'	-6.27	112.42	121.20
46	B	643	U	O4'-C1'-N1	6.26	113.21	108.20
46	CM	608	G	C8-N9-C1'	-6.26	118.86	127.00
46	B	1364	U	C2-N1-C1'	6.25	125.20	117.70
46	B	1624	C	O4'-C1'-N1	-6.25	103.20	108.20
1	AS	1562	G	C8-N9-C4	-6.25	103.90	106.40
46	CM	825	U	C5-C6-N1	-6.24	119.58	122.70
1	1	1217	A	C2-N3-C4	-6.24	107.48	110.60
1	AS	2215	C	N3-C2-O2	-6.21	117.55	121.90
46	B	821	U	C6-N1-C2	-6.21	117.28	121.00
62	R	80	LEU	CA-CB-CG	6.20	129.56	115.30
46	CM	1742	A	O4'-C1'-N9	6.20	113.16	108.20
1	AS	1349	U	N1-C2-O2	6.19	127.13	122.80
1	1	245	G	C4-C5-N7	6.17	113.27	110.80
1	1	1026	A	O4'-C1'-N9	-6.17	103.27	108.20
1	1	3182	C	N1-C2-O2	6.15	122.59	118.90
1	1	483	U	O4'-C1'-N1	6.14	113.11	108.20
1	AS	522	C	P-O3'-C3'	-6.13	112.34	119.70
46	CM	505	U	P-O3'-C3'	6.13	127.06	119.70
1	AS	2814	U	C6-N1-C1'	-6.13	112.62	121.20
46	CM	696	U	O5'-P-OP1	-6.12	100.19	105.70
46	B	671	G	O4'-C1'-N9	6.11	113.09	108.20
1	1	3088	G	O4'-C1'-N9	6.11	113.09	108.20
1	1	3160	C	C2-N1-C1'	6.10	125.51	118.80
46	CM	241	G	N3-C4-C5	6.10	131.65	128.60
1	1	2235	C	N1-C2-O2	6.09	122.56	118.90
1	1	1576	A	C6-C5-N7	-6.08	128.04	132.30
46	CM	1703	C	C5'-C4'-O4'	6.08	116.40	109.10
23	BP	37	LEU	CA-CB-CG	6.07	129.27	115.30
50	CQ	183	LEU	CA-CB-CG	6.07	129.27	115.30
1	AS	2482	U	N1-C2-O2	6.07	127.05	122.80
1	1	1446	G	N3-C2-N2	-6.06	115.66	119.90
46	B	485	G	N7-C8-N9	6.06	116.13	113.10
65	U	131	LEU	CA-CB-CG	6.05	129.23	115.30
46	CM	1444	G	N3-C4-N9	6.05	129.63	126.00
1	AS	486	C	C6-N1-C1'	-6.05	113.55	120.80
46	B	1242	U	C2-N1-C1'	6.04	124.95	117.70
46	CM	991	C	C2-N1-C1'	6.04	125.45	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CM	487	C	C6-N1-C2	-6.04	117.89	120.30
46	B	579	U	C2-N1-C1'	6.04	124.94	117.70
46	CM	222	C	C6-N1-C2	-6.02	117.89	120.30
46	CM	1234	U	C2-N1-C1'	6.02	124.93	117.70
1	1	2736	C	O4'-C1'-N1	6.02	113.02	108.20
46	B	991	C	C2-N1-C1'	6.02	125.42	118.80
46	CM	814	A	P-O3'-C3'	6.02	126.92	119.70
1	1	3128	G	O4'-C1'-N9	6.01	113.01	108.20
59	CZ	52	LEU	CA-CB-CG	6.00	129.11	115.30
1	AS	443	G	N3-C4-C5	-6.00	125.60	128.60
1	1	1018	U	O4'-C1'-N1	6.00	113.00	108.20
46	CM	139	U	O5'-P-OP1	-5.99	100.31	105.70
1	AS	478	G	O5'-P-OP2	5.99	117.89	110.70
46	B	1234	U	C2-N1-C1'	5.98	124.88	117.70
54	CU	70	GLN	CA-CB-CG	5.98	126.55	113.40
1	1	481	G	C8-N9-C1'	5.97	134.76	127.00
46	B	561	U	N3-C2-O2	-5.97	118.02	122.20
46	B	656	C	C6-N1-C2	-5.97	117.91	120.30
1	1	1943	G	OP1-P-O3'	5.96	118.32	105.20
23	BP	37	LEU	CB-CG-CD1	-5.96	100.86	111.00
46	CM	234	G	C6-C5-N7	-5.96	126.82	130.40
1	1	3271	U	C2-N1-C1'	5.96	124.85	117.70
1	AS	447	U	P-O3'-C3'	5.96	126.85	119.70
46	B	676	G	C5'-C4'-O4'	5.95	116.24	109.10
46	CM	822	G	C8-N9-C1'	5.95	134.74	127.00
46	B	1327	C	N1-C2-O2	5.94	122.47	118.90
59	O	96	LEU	CA-CB-CG	5.94	128.96	115.30
1	AS	1558	G	N3-C4-N9	5.94	129.56	126.00
46	CM	218	A	P-O3'-C3'	-5.94	112.58	119.70
46	B	671	G	N3-C4-N9	5.93	129.56	126.00
1	1	245	G	C4-N9-C1'	5.92	134.20	126.50
46	CM	698	C	C2-N1-C1'	5.90	125.29	118.80
1	AS	3243	C	N1-C2-O2	5.90	122.44	118.90
46	B	656	C	C5-C6-N1	5.90	123.95	121.00
1	AS	2485	U	C5-C6-N1	5.88	125.64	122.70
46	B	608	G	C4-N9-C1'	5.88	134.14	126.50
46	CM	985	C	C6-N1-C2	-5.87	117.95	120.30
1	1	2698	C	C2-N1-C1'	5.86	125.24	118.80
46	CM	226	G	N9-C4-C5	-5.85	103.06	105.40
20	z	150	LEU	CA-CB-CG	5.84	128.74	115.30
1	1	1638	A	O4'-C1'-N9	-5.84	103.53	108.20
46	B	1703	C	P-O3'-C3'	5.83	126.70	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AS	2814	U	N1-C2-O2	5.83	126.88	122.80
1	1	1573	C	C2-N1-C1'	5.83	125.21	118.80
46	B	814	A	P-O3'-C3'	5.83	126.70	119.70
1	1	526	G	C8-N9-C4	5.82	108.73	106.40
1	AS	1576	A	C8-N9-C4	-5.82	103.47	105.80
46	CM	1444	G	C4-N9-C1'	5.82	134.07	126.50
1	AS	1346	U	P-O3'-C3'	5.82	126.68	119.70
1	AS	2745	C	C6-N1-C2	-5.81	117.97	120.30
46	CM	1703	C	O4'-C1'-N1	5.80	112.84	108.20
46	CM	1742	A	C8-N9-C4	-5.79	103.48	105.80
1	1	2441	G	OP1-P-O3'	5.79	117.93	105.20
1	AS	2509	C	N1-C2-O2	5.79	122.37	118.90
46	B	1290	U	N3-C2-O2	-5.78	118.15	122.20
1	AS	2235	C	C6-N1-C2	-5.78	117.99	120.30
1	AS	2419	A	O4'-C1'-N9	5.78	112.82	108.20
3	AU	39	G	O4'-C1'-N9	5.77	112.81	108.20
1	1	401	U	C6-N1-C1'	-5.76	113.14	121.20
1	1	481	G	C4-N9-C1'	-5.75	119.02	126.50
46	B	651	C	O4'-C1'-N1	-5.75	103.60	108.20
79	DT	249	LEU	CA-CB-CG	5.75	128.52	115.30
5	AX	140	ASP	CB-CG-OD2	5.74	123.46	118.30
1	AS	480	G	N3-C4-C5	-5.73	125.73	128.60
1	AS	1721	C	O4'-C1'-N1	5.73	112.78	108.20
46	CM	579	U	C2-N1-C1'	5.73	124.58	117.70
46	B	675	U	C6-N1-C2	-5.73	117.56	121.00
46	CM	70	C	P-O3'-C3'	-5.73	112.83	119.70
46	B	1444	G	C4-N9-C1'	5.73	133.94	126.50
46	B	1375	C	N3-C2-O2	-5.72	117.89	121.90
1	1	1853	C	C6-N1-C2	-5.72	118.01	120.30
46	CM	218	A	O4'-C1'-N9	-5.72	103.63	108.20
46	CM	1457	A	C8-N9-C4	-5.71	103.51	105.80
35	CB	111	LYS	CD-CE-NZ	-5.71	98.57	111.70
46	CM	222	C	C2-N3-C4	5.71	122.75	119.90
79	DT	19	TRP	CA-CB-CG	5.71	124.54	113.70
1	1	1033	C	C2-N1-C1'	5.70	125.07	118.80
46	B	1672	G	O4'-C1'-N9	5.70	112.76	108.20
76	f	39	CYS	CB-CA-C	-5.70	99.00	110.40
20	BM	177	LEU	CA-CB-CG	5.70	128.40	115.30
1	1	1224	C	C2-N1-C1'	5.69	125.06	118.80
46	CM	1231	C	C2-N1-C1'	5.69	125.06	118.80
46	CM	1375	C	C6-N1-C1'	-5.69	113.97	120.80
23	BP	87	LEU	CA-CB-CG	5.69	128.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	1462	C	C2-N1-C1'	5.68	125.05	118.80
1	1	1273	C	N1-C2-O2	5.68	122.31	118.90
1	AS	2482	U	N3-C2-O2	-5.68	118.22	122.20
1	AS	2968	U	C2-N1-C1'	5.68	124.51	117.70
46	CM	499	U	P-O3'-C3'	-5.67	112.90	119.70
1	1	2515	G	P-O3'-C3'	5.66	126.50	119.70
1	AS	440	U	P-O3'-C3'	-5.66	112.91	119.70
46	B	505	U	O4'-C1'-N1	5.65	112.72	108.20
46	B	1444	G	C6-C5-N7	-5.65	127.01	130.40
46	CM	648	U	OP1-P-OP2	5.65	128.07	119.60
46	CM	233	G	N9-C4-C5	-5.64	103.14	105.40
46	B	824	U	P-O5'-C5'	-5.63	111.89	120.90
46	CM	846	U	C2-N1-C1'	5.63	124.46	117.70
46	CM	825	U	P-O3'-C3'	5.63	126.45	119.70
1	1	1525	A	C8-N9-C1'	-5.63	117.57	127.70
1	1	2474	C	N1-C2-O2	5.63	122.28	118.90
1	1	2474	C	N3-C2-O2	-5.62	117.97	121.90
1	1	2698	C	O4'-C1'-N1	5.61	112.68	108.20
46	B	4	C	N1-C2-O2	5.61	122.26	118.90
1	1	599	U	P-O5'-C5'	5.60	129.86	120.90
1	1	3102	A	O4'-C1'-N9	5.59	112.67	108.20
1	AS	478	G	C8-N9-C4	-5.59	104.16	106.40
46	B	919	C	N1-C2-O2	5.59	122.25	118.90
46	B	451	C	C6-N1-C1'	-5.58	114.11	120.80
46	CM	218	A	N7-C8-N9	5.56	116.58	113.80
1	AS	3134	C	C2-N1-C1'	5.56	124.92	118.80
43	CJ	43	TYR	CA-CB-CG	5.55	123.95	113.40
1	AS	976	A	C8-N9-C4	-5.55	103.58	105.80
46	B	1547	U	N3-C2-O2	-5.55	118.32	122.20
1	1	1217	A	O4'-C1'-N9	-5.54	103.77	108.20
46	CM	505	U	O4'-C1'-N1	5.54	112.63	108.20
46	CM	1375	C	N1-C2-O2	5.54	122.22	118.90
46	B	1444	G	N3-C4-C5	-5.54	125.83	128.60
50	CQ	60	LEU	CA-CB-CG	5.53	128.02	115.30
1	1	3164	U	OP1-P-O3'	5.53	117.36	105.20
46	CM	451	C	C6-N1-C1'	-5.53	114.17	120.80
48	CO	115	ARG	CA-CB-CG	-5.53	101.24	113.40
1	1	112	C	C2-N1-C1'	5.52	124.88	118.80
1	1	2396	G	C4-N9-C1'	5.52	133.68	126.50
1	1	956	U	C2-N1-C1'	5.51	124.31	117.70
45	i	38	LYS	CG-CD-CE	5.51	128.43	111.90
46	B	1237	C	C2-N1-C1'	5.51	124.86	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AS	1738	U	C5-C6-N1	5.50	125.45	122.70
46	B	218	A	O4'-C1'-N9	5.50	112.60	108.20
1	AS	451	C	C6-N1-C1'	-5.50	114.20	120.80
1	1	2373	G	N3-C2-N2	-5.49	116.06	119.90
1	AS	539	G	N9-C4-C5	-5.49	103.21	105.40
1	1	1569	C	C2-N1-C1'	5.48	124.83	118.80
1	AS	1568	U	O4'-C1'-N1	5.48	112.58	108.20
79	DT	105	VAL	CG1-CB-CG2	5.48	119.67	110.90
1	AS	1562	G	N7-C8-N9	5.48	115.84	113.10
1	1	3030	U	C2-N1-C1'	5.48	124.27	117.70
51	G	56	LEU	CA-CB-CG	5.47	127.89	115.30
1	AS	3165	U	C5'-C4'-O4'	-5.47	102.53	109.10
48	CO	70	LEU	CA-CB-CG	5.47	127.87	115.30
59	CZ	101	ALA	C-N-CA	-5.46	110.82	122.30
46	B	218	A	C8-N9-C4	-5.46	103.62	105.80
1	AS	2235	C	C2-N1-C1'	5.46	124.81	118.80
78	h	159	LEU	CA-CB-CG	5.45	127.83	115.30
1	AS	451	C	N1-C2-O2	5.45	122.17	118.90
46	B	1703	C	N3-C2-O2	-5.44	118.09	121.90
52	CS	174	LEU	CA-CB-CG	5.44	127.82	115.30
48	CO	43	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	AS	2484	U	C6-N1-C1'	-5.43	113.59	121.20
46	CM	500	U	O4'-C1'-N1	5.43	112.54	108.20
46	CM	4	C	N1-C2-O2	5.43	122.16	118.90
50	CQ	216	ASP	CB-CG-OD1	5.43	123.19	118.30
1	1	1347	U	N1-C2-O2	5.43	126.60	122.80
1	1	2484	U	P-O3'-C3'	5.42	126.21	119.70
46	B	849	U	N3-C2-O2	-5.42	118.40	122.20
1	AS	437	G	N3-C4-N9	-5.42	122.75	126.00
1	1	1001	G	N3-C4-N9	-5.42	122.75	126.00
46	B	671	G	N3-C4-C5	-5.42	125.89	128.60
1	AS	161	G	N3-C4-N9	-5.42	122.75	126.00
46	B	1057	C	C2-N1-C1'	5.42	124.76	118.80
82	12	112	ILE	CG1-CB-CG2	-5.41	99.50	111.40
46	B	823	G	N9-C1'-C2'	5.41	121.03	114.00
46	CM	1742	A	C4-C5-N7	-5.41	108.00	110.70
1	1	2484	U	N1-C2-N3	5.39	118.13	114.90
1	1	406	G	O4'-C1'-N9	5.38	112.51	108.20
1	AS	956	U	C2-N1-C1'	5.38	124.16	117.70
1	AS	1001	G	N3-C4-N9	-5.38	122.77	126.00
46	CM	822	G	N3-C4-N9	-5.38	122.77	126.00
1	1	1197	C	N1-C2-O2	5.38	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CM	241	G	N3-C4-N9	-5.38	122.77	126.00
1	1	831	G	O4'-C1'-N9	5.38	112.50	108.20
1	1	242	C	N1-C2-O2	5.37	122.12	118.90
1	1	1347	U	N3-C2-O2	-5.37	118.44	122.20
46	B	505	U	P-O3'-C3'	5.37	126.14	119.70
1	AS	2519	A	P-O3'-C3'	5.36	126.13	119.70
1	AS	1197	C	O4'-C1'-N1	5.35	112.48	108.20
1	AS	1552	C	C2-N1-C1'	5.35	124.68	118.80
1	1	2215	C	N1-C2-O2	5.34	122.11	118.90
45	i	38	LYS	CA-CB-CG	5.34	125.16	113.40
59	CZ	137	LEU	CA-CB-CG	5.34	127.59	115.30
46	CM	1067	C	C2-N1-C1'	5.34	124.68	118.80
1	AS	441	U	O5'-C5'-C4'	5.34	121.84	111.70
79	DT	201	LEU	CB-CG-CD2	5.34	120.08	111.00
3	4	39	G	O4'-C1'-N9	5.34	112.47	108.20
76	f	24	CYS	CA-CB-SG	5.34	123.61	114.00
1	AS	1678	U	N1-C2-O2	-5.34	119.06	122.80
1	1	601	U	P-O3'-C3'	-5.33	113.30	119.70
76	f	21	CYS	CA-CB-SG	5.33	123.60	114.00
1	AS	3159	A	P-O3'-C3'	5.33	126.10	119.70
46	B	1242	U	N1-C2-O2	5.33	126.53	122.80
64	T	73	LEU	CA-CB-CG	5.33	127.56	115.30
1	AS	443	G	N3-C4-N9	5.33	129.20	126.00
46	CM	500	U	C5'-C4'-O4'	5.33	115.49	109.10
1	AS	1558	G	C4-N9-C1'	5.32	133.42	126.50
46	CM	1444	G	C8-N9-C1'	-5.32	120.09	127.00
5	AX	142	LYS	CA-CB-CG	5.32	125.10	113.40
46	CM	81	G	C4-C5-N7	5.31	112.93	110.80
46	CM	825	U	O4'-C1'-N1	5.31	112.45	108.20
46	CM	1742	A	C6-C5-N7	5.31	136.02	132.30
46	B	1457	A	C8-N9-C4	-5.30	103.68	105.80
46	CM	1292	U	C2-N1-C1'	5.30	124.06	117.70
46	B	485	G	C4-C5-N7	5.30	112.92	110.80
1	AS	2215	C	C6-N1-C2	-5.30	118.18	120.30
66	V	114	LEU	CA-CB-CG	5.29	127.48	115.30
46	CM	1369	G	P-O3'-C3'	5.29	126.05	119.70
1	AS	3271	U	C2-N1-C1'	5.29	124.05	117.70
1	1	912	G	P-O3'-C3'	5.28	126.03	119.70
1	AS	1567	U	O4'-C1'-N1	-5.28	103.98	108.20
46	CM	696	U	C5-C6-N1	5.27	125.34	122.70
1	1	1197	C	C2-N1-C1'	5.27	124.60	118.80
1	1	2441	G	P-O3'-C3'	5.27	126.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	CM	81	G	N1-C6-O6	5.27	123.06	119.90
46	CM	823	G	C4-N9-C1'	5.27	133.35	126.50
1	1	1388	G	O4'-C1'-N9	5.26	112.41	108.20
46	B	675	U	O4'-C1'-N1	5.26	112.41	108.20
1	1	2235	C	N3-C2-O2	-5.26	118.22	121.90
46	B	1457	A	C8-N9-C1'	-5.26	118.23	127.70
1	AS	1197	C	C2-N1-C1'	5.26	124.59	118.80
46	B	137	A	P-O3'-C3'	5.26	126.01	119.70
1	AS	1558	G	C8-N9-C1'	-5.26	120.17	127.00
1	AS	3182	C	C6-N1-C1'	-5.25	114.50	120.80
46	CM	816	U	N3-C4-O4	-5.25	115.72	119.40
1	1	2957	C	C6-N1-C2	-5.24	118.20	120.30
46	CM	824	U	O4'-C1'-N1	-5.24	104.01	108.20
1	AS	1026	A	C4-N9-C1'	5.24	135.72	126.30
46	CM	656	C	N1-C2-O2	5.24	122.04	118.90
46	B	671	G	C4-N9-C1'	5.23	133.30	126.50
46	CM	1442	C	C2-N1-C1'	5.23	124.55	118.80
1	AS	1099	A	OP2-P-O3'	5.23	116.70	105.20
46	CM	1067	C	N1-C2-O2	5.23	122.04	118.90
1	AS	3160	C	OP1-P-O3'	5.22	116.69	105.20
46	CM	1704	C	O4'-C1'-N1	5.22	112.38	108.20
1	1	2666	A	P-O3'-C3'	5.22	125.96	119.70
46	B	75	U	C2-N1-C1'	5.22	123.96	117.70
1	AS	112	C	C2-N1-C1'	5.22	124.54	118.80
46	CM	821	U	C2-N1-C1'	5.21	123.96	117.70
1	AS	1228	C	C2-N1-C1'	5.21	124.53	118.80
1	AS	3164	U	O4'-C1'-N1	-5.21	104.03	108.20
46	B	1242	U	N3-C2-O2	-5.21	118.56	122.20
1	AS	3030	U	C2-N1-C1'	5.21	123.95	117.70
46	B	1231	C	C2-N1-C1'	5.20	124.52	118.80
46	CM	739	A	P-O3'-C3'	5.20	125.94	119.70
46	B	1364	U	O4'-C1'-N1	5.19	112.36	108.20
46	CM	1327	C	N1-C2-O2	5.19	122.02	118.90
1	AS	1563	A	O4'-C1'-N9	5.19	112.35	108.20
46	CM	137	A	P-O3'-C3'	5.19	125.92	119.70
46	B	482	C	O4'-C1'-N1	5.18	112.35	108.20
1	AS	3243	C	N3-C2-O2	-5.18	118.27	121.90
46	B	485	G	N1-C6-O6	5.18	123.01	119.90
46	B	1082	U	O4'-C1'-N1	5.18	112.34	108.20
1	AS	1349	U	N3-C2-O2	-5.18	118.57	122.20
1	AS	3327	A	O4'-C1'-N9	5.18	112.34	108.20
1	1	977	U	C6-N1-C1'	-5.18	113.95	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	478	G	N3-C4-N9	-5.18	122.89	126.00
1	AS	1720	U	O4'-C1'-N1	5.18	112.34	108.20
46	CM	500	U	P-O3'-C3'	-5.17	113.49	119.70
1	1	1573	C	C6-N1-C1'	-5.17	114.60	120.80
1	1	3347	U	C2-N1-C1'	5.16	123.89	117.70
46	CM	4	C	C2-N1-C1'	5.16	124.48	118.80
46	B	1446	A	O4'-C1'-N9	5.16	112.33	108.20
46	CM	1468	C	C5-C6-N1	5.15	123.58	121.00
1	1	376	G	O4'-C1'-N9	5.15	112.32	108.20
1	1	1228	C	C2-N1-C1'	5.15	124.46	118.80
1	1	1363	G	C4-N9-C1'	5.15	133.19	126.50
46	B	656	C	N3-C2-O2	-5.15	118.30	121.90
46	B	216	A	OP1-P-O3'	5.14	116.51	105.20
1	1	35	C	N3-C2-O2	-5.14	118.30	121.90
46	CM	561	U	N3-C2-O2	-5.14	118.61	122.20
46	B	1546	G	O4'-C1'-N9	5.13	112.30	108.20
46	CM	919	C	N1-C2-O2	5.13	121.98	118.90
1	1	2968	U	C2-N1-C1'	5.12	123.85	117.70
1	AS	1349	U	C6-N1-C1'	-5.12	114.03	121.20
1	1	918	U	N1-C2-O2	5.12	126.38	122.80
1	1	1099	A	OP2-P-O3'	5.12	116.46	105.20
1	AS	1576	A	C5-N7-C8	-5.12	101.34	103.90
20	z	66	LEU	CA-CB-CG	5.12	127.07	115.30
20	z	157	GLU	CA-CB-CG	5.12	124.65	113.40
1	AS	406	G	O4'-C1'-N9	5.11	112.29	108.20
1	AS	1492	C	C6-N1-C1'	-5.11	114.67	120.80
46	B	4	C	C2-N1-C1'	5.11	124.42	118.80
1	AS	1885	G	C4-N9-C1'	5.11	133.14	126.50
23	BP	56	ILE	CA-CB-CG1	-5.11	101.30	111.00
1	AS	1226	G	O4'-C1'-N9	5.10	112.28	108.20
1	1	3030	U	N3-C2-O2	-5.10	118.63	122.20
46	B	579	U	N1-C2-O2	5.10	126.37	122.80
1	1	1552	C	C2-N1-C1'	5.09	124.40	118.80
46	CM	1237	C	N3-C2-O2	-5.09	118.33	121.90
1	1	3327	A	O4'-C1'-N9	5.09	112.27	108.20
59	CZ	62	LEU	CA-CB-CG	5.09	127.01	115.30
46	CM	480	U	N3-C2-O2	-5.09	118.64	122.20
1	1	35	C	N1-C2-O2	5.08	121.95	118.90
46	B	500	U	C5'-C4'-O4'	5.08	115.20	109.10
46	CM	1364	U	C2-N1-C1'	5.08	123.80	117.70
1	1	1018	U	O5'-P-OP1	-5.08	101.13	105.70
1	AS	2090	U	P-O3'-C3'	5.08	125.79	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BC	62	GLN	CB-CG-CD	5.08	124.80	111.60
54	CU	40	LYS	CA-CB-CG	5.08	124.57	113.40
1	AS	2589	U	N3-C2-O2	-5.07	118.65	122.20
1	AS	3151	C	C2-N1-C1'	5.07	124.38	118.80
25	BR	109	LEU	CB-CG-CD2	5.07	119.63	111.00
1	1	3167	G	N3-C4-N9	5.07	129.04	126.00
1	1	2814	U	C5-C6-N1	5.07	125.23	122.70
46	B	985	C	C6-N1-C2	-5.07	118.27	120.30
1	AS	912	G	P-O3'-C3'	5.07	125.78	119.70
46	CM	1444	G	C6-C5-N7	-5.07	127.36	130.40
1	1	1228	C	C6-N1-C1'	-5.07	114.72	120.80
46	CM	240	U	P-O3'-C3'	-5.06	113.63	119.70
46	B	1283	U	O3'-P-O5'	5.05	113.60	104.00
1	AS	977	U	C6-N1-C1'	-5.05	114.12	121.20
1	1	2455	G	C3'-C2'-C1'	5.05	105.54	101.50
1	AS	1562	G	C8-N9-C1'	-5.05	120.44	127.00
3	AU	21	C	O4'-C1'-N1	5.05	112.24	108.20
46	B	879	U	N1-C2-O2	5.05	126.33	122.80
1	AS	1576	A	C4-C5-C6	5.05	119.52	117.00
46	CM	234	G	N1-C6-O6	5.05	122.93	119.90
46	CM	681	C	C6-N1-C2	-5.05	118.28	120.30
1	AS	2484	U	N3-C4-O4	5.04	122.93	119.40
46	CM	1231	C	O4'-C1'-N1	5.04	112.23	108.20
46	CM	739	A	O4'-C1'-N9	5.04	112.23	108.20
1	1	2697	U	O4'-C1'-N1	5.04	112.23	108.20
46	B	1360	C	C2-N1-C1'	5.04	124.34	118.80
1	AS	115	A	O4'-C1'-N9	5.03	112.23	108.20
1	AS	2484	U	C5-C4-O4	-5.03	122.88	125.90
46	B	676	G	C2-N3-C4	5.03	114.42	111.90
1	AS	1099	A	P-O3'-C3'	5.03	125.73	119.70
46	CM	493	U	C2-N1-C1'	5.03	123.73	117.70
1	1	2509	C	N1-C2-O2	5.02	121.91	118.90
28	BU	57	MET	C-N-CA	-5.02	109.16	121.70
1	AS	1026	A	C8-N9-C1'	-5.01	118.68	127.70
1	AS	3317	U	P-O3'-C3'	5.01	125.71	119.70
46	B	1067	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AW	247/254 (97%)	240 (97%)	7 (3%)	0	100	100
4	j	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
5	k	384/389 (99%)	374 (97%)	9 (2%)	1 (0%)	37	68
6	AY	357/363 (98%)	349 (98%)	8 (2%)	0	100	100
6	l	357/363 (98%)	346 (97%)	10 (3%)	1 (0%)	37	68
7	AZ	290/298 (97%)	280 (97%)	10 (3%)	0	100	100
7	m	292/298 (98%)	281 (96%)	11 (4%)	0	100	100
8	BA	149/176 (85%)	147 (99%)	2 (1%)	0	100	100
8	n	153/176 (87%)	150 (98%)	3 (2%)	0	100	100
9	BB	224/241 (93%)	218 (97%)	5 (2%)	1 (0%)	30	64
9	o	227/241 (94%)	220 (97%)	7 (3%)	0	100	100
10	BC	231/262 (88%)	210 (91%)	16 (7%)	5 (2%)	5	31
10	p	234/262 (89%)	225 (96%)	8 (3%)	1 (0%)	30	64
11	BD	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
11	q	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
12	r	203/219 (93%)	201 (99%)	2 (1%)	0	100	100
13	BF	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	179 (90%)	12 (6%)	7 (4%)	3	24
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BH	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
15	u	126/131 (96%)	123 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	170/185 (92%)	166 (98%)	4 (2%)	0	100	100
18	x	165/185 (89%)	160 (97%)	5 (3%)	0	100	100
19	BL	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
19	y	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
20	BM	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
20	z	177/190 (93%)	172 (97%)	5 (3%)	0	100	100
21	0	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
21	BN	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
22	2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
22	BO	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	5	98/124 (79%)	90 (92%)	6 (6%)	2 (2%)	6	33
23	BP	97/124 (78%)	75 (77%)	16 (16%)	6 (6%)	1	12
24	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	114/155 (74%)	89 (78%)	25 (22%)	0	100	100
25	BR	105/155 (68%)	90 (86%)	14 (13%)	1 (1%)	13	46
26	8	118/142 (83%)	117 (99%)	1 (1%)	0	100	100
26	BS	117/142 (82%)	111 (95%)	5 (4%)	1 (1%)	14	49
27	9	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
27	BT	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	116 (87%)	15 (11%)	2 (2%)	8	39
29	AB	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	56/63 (89%)	52 (93%)	1 (2%)	3 (5%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BW	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
31	AD	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	BX	92/106 (87%)	90 (98%)	2 (2%)	0	100	100
32	AE	106/112 (95%)	104 (98%)	2 (2%)	0	100	100
32	BY	106/112 (95%)	103 (97%)	2 (2%)	1 (1%)	14	49
33	AF	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
33	BZ	120/131 (92%)	120 (100%)	0	0	100	100
34	AG	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
34	CA	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	108/122 (88%)	105 (97%)	3 (3%)	0	100	100
36	AI	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
36	CC	115/120 (96%)	111 (96%)	3 (3%)	1 (1%)	14	49
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	93/99 (94%)	85 (91%)	8 (9%)	0	100	100
38	AK	84/90 (93%)	80 (95%)	4 (5%)	0	100	100
38	CE	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	2	20
40	AM	48/51 (94%)	48 (100%)	0	0	100	100
40	CG	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	AN	48/52 (92%)	48 (100%)	0	0	100	100
41	CH	48/52 (92%)	46 (96%)	1 (2%)	1 (2%)	5	32
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	CI	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
43	CJ	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	CK	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	CL	116/267 (43%)	72 (62%)	34 (29%)	10 (9%)	0	7
45	i	104/267 (39%)	51 (49%)	35 (34%)	18 (17%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	C	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
47	CN	206/261 (79%)	199 (97%)	7 (3%)	0	100	100
48	CO	211/256 (82%)	191 (90%)	14 (7%)	6 (3%)	4	27
48	D	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
49	CP	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
49	E	215/249 (86%)	208 (97%)	7 (3%)	0	100	100
50	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
50	F	221/251 (88%)	214 (97%)	7 (3%)	0	100	100
51	CR	258/262 (98%)	255 (99%)	3 (1%)	0	100	100
51	G	256/262 (98%)	252 (98%)	4 (2%)	0	100	100
52	CS	203/225 (90%)	180 (89%)	20 (10%)	3 (2%)	8	39
52	H	204/225 (91%)	193 (95%)	11 (5%)	0	100	100
53	CT	234/236 (99%)	228 (97%)	6 (3%)	0	100	100
53	I	221/236 (94%)	217 (98%)	4 (2%)	0	100	100
54	CU	177/186 (95%)	150 (85%)	21 (12%)	6 (3%)	3	24
54	J	180/186 (97%)	171 (95%)	9 (5%)	0	100	100
55	CV	201/206 (98%)	199 (99%)	2 (1%)	0	100	100
55	K	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
56	CW	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
56	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	CX	92/118 (78%)	86 (94%)	6 (6%)	0	100	100
57	M	96/118 (81%)	82 (85%)	12 (12%)	2 (2%)	5	32
58	CY	139/155 (90%)	133 (96%)	6 (4%)	0	100	100
58	N	142/155 (92%)	136 (96%)	6 (4%)	0	100	100
59	CZ	117/143 (82%)	75 (64%)	36 (31%)	6 (5%)	1	16
59	O	114/143 (80%)	88 (77%)	24 (21%)	2 (2%)	7	35
60	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	P	146/151 (97%)	144 (99%)	2 (1%)	0	100	100
61	DB	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
61	Q	125/132 (95%)	121 (97%)	3 (2%)	1 (1%)	16	51
62	DC	128/142 (90%)	97 (76%)	27 (21%)	4 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	R	129/142 (91%)	110 (85%)	17 (13%)	2 (2%)	8	38
63	DD	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
63	S	137/142 (96%)	130 (95%)	7 (5%)	0	100	100
64	DE	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
64	T	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
65	DF	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
65	U	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
66	DG	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
66	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
67	DH	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
67	W	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
68	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
69	DJ	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
69	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	DK	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
70	Z	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
71	DL	130/135 (96%)	130 (100%)	0	0	100	100
71	a	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
72	DM	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
72	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	DN	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
73	c	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
74	DO	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
74	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	DP	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
75	e	58/67 (87%)	55 (95%)	3 (5%)	0	100	100
76	DQ	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
76	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
77	DR	57/63 (90%)	50 (88%)	6 (10%)	1 (2%)	7	35
77	g	58/63 (92%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	DS	64/193 (33%)	31 (48%)	23 (36%)	10 (16%)	0	2
78	h	68/193 (35%)	56 (82%)	11 (16%)	1 (2%)	8	39
79	AR	309/317 (98%)	291 (94%)	17 (6%)	1 (0%)	37	68
79	DT	303/317 (96%)	221 (73%)	65 (22%)	17 (6%)	1	14
80	BE	201/220 (91%)	197 (98%)	4 (2%)	0	100	100
81	P0	105/312 (34%)	69 (66%)	27 (26%)	9 (9%)	0	7
82	12	61/165 (37%)	36 (59%)	22 (36%)	3 (5%)	2	16
All	All	22176/24752 (90%)	21009 (95%)	1028 (5%)	139 (1%)	22	56

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	267	SER
10	p	205	ASN
45	i	36	SER
45	i	37	LYS
45	i	44	ALA
45	i	50	LYS
45	i	52	LYS
45	i	66	ASN
45	i	72	ASP
45	i	76	PRO
45	i	112	LYS
59	O	130	SER
61	Q	119	ASP
14	BG	17	HIS
14	BG	48	PRO
14	BG	127	ASP
14	BG	154	PRO
23	BP	61	ASP
28	BU	128	LYS
39	CF	72	THR
41	CH	4	PRO
45	CL	41	ALA
45	CL	43	PRO
45	CL	48	PRO
45	CL	160	LEU
48	CO	43	VAL
48	CO	59	ASP
48	CO	212	ILE

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Mol	Chain	Res	Type
52	CS	101	GLY
52	CS	206	SER
54	CU	83	ASP
54	CU	128	PRO
59	CZ	69	GLU
59	CZ	70	SER
59	CZ	117	GLY
62	DC	18	LYS
62	DC	129	GLY
78	DS	162	GLU
78	DS	167	THR
78	DS	174	MET
79	DT	5	GLU
79	DT	162	GLN
79	DT	265	ARG
79	DT	277	VAL
81	P0	72	GLU
82	12	160	ILE
30	AC	58	ARG
45	i	57	PRO
45	i	81	THR
57	M	88	PRO
10	BC	183	GLY
10	BC	226	LYS
23	BP	64	VAL
28	BU	127	ASN
39	CF	71	PRO
45	CL	55	LYS
45	CL	64	LEU
54	CU	100	ARG
54	CU	159	ASP
59	CZ	81	GLU
59	CZ	82	PRO
59	CZ	121	VAL
62	DC	7	PRO
77	DR	33	ARG
78	DS	158	ARG
78	DS	182	TYR
79	DT	21	THR
79	DT	102	GLN
79	DT	157	ILE
79	DT	163	SER

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Mol	Chain	Res	Type
79	DT	247	TYR
81	P0	3	GLY
81	P0	75	LYS
81	P0	77	LEU
81	P0	101	VAL
45	i	51	ALA
45	i	114	GLU
62	R	7	PRO
10	BC	100	PRO
23	BP	25	ASN
26	BS	117	ASN
52	CS	153	GLY
79	DT	31	ASP
79	DT	241	ALA
79	DT	263	GLN
81	P0	100	VAL
23	5	20	ALA
9	BB	230	GLU
10	BC	127	SER
14	BG	166	GLN
23	BP	24	GLU
32	BY	83	ASP
39	CF	21	LYS
45	CL	46	ALA
45	CL	56	SER
45	CL	62	ALA
48	CO	29	TRP
48	CO	80	SER
79	DT	160	SER
79	DT	296	GLN
81	P0	107	ALA
23	5	11	SER
45	i	47	ASP
57	M	92	LEU
59	O	104	CYS
14	BG	164	PRO
23	BP	13	LYS
25	BR	97	LYS
48	CO	51	SER
54	CU	51	LYS
62	DC	16	SER
78	DS	142	LEU

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Mol	Chain	Res	Type
78	DS	143	ALA
78	DS	164	PRO
78	DS	179	ASP
79	DT	262	LEU
82	12	105	PRO
82	12	106	LEU
5	k	139	THR
30	AC	3	LYS
45	i	61	GLU
45	i	65	LYS
45	i	69	PHE
78	h	141	LYS
79	AR	203	PRO
10	BC	128	PRO
14	BG	49	ARG
45	CL	88	PHE
54	CU	82	PRO
79	DT	74	ILE
79	DT	95	LEU
45	i	73	VAL
23	BP	68	VAL
36	CC	39	PRO
81	P0	28	VAL
30	AC	21	ILE
62	R	2	VAL
81	P0	25	ILE
78	DS	129	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AW	190/194 (98%)	190 (100%)	0	100	100
4	j	190/194 (98%)	190 (100%)	0	100	100
5	AX	325/328 (99%)	324 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	k	325/328 (99%)	324 (100%)	1 (0%)	91	96
6	AY	288/292 (99%)	285 (99%)	3 (1%)	73	84
6	l	288/292 (99%)	286 (99%)	2 (1%)	81	89
7	AZ	247/252 (98%)	244 (99%)	3 (1%)	67	82
7	m	248/252 (98%)	246 (99%)	2 (1%)	79	88
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	135 (99%)	1 (1%)	81	89
9	BB	190/204 (93%)	189 (100%)	1 (0%)	86	93
9	o	193/204 (95%)	191 (99%)	2 (1%)	73	84
10	BC	193/216 (89%)	190 (98%)	3 (2%)	58	76
10	p	196/216 (91%)	195 (100%)	1 (0%)	86	93
11	BD	169/170 (99%)	169 (100%)	0	100	100
11	q	169/170 (99%)	169 (100%)	0	100	100
12	r	177/185 (96%)	176 (99%)	1 (1%)	84	91
13	BF	146/149 (98%)	144 (99%)	2 (1%)	62	79
13	s	146/149 (98%)	144 (99%)	2 (1%)	62	79
14	BG	166/168 (99%)	164 (99%)	2 (1%)	67	82
14	t	166/168 (99%)	165 (99%)	1 (1%)	84	91
15	BH	108/109 (99%)	108 (100%)	0	100	100
15	u	107/109 (98%)	106 (99%)	1 (1%)	75	86
16	BI	177/178 (99%)	177 (100%)	0	100	100
16	v	177/178 (99%)	176 (99%)	1 (1%)	84	91
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	165 (99%)	1 (1%)	84	91
18	BK	145/154 (94%)	143 (99%)	2 (1%)	62	79
18	x	140/154 (91%)	139 (99%)	1 (1%)	81	89
19	BL	153/154 (99%)	152 (99%)	1 (1%)	81	89
19	y	153/154 (99%)	153 (100%)	0	100	100
20	BM	146/153 (95%)	142 (97%)	4 (3%)	40	65
20	z	146/153 (95%)	144 (99%)	2 (1%)	62	79
21	0	155/157 (99%)	153 (99%)	2 (1%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	BN	155/157 (99%)	154 (99%)	1 (1%)	84	91
22	2	133/134 (99%)	133 (100%)	0	100	100
22	BO	133/134 (99%)	132 (99%)	1 (1%)	79	88
23	5	91/112 (81%)	89 (98%)	2 (2%)	47	70
23	BP	90/112 (80%)	87 (97%)	3 (3%)	33	61
24	6	101/104 (97%)	100 (99%)	1 (1%)	73	84
24	BQ	101/104 (97%)	100 (99%)	1 (1%)	73	84
25	7	97/127 (76%)	94 (97%)	3 (3%)	35	63
25	BR	91/127 (72%)	90 (99%)	1 (1%)	70	83
26	8	107/121 (88%)	106 (99%)	1 (1%)	75	86
26	BS	107/121 (88%)	106 (99%)	1 (1%)	75	86
27	9	111/112 (99%)	109 (98%)	2 (2%)	54	74
27	BT	111/112 (99%)	109 (98%)	2 (2%)	54	74
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	115 (98%)	2 (2%)	56	75
29	AB	120/121 (99%)	119 (99%)	1 (1%)	79	88
29	BV	120/121 (99%)	119 (99%)	1 (1%)	79	88
30	AC	45/49 (92%)	45 (100%)	0	100	100
30	BW	47/49 (96%)	47 (100%)	0	100	100
31	AD	83/90 (92%)	81 (98%)	2 (2%)	44	68
31	BX	79/90 (88%)	78 (99%)	1 (1%)	65	81
32	AE	97/100 (97%)	96 (99%)	1 (1%)	73	84
32	BY	97/100 (97%)	97 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	109/115 (95%)	109 (100%)	0	100	100
34	AG	91/92 (99%)	90 (99%)	1 (1%)	70	83
34	CA	91/92 (99%)	90 (99%)	1 (1%)	70	83
35	AH	95/102 (93%)	93 (98%)	2 (2%)	48	71
35	CB	93/102 (91%)	92 (99%)	1 (1%)	70	83
36	AI	104/106 (98%)	104 (100%)	0	100	100
36	CC	105/106 (99%)	102 (97%)	3 (3%)	37	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AJ	77/79 (98%)	76 (99%)	1 (1%)	65	81
37	CD	75/79 (95%)	73 (97%)	2 (3%)	40	65
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	68/69 (99%)	66 (97%)	2 (3%)	37	64
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	46/47 (98%)	46 (100%)	0	100	100
41	AN	45/47 (96%)	45 (100%)	0	100	100
41	CH	45/47 (96%)	45 (100%)	0	100	100
42	AO	24/24 (100%)	23 (96%)	1 (4%)	25	54
42	CI	23/24 (96%)	23 (100%)	0	100	100
43	AP	88/91 (97%)	87 (99%)	1 (1%)	70	83
43	CJ	88/91 (97%)	87 (99%)	1 (1%)	70	83
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	72 (100%)	0	100	100
45	CL	99/212 (47%)	97 (98%)	2 (2%)	50	72
45	i	86/212 (41%)	79 (92%)	7 (8%)	9	33
47	C	176/215 (82%)	174 (99%)	2 (1%)	70	83
47	CN	176/215 (82%)	173 (98%)	3 (2%)	56	75
48	CO	193/229 (84%)	187 (97%)	6 (3%)	35	63
48	D	194/229 (85%)	194 (100%)	0	100	100
49	CP	175/198 (88%)	174 (99%)	1 (1%)	84	91
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	169 (97%)	5 (3%)	37	64
50	F	174/196 (89%)	172 (99%)	2 (1%)	70	83
51	CR	218/220 (99%)	217 (100%)	1 (0%)	86	93
51	G	217/220 (99%)	217 (100%)	0	100	100
52	CS	177/197 (90%)	170 (96%)	7 (4%)	27	56
52	H	178/197 (90%)	178 (100%)	0	100	100
53	CT	204/204 (100%)	202 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	I	193/204 (95%)	192 (100%)	1 (0%)	86	93
54	CU	161/167 (96%)	158 (98%)	3 (2%)	52	73
54	J	163/167 (98%)	162 (99%)	1 (1%)	84	91
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	156 (99%)	1 (1%)	84	91
56	CW	153/160 (96%)	153 (100%)	0	100	100
56	L	153/160 (96%)	153 (100%)	0	100	100
57	CX	88/104 (85%)	88 (100%)	0	100	100
57	M	90/104 (86%)	90 (100%)	0	100	100
58	CY	122/134 (91%)	120 (98%)	2 (2%)	58	76
58	N	124/134 (92%)	121 (98%)	3 (2%)	44	68
59	CZ	101/123 (82%)	97 (96%)	4 (4%)	27	56
59	O	98/123 (80%)	90 (92%)	8 (8%)	9	33
60	DA	129/130 (99%)	128 (99%)	1 (1%)	79	88
60	P	128/130 (98%)	128 (100%)	0	100	100
61	DB	93/102 (91%)	93 (100%)	0	100	100
61	Q	97/102 (95%)	96 (99%)	1 (1%)	73	84
62	DC	112/121 (93%)	108 (96%)	4 (4%)	30	59
62	R	112/121 (93%)	110 (98%)	2 (2%)	54	74
63	DD	113/116 (97%)	111 (98%)	2 (2%)	54	74
63	S	113/116 (97%)	111 (98%)	2 (2%)	54	74
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	112/122 (92%)	110 (98%)	2 (2%)	54	74
65	DF	125/129 (97%)	121 (97%)	4 (3%)	34	62
65	U	128/129 (99%)	125 (98%)	3 (2%)	45	69
66	DG	113/117 (97%)	113 (100%)	0	100	100
66	V	113/117 (97%)	113 (100%)	0	100	100
67	DH	87/105 (83%)	85 (98%)	2 (2%)	45	69
67	W	92/105 (88%)	89 (97%)	3 (3%)	33	61
68	DI	71/71 (100%)	71 (100%)	0	100	100
68	X	71/71 (100%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	DJ	112/113 (99%)	111 (99%)	1 (1%)	75	86
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	115 (99%)	1 (1%)	75	86
70	Z	116/118 (98%)	115 (99%)	1 (1%)	75	86
71	DL	109/112 (97%)	109 (100%)	0	100	100
71	a	111/112 (99%)	111 (100%)	0	100	100
72	DM	63/85 (74%)	63 (100%)	0	100	100
72	b	64/85 (75%)	64 (100%)	0	100	100
73	DN	84/102 (82%)	83 (99%)	1 (1%)	67	82
73	c	83/102 (81%)	81 (98%)	2 (2%)	44	68
74	DO	72/73 (99%)	72 (100%)	0	100	100
74	d	72/73 (99%)	72 (100%)	0	100	100
75	DP	53/58 (91%)	53 (100%)	0	100	100
75	e	52/58 (90%)	51 (98%)	1 (2%)	52	73
76	DQ	47/48 (98%)	44 (94%)	3 (6%)	14	41
76	f	47/48 (98%)	43 (92%)	4 (8%)	8	32
77	DR	51/54 (94%)	49 (96%)	2 (4%)	27	56
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	60/175 (34%)	57 (95%)	3 (5%)	20	49
78	h	62/175 (35%)	60 (97%)	2 (3%)	34	62
79	AR	259/263 (98%)	258 (100%)	1 (0%)	89	95
79	DT	255/263 (97%)	242 (95%)	13 (5%)	20	48
80	BE	175/186 (94%)	174 (99%)	1 (1%)	84	91
81	P0	92/247 (37%)	89 (97%)	3 (3%)	33	61
82	12	53/137 (39%)	48 (91%)	5 (9%)	7	29
All	All	19011/20831 (91%)	18794 (99%)	217 (1%)	70	83

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	k	386	ASP
6	l	99	ARG
6	l	121	TYR

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Mol	Chain	Res	Type
7	m	7	PHE
7	m	45	ASN
8	n	140	SER
9	o	13	LYS
9	o	14	GLU
10	p	27	LEU
12	r	92	HIS
13	s	13	ARG
13	s	68	HIS
14	t	4	SER
15	u	121	ARG
16	v	178	HIS
17	w	83	LYS
18	x	180	LYS
20	z	162	ARG
20	z	165	ARG
21	0	26	ARG
21	0	113	ARG
23	5	13	LYS
23	5	103	GLN
24	6	86	ARG
25	7	56	ARG
25	7	117	LYS
25	7	124	LYS
26	8	138	ARG
27	9	3	LYS
27	9	5	SER
29	AB	25	HIS
31	AD	10	GLU
31	AD	11	ASN
32	AE	16	HIS
34	AG	92	LYS
35	AH	67	LYS
35	AH	81	CYS
37	AJ	98	ARG
42	AO	2	ARG
43	AP	45	ARG
45	i	89	ASP
45	i	90	ARG
45	i	101	LYS
45	i	109	GLN
45	i	115	LEU

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Mol	Chain	Res	Type
45	i	135	GLU
45	i	137	ASP
47	C	18	LEU
47	C	179	ARG
50	F	77	ARG
50	F	167	ASP
53	I	25	ARG
54	J	30	LEU
55	K	125	LYS
58	N	29	LYS
58	N	46	LYS
58	N	67	ARG
59	O	33	ARG
59	O	36	LEU
59	O	38	HIS
59	O	39	ASP
59	O	41	LEU
59	O	109	ASP
59	O	129	ASP
59	O	137	LEU
61	Q	31	LYS
62	R	28	MET
62	R	130	ARG
63	S	38	VAL
63	S	39	GLN
64	T	48	ASN
64	T	80	ARG
65	U	87	ASN
65	U	115	ARG
65	U	138	THR
67	W	51	LYS
67	W	88	ARG
67	W	100	LYS
70	Z	107	PHE
73	c	5	ARG
73	c	89	ARG
75	e	18	ARG
76	f	24	CYS
76	f	36	LEU
76	f	38	LEU
76	f	39	CYS
78	h	168	CYS

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Mol	Chain	Res	Type
78	h	177	MET
79	AR	121	ARG
5	AX	5	LYS
6	AY	59	HIS
6	AY	99	ARG
6	AY	195	LEU
7	AZ	81	HIS
7	AZ	136	GLU
7	AZ	244	HIS
9	BB	198	ASN
10	BC	182	LYS
10	BC	217	SER
10	BC	224	ILE
80	BE	203	LYS
13	BF	13	ARG
13	BF	168	ASP
14	BG	48	PRO
14	BG	194	GLU
18	BK	118	GLN
18	BK	180	LYS
19	BL	113	ARG
20	BM	130	ASN
20	BM	167	ARG
20	BM	170	ARG
20	BM	174	GLN
21	BN	52	LYS
22	BO	83	ARG
23	BP	62	ASN
23	BP	78	TYR
23	BP	107	LYS
24	BQ	80	ARG
25	BR	123	ARG
26	BS	47	GLN
27	BT	3	LYS
27	BT	64	LYS
28	BU	74	LEU
28	BU	136	PHE
29	BV	25	HIS
31	BX	96	ASP
34	CA	106	ASN
35	CB	64	GLN
36	CC	38	ARG

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Mol	Chain	Res	Type
36	CC	40	SER
36	CC	59	ASN
37	CD	11	ASN
37	CD	40	ARG
39	CF	3	ARG
39	CF	37	LYS
43	CJ	18	ARG
45	CL	47	ASP
45	CL	99	SER
47	CN	79	ARG
47	CN	205	ARG
47	CN	206	ASP
48	CO	30	PHE
48	CO	85	LYS
48	CO	128	LYS
48	CO	130	SER
48	CO	131	ASP
48	CO	186	SER
49	CP	74	ASP
50	CQ	77	ARG
50	CQ	107	LYS
50	CQ	155	ASP
50	CQ	179	ARG
50	CQ	198	PHE
51	CR	10	LYS
52	CS	23	VAL
52	CS	54	LYS
52	CS	72	HIS
52	CS	86	GLN
52	CS	104	ASN
52	CS	180	ARG
52	CS	183	SER
53	CT	93	LYS
53	CT	155	ASP
54	CU	13	LEU
54	CU	15	LEU
54	CU	39	PHE
58	CY	46	LYS
58	CY	67	ARG
59	CZ	60	CYS
59	CZ	93	ASP
59	CZ	129	ASP

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Mol	Chain	Res	Type
59	CZ	137	LEU
60	DA	80	LEU
62	DC	10	ARG
62	DC	46	SER
62	DC	51	SER
62	DC	130	ARG
63	DD	33	SER
63	DD	65	ARG
65	DF	25	ARG
65	DF	36	ARG
65	DF	41	ARG
65	DF	138	THR
67	DH	51	LYS
67	DH	100	LYS
69	DJ	37	PHE
70	DK	13	ARG
73	DN	74	CYS
76	DQ	8	PHE
76	DQ	42	CYS
76	DQ	54	LYS
77	DR	29	LYS
77	DR	31	GLN
78	DS	141	LYS
78	DS	149	LYS
78	DS	163	CYS
79	DT	20	VAL
79	DT	22	SER
79	DT	65	HIS
79	DT	66	SER
79	DT	75	SER
79	DT	92	LEU
79	DT	93	TRP
79	DT	102	GLN
79	DT	160	SER
79	DT	161	ASP
79	DT	275	PHE
79	DT	294	ASP
79	DT	311	GLN
81	P0	13	SER
81	P0	46	ARG
81	P0	103	ASN
82	12	103	ASN

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Mol	Chain	Res	Type
82	12	104	ILE
82	12	106	LEU
82	12	114	ARG
82	12	146	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
5	k	184	ASN
23	5	30	GLN
31	AD	11	ASN
40	AM	33	ASN
45	i	109	GLN
47	C	30	GLN
47	C	33	ASN
47	C	49	ASN
52	H	37	GLN
52	H	63	GLN
62	R	79	HIS
63	S	39	GLN
79	AR	16	HIS
79	AR	53	ASN
6	AY	46	ASN
6	AY	111	ASN
9	BB	218	GLN
10	BC	39	GLN
10	BC	62	GLN
10	BC	139	HIS
10	BC	156	ASN
10	BC	244	ASN
11	BD	129	HIS
11	BD	140	GLN
13	BF	47	GLN
13	BF	109	HIS
20	BM	134	HIS
20	BM	175	GLN
22	BO	95	HIS
22	BO	112	ASN
23	BP	71	ASN
26	BS	47	GLN
34	CA	106	ASN
37	CD	11	ASN

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Mol	Chain	Res	Type
37	CD	34	GLN
37	CD	79	HIS
45	CL	83	HIS
48	CO	99	ASN
48	CO	220	GLN
50	CQ	33	GLN
52	CS	103	ASN
52	CS	104	ASN
52	CS	169	ASN
53	CT	200	GLN
54	CU	19	GLN
57	CX	58	GLN
59	CZ	134	ASN
63	DD	138	GLN
67	DH	43	ASN
69	DJ	92	ASN
72	DM	38	HIS
77	DR	31	GLN
79	DT	16	HIS
79	DT	29	HIS
79	DT	107	HIS
81	P0	10	GLN
82	12	103	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3215/3359 (95%)	607 (18%)	45 (1%)
1	AS	3093/3359 (92%)	528 (17%)	39 (1%)
2	3	120/121 (99%)	9 (7%)	0
2	AT	120/121 (99%)	9 (7%)	0
3	4	155/158 (98%)	22 (14%)	2 (1%)
3	AU	157/158 (99%)	23 (14%)	3 (1%)
46	B	1702/1787 (95%)	405 (23%)	45 (2%)
46	CM	1722/1787 (96%)	430 (24%)	48 (2%)
All	All	10284/10850 (94%)	2033 (19%)	182 (1%)

All (2033) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	15	A

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Mol	Chain	Res	Type
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A
1	1	42	A
1	1	48	A
1	1	56	A
1	1	58	G
1	1	59	A
1	1	64	A
1	1	65	A
1	1	91	G
1	1	98	A
1	1	104	C
1	1	108	A
1	1	109	G
1	1	110	C
1	1	121	A
1	1	134	U
1	1	135	G
1	1	155	A
1	1	156	A
1	1	164	U
1	1	169	G
1	1	172	C
1	1	173	C
1	1	175	G
1	1	186	A
1	1	189	U
1	1	190	U
1	1	199	C
1	1	205	G
1	1	209	C
1	1	212	A
1	1	217	G
1	1	218	A
1	1	219	G
1	1	230	G
1	1	236	A
1	1	239	A
1	1	240	C
1	1	243	G

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Mol	Chain	Res	Type
1	1	245	G
1	1	249	G
1	1	250	U
1	1	269	G
1	1	286	U
1	1	295	A
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	337	G
1	1	338	A
1	1	339	C
1	1	349	A
1	1	350	C
1	1	376	G
1	1	377	A
1	1	387	A
1	1	395	A
1	1	398	A
1	1	402	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	448	U
1	1	450	G
1	1	451	C
1	1	481	G
1	1	482	U
1	1	506	A
1	1	517	A
1	1	519	U
1	1	531	G
1	1	532	U
1	1	538	G
1	1	539	G
1	1	540	C
1	1	541	U

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Mol	Chain	Res	Type
1	1	542	U
1	1	543	C
1	1	544	U
1	1	545	G
1	1	546	C
1	1	555	A
1	1	556	U
1	1	557	A
1	1	564	G
1	1	577	G
1	1	589	G
1	1	590	A
1	1	598	U
1	1	600	U
1	1	601	U
1	1	602	A
1	1	609	A
1	1	618	U
1	1	619	A
1	1	620	A
1	1	635	C
1	1	647	A
1	1	658	A
1	1	675	A
1	1	679	U
1	1	681	U
1	1	688	A
1	1	689	A
1	1	703	A
1	1	710	G
1	1	713	A
1	1	717	A
1	1	723	G
1	1	730	A
1	1	732	U
1	1	760	U
1	1	763	U
1	1	772	U
1	1	773	U
1	1	776	A
1	1	777	G
1	1	780	A

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Mol	Chain	Res	Type
1	1	781	G
1	1	802	A
1	1	812	A
1	1	813	A
1	1	826	A
1	1	845	C
1	1	857	C
1	1	861	U
1	1	870	U
1	1	875	U
1	1	903	G
1	1	904	G
1	1	910	A
1	1	912	G
1	1	913	A
1	1	917	A
1	1	919	C
1	1	921	A
1	1	933	G
1	1	940	C
1	1	949	G
1	1	955	C
1	1	956	U
1	1	958	A
1	1	959	G
1	1	977	U
1	1	990	G
1	1	991	U
1	1	996	C
1	1	997	G
1	1	998	A
1	1	1006	G
1	1	1011	C
1	1	1012	U
1	1	1013	U
1	1	1014	G
1	1	1018	U
1	1	1019	U
1	1	1020	G
1	1	1021	A
1	1	1023	A
1	1	1024	U

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Mol	Chain	Res	Type
1	1	1027	C
1	1	1030	U
1	1	1033	C
1	1	1043	A
1	1	1045	C
1	1	1060	A
1	1	1061	A
1	1	1068	G
1	1	1077	U
1	1	1078	U
1	1	1089	A
1	1	1090	A
1	1	1091	U
1	1	1092	U
1	1	1094	A
1	1	1099	A
1	1	1100	G
1	1	1113	G
1	1	1127	G
1	1	1140	U
1	1	1149	A
1	1	1150	A
1	1	1151	C
1	1	1155	A
1	1	1156	C
1	1	1164	U
1	1	1174	G
1	1	1176	A
1	1	1177	U
1	1	1178	G
1	1	1188	C
1	1	1189	A
1	1	1192	C
1	1	1197	C
1	1	1204	U
1	1	1205	G
1	1	1218	G
1	1	1223	C
1	1	1224	C
1	1	1229	G
1	1	1230	G
1	1	1231	U

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Mol	Chain	Res	Type
1	1	1232	G
1	1	1239	G
1	1	1240	A
1	1	1241	A
1	1	1242	G
1	1	1243	U
1	1	1244	C
1	1	1245	G
1	1	1246	G
1	1	1247	A
1	1	1249	U
1	1	1250	C
1	1	1252	G
1	1	1254	U
1	1	1255	A
1	1	1257	G
1	1	1258	G
1	1	1259	A
1	1	1262	G
1	1	1263	U
1	1	1264	G
1	1	1265	U
1	1	1266	A
1	1	1269	A
1	1	1270	A
1	1	1271	C
1	1	1273	C
1	1	1274	A
1	1	1278	G
1	1	1303	G
1	1	1304	A
1	1	1305	U
1	1	1309	G
1	1	1312	C
1	1	1326	A
1	1	1345	G
1	1	1346	U
1	1	1347	U
1	1	1348	U
1	1	1349	U
1	1	1382	A
1	1	1395	U

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Mol	Chain	Res	Type
1	1	1415	A
1	1	1417	G
1	1	1421	U
1	1	1427	G
1	1	1430	G
1	1	1433	C
1	1	1442	A
1	1	1446	G
1	1	1465	C
1	1	1471	A
1	1	1477	A
1	1	1484	G
1	1	1498	C
1	1	1504	C
1	1	1520	A
1	1	1523	C
1	1	1525	A
1	1	1526	U
1	1	1532	G
1	1	1535	A
1	1	1552	C
1	1	1556	G
1	1	1558	G
1	1	1559	C
1	1	1560	U
1	1	1561	U
1	1	1562	G
1	1	1563	A
1	1	1565	U
1	1	1566	U
1	1	1567	U
1	1	1568	U
1	1	1569	C
1	1	1571	G
1	1	1572	G
1	1	1574	C
1	1	1576	A
1	1	1577	C
1	1	1585	A
1	1	1589	A
1	1	1601	A
1	1	1603	U

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Mol	Chain	Res	Type
1	1	1624	C
1	1	1625	U
1	1	1635	C
1	1	1638	A
1	1	1639	A
1	1	1641	U
1	1	1648	G
1	1	1653	C
1	1	1654	G
1	1	1679	A
1	1	1720	U
1	1	1721	C
1	1	1732	G
1	1	1746	A
1	1	1747	G
1	1	1755	U
1	1	1756	A
1	1	1757	A
1	1	1758	U
1	1	1759	U
1	1	1760	U
1	1	1761	U
1	1	1762	G
1	1	1763	C
1	1	1776	G
1	1	1793	A
1	1	1804	G
1	1	1809	A
1	1	1810	A
1	1	1811	U
1	1	1812	A
1	1	1814	U
1	1	1815	U
1	1	1816	U
1	1	1817	U
1	1	1837	A
1	1	1838	A
1	1	1842	C
1	1	1845	C
1	1	1862	C
1	1	1874	G
1	1	1882	A

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Mol	Chain	Res	Type
1	1	1889	A
1	1	1902	G
1	1	1944	G
1	1	1949	G
1	1	2068	U
1	1	2069	U
1	1	2070	A
1	1	2071	A
1	1	2078	A
1	1	2088	G
1	1	2089	G
1	1	2091	A
1	1	2092	C
1	1	2099	G
1	1	2100	G
1	1	2109	A
1	1	2118	U
1	1	2122	A
1	1	2136	A
1	1	2147	G
1	1	2149	G
1	1	2183	U
1	1	2184	G
1	1	2185	A
1	1	2186	A
1	1	2187	U
1	1	2188	G
1	1	2222	A
1	1	2227	G
1	1	2233	A
1	1	2234	A
1	1	2235	C
1	1	2250	G
1	1	2251	G
1	1	2259	A
1	1	2260	U
1	1	2276	U
1	1	2285	G
1	1	2286	C
1	1	2288	U
1	1	2291	A
1	1	2292	U

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Mol	Chain	Res	Type
1	1	2293	G
1	1	2313	G
1	1	2314	U
1	1	2341	A
1	1	2351	A
1	1	2352	C
1	1	2353	G
1	1	2363	G
1	1	2366	U
1	1	2371	G
1	1	2372	G
1	1	2375	A
1	1	2380	A
1	1	2381	G
1	1	2382	A
1	1	2389	U
1	1	2396	G
1	1	2397	A
1	1	2413	G
1	1	2415	G
1	1	2420	G
1	1	2421	A
1	1	2422	C
1	1	2426	G
1	1	2427	A
1	1	2430	G
1	1	2431	U
1	1	2432	G
1	1	2433	U
1	1	2437	A
1	1	2438	U
1	1	2439	A
1	1	2441	G
1	1	2442	U
1	1	2443	G
1	1	2444	G
1	1	2445	G
1	1	2446	A
1	1	2448	C
1	1	2449	U
1	1	2450	U
1	1	2451	C

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Mol	Chain	Res	Type
1	1	2452	G
1	1	2453	G
1	1	2454	C
1	1	2455	G
1	1	2456	C
1	1	2457	C
1	1	2459	G
1	1	2460	U
1	1	2464	A
1	1	2465	U
1	1	2466	A
1	1	2467	C
1	1	2468	C
1	1	2470	C
1	1	2471	U
1	1	2472	A
1	1	2473	C
1	1	2475	U
1	1	2476	C
1	1	2477	U
1	1	2480	A
1	1	2482	U
1	1	2483	U
1	1	2484	U
1	1	2485	U
1	1	2489	A
1	1	2492	U
1	1	2493	A
1	1	2511	G
1	1	2513	A
1	1	2515	G
1	1	2516	U
1	1	2517	C
1	1	2518	A
1	1	2519	A
1	1	2520	A
1	1	2521	C
1	1	2529	U
1	1	2530	C
1	1	2533	G
1	1	2536	U
1	1	2538	A

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Mol	Chain	Res	Type
1	1	2545	C
1	1	2546	U
1	1	2554	C
1	1	2557	G
1	1	2565	A
1	1	2566	C
1	1	2578	G
1	1	2579	G
1	1	2586	G
1	1	2598	A
1	1	2623	G
1	1	2624	U
1	1	2628	A
1	1	2644	G
1	1	2646	A
1	1	2649	G
1	1	2661	A
1	1	2662	G
1	1	2663	A
1	1	2664	A
1	1	2666	A
1	1	2668	A
1	1	2676	A
1	1	2677	A
1	1	2686	G
1	1	2691	U
1	1	2699	A
1	1	2700	G
1	1	2701	U
1	1	2724	U
1	1	2725	G
1	1	2734	A
1	1	2745	C
1	1	2749	G
1	1	2750	G
1	1	2768	G
1	1	2771	A
1	1	2772	G
1	1	2773	A
1	1	2774	A
1	1	2782	C
1	1	2786	G

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Mol	Chain	Res	Type
1	1	2789	A
1	1	2790	U
1	1	2814	U
1	1	2815	U
1	1	2817	A
1	1	2833	U
1	1	2839	C
1	1	2843	G
1	1	2844	A
1	1	2847	U
1	1	2859	A
1	1	2861	C
1	1	2866	C
1	1	2870	G
1	1	2871	C
1	1	2886	G
1	1	2895	U
1	1	2900	C
1	1	2907	U
1	1	2908	A
1	1	2911	G
1	1	2914	C
1	1	2919	G
1	1	2920	C
1	1	2923	G
1	1	2926	U
1	1	2943	A
1	1	2955	C
1	1	2960	C
1	1	2962	G
1	1	2969	G
1	1	2984	A
1	1	3021	A
1	1	3028	U
1	1	3031	G
1	1	3050	A
1	1	3051	C
1	1	3052	G
1	1	3058	A
1	1	3064	C
1	1	3073	G
1	1	3094	A

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Mol	Chain	Res	Type
1	1	3101	A
1	1	3102	A
1	1	3103	U
1	1	3114	A
1	1	3115	C
1	1	3125	U
1	1	3127	U
1	1	3143	G
1	1	3144	A
1	1	3146	G
1	1	3149	U
1	1	3151	C
1	1	3157	A
1	1	3160	C
1	1	3161	U
1	1	3162	U
1	1	3163	U
1	1	3164	U
1	1	3165	U
1	1	3166	A
1	1	3171	C
1	1	3172	U
1	1	3182	C
1	1	3183	A
1	1	3184	G
1	1	3194	G
1	1	3208	A
1	1	3210	A
1	1	3212	G
1	1	3214	U
1	1	3221	G
1	1	3224	U
1	1	3228	G
1	1	3235	A
1	1	3241	G
1	1	3246	C
1	1	3252	C
1	1	3259	A
1	1	3260	A
1	1	3268	G
1	1	3269	C
1	1	3272	A

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Mol	Chain	Res	Type
1	1	3278	U
1	1	3281	A
1	1	3284	U
1	1	3285	A
1	1	3306	U
1	1	3307	A
1	1	3309	A
1	1	3310	G
1	1	3316	U
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	U
1	1	3321	G
1	1	3334	G
1	1	3343	C
1	1	3351	G
1	1	3361	U
2	3	7	G
2	3	22	A
2	3	54	U
2	3	55	A
2	3	65	G
2	3	73	C
2	3	76	A
2	3	102	A
2	3	112	G
3	4	23	U
3	4	34	U
3	4	35	C
3	4	59	A
3	4	62	C
3	4	63	G
3	4	81	A
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	92	A
3	4	95	G
3	4	102	U
3	4	104	A

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Mol	Chain	Res	Type
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	148	G
3	4	152	G
46	B	17	C
46	B	25	C
46	B	26	A
46	B	27	U
46	B	34	G
46	B	47	A
46	B	57	G
46	B	66	U
46	B	74	U
46	B	75	U
46	B	76	A
46	B	78	A
46	B	79	C
46	B	81	G
46	B	84	A
46	B	93	A
46	B	104	A
46	B	114	C
46	B	115	G
46	B	123	G
46	B	126	A
46	B	127	G
46	B	128	U
46	B	138	C
46	B	139	U
46	B	142	G
46	B	143	A
46	B	150	U
46	B	151	G
46	B	152	G
46	B	154	A
46	B	159	U
46	B	166	A
46	B	168	U
46	B	173	G

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Mol	Chain	Res	Type
46	B	174	C
46	B	176	U
46	B	177	A
46	B	179	A
46	B	190	U
46	B	191	U
46	B	193	G
46	B	199	G
46	B	200	A
46	B	202	G
46	B	206	U
46	B	211	A
46	B	213	A
46	B	214	U
46	B	215	A
46	B	216	A
46	B	217	A
46	B	218	A
46	B	224	A
46	B	226	G
46	B	229	U
46	B	230	U
46	B	231	C
46	B	236	U
46	B	237	C
46	B	247	U
46	B	255	A
46	B	259	U
46	B	260	U
46	B	261	C
46	B	262	G
46	B	266	C
46	B	269	A
46	B	270	U
46	B	274	C
46	B	276	U
46	B	277	G
46	B	278	U
46	B	279	G
46	B	283	G
46	B	285	G
46	B	297	A

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Mol	Chain	Res	Type
46	B	312	C
46	B	314	A
46	B	318	U
46	B	319	C
46	B	320	G
46	B	335	G
46	B	336	C
46	B	350	A
46	B	357	A
46	B	358	A
46	B	359	C
46	B	388	G
46	B	398	A
46	B	400	C
46	B	402	G
46	B	414	A
46	B	416	G
46	B	421	G
46	B	422	C
46	B	423	A
46	B	424	G
46	B	432	G
46	B	437	U
46	B	442	C
46	B	446	C
46	B	452	A
46	B	458	A
46	B	466	A
46	B	475	A
46	B	480	U
46	B	483	A
46	B	485	G
46	B	487	C
46	B	490	U
46	B	491	U
46	B	493	U
46	B	499	U
46	B	503	A
46	B	505	U
46	B	506	U
46	B	509	A
46	B	512	G

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Mol	Chain	Res	Type
46	B	513	A
46	B	515	U
46	B	518	A
46	B	519	A
46	B	525	A
46	B	530	U
46	B	534	C
46	B	536	A
46	B	537	G
46	B	539	A
46	B	540	A
46	B	547	G
46	B	553	A
46	B	554	A
46	B	555	G
46	B	556	U
46	B	557	C
46	B	563	C
46	B	566	G
46	B	575	G
46	B	576	U
46	B	580	U
46	B	592	A
46	B	593	G
46	B	604	A
46	B	609	U
46	B	617	A
46	B	618	A
46	B	620	A
46	B	621	A
46	B	639	G
46	B	643	U
46	B	645	G
46	B	647	C
46	B	648	U
46	B	649	G
46	B	650	G
46	B	651	C
46	B	652	C
46	B	653	G
46	B	657	C
46	B	670	C

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Mol	Chain	Res	Type
46	B	671	G
46	B	672	U
46	B	673	A
46	B	674	C
46	B	675	U
46	B	677	G
46	B	678	A
46	B	679	C
46	B	680	C
46	B	681	C
46	B	682	A
46	B	688	G
46	B	695	C
46	B	729	U
46	B	739	A
46	B	740	A
46	B	741	A
46	B	750	G
46	B	751	U
46	B	756	A
46	B	759	A
46	B	760	G
46	B	762	C
46	B	764	U
46	B	765	U
46	B	766	U
46	B	767	G
46	B	768	C
46	B	770	C
46	B	771	G
46	B	773	A
46	B	775	A
46	B	778	U
46	B	779	U
46	B	796	A
46	B	798	A
46	B	799	G
46	B	802	C
46	B	803	G
46	B	804	U
46	B	805	U
46	B	807	U

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Mol	Chain	Res	Type
46	B	808	G
46	B	813	U
46	B	815	U
46	B	817	U
46	B	819	G
46	B	820	U
46	B	821	U
46	B	823	G
46	B	824	U
46	B	825	U
46	B	826	U
46	B	827	C
46	B	828	U
46	B	829	A
46	B	831	G
46	B	840	A
46	B	842	U
46	B	847	A
46	B	848	A
46	B	856	G
46	B	857	G
46	B	869	A
46	B	871	U
46	B	875	C
46	B	877	G
46	B	878	U
46	B	879	U
46	B	881	U
46	B	891	A
46	B	909	A
46	B	910	G
46	B	911	A
46	B	918	A
46	B	920	U
46	B	927	G
46	B	945	U
46	B	951	A
46	B	973	A
46	B	975	C
46	B	977	A
46	B	988	A
46	B	989	U

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Mol	Chain	Res	Type
46	B	990	A
46	B	997	U
46	B	998	A
46	B	1004	A
46	B	1005	A
46	B	1011	A
46	B	1013	C
46	B	1017	G
46	B	1024	A
46	B	1025	G
46	B	1039	U
46	B	1042	U
46	B	1043	U
46	B	1055	A
46	B	1056	U
46	B	1057	C
46	B	1058	G
46	B	1059	G
46	B	1060	C
46	B	1061	A
46	B	1067	C
46	B	1077	A
46	B	1081	C
46	B	1085	G
46	B	1123	A
46	B	1135	G
46	B	1143	C
46	B	1145	A
46	B	1152	G
46	B	1168	A
46	B	1169	A
46	B	1170	U
46	B	1179	A
46	B	1181	A
46	B	1184	G
46	B	1185	G
46	B	1186	G
46	B	1187	A
46	B	1193	A
46	B	1202	A
46	B	1203	G
46	B	1206	A

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Mol	Chain	Res	Type
46	B	1207	C
46	B	1212	A
46	B	1215	A
46	B	1219	A
46	B	1220	C
46	B	1221	A
46	B	1229	A
46	B	1230	G
46	B	1231	C
46	B	1236	U
46	B	1243	U
46	B	1250	G
46	B	1270	U
46	B	1299	U
46	B	1300	U
46	B	1301	G
46	B	1306	A
46	B	1325	U
46	B	1330	A
46	B	1336	G
46	B	1339	G
46	B	1342	A
46	B	1343	G
46	B	1345	A
46	B	1346	U
46	B	1348	U
46	B	1349	G
46	B	1352	G
46	B	1355	A
46	B	1356	U
46	B	1357	A
46	B	1359	U
46	B	1360	C
46	B	1364	U
46	B	1369	G
46	B	1370	A
46	B	1376	U
46	B	1380	G
46	B	1381	A
46	B	1382	U
46	B	1384	U
46	B	1385	C

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Mol	Chain	Res	Type
46	B	1392	A
46	B	1397	A
46	B	1398	G
46	B	1399	U
46	B	1400	U
46	B	1401	U
46	B	1410	A
46	B	1413	A
46	B	1414	G
46	B	1415	G
46	B	1422	A
46	B	1431	G
46	B	1433	C
46	B	1445	C
46	B	1446	A
46	B	1455	A
46	B	1457	A
46	B	1458	C
46	B	1461	A
46	B	1462	C
46	B	1463	G
46	B	1468	C
46	B	1476	A
46	B	1477	U
46	B	1480	G
46	B	1483	U
46	B	1485	G
46	B	1491	G
46	B	1502	A
46	B	1503	A
46	B	1508	G
46	B	1510	G
46	B	1511	A
46	B	1523	G
46	B	1524	C
46	B	1529	G
46	B	1530	A
46	B	1541	U
46	B	1544	U
46	B	1546	G
46	B	1560	A
46	B	1561	G

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Mol	Chain	Res	Type
46	B	1571	G
46	B	1574	A
46	B	1575	G
46	B	1577	G
46	B	1580	A
46	B	1582	U
46	B	1584	A
46	B	1588	G
46	B	1621	C
46	B	1644	U
46	B	1645	G
46	B	1665	C
46	B	1667	G
46	B	1670	U
46	B	1671	G
46	B	1672	G
46	B	1673	U
46	B	1702	A
46	B	1704	C
46	B	1737	A
46	B	1742	A
46	B	1743	A
46	B	1744	G
46	B	1747	G
46	B	1749	A
46	B	1753	A
46	B	1756	U
46	B	1767	G
46	B	1770	C
46	B	1779	G
46	B	1780	G
46	B	1781	A
46	B	1782	U
46	B	1783	C
1	AS	24	U
1	AS	25	A
1	AS	29	G
1	AS	39	A
1	AS	42	A
1	AS	48	A
1	AS	56	A
1	AS	58	G

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Mol	Chain	Res	Type
1	AS	59	A
1	AS	64	A
1	AS	65	A
1	AS	91	G
1	AS	98	A
1	AS	104	C
1	AS	108	A
1	AS	109	G
1	AS	110	C
1	AS	121	A
1	AS	134	U
1	AS	135	G
1	AS	155	A
1	AS	156	A
1	AS	164	U
1	AS	169	G
1	AS	172	C
1	AS	173	C
1	AS	175	G
1	AS	186	A
1	AS	189	U
1	AS	190	U
1	AS	199	C
1	AS	205	G
1	AS	209	C
1	AS	212	A
1	AS	217	G
1	AS	218	A
1	AS	219	G
1	AS	230	G
1	AS	236	A
1	AS	239	A
1	AS	240	C
1	AS	243	G
1	AS	245	G
1	AS	249	G
1	AS	250	U
1	AS	269	G
1	AS	286	U
1	AS	295	A
1	AS	305	U
1	AS	311	C

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Mol	Chain	Res	Type
1	AS	323	A
1	AS	329	U
1	AS	337	G
1	AS	338	A
1	AS	339	C
1	AS	343	U
1	AS	349	A
1	AS	350	C
1	AS	376	G
1	AS	377	A
1	AS	395	A
1	AS	398	A
1	AS	402	A
1	AS	403	C
1	AS	404	G
1	AS	420	G
1	AS	421	G
1	AS	422	A
1	AS	438	A
1	AS	439	C
1	AS	445	A
1	AS	447	U
1	AS	448	U
1	AS	449	U
1	AS	450	G
1	AS	451	C
1	AS	478	G
1	AS	479	C
1	AS	480	G
1	AS	481	G
1	AS	482	U
1	AS	483	U
1	AS	484	U
1	AS	486	C
1	AS	487	C
1	AS	488	G
1	AS	506	A
1	AS	517	A
1	AS	519	U
1	AS	531	G
1	AS	532	U
1	AS	538	G

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Mol	Chain	Res	Type
1	AS	539	G
1	AS	540	C
1	AS	541	U
1	AS	555	A
1	AS	556	U
1	AS	557	A
1	AS	564	G
1	AS	576	A
1	AS	577	G
1	AS	589	G
1	AS	590	A
1	AS	598	U
1	AS	600	U
1	AS	601	U
1	AS	602	A
1	AS	609	A
1	AS	618	U
1	AS	619	A
1	AS	620	A
1	AS	635	C
1	AS	647	A
1	AS	658	A
1	AS	675	A
1	AS	679	U
1	AS	688	A
1	AS	689	A
1	AS	703	A
1	AS	710	G
1	AS	713	A
1	AS	717	A
1	AS	723	G
1	AS	730	A
1	AS	732	U
1	AS	760	U
1	AS	763	U
1	AS	772	U
1	AS	773	U
1	AS	776	A
1	AS	777	G
1	AS	780	A
1	AS	781	G
1	AS	802	A

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Mol	Chain	Res	Type
1	AS	813	A
1	AS	826	A
1	AS	845	C
1	AS	857	C
1	AS	861	U
1	AS	870	U
1	AS	875	U
1	AS	892	A
1	AS	903	G
1	AS	904	G
1	AS	910	A
1	AS	912	G
1	AS	913	A
1	AS	917	A
1	AS	919	C
1	AS	921	A
1	AS	933	G
1	AS	940	C
1	AS	949	G
1	AS	955	C
1	AS	956	U
1	AS	959	G
1	AS	970	G
1	AS	976	A
1	AS	977	U
1	AS	990	G
1	AS	991	U
1	AS	996	C
1	AS	997	G
1	AS	998	A
1	AS	1006	G
1	AS	1011	C
1	AS	1012	U
1	AS	1014	G
1	AS	1019	U
1	AS	1020	G
1	AS	1026	A
1	AS	1027	C
1	AS	1030	U
1	AS	1033	C
1	AS	1043	A
1	AS	1045	C

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Mol	Chain	Res	Type
1	AS	1060	A
1	AS	1061	A
1	AS	1068	G
1	AS	1077	U
1	AS	1078	U
1	AS	1089	A
1	AS	1090	A
1	AS	1091	U
1	AS	1092	U
1	AS	1094	A
1	AS	1099	A
1	AS	1100	G
1	AS	1113	G
1	AS	1127	G
1	AS	1140	U
1	AS	1149	A
1	AS	1150	A
1	AS	1151	C
1	AS	1155	A
1	AS	1156	C
1	AS	1164	U
1	AS	1174	G
1	AS	1176	A
1	AS	1177	U
1	AS	1178	G
1	AS	1188	C
1	AS	1189	A
1	AS	1192	C
1	AS	1197	C
1	AS	1204	U
1	AS	1205	G
1	AS	1218	G
1	AS	1219	A
1	AS	1224	C
1	AS	1228	C
1	AS	1303	G
1	AS	1304	A
1	AS	1305	U
1	AS	1309	G
1	AS	1326	A
1	AS	1345	G
1	AS	1346	U

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Mol	Chain	Res	Type
1	AS	1347	U
1	AS	1348	U
1	AS	1382	A
1	AS	1395	U
1	AS	1415	A
1	AS	1417	G
1	AS	1421	U
1	AS	1427	G
1	AS	1430	G
1	AS	1433	C
1	AS	1442	A
1	AS	1446	G
1	AS	1465	C
1	AS	1471	A
1	AS	1477	A
1	AS	1484	G
1	AS	1498	C
1	AS	1504	C
1	AS	1520	A
1	AS	1523	C
1	AS	1532	G
1	AS	1535	A
1	AS	1552	C
1	AS	1556	G
1	AS	1558	G
1	AS	1559	C
1	AS	1560	U
1	AS	1561	U
1	AS	1562	G
1	AS	1563	A
1	AS	1564	U
1	AS	1568	U
1	AS	1569	C
1	AS	1571	G
1	AS	1572	G
1	AS	1574	C
1	AS	1576	A
1	AS	1577	C
1	AS	1585	A
1	AS	1589	A
1	AS	1601	A
1	AS	1603	U

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Mol	Chain	Res	Type
1	AS	1624	C
1	AS	1625	U
1	AS	1635	C
1	AS	1638	A
1	AS	1639	A
1	AS	1641	U
1	AS	1648	G
1	AS	1654	G
1	AS	1679	A
1	AS	1720	U
1	AS	1721	C
1	AS	1732	G
1	AS	1746	A
1	AS	1747	G
1	AS	1755	U
1	AS	1756	A
1	AS	1757	A
1	AS	1758	U
1	AS	1759	U
1	AS	1761	U
1	AS	1762	G
1	AS	1763	C
1	AS	1776	G
1	AS	1793	A
1	AS	1804	G
1	AS	1809	A
1	AS	1810	A
1	AS	1811	U
1	AS	1812	A
1	AS	1814	U
1	AS	1815	U
1	AS	1816	U
1	AS	1817	U
1	AS	1835	A
1	AS	1838	A
1	AS	1842	C
1	AS	1845	C
1	AS	1862	C
1	AS	1874	G
1	AS	1882	A
1	AS	1889	A
1	AS	1902	G

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Mol	Chain	Res	Type
1	AS	1944	G
1	AS	1949	G
1	AS	2071	A
1	AS	2078	A
1	AS	2088	G
1	AS	2089	G
1	AS	2091	A
1	AS	2092	C
1	AS	2099	G
1	AS	2100	G
1	AS	2109	A
1	AS	2118	U
1	AS	2122	A
1	AS	2136	A
1	AS	2147	G
1	AS	2149	G
1	AS	2183	U
1	AS	2184	G
1	AS	2185	A
1	AS	2186	A
1	AS	2187	U
1	AS	2188	G
1	AS	2201	A
1	AS	2222	A
1	AS	2227	G
1	AS	2233	A
1	AS	2234	A
1	AS	2250	G
1	AS	2251	G
1	AS	2257	A
1	AS	2259	A
1	AS	2260	U
1	AS	2276	U
1	AS	2285	G
1	AS	2286	C
1	AS	2288	U
1	AS	2291	A
1	AS	2292	U
1	AS	2293	G
1	AS	2312	U
1	AS	2313	G
1	AS	2314	U

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Mol	Chain	Res	Type
1	AS	2341	A
1	AS	2351	A
1	AS	2352	C
1	AS	2353	G
1	AS	2363	G
1	AS	2366	U
1	AS	2371	G
1	AS	2372	G
1	AS	2375	A
1	AS	2380	A
1	AS	2381	G
1	AS	2382	A
1	AS	2389	U
1	AS	2396	G
1	AS	2397	A
1	AS	2413	G
1	AS	2419	A
1	AS	2421	A
1	AS	2422	C
1	AS	2425	G
1	AS	2426	G
1	AS	2427	A
1	AS	2428	G
1	AS	2429	G
1	AS	2430	G
1	AS	2431	U
1	AS	2482	U
1	AS	2483	U
1	AS	2484	U
1	AS	2489	A
1	AS	2492	U
1	AS	2493	A
1	AS	2510	U
1	AS	2511	G
1	AS	2513	A
1	AS	2515	G
1	AS	2516	U
1	AS	2517	C
1	AS	2518	A
1	AS	2519	A
1	AS	2520	A
1	AS	2521	C

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Mol	Chain	Res	Type
1	AS	2529	U
1	AS	2530	C
1	AS	2533	G
1	AS	2536	U
1	AS	2538	A
1	AS	2545	C
1	AS	2546	U
1	AS	2554	C
1	AS	2557	G
1	AS	2565	A
1	AS	2566	C
1	AS	2578	G
1	AS	2579	G
1	AS	2586	G
1	AS	2598	A
1	AS	2623	G
1	AS	2624	U
1	AS	2628	A
1	AS	2646	A
1	AS	2649	G
1	AS	2661	A
1	AS	2662	G
1	AS	2663	A
1	AS	2666	A
1	AS	2668	A
1	AS	2676	A
1	AS	2677	A
1	AS	2686	G
1	AS	2699	A
1	AS	2700	G
1	AS	2701	U
1	AS	2724	U
1	AS	2725	G
1	AS	2734	A
1	AS	2745	C
1	AS	2749	G
1	AS	2750	G
1	AS	2768	G
1	AS	2771	A
1	AS	2772	G
1	AS	2773	A
1	AS	2774	A

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Mol	Chain	Res	Type
1	AS	2782	C
1	AS	2786	G
1	AS	2789	A
1	AS	2790	U
1	AS	2814	U
1	AS	2815	U
1	AS	2817	A
1	AS	2833	U
1	AS	2839	C
1	AS	2843	G
1	AS	2844	A
1	AS	2847	U
1	AS	2859	A
1	AS	2861	C
1	AS	2866	C
1	AS	2870	G
1	AS	2871	C
1	AS	2886	G
1	AS	2895	U
1	AS	2907	U
1	AS	2908	A
1	AS	2911	G
1	AS	2914	C
1	AS	2919	G
1	AS	2920	C
1	AS	2923	G
1	AS	2926	U
1	AS	2943	A
1	AS	2955	C
1	AS	2960	C
1	AS	2962	G
1	AS	2969	G
1	AS	2984	A
1	AS	3021	A
1	AS	3028	U
1	AS	3031	G
1	AS	3050	A
1	AS	3051	C
1	AS	3052	G
1	AS	3058	A
1	AS	3064	C
1	AS	3076	U

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Mol	Chain	Res	Type
1	AS	3094	A
1	AS	3101	A
1	AS	3102	A
1	AS	3103	U
1	AS	3114	A
1	AS	3115	C
1	AS	3134	C
1	AS	3143	G
1	AS	3144	A
1	AS	3146	G
1	AS	3149	U
1	AS	3151	C
1	AS	3157	A
1	AS	3160	C
1	AS	3161	U
1	AS	3163	U
1	AS	3164	U
1	AS	3166	A
1	AS	3167	G
1	AS	3171	C
1	AS	3172	U
1	AS	3182	C
1	AS	3183	A
1	AS	3184	G
1	AS	3194	G
1	AS	3208	A
1	AS	3210	A
1	AS	3212	G
1	AS	3214	U
1	AS	3224	U
1	AS	3228	G
1	AS	3235	A
1	AS	3241	G
1	AS	3246	C
1	AS	3252	C
1	AS	3259	A
1	AS	3260	A
1	AS	3268	G
1	AS	3269	C
1	AS	3272	A
1	AS	3278	U
1	AS	3281	A

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Mol	Chain	Res	Type
1	AS	3284	U
1	AS	3285	A
1	AS	3306	U
1	AS	3307	A
1	AS	3309	A
1	AS	3310	G
1	AS	3316	U
1	AS	3317	U
1	AS	3318	G
1	AS	3319	U
1	AS	3320	U
1	AS	3321	G
1	AS	3334	G
1	AS	3343	C
1	AS	3351	G
1	AS	3361	U
2	AT	7	G
2	AT	22	A
2	AT	54	U
2	AT	55	A
2	AT	65	G
2	AT	73	C
2	AT	76	A
2	AT	102	A
2	AT	112	G
3	AU	23	U
3	AU	34	U
3	AU	35	C
3	AU	59	A
3	AU	62	C
3	AU	63	G
3	AU	81	A
3	AU	84	C
3	AU	85	G
3	AU	86	U
3	AU	87	G
3	AU	92	A
3	AU	95	G
3	AU	102	U
3	AU	104	A
3	AU	105	A
3	AU	106	C

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Mol	Chain	Res	Type
3	AU	111	A
3	AU	113	U
3	AU	125	U
3	AU	126	A
3	AU	152	G
3	AU	157	U
46	CM	17	C
46	CM	25	C
46	CM	26	A
46	CM	27	U
46	CM	34	G
46	CM	47	A
46	CM	57	G
46	CM	66	U
46	CM	72	A
46	CM	73	U
46	CM	74	U
46	CM	75	U
46	CM	76	A
46	CM	78	A
46	CM	79	C
46	CM	81	G
46	CM	84	A
46	CM	104	A
46	CM	114	C
46	CM	115	G
46	CM	123	G
46	CM	126	A
46	CM	127	G
46	CM	128	U
46	CM	138	C
46	CM	139	U
46	CM	142	G
46	CM	143	A
46	CM	150	U
46	CM	151	G
46	CM	152	G
46	CM	154	A
46	CM	159	U
46	CM	166	A
46	CM	168	U
46	CM	173	G

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Mol	Chain	Res	Type
46	CM	176	U
46	CM	177	A
46	CM	190	U
46	CM	193	G
46	CM	199	G
46	CM	200	A
46	CM	202	G
46	CM	206	U
46	CM	211	A
46	CM	214	U
46	CM	215	A
46	CM	216	A
46	CM	217	A
46	CM	219	A
46	CM	220	A
46	CM	221	U
46	CM	222	C
46	CM	224	A
46	CM	225	U
46	CM	226	G
46	CM	228	C
46	CM	229	U
46	CM	230	U
46	CM	231	C
46	CM	234	G
46	CM	235	C
46	CM	236	U
46	CM	237	C
46	CM	238	U
46	CM	239	U
46	CM	240	U
46	CM	247	U
46	CM	255	A
46	CM	259	U
46	CM	260	U
46	CM	261	C
46	CM	262	G
46	CM	266	C
46	CM	269	A
46	CM	270	U
46	CM	274	C
46	CM	276	U

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Mol	Chain	Res	Type
46	CM	277	G
46	CM	278	U
46	CM	279	G
46	CM	283	G
46	CM	285	G
46	CM	297	A
46	CM	312	C
46	CM	314	A
46	CM	318	U
46	CM	319	C
46	CM	320	G
46	CM	335	G
46	CM	336	C
46	CM	350	A
46	CM	357	A
46	CM	358	A
46	CM	359	C
46	CM	388	G
46	CM	398	A
46	CM	400	C
46	CM	402	G
46	CM	414	A
46	CM	416	G
46	CM	421	G
46	CM	422	C
46	CM	423	A
46	CM	424	G
46	CM	432	G
46	CM	437	U
46	CM	442	C
46	CM	446	C
46	CM	452	A
46	CM	458	A
46	CM	462	A
46	CM	466	A
46	CM	475	A
46	CM	480	U
46	CM	489	C
46	CM	490	U
46	CM	491	U
46	CM	495	G
46	CM	498	C

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Mol	Chain	Res	Type
46	CM	499	U
46	CM	503	A
46	CM	504	A
46	CM	505	U
46	CM	506	U
46	CM	509	A
46	CM	512	G
46	CM	513	A
46	CM	515	U
46	CM	518	A
46	CM	519	A
46	CM	525	A
46	CM	530	U
46	CM	534	C
46	CM	536	A
46	CM	537	G
46	CM	539	A
46	CM	540	A
46	CM	547	G
46	CM	553	A
46	CM	554	A
46	CM	555	G
46	CM	556	U
46	CM	557	C
46	CM	563	C
46	CM	566	G
46	CM	576	U
46	CM	592	A
46	CM	593	G
46	CM	604	A
46	CM	609	U
46	CM	617	A
46	CM	618	A
46	CM	620	A
46	CM	621	A
46	CM	633	A
46	CM	639	G
46	CM	645	G
46	CM	648	U
46	CM	649	G
46	CM	650	G
46	CM	652	C

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Mol	Chain	Res	Type
46	CM	653	G
46	CM	654	G
46	CM	655	U
46	CM	658	A
46	CM	659	U
46	CM	668	U
46	CM	669	G
46	CM	670	C
46	CM	671	G
46	CM	672	U
46	CM	673	A
46	CM	674	C
46	CM	675	U
46	CM	676	G
46	CM	678	A
46	CM	680	C
46	CM	681	C
46	CM	682	A
46	CM	688	G
46	CM	691	U
46	CM	694	C
46	CM	695	C
46	CM	696	U
46	CM	697	U
46	CM	700	G
46	CM	701	G
46	CM	702	G
46	CM	703	U
46	CM	719	A
46	CM	720	C
46	CM	722	A
46	CM	723	G
46	CM	724	G
46	CM	729	U
46	CM	739	A
46	CM	740	A
46	CM	741	A
46	CM	750	G
46	CM	751	U
46	CM	756	A
46	CM	759	A
46	CM	760	G

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Mol	Chain	Res	Type
46	CM	762	C
46	CM	764	U
46	CM	765	U
46	CM	766	U
46	CM	767	G
46	CM	768	C
46	CM	770	C
46	CM	771	G
46	CM	773	A
46	CM	775	A
46	CM	778	U
46	CM	779	U
46	CM	796	A
46	CM	798	A
46	CM	799	G
46	CM	802	C
46	CM	803	G
46	CM	804	U
46	CM	805	U
46	CM	807	U
46	CM	808	G
46	CM	812	C
46	CM	813	U
46	CM	814	A
46	CM	815	U
46	CM	816	U
46	CM	818	U
46	CM	819	G
46	CM	820	U
46	CM	821	U
46	CM	823	G
46	CM	824	U
46	CM	825	U
46	CM	826	U
46	CM	827	C
46	CM	828	U
46	CM	829	A
46	CM	840	A
46	CM	842	U
46	CM	848	A
46	CM	856	G
46	CM	857	G

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Mol	Chain	Res	Type
46	CM	869	A
46	CM	871	U
46	CM	875	C
46	CM	877	G
46	CM	878	U
46	CM	879	U
46	CM	881	U
46	CM	891	A
46	CM	909	A
46	CM	910	G
46	CM	911	A
46	CM	918	A
46	CM	920	U
46	CM	927	G
46	CM	945	U
46	CM	951	A
46	CM	973	A
46	CM	975	C
46	CM	977	A
46	CM	988	A
46	CM	989	U
46	CM	990	A
46	CM	997	U
46	CM	998	A
46	CM	1004	A
46	CM	1005	A
46	CM	1011	A
46	CM	1013	C
46	CM	1017	G
46	CM	1024	A
46	CM	1025	G
46	CM	1039	U
46	CM	1042	U
46	CM	1043	U
46	CM	1055	A
46	CM	1056	U
46	CM	1057	C
46	CM	1058	G
46	CM	1059	G
46	CM	1060	C
46	CM	1061	A
46	CM	1067	C

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Mol	Chain	Res	Type
46	CM	1074	U
46	CM	1077	A
46	CM	1081	C
46	CM	1085	G
46	CM	1123	A
46	CM	1135	G
46	CM	1143	C
46	CM	1145	A
46	CM	1152	G
46	CM	1168	A
46	CM	1169	A
46	CM	1170	U
46	CM	1179	A
46	CM	1181	A
46	CM	1184	G
46	CM	1185	G
46	CM	1186	G
46	CM	1187	A
46	CM	1193	A
46	CM	1202	A
46	CM	1203	G
46	CM	1206	A
46	CM	1207	C
46	CM	1212	A
46	CM	1215	A
46	CM	1219	A
46	CM	1220	C
46	CM	1221	A
46	CM	1229	A
46	CM	1230	G
46	CM	1231	C
46	CM	1236	U
46	CM	1243	U
46	CM	1250	G
46	CM	1270	U
46	CM	1284	G
46	CM	1299	U
46	CM	1300	U
46	CM	1301	G
46	CM	1306	A
46	CM	1325	U
46	CM	1330	A

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Mol	Chain	Res	Type
46	CM	1336	G
46	CM	1339	G
46	CM	1342	A
46	CM	1343	G
46	CM	1345	A
46	CM	1346	U
46	CM	1348	U
46	CM	1349	G
46	CM	1352	G
46	CM	1355	A
46	CM	1356	U
46	CM	1357	A
46	CM	1358	G
46	CM	1359	U
46	CM	1360	C
46	CM	1364	U
46	CM	1365	C
46	CM	1369	G
46	CM	1370	A
46	CM	1376	U
46	CM	1380	G
46	CM	1381	A
46	CM	1382	U
46	CM	1384	U
46	CM	1385	C
46	CM	1392	A
46	CM	1397	A
46	CM	1398	G
46	CM	1399	U
46	CM	1400	U
46	CM	1401	U
46	CM	1410	A
46	CM	1413	A
46	CM	1414	G
46	CM	1415	G
46	CM	1422	A
46	CM	1431	G
46	CM	1433	C
46	CM	1445	C
46	CM	1446	A
46	CM	1455	A
46	CM	1457	A

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Mol	Chain	Res	Type
46	CM	1458	C
46	CM	1461	A
46	CM	1462	C
46	CM	1463	G
46	CM	1468	C
46	CM	1476	A
46	CM	1477	U
46	CM	1480	G
46	CM	1483	U
46	CM	1491	G
46	CM	1502	A
46	CM	1503	A
46	CM	1508	G
46	CM	1510	G
46	CM	1511	A
46	CM	1523	G
46	CM	1524	C
46	CM	1529	G
46	CM	1530	A
46	CM	1541	U
46	CM	1544	U
46	CM	1546	G
46	CM	1556	A
46	CM	1560	A
46	CM	1561	G
46	CM	1571	G
46	CM	1574	A
46	CM	1575	G
46	CM	1577	G
46	CM	1580	A
46	CM	1582	U
46	CM	1584	A
46	CM	1588	G
46	CM	1621	C
46	CM	1644	U
46	CM	1645	G
46	CM	1665	C
46	CM	1667	G
46	CM	1670	U
46	CM	1671	G
46	CM	1673	U
46	CM	1702	A

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Mol	Chain	Res	Type
46	CM	1704	C
46	CM	1737	A
46	CM	1742	A
46	CM	1743	A
46	CM	1744	G
46	CM	1747	G
46	CM	1749	A
46	CM	1753	A
46	CM	1756	U
46	CM	1767	G
46	CM	1770	C
46	CM	1779	G
46	CM	1780	G
46	CM	1781	A
46	CM	1782	U
46	CM	1783	C

All (182) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	172	C
1	1	403	C
1	1	538	G
1	1	563	U
1	1	601	U
1	1	759	G
1	1	912	G
1	1	1011	C
1	1	1012	U
1	1	1029	U
1	1	1060	A
1	1	1099	A
1	1	1346	U
1	1	1347	U
1	1	1559	C
1	1	1561	U
1	1	1576	A
1	1	1762	G
1	1	1815	U
1	1	1943	G
1	1	2090	U
1	1	2182	C

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Mol	Chain	Res	Type
1	1	2183	U
1	1	2441	G
1	1	2442	U
1	1	2443	G
1	1	2447	G
1	1	2455	G
1	1	2465	U
1	1	2476	C
1	1	2515	G
1	1	2519	A
1	1	2545	C
1	1	2789	A
1	1	2790	U
1	1	3093	U
1	1	3163	U
1	1	3164	U
1	1	3165	U
1	1	3193	C
1	1	3234	U
1	1	3240	U
1	1	3284	U
1	1	3309	A
1	1	3317	U
3	4	85	G
3	4	125	U
46	B	25	C
46	B	78	A
46	B	137	A
46	B	151	G
46	B	176	U
46	B	215	A
46	B	216	A
46	B	235	C
46	B	259	U
46	B	265	U
46	B	278	U
46	B	415	A
46	B	451	C
46	B	505	U
46	B	514	G
46	B	518	A
46	B	529	C

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Mol	Chain	Res	Type
46	B	533	A
46	B	553	A
46	B	556	U
46	B	638	U
46	B	740	A
46	B	763	C
46	B	769	U
46	B	814	A
46	B	820	U
46	B	855	C
46	B	874	U
46	B	876	A
46	B	1168	A
46	B	1335	U
46	B	1355	A
46	B	1369	G
46	B	1396	A
46	B	1398	G
46	B	1457	A
46	B	1467	C
46	B	1479	A
46	B	1484	U
46	B	1523	G
46	B	1573	A
46	B	1579	A
46	B	1581	G
46	B	1703	C
46	B	1743	A
1	AS	172	C
1	AS	403	C
1	AS	447	U
1	AS	487	C
1	AS	538	G
1	AS	563	U
1	AS	601	U
1	AS	759	G
1	AS	912	G
1	AS	1029	U
1	AS	1060	A
1	AS	1099	A
1	AS	1346	U
1	AS	1347	U

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Mol	Chain	Res	Type
1	AS	1559	C
1	AS	1576	A
1	AS	1762	G
1	AS	1815	U
1	AS	1943	G
1	AS	2090	U
1	AS	2182	C
1	AS	2183	U
1	AS	2430	G
1	AS	2515	G
1	AS	2519	A
1	AS	2545	C
1	AS	2667	A
1	AS	2789	A
1	AS	2790	U
1	AS	3093	U
1	AS	3159	A
1	AS	3160	C
1	AS	3193	C
1	AS	3234	U
1	AS	3240	U
1	AS	3284	U
1	AS	3309	A
1	AS	3315	C
1	AS	3317	U
3	AU	85	G
3	AU	125	U
3	AU	156	U
46	CM	25	C
46	CM	65	A
46	CM	74	U
46	CM	78	A
46	CM	137	A
46	CM	151	G
46	CM	176	U
46	CM	214	U
46	CM	237	C
46	CM	259	U
46	CM	265	U
46	CM	415	A
46	CM	451	C
46	CM	504	A

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Mol	Chain	Res	Type
46	CM	505	U
46	CM	514	G
46	CM	518	A
46	CM	529	C
46	CM	533	A
46	CM	553	A
46	CM	556	U
46	CM	638	U
46	CM	680	C
46	CM	690	C
46	CM	695	C
46	CM	740	A
46	CM	763	C
46	CM	769	U
46	CM	814	A
46	CM	817	U
46	CM	855	C
46	CM	874	U
46	CM	876	A
46	CM	1168	A
46	CM	1335	U
46	CM	1359	U
46	CM	1369	G
46	CM	1396	A
46	CM	1398	G
46	CM	1457	A
46	CM	1467	C
46	CM	1479	A
46	CM	1523	G
46	CM	1555	C
46	CM	1573	A
46	CM	1579	A
46	CM	1581	G
46	CM	1742	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1152 ligands modelled in this entry, 1148 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	3K5	1	3401	-	62,63,63	0.21	0	82,95,95	0.46	1 (1%)
86	GET	B	1851	-	33,36,36	0.45	0	43,55,55	0.60	1 (2%)
83	3K5	AS	3401	-	62,63,63	0.30	0	82,95,95	0.92	3 (3%)
86	GET	CM	1822	-	33,36,36	0.43	0	43,55,55	0.63	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	3K5	1	3401	-	-	4/29/121/121	0/7/7/7
86	GET	B	1851	-	-	3/13/74/74	0/3/3/3
83	3K5	AS	3401	-	-	4/29/121/121	0/7/7/7
86	GET	CM	1822	-	-	2/13/74/74	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	AS	3401	3K5	C34-O14-C38	4.26	124.32	117.72
83	AS	3401	3K5	O14-C34-C35	3.95	116.71	107.70
83	AS	3401	3K5	O14-C34-C33	3.42	115.51	107.70
86	CM	1822	GET	O11-C11-C21	3.18	113.70	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	B	1851	GET	O11-C11-C21	2.59	112.67	108.22
83	1	3401	3K5	O1-C5-C1	2.25	110.42	107.23

There are no chirality outliers.

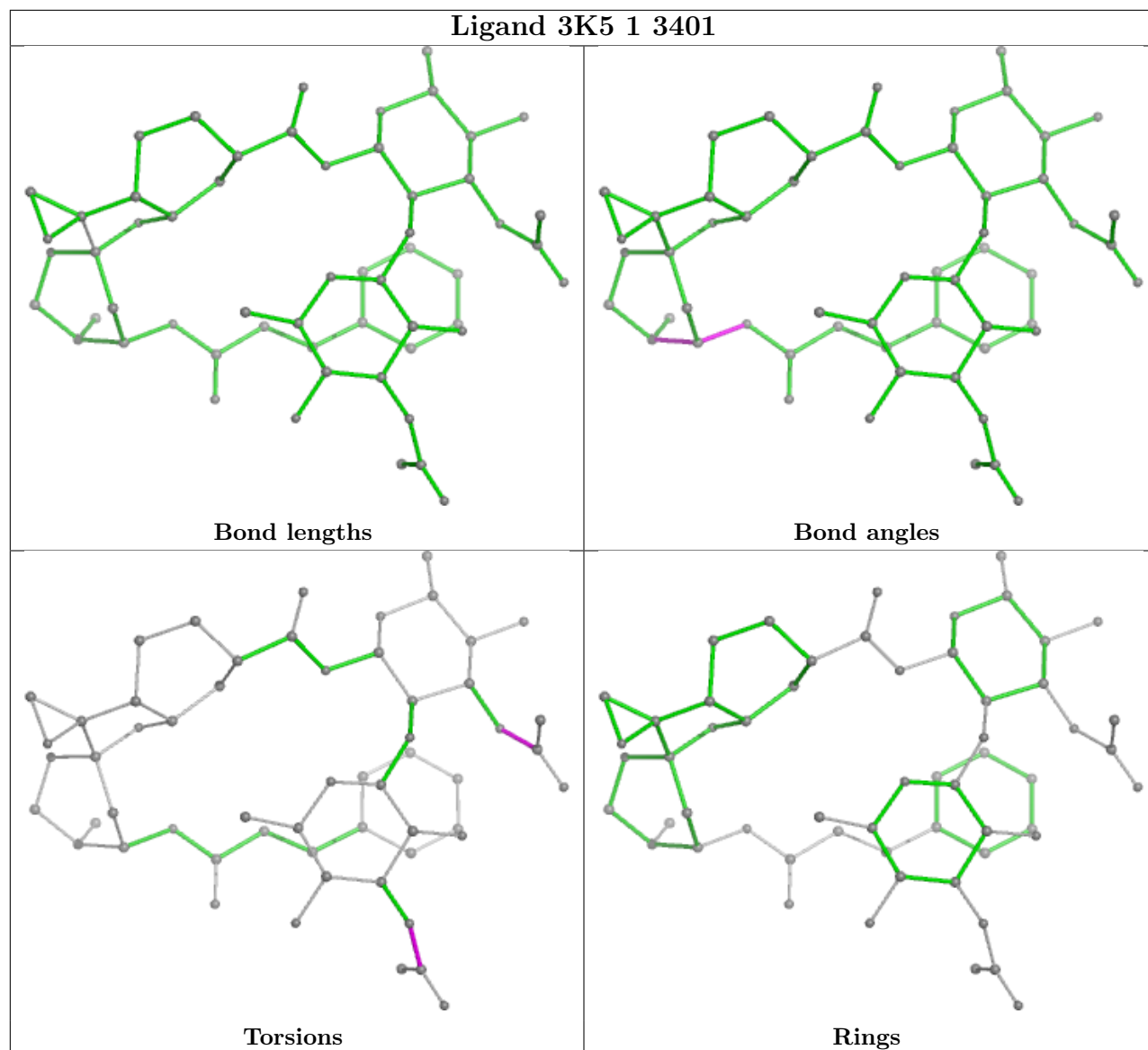
All (13) torsion outliers are listed below:

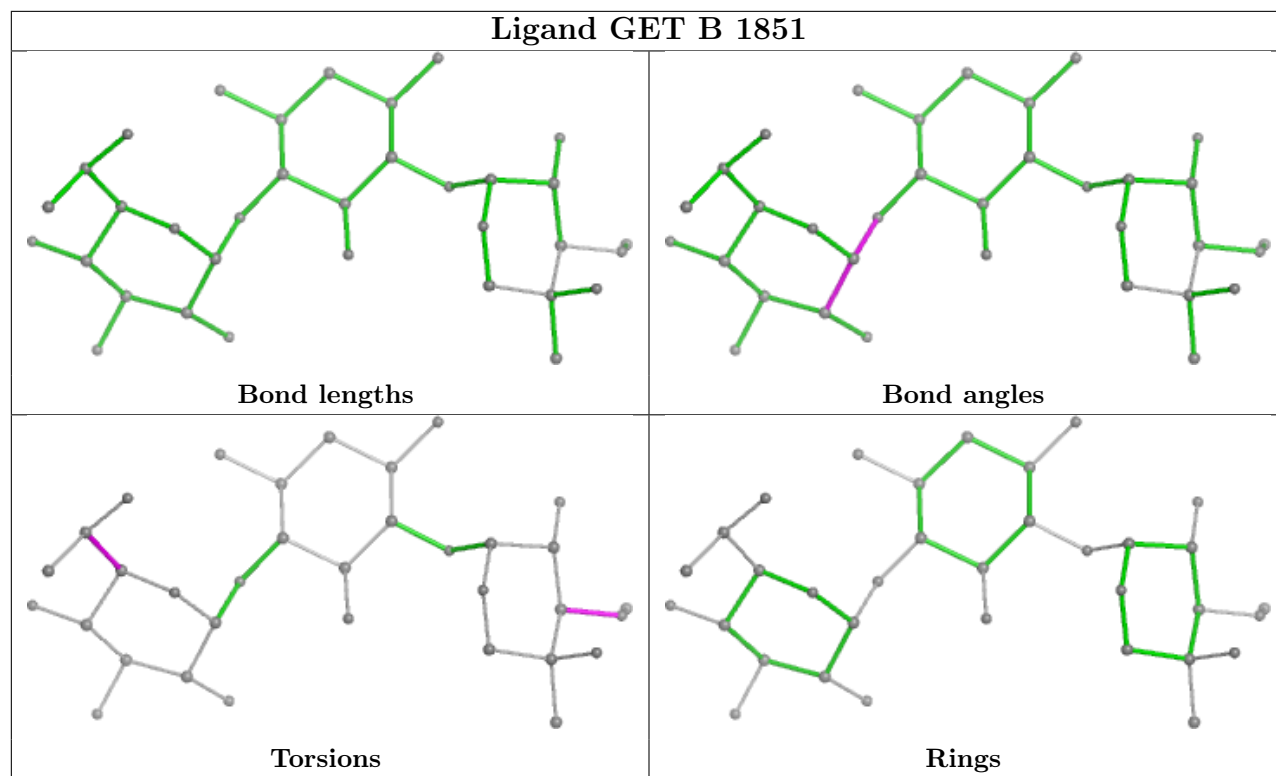
Mol	Chain	Res	Type	Atoms
86	B	1851	GET	O51-C51-C61-O61
86	B	1851	GET	C23-C33-N33-C93
86	CM	1822	GET	C23-C33-N33-C93
83	1	3401	3K5	C39-C38-O14-C34
83	1	3401	3K5	C31-C30-O9-C26
83	1	3401	3K5	O15-C38-O14-C34
83	1	3401	3K5	O10-C30-O9-C26
83	AS	3401	3K5	C39-C38-O14-C34
83	AS	3401	3K5	O15-C38-O14-C34
83	AS	3401	3K5	C33-C34-O14-C38
86	CM	1822	GET	O51-C11-O11-C42
83	AS	3401	3K5	O7-C24-O6-C23
86	B	1851	GET	C41-C51-C61-C71

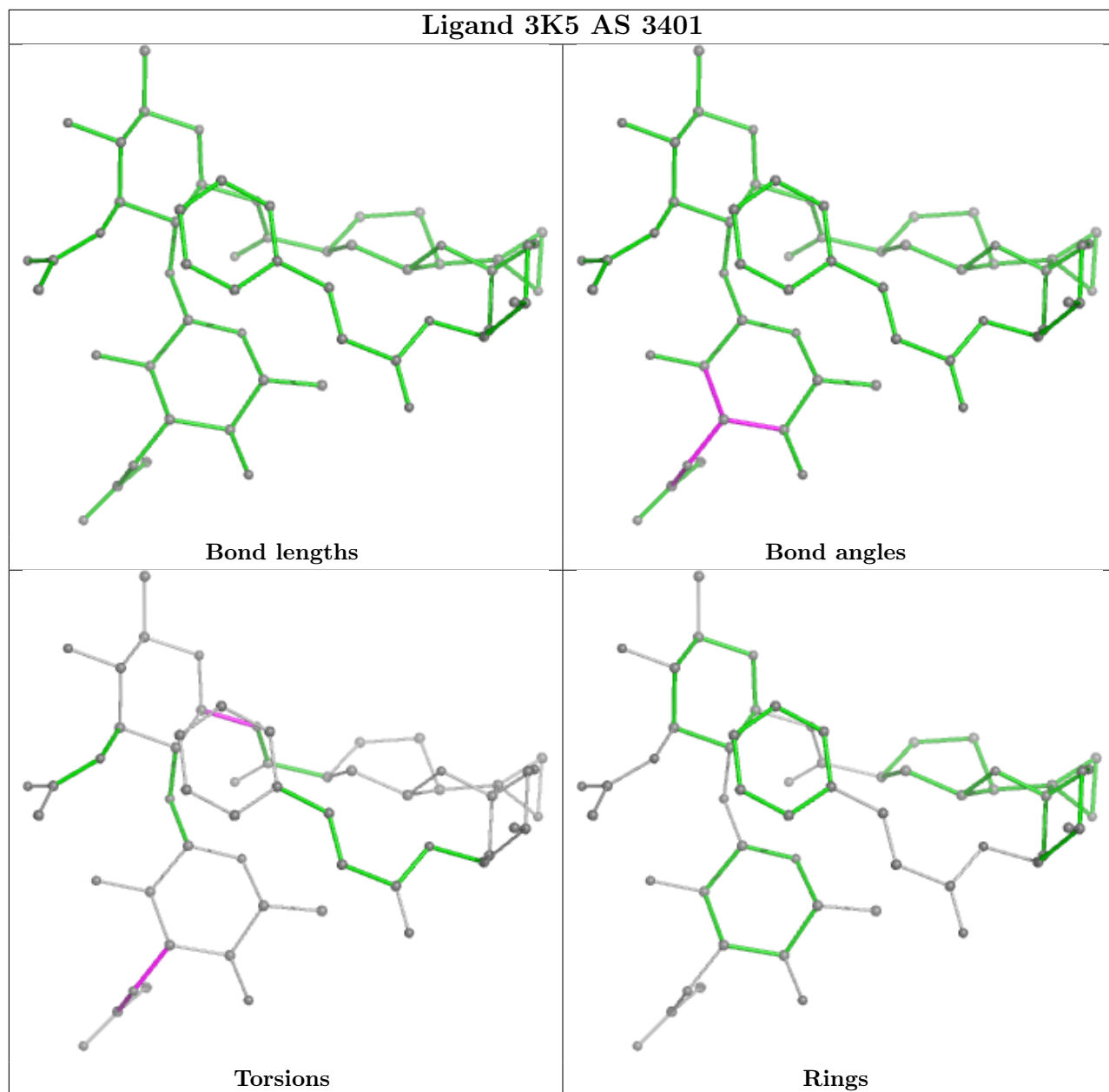
There are no ring outliers.

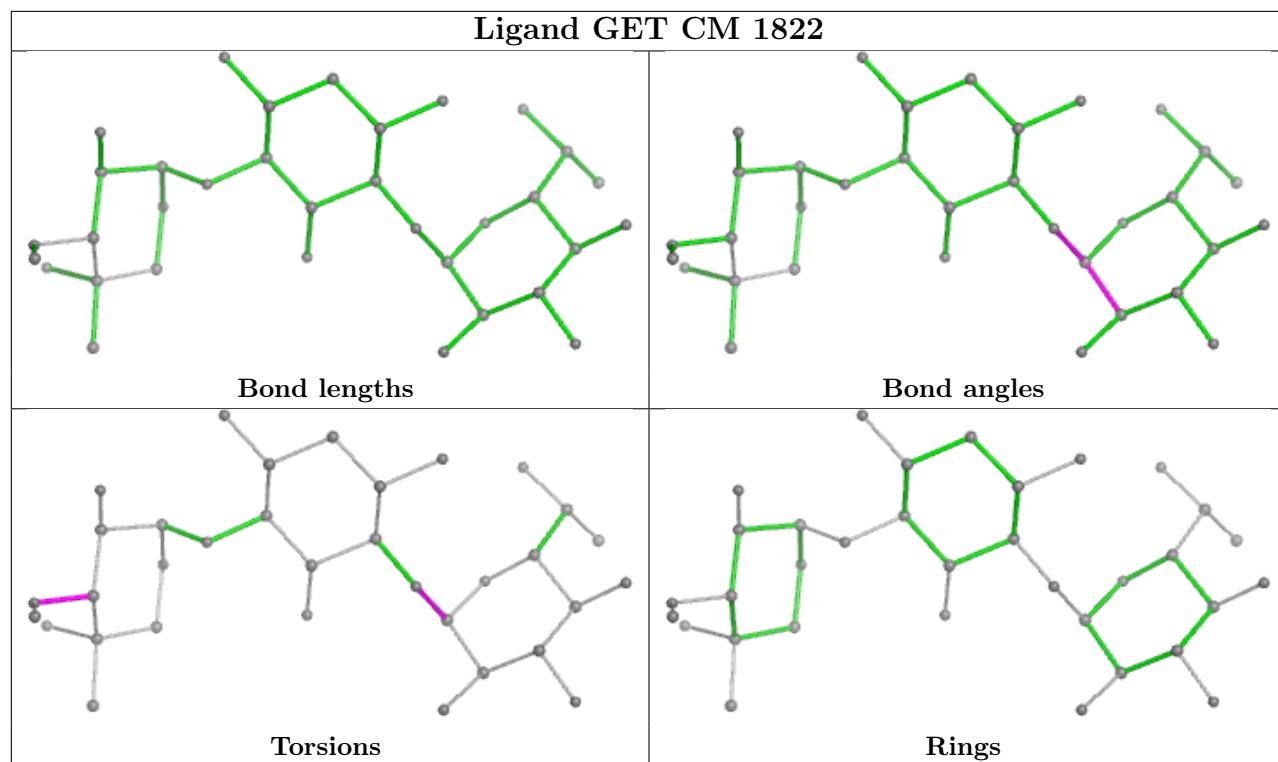
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1	3218/3359 (95%)	-0.02	72 (2%) 62 43	67, 107, 226, 432	0
1	AS	3101/3359 (92%)	0.10	92 (2%) 52 35	74, 119, 222, 327	0
2	3	121/121 (100%)	-0.27	2 (1%) 69 49	81, 112, 128, 178	0
2	AT	121/121 (100%)	-0.14	1 (0%) 82 67	86, 122, 141, 189	0
3	4	156/158 (98%)	-0.10	4 (2%) 57 39	88, 119, 158, 213	0
3	AU	158/158 (100%)	0.07	6 (3%) 44 30	103, 142, 189, 269	0
4	AW	249/254 (98%)	0.35	21 (8%) 18 14	88, 128, 152, 164	0
4	j	249/254 (98%)	0.34	13 (5%) 34 24	67, 103, 134, 178	0
5	AX	386/389 (99%)	0.27	26 (6%) 25 19	61, 100, 137, 204	0
5	k	386/389 (99%)	0.25	16 (4%) 42 28	59, 100, 127, 167	0
6	AY	359/363 (98%)	0.54	42 (11%) 10 9	76, 125, 157, 177	0
6	l	359/363 (98%)	0.42	25 (6%) 24 19	58, 111, 144, 177	0
7	AZ	292/298 (97%)	0.54	26 (8%) 17 13	88, 141, 175, 185	0
7	m	294/298 (98%)	0.12	17 (5%) 30 22	88, 123, 160, 181	0
8	BA	153/176 (86%)	0.48	12 (7%) 20 16	92, 129, 157, 192	0
8	n	157/176 (89%)	0.17	5 (3%) 50 34	93, 124, 156, 186	0
9	BB	226/241 (93%)	0.38	19 (8%) 18 14	75, 107, 144, 180	0
9	o	229/241 (95%)	0.10	11 (4%) 36 26	70, 97, 140, 210	0
10	BC	233/262 (88%)	0.14	8 (3%) 48 32	132, 169, 208, 223	0
10	p	236/262 (90%)	0.05	6 (2%) 58 40	101, 134, 180, 207	0
11	BD	190/191 (99%)	0.06	9 (4%) 37 26	97, 127, 155, 192	0
11	q	190/191 (99%)	0.01	1 (0%) 87 75	84, 115, 139, 174	0
12	r	207/219 (94%)	0.07	7 (3%) 48 32	57, 93, 137, 168	0
13	BF	171/174 (98%)	0.07	5 (2%) 54 36	91, 132, 162, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	s	171/174 (98%)	0.17	10 (5%) 30 22	82, 126, 154, 168	0
14	BG	200/202 (99%)	0.14	7 (3%) 47 32	88, 140, 182, 202	0
14	t	200/202 (99%)	0.04	7 (3%) 47 32	68, 122, 169, 194	0
15	BH	130/131 (99%)	0.07	3 (2%) 61 42	90, 123, 153, 167	0
15	u	128/131 (97%)	0.07	8 (6%) 27 20	87, 112, 136, 151	0
16	BI	203/204 (99%)	1.05	30 (14%) 7 6	93, 134, 156, 171	0
16	v	203/204 (99%)	0.87	32 (15%) 6 6	74, 104, 123, 140	0
17	BJ	199/200 (99%)	0.27	14 (7%) 24 19	74, 100, 145, 164	0
17	w	199/200 (99%)	0.27	7 (3%) 47 32	69, 96, 136, 157	0
18	BK	174/185 (94%)	0.34	6 (3%) 48 32	82, 114, 142, 165	0
18	x	169/185 (91%)	0.41	8 (4%) 37 26	75, 105, 153, 171	0
19	BL	185/186 (99%)	0.58	16 (8%) 18 14	91, 120, 141, 159	0
19	y	185/186 (99%)	0.39	15 (8%) 19 15	75, 106, 131, 150	0
20	BM	179/190 (94%)	0.31	11 (6%) 28 21	103, 134, 198, 217	0
20	z	179/190 (94%)	0.45	12 (6%) 25 19	91, 120, 185, 204	0
21	0	170/172 (98%)	-0.00	3 (1%) 67 48	75, 96, 124, 174	0
21	BN	170/172 (98%)	0.05	0 100 100	81, 110, 135, 159	0
22	2	159/160 (99%)	0.25	10 (6%) 27 20	74, 97, 165, 186	0
22	BO	159/160 (99%)	0.58	16 (10%) 14 11	80, 109, 165, 203	0
23	5	100/124 (80%)	-0.15	0 100 100	122, 159, 188, 195	0
23	BP	99/124 (79%)	-0.40	0 100 100	137, 175, 196, 243	0
24	6	131/137 (95%)	0.40	6 (4%) 38 27	69, 92, 121, 137	0
24	BQ	131/137 (95%)	0.29	4 (3%) 51 35	58, 94, 121, 142	0
25	7	118/155 (76%)	-0.13	0 100 100	80, 126, 175, 186	0
25	BR	109/155 (70%)	0.05	4 (3%) 45 30	84, 117, 150, 174	0
26	8	120/142 (84%)	0.32	11 (9%) 16 12	93, 123, 143, 156	0
26	BS	119/142 (83%)	0.22	3 (2%) 58 40	118, 146, 163, 176	0
27	9	126/127 (99%)	0.16	2 (1%) 70 51	92, 126, 155, 164	0
27	BT	126/127 (99%)	0.29	7 (5%) 31 23	110, 143, 174, 191	0
28	AA	135/136 (99%)	0.08	2 (1%) 71 53	112, 141, 166, 198	0
28	BU	135/136 (99%)	-0.13	1 (0%) 84 69	138, 171, 197, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	AB	148/149 (99%)	0.50	12 (8%) 19 15	70, 101, 132, 161	0
29	BV	148/149 (99%)	0.51	8 (5%) 32 23	77, 124, 153, 170	0
30	AC	58/63 (92%)	0.53	9 (15%) 6 6	69, 114, 142, 164	0
30	BW	60/63 (95%)	0.81	8 (13%) 8 7	87, 130, 167, 194	0
31	AD	98/106 (92%)	-0.00	0 100 100	99, 130, 149, 153	0
31	BX	94/106 (88%)	-0.17	0 100 100	129, 160, 181, 199	0
32	AE	108/112 (96%)	0.17	5 (4%) 38 27	86, 115, 163, 184	0
32	BY	108/112 (96%)	0.36	8 (7%) 22 17	87, 120, 164, 203	0
33	AF	124/131 (94%)	0.69	14 (11%) 11 9	64, 105, 131, 151	0
33	BZ	122/131 (93%)	0.69	8 (6%) 26 19	88, 112, 140, 154	0
34	AG	106/107 (99%)	0.35	7 (6%) 26 19	76, 102, 120, 142	0
34	CA	106/107 (99%)	0.14	1 (0%) 81 64	85, 106, 127, 144	0
35	AH	112/122 (91%)	0.92	21 (18%) 4 4	87, 121, 168, 190	0
35	CB	110/122 (90%)	0.93	19 (17%) 5 5	112, 146, 194, 201	0
36	AI	115/120 (95%)	0.17	6 (5%) 34 24	105, 131, 157, 175	0
36	CC	117/120 (97%)	0.29	7 (5%) 29 22	127, 155, 175, 210	0
37	AJ	97/99 (97%)	-0.06	1 (1%) 79 61	103, 119, 155, 199	0
37	CD	95/99 (95%)	0.03	2 (2%) 63 44	115, 148, 174, 197	0
38	AK	86/90 (95%)	0.46	5 (5%) 30 22	81, 102, 141, 152	0
38	CE	86/90 (95%)	0.44	6 (6%) 24 19	88, 120, 160, 169	0
39	AL	77/78 (98%)	0.22	1 (1%) 74 56	113, 152, 178, 207	0
39	CF	77/78 (98%)	-0.13	2 (2%) 57 39	140, 167, 202, 208	0
40	AM	50/51 (98%)	0.53	3 (6%) 29 22	84, 111, 135, 143	0
40	CG	50/51 (98%)	0.57	5 (10%) 14 11	95, 125, 143, 147	0
41	AN	50/52 (96%)	0.70	5 (10%) 14 11	113, 149, 165, 169	0
41	CH	50/52 (96%)	0.79	7 (14%) 7 6	121, 154, 169, 181	0
42	AO	25/25 (100%)	0.96	4 (16%) 6 5	99, 107, 123, 130	0
42	CI	24/25 (96%)	1.02	4 (16%) 5 5	93, 112, 125, 132	0
43	AP	103/106 (97%)	0.05	2 (1%) 66 46	73, 100, 143, 158	0
43	CJ	103/106 (97%)	0.26	6 (5%) 30 22	91, 124, 160, 171	0
44	AQ	91/92 (98%)	0.30	5 (5%) 32 23	79, 111, 140, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CK	91/92 (98%)	-0.12	1 (1%) 77 59	106, 130, 160, 174	0
45	CL	120/267 (44%)	0.01	6 (5%) 35 25	100, 143, 178, 186	0
45	i	106/267 (39%)	0.35	6 (5%) 30 23	108, 150, 178, 201	0
46	B	1708/1787 (95%)	0.13	74 (4%) 40 27	83, 128, 212, 439	0
46	CM	1728/1787 (96%)	-0.02	33 (1%) 66 46	86, 131, 222, 410	0
47	C	208/261 (79%)	0.16	8 (3%) 44 30	127, 161, 191, 201	0
47	CN	208/261 (79%)	0.08	9 (4%) 40 27	101, 152, 181, 215	0
48	CO	213/256 (83%)	-0.24	5 (2%) 61 42	124, 173, 195, 212	0
48	D	214/256 (83%)	-0.02	4 (1%) 66 46	110, 144, 167, 178	0
49	CP	217/249 (87%)	0.08	8 (3%) 45 30	83, 124, 152, 171	0
49	E	217/249 (87%)	0.22	18 (8%) 19 14	106, 137, 164, 187	0
50	CQ	223/251 (88%)	0.07	10 (4%) 39 27	99, 130, 186, 216	0
50	F	223/251 (88%)	0.33	14 (6%) 27 20	103, 143, 197, 215	0
51	CR	260/262 (99%)	0.04	15 (5%) 30 22	103, 130, 156, 184	0
51	G	258/262 (98%)	0.61	25 (9%) 15 11	110, 145, 166, 192	0
52	CS	205/225 (91%)	0.05	11 (5%) 32 23	124, 155, 189, 241	0
52	H	206/225 (91%)	0.38	18 (8%) 17 13	107, 146, 181, 213	0
53	CT	236/236 (100%)	0.16	9 (3%) 44 30	94, 143, 182, 203	0
53	I	223/236 (94%)	0.31	24 (10%) 12 10	97, 143, 178, 222	0
54	CU	179/186 (96%)	-0.20	3 (1%) 69 49	123, 179, 214, 226	0
54	J	182/186 (97%)	0.24	11 (6%) 29 22	118, 180, 204, 219	0
55	CV	203/206 (98%)	0.41	17 (8%) 18 14	82, 121, 170, 195	0
55	K	203/206 (98%)	0.19	14 (6%) 24 19	89, 129, 173, 189	0
56	CW	178/189 (94%)	0.18	10 (5%) 31 23	101, 137, 167, 188	0
56	L	178/189 (94%)	0.63	22 (12%) 9 8	118, 151, 173, 185	0
57	CX	94/118 (79%)	-0.20	0 100 100	104, 147, 177, 208	0
57	M	98/118 (83%)	0.18	2 (2%) 64 45	108, 154, 188, 204	0
58	CY	141/155 (90%)	-0.01	0 100 100	83, 118, 151, 197	0
58	N	144/155 (92%)	0.34	10 (6%) 24 19	102, 129, 165, 189	0
59	CZ	119/143 (83%)	-0.13	0 100 100	178, 214, 225, 231	0
59	O	116/143 (81%)	0.04	4 (3%) 48 32	193, 225, 239, 248	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	DA	150/151 (99%)	0.13	5 (3%) 49 33	103, 146, 173, 183	0
60	P	148/151 (98%)	0.41	11 (7%) 22 17	101, 140, 167, 179	0
61	DB	122/132 (92%)	-0.06	3 (2%) 58 40	98, 153, 179, 189	0
61	Q	127/132 (96%)	0.23	8 (6%) 27 20	97, 129, 152, 162	0
62	DC	130/142 (91%)	0.34	3 (2%) 61 42	115, 155, 184, 195	0
62	R	131/142 (92%)	0.25	6 (4%) 38 27	94, 138, 178, 202	0
63	DD	139/142 (97%)	0.52	15 (10%) 12 10	108, 152, 179, 189	0
63	S	139/142 (97%)	0.44	11 (7%) 20 16	110, 149, 184, 201	0
64	DE	124/137 (90%)	0.28	5 (4%) 43 29	104, 163, 207, 216	0
64	T	124/137 (90%)	0.28	4 (3%) 50 34	128, 167, 217, 226	0
65	DF	141/145 (97%)	0.14	1 (0%) 84 69	115, 153, 182, 210	0
65	U	144/145 (99%)	0.11	3 (2%) 63 44	96, 126, 165, 179	0
66	DG	141/145 (97%)	0.13	4 (2%) 55 37	117, 150, 175, 193	0
66	V	141/145 (97%)	0.14	1 (0%) 84 69	110, 137, 176, 196	0
67	DH	97/119 (81%)	0.42	9 (9%) 16 12	97, 147, 182, 194	0
67	W	102/119 (85%)	0.49	9 (8%) 17 13	96, 164, 192, 198	0
68	DI	87/87 (100%)	-0.01	2 (2%) 61 42	106, 144, 173, 193	0
68	X	87/87 (100%)	-0.02	2 (2%) 61 42	111, 147, 172, 181	0
69	DJ	129/130 (99%)	0.12	0 100 100	104, 127, 144, 151	0
69	Y	129/130 (99%)	0.42	5 (3%) 44 30	112, 133, 148, 154	0
70	DK	143/145 (98%)	0.36	9 (6%) 27 20	79, 104, 131, 156	0
70	Z	143/145 (98%)	0.43	10 (6%) 24 19	85, 110, 132, 158	0
71	DL	132/135 (97%)	-0.15	1 (0%) 82 67	114, 150, 176, 204	0
71	a	134/135 (99%)	0.10	6 (4%) 39 27	115, 152, 175, 189	0
72	DM	71/105 (67%)	-0.13	1 (1%) 73 53	149, 175, 195, 201	0
72	b	72/105 (68%)	-0.23	1 (1%) 73 53	120, 150, 179, 193	0
73	DN	98/119 (82%)	0.15	6 (6%) 28 21	109, 136, 188, 195	0
73	c	97/119 (81%)	0.32	9 (9%) 16 12	100, 133, 168, 197	0
74	DO	81/82 (98%)	-0.14	1 (1%) 76 57	125, 163, 219, 233	0
74	d	81/82 (98%)	0.19	4 (4%) 36 25	120, 154, 198, 218	0
75	DP	61/67 (91%)	-0.28	1 (1%) 70 51	133, 162, 183, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	e	60/67 (89%)	0.15	3 (5%) 35 25	125, 156, 185, 191	0
76	DQ	54/56 (96%)	0.34	2 (3%) 45 30	95, 116, 149, 169	0
76	f	55/56 (98%)	0.71	8 (14%) 7 6	98, 118, 141, 175	0
77	DR	59/63 (93%)	0.33	5 (8%) 18 14	98, 140, 207, 220	0
77	g	60/63 (95%)	0.47	7 (11%) 10 9	117, 147, 202, 222	0
78	DS	68/193 (35%)	0.04	4 (5%) 29 22	154, 226, 246, 252	0
78	h	70/193 (36%)	0.30	6 (8%) 18 14	163, 211, 237, 252	0
79	AR	311/317 (98%)	0.11	9 (2%) 54 36	162, 200, 225, 242	0
79	DT	307/317 (96%)	-0.17	2 (0%) 84 69	162, 200, 221, 236	0
80	BE	205/220 (93%)	0.02	6 (2%) 54 36	64, 97, 143, 172	0
81	P0	107/312 (34%)	-0.22	1 (0%) 81 64	155, 176, 191, 202	0
82	12	63/165 (38%)	-0.27	0 100 100	159, 180, 196, 207	0
All	All	32813/35602 (92%)	0.17	1492 (4%) 39 27	57, 128, 201, 439	0

All (1492) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	G	39	ARG	9.2
53	I	79	LYS	8.9
53	CT	79	LYS	8.8
60	P	7	SER	8.6
35	CB	33	GLN	8.6
6	l	55	GLU	8.3
6	AY	363	ASN	8.3
70	Z	27	GLN	7.9
63	DD	129	GLY	7.8
16	v	185	ALA	7.8
13	BF	143	ARG	7.6
8	n	1	MET	7.5
16	v	184	LYS	7.4
63	DD	137	PHE	7.2
67	DH	76	LYS	7.2
29	AB	46	ASP	7.1
16	v	193	LYS	7.1
6	AY	66	TRP	7.0
7	AZ	150	LEU	7.0
35	CB	21	LYS	6.8
35	AH	61	GLN	6.8

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Mol	Chain	Res	Type	RSRZ
32	BY	26	LYS	6.7
1	AS	132	U	6.7
76	f	54	LYS	6.6
51	CR	2	ALA	6.5
53	I	86	PRO	6.5
78	DS	127	TYR	6.4
51	G	6	LYS	6.3
66	DG	92	LYS	6.3
70	DK	27	GLN	6.3
35	CB	20	ILE	6.2
5	AX	245	GLY	6.2
36	CC	83	LYS	6.2
40	AM	34	LYS	6.2
7	AZ	27	LYS	6.1
53	I	80	GLY	6.1
53	I	77	LEU	6.0
6	AY	70	ARG	5.9
46	CM	1270	U	5.9
6	AY	199	ARG	5.8
6	AY	110	TRP	5.8
55	CV	53	GLN	5.8
16	BI	89	VAL	5.7
29	BV	110	GLY	5.7
33	BZ	35	LYS	5.7
1	1	1127	G	5.7
19	BL	168	LYS	5.7
7	AZ	149	GLY	5.7
36	CC	88	LEU	5.7
5	k	23	ALA	5.6
17	w	30	ASN	5.6
51	G	14	ALA	5.5
9	BB	126	LYS	5.5
8	n	2	SER	5.5
68	DI	20	THR	5.5
50	F	188	LYS	5.5
6	AY	197	GLY	5.4
63	DD	131	ARG	5.4
38	AK	51	LEU	5.4
33	AF	53	GLN	5.4
6	AY	361	LEU	5.4
46	B	1078	A	5.4
22	BO	79	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
55	CV	40	PRO	5.4
49	CP	86	ARG	5.4
20	BM	12	ALA	5.3
18	x	128	ARG	5.3
35	CB	36	LYS	5.3
1	AS	134	U	5.3
22	BO	81	GLY	5.3
63	DD	128	PHE	5.3
67	DH	78	TRP	5.3
46	B	1016	U	5.3
35	CB	35	VAL	5.2
20	z	54	PRO	5.2
63	S	129	GLY	5.1
35	CB	31	VAL	5.1
19	BL	160	GLY	5.1
16	BI	189	HIS	5.1
53	I	96	SER	5.1
1	AS	368	G	5.0
70	Z	31	ALA	5.0
7	AZ	53	VAL	5.0
35	CB	32	ALA	5.0
46	B	1099	G	5.0
35	CB	61	GLN	5.0
30	BW	32	LEU	5.0
6	l	105	LYS	4.9
35	AH	21	LYS	4.9
55	CV	19	ALA	4.9
63	DD	136	ARG	4.9
4	j	195	SER	4.9
51	G	2	ALA	4.9
6	AY	55	GLU	4.9
47	C	97	ALA	4.9
16	BI	191	TRP	4.8
35	CB	34	HIS	4.8
6	AY	52	ALA	4.8
20	BM	93	VAL	4.8
29	BV	127	ALA	4.8
38	CE	18	LEU	4.8
53	CT	158	VAL	4.7
16	v	192	LYS	4.7
20	z	51	VAL	4.7
6	l	199	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
67	DH	77	THR	4.7
6	l	110	TRP	4.6
53	I	97	VAL	4.6
55	K	45	SER	4.6
46	B	1399	U	4.6
56	L	51	LYS	4.6
4	AW	235	ALA	4.5
77	g	35	TYR	4.5
1	AS	1927	U	4.5
60	P	121	ARG	4.5
1	AS	1850	C	4.5
47	CN	74	ALA	4.5
7	m	92	LEU	4.5
49	E	80	SER	4.5
46	B	1270	U	4.5
35	AH	29	LYS	4.4
1	1	1188	C	4.4
62	R	17	PHE	4.4
16	v	174	ILE	4.4
67	DH	63	LYS	4.4
5	AX	242	THR	4.4
46	B	357	A	4.4
56	L	13	SER	4.4
77	g	39	LEU	4.4
4	AW	228	GLY	4.4
55	K	53	GLN	4.4
46	CM	1571	G	4.4
1	AS	826	A	4.3
52	H	71	SER	4.3
32	BY	30	LYS	4.3
15	BH	52	LEU	4.3
47	CN	134	LYS	4.3
53	I	135	PRO	4.3
70	Z	24	TRP	4.3
33	BZ	37	LYS	4.3
9	o	90	ILE	4.3
50	F	167	ASP	4.3
52	CS	71	SER	4.3
6	l	59	HIS	4.3
24	6	137	VAL	4.3
5	AX	10	ARG	4.2
7	AZ	61	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
52	H	84	LYS	4.2
35	AH	38	ALA	4.2
45	CL	103	LEU	4.2
6	AY	84	HIS	4.2
46	B	75	U	4.2
1	1	949	G	4.2
70	Z	30	LYS	4.2
29	AB	17	ALA	4.2
51	G	13	ALA	4.2
10	BC	67	SER	4.2
16	BI	81	TYR	4.1
45	i	103	LEU	4.1
15	u	128	LEU	4.1
9	BB	96	LYS	4.1
52	H	76	LYS	4.1
6	AY	106	THR	4.1
7	AZ	38	THR	4.1
3	AU	111	A	4.1
46	B	298	A	4.1
70	Z	21	ASN	4.1
29	AB	68	PHE	4.0
70	DK	21	ASN	4.0
18	x	126	ARG	4.0
29	BV	68	PHE	4.0
6	l	104	THR	4.0
36	CC	92	LEU	4.0
9	BB	98	ARG	4.0
16	BI	146	ALA	4.0
51	CR	39	ARG	4.0
51	G	15	PRO	4.0
55	CV	45	SER	4.0
80	BE	199	PHE	4.0
46	B	482	C	4.0
1	AS	1483	G	4.0
35	AH	22	VAL	4.0
6	AY	188	LEU	4.0
67	W	76	LYS	4.0
25	BR	86	SER	4.0
46	B	1571	G	4.0
46	CM	1099	G	4.0
63	DD	130	GLY	4.0
54	J	89	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
74	d	24	LEU	3.9
6	l	195	LEU	3.9
22	BO	86	GLU	3.9
52	H	70	VAL	3.9
1	AS	1192	C	3.9
1	AS	1862	C	3.9
51	G	45	VAL	3.9
63	DD	126	LYS	3.9
51	G	40	GLU	3.9
36	CC	84	LYS	3.9
19	y	69	ARG	3.8
79	AR	134	VAL	3.8
6	AY	353	SER	3.8
46	B	1404	G	3.8
1	AS	1775	C	3.8
1	AS	2379	A	3.8
46	B	929	A	3.8
16	BI	174	ILE	3.8
51	G	47	PHE	3.8
4	j	110	GLY	3.8
47	C	130	ALA	3.8
16	BI	184	LYS	3.8
51	G	22	LYS	3.8
1	l	1781	C	3.8
49	E	79	ARG	3.8
56	L	14	VAL	3.8
16	v	153	ASN	3.8
22	2	77	ASN	3.8
46	CM	1404	G	3.8
11	BD	9	ILE	3.8
52	CS	113	ILE	3.8
54	J	132	ILE	3.8
78	h	126	VAL	3.8
4	j	153	GLY	3.7
79	AR	138	ILE	3.7
17	w	11	ASP	3.7
1	AS	1188	C	3.7
27	BT	16	ARG	3.7
46	B	938	G	3.7
7	AZ	62	ALA	3.7
5	AX	246	LEU	3.7
45	CL	84	SER	3.7

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Mol	Chain	Res	Type	RSRZ
51	G	38	LEU	3.7
19	BL	159	LYS	3.7
33	AF	35	LYS	3.7
1	1	1197	C	3.7
53	CT	135	PRO	3.7
60	P	9	LYS	3.7
6	l	61	THR	3.7
52	H	177	ILE	3.7
1	AS	2943	A	3.7
76	f	43	PHE	3.7
16	BI	43	SER	3.6
3	AU	38	U	3.6
22	BO	63	ILE	3.6
11	BD	10	LEU	3.6
32	AE	15	LEU	3.6
56	CW	104	PHE	3.6
15	u	13	VAL	3.6
46	CM	1618	A	3.6
51	CR	23	LEU	3.6
63	S	137	PHE	3.6
20	BM	19	LYS	3.6
46	B	381	G	3.6
68	X	58	TYR	3.6
50	CQ	185	ILE	3.6
38	CE	48	ASN	3.6
6	l	91	PHE	3.6
19	y	180	ARG	3.6
60	P	5	HIS	3.6
3	AU	22	U	3.6
24	BQ	49	LEU	3.6
6	l	66	TRP	3.6
16	BI	193	LYS	3.6
70	Z	28	ALA	3.6
49	CP	210	PHE	3.6
46	CM	382	G	3.6
1	AS	895	U	3.6
41	CH	37	ARG	3.6
10	BC	151	LEU	3.6
22	2	81	GLY	3.5
35	CB	22	VAL	3.5
51	CR	31	PRO	3.5
78	DS	126	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
46	B	1135	G	3.5
6	AY	234	LEU	3.5
13	s	19	LEU	3.5
46	CM	1703	C	3.5
6	AY	362	LYS	3.5
7	AZ	54	ARG	3.5
36	AI	84	LYS	3.5
46	CM	504	A	3.5
49	E	203	GLU	3.5
8	BA	69	LYS	3.5
1	AS	827	G	3.5
1	AS	1888	G	3.5
63	DD	135	ALA	3.5
7	m	55	PHE	3.5
33	BZ	36	GLN	3.5
80	BE	175	PRO	3.5
36	CC	91	LYS	3.5
49	CP	156	LYS	3.5
75	e	49	ARG	3.5
1	AS	775	G	3.5
1	1	110	C	3.5
67	W	79	ASP	3.5
55	CV	20	GLN	3.5
63	DD	127	LYS	3.5
52	H	152	SER	3.5
1	1	1934	U	3.5
29	AB	129	PHE	3.5
5	AX	12	GLY	3.5
1	1	2454	C	3.5
11	BD	8	GLN	3.5
38	CE	23	GLY	3.5
29	AB	45	LEU	3.5
61	DB	85	LYS	3.5
79	AR	82	LEU	3.5
22	BO	77	ASN	3.4
19	BL	84	VAL	3.4
41	CH	23	CYS	3.4
46	B	1570	A	3.4
56	CW	10	LYS	3.4
16	v	173	GLY	3.4
18	x	22	LEU	3.4
7	AZ	69	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
29	AB	65	GLN	3.4
3	4	21	C	3.4
49	E	178	VAL	3.4
5	AX	236	LYS	3.4
52	CS	177	ILE	3.4
58	N	70	ILE	3.4
33	AF	36	GLN	3.4
56	L	47	PHE	3.4
14	t	4	SER	3.4
67	DH	81	TYR	3.4
22	BO	32	LYS	3.4
53	I	73	VAL	3.4
63	S	68	VAL	3.4
9	BB	103	LEU	3.4
17	BJ	53	LEU	3.4
7	m	24	GLN	3.4
47	CN	107	PHE	3.4
5	k	217	VAL	3.4
1	1	2090	U	3.4
46	B	1359	U	3.4
19	BL	5	HIS	3.4
49	E	214	GLY	3.4
6	AY	224	PRO	3.4
6	l	90	ALA	3.4
51	G	52	LEU	3.4
8	BA	66	GLY	3.4
46	B	259	U	3.4
1	1	29	G	3.4
56	CW	15	PRO	3.4
1	AS	1891	A	3.4
33	AF	37	LYS	3.4
24	BQ	15	LEU	3.4
42	CI	10	VAL	3.4
22	2	86	GLU	3.3
55	CV	51	GLY	3.3
2	AT	73	C	3.3
26	8	66	PRO	3.3
9	BB	101	LEU	3.3
64	T	9	VAL	3.3
22	2	84	TYR	3.3
13	s	147	THR	3.3
30	BW	5	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
16	BI	175	ASN	3.3
27	BT	76	LEU	3.3
33	AF	43	VAL	3.3
50	F	207	VAL	3.3
29	BV	72	GLU	3.3
4	j	13	GLY	3.3
20	BM	13	SER	3.3
34	AG	95	GLY	3.3
5	AX	4	ARG	3.3
6	l	56	ASN	3.3
7	m	150	LEU	3.3
16	BI	74	PRO	3.3
24	6	22	VAL	3.3
45	CL	98	ASP	3.3
20	z	52	LYS	3.3
49	E	77	LYS	3.3
46	B	258	U	3.3
17	BJ	44	ILE	3.3
51	CR	6	LYS	3.3
73	c	29	CYS	3.3
18	BK	77	GLY	3.3
63	DD	134	ARG	3.3
16	v	196	THR	3.3
49	E	196	SER	3.3
78	DS	133	ILE	3.3
67	W	81	TYR	3.3
5	k	24	LYS	3.3
7	m	82	GLU	3.3
6	AY	77	ARG	3.3
76	f	40	ARG	3.3
9	o	132	VAL	3.2
50	F	150	SER	3.2
56	L	2	PRO	3.2
35	AH	32	ALA	3.2
52	H	181	GLU	3.2
1	AS	1117	U	3.2
5	AX	249	VAL	3.2
26	BS	60	HIS	3.2
78	DS	128	THR	3.2
12	r	166	ILE	3.2
17	BJ	45	SER	3.2
35	AH	36	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
10	BC	200	ALA	3.2
45	i	42	ALA	3.2
47	CN	130	ALA	3.2
49	E	161	ALA	3.2
77	DR	35	TYR	3.2
52	H	86	GLN	3.2
14	t	20	GLU	3.2
5	k	107	ALA	3.2
49	E	210	PHE	3.2
55	CV	79	ALA	3.2
4	AW	2	GLY	3.2
5	AX	263	THR	3.2
56	L	104	PHE	3.2
1	AS	774	U	3.2
1	1	1192	C	3.2
20	z	128	LYS	3.2
38	CE	2	GLY	3.2
5	AX	250	ALA	3.2
52	H	61	TYR	3.1
47	C	134	LYS	3.1
19	BL	156	GLY	3.1
20	z	17	VAL	3.1
33	AF	32	ASN	3.1
1	1	1138	G	3.1
46	B	1392	A	3.1
16	BI	197	LEU	3.1
52	H	87	CYS	3.1
52	CS	70	VAL	3.1
6	AY	122	ALA	3.1
13	BF	76	ALA	3.1
77	DR	34	ALA	3.1
9	o	96	LYS	3.1
52	CS	115	LYS	3.1
79	AR	137	THR	3.1
1	AS	1217	A	3.1
20	BM	16	GLY	3.1
35	AH	14	ASN	3.1
35	AH	30	LEU	3.1
54	J	55	ALA	3.1
15	BH	50	ILE	3.1
34	AG	14	ILE	3.1
50	F	40	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
54	J	69	VAL	3.1
16	v	108	ARG	3.1
4	AW	236	GLY	3.1
1	AS	1906	A	3.1
1	AS	2382	A	3.1
46	B	504	A	3.1
53	I	75	LEU	3.1
11	BD	53	ILE	3.1
67	DH	67	ARG	3.1
4	AW	250	GLN	3.1
15	u	122	PHE	3.1
56	L	118	LEU	3.1
19	y	185	LYS	3.1
29	BV	126	LYS	3.1
1	AS	2098	A	3.1
11	q	71	VAL	3.1
16	BI	108	ARG	3.1
19	BL	178	ARG	3.1
38	CE	29	VAL	3.1
6	AY	200	PHE	3.0
4	AW	47	GLN	3.0
20	z	7	GLN	3.0
77	DR	39	LEU	3.0
44	AQ	6	LYS	3.0
73	c	19	LYS	3.0
1	AS	171	G	3.0
1	AS	3320	U	3.0
7	AZ	84	PRO	3.0
29	AB	66	ASN	3.0
4	AW	3	ARG	3.0
33	BZ	45	ARG	3.0
55	CV	8	ARG	3.0
16	v	183	THR	3.0
44	AQ	29	LEU	3.0
56	L	48	GLN	3.0
1	AS	780	A	3.0
40	AM	32	ASP	3.0
40	CG	32	ASP	3.0
53	I	78	SER	3.0
53	I	74	ARG	3.0
16	BI	195	ASN	3.0
76	f	52	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	AS	1138	G	3.0
4	AW	155	LYS	3.0
19	y	159	LYS	3.0
45	CL	100	LYS	3.0
54	J	122	LEU	3.0
56	L	116	LEU	3.0
6	l	107	TRP	3.0
17	BJ	129	ARG	3.0
24	6	87	ARG	3.0
28	AA	25	ILE	3.0
60	DA	84	ILE	3.0
70	Z	32	ARG	3.0
1	1	780	A	3.0
1	AS	2364	A	3.0
5	k	331	VAL	3.0
9	o	84	VAL	3.0
43	CJ	84	PRO	3.0
56	CW	2	PRO	3.0
33	BZ	21	HIS	3.0
49	E	202	THR	3.0
46	B	1615	U	3.0
37	CD	8	ALA	3.0
26	8	123	TYR	3.0
51	G	82	TYR	3.0
70	Z	17	VAL	3.0
1	AS	402	A	3.0
10	BC	199	ALA	3.0
30	BW	14	ARG	3.0
33	BZ	53	GLN	3.0
67	DH	93	GLN	3.0
56	L	45	ILE	3.0
46	CM	1292	U	3.0
19	BL	161	LYS	3.0
35	CB	8	ARG	3.0
74	DO	27	GLN	3.0
1	1	102	G	2.9
69	Y	41	MET	3.0
30	BW	33	LYS	2.9
1	1	2466	A	2.9
46	B	1390	C	2.9
1	1	78	U	2.9
16	v	73	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
12	r	167	ILE	2.9
38	CE	10	LYS	2.9
44	AQ	61	LYS	2.9
9	BB	123	GLU	2.9
27	BT	73	VAL	2.9
1	1	2700	G	2.9
51	CR	4	GLY	2.9
79	DT	106	GLY	2.9
36	CC	82	ALA	2.9
16	BI	77	LYS	2.9
16	BI	176	LYS	2.9
17	BJ	93	THR	2.9
26	8	49	LYS	2.9
63	S	67	LYS	2.9
26	8	82	LEU	2.9
18	x	136	ILE	2.9
8	BA	157	GLN	2.9
53	CT	153	VAL	2.9
58	N	94	VAL	2.9
1	AS	1585	A	2.9
1	1	659	G	2.9
1	1	1405	G	2.9
46	B	393	U	2.9
73	c	20	PRO	2.9
78	h	130	PRO	2.9
4	AW	219	ILE	2.9
7	m	64	ILE	2.9
50	F	159	ILE	2.9
72	b	34	ASP	2.9
20	z	16	GLY	2.9
50	CQ	186	LYS	2.9
19	y	71	LEU	2.9
4	AW	6	ARG	2.9
55	CV	22	ARG	2.9
1	AS	133	U	2.9
46	B	502	U	2.9
53	I	156	PHE	2.9
77	g	38	LEU	2.9
30	AC	31	SER	2.9
1	AS	1419	C	2.9
4	AW	73	GLU	2.9
7	m	25	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
35	AH	8	ARG	2.9
9	o	126	LYS	2.9
67	W	63	LYS	2.9
73	c	31	PRO	2.8
6	AY	67	GLY	2.8
8	BA	143	ALA	2.8
51	G	9	LEU	2.8
63	DD	133	ALA	2.8
35	AH	23	VAL	2.8
37	CD	10	VAL	2.8
58	N	97	TYR	2.8
70	DK	39	LYS	2.8
78	h	123	LYS	2.8
1	AS	174	C	2.8
56	L	101	PRO	2.8
35	CB	30	LEU	2.8
6	AY	87	GLY	2.8
1	AS	883	G	2.8
8	BA	51	VAL	2.8
46	B	1068	G	2.8
49	E	81	VAL	2.8
60	DA	65	VAL	2.8
16	v	189	HIS	2.8
16	BI	144	ARG	2.8
7	AZ	39	GLN	2.8
19	y	168	LYS	2.8
39	CF	76	THR	2.8
35	AH	33	GLN	2.8
35	CB	3	GLN	2.8
49	E	207	LYS	2.8
56	L	130	THR	2.8
52	H	100	ASN	2.8
49	E	78	ILE	2.8
49	CP	78	ILE	2.8
7	m	163	LEU	2.8
54	CU	63	LEU	2.8
1	1	1933	U	2.8
1	1	2701	U	2.8
1	AS	1374	U	2.8
46	CM	1459	U	2.8
47	C	102	PHE	2.8
14	BG	124	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
55	K	22	ARG	2.8
1	AS	1197	C	2.8
5	AX	237	LYS	2.8
36	AI	91	LYS	2.8
6	AY	359	GLU	2.8
4	j	246	LEU	2.8
51	CR	9	LEU	2.8
7	AZ	170	GLY	2.8
55	K	183	GLY	2.8
55	K	8	ARG	2.8
30	AC	22	LYS	2.8
68	DI	58	TYR	2.8
73	c	3	LYS	2.8
42	AO	3	ASP	2.8
42	CI	3	ASP	2.8
46	B	740	A	2.8
46	B	1061	A	2.8
30	BW	31	SER	2.8
33	AF	51	ILE	2.8
2	3	10	C	2.8
46	CM	674	C	2.8
14	BG	2	ALA	2.8
50	F	206	ALA	2.8
6	l	48	ARG	2.8
22	2	79	VAL	2.8
35	CB	28	GLY	2.8
73	c	18	VAL	2.8
29	AB	11	HIS	2.8
30	AC	21	ILE	2.8
46	CM	1672	G	2.8
7	AZ	146	LEU	2.8
9	o	222	GLN	2.8
22	BO	149	GLN	2.8
43	CJ	56	GLN	2.8
7	AZ	25	GLU	2.8
41	CH	3	GLU	2.8
56	L	114	PHE	2.8
1	AS	1890	U	2.8
46	B	9	U	2.8
46	B	797	U	2.8
1	1	108	A	2.8
5	AX	19	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
9	BB	16	ALA	2.8
35	AH	35	VAL	2.8
46	B	1066	A	2.8
15	u	117	LYS	2.8
35	AH	37	LYS	2.8
46	CM	1514	C	2.7
62	DC	84	ILE	2.7
70	DK	24	TRP	2.7
77	g	36	MET	2.7
79	AR	123	ILE	2.7
13	s	145	ARG	2.7
5	AX	8	ALA	2.7
62	R	76	VAL	2.7
77	DR	30	PRO	2.7
7	AZ	49	TYR	2.7
46	CM	1322	A	2.7
67	W	78	TRP	2.7
6	l	200	PHE	2.7
16	BI	11	GLN	2.7
38	AK	54	LYS	2.7
41	CH	29	PRO	2.7
61	Q	116	VAL	2.7
1	1	2467	C	2.7
1	AS	3054	C	2.7
9	o	223	GLY	2.7
5	AX	6	TYR	2.7
36	AI	92	LEU	2.7
6	AY	47	LYS	2.7
6	AY	186	LYS	2.7
46	CM	1614	U	2.7
4	j	250	GLN	2.7
29	BV	46	ASP	2.7
1	1	369	A	2.7
1	1	402	A	2.7
1	1	947	A	2.7
4	AW	225	ILE	2.7
48	D	120	LEU	2.7
3	4	91	C	2.7
13	s	102	PHE	2.7
18	x	135	ARG	2.7
64	T	5	ARG	2.7
6	AY	72	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
10	BC	62	GLN	2.7
43	CJ	47	GLN	2.7
1	AS	825	U	2.7
3	AU	23	U	2.7
46	CM	1590	U	2.7
22	BO	84	TYR	2.7
1	1	703	A	2.7
5	AX	240	ARG	2.7
55	K	75	LYS	2.7
71	a	23	PHE	2.7
1	1	79	G	2.7
1	AS	29	G	2.7
26	8	51	VAL	2.7
29	BV	11	HIS	2.7
24	6	55	GLY	2.7
5	AX	17	LEU	2.7
47	C	173	ILE	2.7
51	G	24	SER	2.7
56	L	12	TYR	2.7
66	V	18	TYR	2.7
16	BI	72	LYS	2.7
30	AC	6	ASN	2.7
41	CH	43	ASN	2.7
1	1	1602	U	2.7
46	B	1614	U	2.7
53	I	83	CYS	2.7
13	s	130	VAL	2.6
33	BZ	43	VAL	2.6
55	CV	46	VAL	2.6
64	T	4	VAL	2.6
1	AS	2323	A	2.6
12	r	114	GLY	2.6
49	E	213	ILE	2.6
80	BE	131	ILE	2.6
1	AS	863	G	2.6
60	P	109	LYS	2.6
69	Y	80	ASN	2.6
46	B	1067	C	2.6
46	CM	1144	C	2.6
1	1	329	U	2.6
1	AS	1661	U	2.6
46	B	1376	U	2.6

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Mol	Chain	Res	Type	RSRZ
53	CT	91	GLU	2.6
54	J	149	LEU	2.6
55	CV	24	LYS	2.6
73	c	90	THR	2.6
51	G	3	ARG	2.6
45	i	137	ASP	2.6
1	AS	917	A	2.6
46	B	621	A	2.6
46	B	1410	A	2.6
11	BD	158	ALA	2.6
55	CV	185	CYS	2.6
9	BB	127	LEU	2.6
17	BJ	20	LEU	2.6
35	AH	57	LEU	2.6
11	BD	48	ILE	2.6
1	AS	2383	C	2.6
4	j	210	PRO	2.6
44	AQ	28	LYS	2.6
46	CM	1704	C	2.6
53	I	88	ARG	2.6
10	BC	111	THR	2.6
53	I	89	THR	2.6
1	1	875	U	2.6
1	1	962	U	2.6
3	4	23	U	2.6
6	AY	223	VAL	2.6
17	BJ	128	LEU	2.6
48	D	156	ALA	2.6
75	e	54	LEU	2.6
1	AS	824	A	2.6
40	CG	34	LYS	2.6
46	CM	1570	A	2.6
47	CN	127	ARG	2.6
14	BG	89	TYR	2.6
28	BU	26	VAL	2.6
1	1	1406	C	2.6
1	1	3054	C	2.6
26	BS	50	SER	2.6
42	CI	24	SER	2.6
46	CM	656	C	2.6
1	AS	980	G	2.6
22	BO	91	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
46	B	382	G	2.6
58	N	91	LEU	2.6
46	B	1114	U	2.6
70	DK	119	GLY	2.6
29	AB	72	GLU	2.6
77	DR	27	PRO	2.6
16	BI	80	THR	2.6
1	AS	1889	A	2.6
47	CN	121	VAL	2.6
61	Q	78	LEU	2.6
67	DH	79	ASP	2.6
5	AX	252	ILE	2.6
8	BA	65	SER	2.6
8	BA	80	ALA	2.6
16	v	182	LYS	2.6
14	BG	85	ILE	2.6
16	BI	185	ALA	2.6
21	0	116	ALA	2.6
42	AO	16	LYS	2.6
63	S	46	LYS	2.6
22	BO	5	ARG	2.6
33	AF	97	ILE	2.6
16	v	104	GLU	2.5
1	1	3240	U	2.5
1	AS	1778	U	2.5
46	B	1292	U	2.5
1	1	63	G	2.5
46	B	494	G	2.5
70	DK	17	VAL	2.5
50	F	47	LEU	2.5
74	d	22	LYS	2.5
5	k	252	ILE	2.5
13	s	136	ALA	2.5
1	1	408	A	2.5
55	CV	35	ASN	2.5
4	AW	4	VAL	2.5
5	AX	337	THR	2.5
8	n	4	VAL	2.5
7	AZ	143	LYS	2.5
36	CC	32	LYS	2.5
40	CG	13	LEU	2.5
50	CQ	70	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
7	AZ	50	ARG	2.5
1	1	1114	C	2.5
46	B	1081	C	2.5
30	AC	11	ASN	2.5
64	DE	68	GLY	2.5
65	U	44	ASN	2.5
17	BJ	122	PRO	2.5
1	1	717	A	2.5
7	m	27	LYS	2.5
20	z	19	LYS	2.5
41	AN	38	LYS	2.5
49	E	235	LEU	2.5
55	K	96	LEU	2.5
22	2	11	THR	2.5
63	S	136	ARG	2.5
4	AW	229	ALA	2.5
7	AZ	77	ALA	2.5
14	t	2	ALA	2.5
17	w	145	ALA	2.5
22	2	24	ALA	2.5
16	v	191	TRP	2.5
10	p	67	SER	2.5
50	F	205	ASP	2.5
1	AS	1851	U	2.5
1	AS	30	C	2.5
44	AQ	7	LYS	2.5
10	p	201	LEU	2.5
10	BC	152	VAL	2.5
14	t	22	VAL	2.5
15	u	52	LEU	2.5
46	CM	726	C	2.5
19	BL	83	VAL	2.5
34	AG	31	GLN	2.5
51	CR	3	ARG	2.5
4	j	157	ILE	2.5
22	2	85	ILE	2.5
32	BY	105	THR	2.5
76	f	50	ILE	2.5
51	CR	47	PHE	2.5
1	1	545	G	2.5
46	CM	1184	G	2.5
20	BM	80	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
60	P	94	LYS	2.5
43	CJ	85	LEU	2.5
52	H	44	ASN	2.5
63	S	43	LEU	2.5
5	AX	28	ARG	2.5
22	BO	72	VAL	2.5
35	AH	16	ARG	2.5
35	AH	31	VAL	2.5
54	J	87	VAL	2.5
2	3	16	U	2.5
46	B	480	U	2.5
18	x	79	THR	2.5
40	CG	39	ALA	2.5
1	1	1352	C	2.5
46	CM	1182	C	2.5
30	AC	23	LYS	2.5
41	CH	22	LYS	2.5
51	CR	22	LYS	2.5
21	0	152	LEU	2.5
51	CR	12	LEU	2.5
25	BR	38	SER	2.5
30	BW	24	PRO	2.5
1	AS	1116	A	2.5
41	AN	43	ASN	2.5
46	CM	105	A	2.5
46	CM	383	A	2.5
1	AS	1664	G	2.4
7	m	151	GLN	2.5
7	AZ	78	ALA	2.4
26	8	65	ALA	2.4
45	i	58	THR	2.4
67	DH	66	THR	2.4
41	AN	23	CYS	2.4
46	CM	1400	U	2.4
5	k	47	LEU	2.4
6	l	197	GLY	2.4
16	v	203	ARG	2.4
48	CO	120	LEU	2.4
49	CP	108	LEU	2.4
56	L	49	LEU	2.4
58	N	71	LEU	2.4
63	S	51	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
50	CQ	224	VAL	2.4
16	v	198	SER	2.4
34	AG	30	ILE	2.4
60	P	84	ILE	2.4
29	AB	44	ASN	2.4
19	BL	6	THR	2.4
30	AC	13	THR	2.4
63	S	114	THR	2.4
46	CM	1357	A	2.4
51	G	127	LYS	2.4
55	K	23	LYS	2.4
66	DG	119	LYS	2.4
22	BO	151	LEU	2.4
77	g	37	ARG	2.4
80	BE	132	GLY	2.4
18	BK	88	VAL	2.4
4	j	219	ILE	2.4
46	B	1402	G	2.4
16	BI	76	PRO	2.4
50	F	171	ILE	2.4
58	N	95	PRO	2.4
1	AS	1817	U	2.4
11	BD	7	ASP	2.4
46	B	615	U	2.4
16	v	171	SER	2.4
33	AF	27	HIS	2.4
35	AH	79	SER	2.4
67	W	75	SER	2.4
6	AY	356	GLN	2.4
48	CO	141	ALA	2.4
55	K	20	GLN	2.4
55	K	41	LYS	2.4
9	o	98	ARG	2.4
13	s	140	ARG	2.4
52	CS	93	LEU	2.4
53	I	87	ARG	2.4
53	I	178	LEU	2.4
57	M	46	LEU	2.4
73	c	89	ARG	2.4
61	Q	110	ILE	2.4
1	AS	1139	A	2.4
6	AY	89	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
9	BB	128	ALA	2.4
16	v	86	ASN	2.4
16	v	175	ASN	2.4
26	8	89	LYS	2.4
35	AH	52	ALA	2.4
45	CL	71	LYS	2.4
56	CW	13	SER	2.4
26	8	85	GLN	2.4
8	BA	42	LEU	2.4
42	AO	6	ARG	2.4
61	DB	132	LEU	2.4
1	AS	2313	G	2.4
46	B	939	G	2.4
19	BL	169	GLY	2.4
61	Q	23	VAL	2.4
62	R	99	GLY	2.4
71	a	24	VAL	2.4
26	BS	123	TYR	2.4
4	AW	210	PRO	2.4
9	BB	130	PRO	2.4
1	1	2317	C	2.4
1	AS	882	C	2.4
1	AS	2745	C	2.4
46	B	261	C	2.4
56	L	10	LYS	2.4
8	BA	136	ALA	2.4
14	BG	86	ALA	2.4
6	l	111	ASN	2.4
8	BA	154	LEU	2.4
16	v	50	ARG	2.4
45	i	60	ASN	2.4
49	E	108	LEU	2.4
52	CS	102	ARG	2.4
53	I	85	ARG	2.4
63	S	131	ARG	2.4
1	1	963	A	2.4
1	1	1499	A	2.4
1	1	2091	A	2.4
62	DC	89	MET	2.4
68	X	20	THR	2.4
26	8	67	ILE	2.4
48	CO	137	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
53	I	157	VAL	2.4
56	CW	42	ILE	2.4
76	DQ	6	VAL	2.4
80	BE	167	ILE	2.4
1	AS	1849	U	2.4
22	BO	34	TYR	2.4
54	J	179	PHE	2.4
16	v	74	PRO	2.4
73	DN	2	PRO	2.4
73	DN	31	PRO	2.4
6	AY	57	ALA	2.4
19	y	102	ALA	2.4
9	BB	122	SER	2.4
1	1	3104	C	2.4
1	AS	3051	C	2.4
19	BL	140	VAL	2.3
46	B	392	C	2.4
56	CW	130	THR	2.3
19	y	183	GLY	2.3
6	l	194	LYS	2.3
7	m	7	PHE	2.3
12	r	171	TRP	2.3
26	8	84	PHE	2.3
30	AC	33	LYS	2.3
38	AK	84	LYS	2.3
47	C	155	TYR	2.3
1	AS	369	A	2.3
6	AY	90	ALA	2.3
37	AJ	7	ALA	2.3
76	f	48	ALA	2.3
6	l	236	LEU	2.3
51	G	8	HIS	2.3
18	x	140	GLN	2.3
25	BR	42	GLN	2.3
5	AX	73	VAL	2.3
18	BK	136	ILE	2.3
50	F	17	VAL	2.3
51	G	76	VAL	2.3
73	c	25	ASN	2.3
10	p	175	GLY	2.3
53	I	146	GLY	2.3
64	DE	8	THR	2.3

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Mol	Chain	Res	Type	RSRZ
42	CI	16	LYS	2.3
49	CP	83	LYS	2.3
64	DE	7	LYS	2.3
1	1	1894	G	2.3
1	AS	1127	G	2.3
1	AS	2089	G	2.3
46	B	507	G	2.3
46	B	1125	G	2.3
5	k	4	ARG	2.3
5	AX	254	ALA	2.3
6	l	54	ALA	2.3
32	BY	27	ARG	2.3
51	G	51	ARG	2.3
73	DN	20	PRO	2.3
10	p	153	LEU	2.3
43	AP	85	LEU	2.3
46	B	1627	C	2.3
69	Y	26	LEU	2.3
4	j	209	HIS	2.3
17	w	15	HIS	2.3
70	DK	48	HIS	2.3
17	BJ	123	GLN	2.3
35	AH	3	GLN	2.3
19	y	4	ASP	2.3
19	BL	30	VAL	2.3
20	z	22	VAL	2.3
27	BT	11	SER	2.3
32	BY	22	VAL	2.3
56	L	148	VAL	2.3
5	k	50	LYS	2.3
1	1	1637	U	2.3
5	k	270	ASN	2.3
32	AE	100	THR	2.3
46	B	1401	U	2.3
50	F	165	THR	2.3
79	AR	98	GLY	2.3
49	E	86	ARG	2.3
6	AY	50	ALA	2.3
13	BF	144	ALA	2.3
14	t	54	LEU	2.3
24	6	15	LEU	2.3
35	CB	63	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
53	CT	161	GLU	2.3
49	E	76	MET	2.3
19	BL	158	HIS	2.3
7	m	52	VAL	2.3
16	v	57	GLN	2.3
16	v	121	VAL	2.3
27	BT	77	LYS	2.3
29	AB	63	LYS	2.3
53	I	153	VAL	2.3
62	R	85	VAL	2.3
75	DP	45	LYS	2.3
1	1	3053	C	2.3
1	AS	1781	C	2.3
16	v	177	GLY	2.3
46	B	1013	C	2.3
46	CM	381	G	2.3
55	CV	109	PHE	2.3
57	M	51	SER	2.3
40	AM	33	ASN	2.3
6	AY	104	THR	2.3
1	AS	776	A	2.3
32	AE	18	ARG	2.3
41	CH	32	THR	2.3
55	CV	67	TRP	2.3
59	O	106	LEU	2.3
60	DA	16	LEU	2.3
5	k	96	PRO	2.3
16	v	55	ALA	2.3
46	B	318	U	2.3
51	G	5	PRO	2.3
62	DC	83	MET	2.3
9	o	221	ILE	2.3
7	AZ	81	HIS	2.3
54	J	178	VAL	2.3
15	BH	111	PHE	2.3
10	p	183	GLY	2.3
47	CN	137	SER	2.3
52	CS	152	SER	2.3
16	BI	149	ASN	2.3
17	BJ	30	ASN	2.3
60	P	80	LEU	2.3
61	DB	84	THR	2.3

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Mol	Chain	Res	Type	RSRZ
67	W	69	THR	2.3
15	u	127	ALA	2.3
50	CQ	103	ALA	2.3
1	1	1775	C	2.3
1	1	1900	C	2.3
46	CM	1619	C	2.3
5	AX	5	LYS	2.3
1	1	2702	G	2.3
1	AS	862	A	2.3
14	BG	22	VAL	2.3
46	B	1126	G	2.3
46	CM	1441	G	2.3
48	D	164	VAL	2.3
1	1	1012	U	2.3
46	B	1613	U	2.3
50	F	168	PHE	2.3
22	BO	88	ARG	2.3
19	y	138	LEU	2.3
48	D	161	LEU	2.3
61	Q	97	LEU	2.3
47	CN	132	ALA	2.3
20	BM	96	MET	2.2
41	AN	47	PRO	2.2
70	DK	38	PHE	2.2
71	a	119	PHE	2.2
20	BM	9	ARG	2.2
29	AB	42	ARG	2.2
53	CT	74	ARG	2.2
74	d	26	GLN	2.2
1	1	940	C	2.2
1	1	2839	C	2.2
1	AS	1114	C	2.2
1	AS	1665	C	2.2
78	h	142	LEU	2.2
1	1	2675	A	2.2
1	AS	1584	A	2.2
47	CN	19	ALA	2.2
52	H	74	ALA	2.2
1	AS	170	G	2.2
6	AY	105	LYS	2.2
19	y	161	LYS	2.2
36	AI	83	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	AW	157	ILE	2.2
69	Y	14	ILE	2.2
13	s	18	VAL	2.2
56	CW	14	VAL	2.2
6	AY	48	ARG	2.2
27	BT	26	GLU	2.2
70	DK	32	ARG	2.2
51	G	44	LEU	2.2
6	AY	88	GLN	2.2
6	l	192	LYS	2.2
60	P	81	ALA	2.2
72	DM	97	LYS	2.2
4	AW	226	SER	2.2
18	x	20	SER	2.2
26	8	41	THR	2.2
34	AG	15	SER	2.2
43	CJ	7	THR	2.2
53	CT	78	SER	2.2
9	BB	94	PRO	2.2
29	BV	29	PRO	2.2
1	1	101	C	2.2
46	B	1602	C	2.2
1	1	82	U	2.2
1	AS	1160	A	2.2
7	AZ	55	PHE	2.2
7	AZ	142	PHE	2.2
3	4	22	U	2.2
46	B	1599	U	2.2
46	B	1618	A	2.2
60	DA	121	ARG	2.2
73	DN	89	ARG	2.2
1	1	1264	G	2.2
1	AS	420	G	2.2
16	BI	78	GLY	2.2
7	AZ	34	LYS	2.2
16	BI	182	LYS	2.2
53	I	143	LYS	2.2
56	L	29	LYS	2.2
6	l	249	ILE	2.2
79	AR	101	THR	2.2
13	s	168	ASP	2.2
16	v	204	SER	2.2

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Mol	Chain	Res	Type	RSRZ
18	BK	113	VAL	2.2
19	y	64	VAL	2.2
28	AA	72	VAL	2.2
33	AF	34	ARG	2.2
35	CB	23	VAL	2.2
51	CR	29	PRO	2.2
55	K	27	PHE	2.2
64	DE	110	VAL	2.2
5	k	324	LEU	2.2
6	AY	290	LEU	2.2
58	N	140	LEU	2.2
76	f	36	LEU	2.2
7	m	170	GLY	2.2
43	CJ	51	GLY	2.2
51	CR	8	HIS	2.2
1	1	30	C	2.2
1	AS	1879	A	2.2
1	AS	2431	U	2.2
46	B	378	U	2.2
46	CM	1412	C	2.2
46	CM	1613	U	2.2
14	BG	44	ALA	2.2
12	r	165	ILE	2.2
50	CQ	173	ILE	2.2
47	C	76	CYS	2.2
8	BA	52	VAL	2.2
32	BY	18	ARG	2.2
55	CV	21	PHE	2.2
58	N	72	THR	2.2
60	P	114	ARG	2.2
56	L	18	PRO	2.2
61	Q	121	THR	2.2
4	AW	208	ASP	2.2
6	l	137	LEU	2.2
19	BL	29	LEU	2.2
25	BR	109	LEU	2.2
51	CR	56	LEU	2.2
56	L	36	LEU	2.2
74	d	21	LEU	2.2
1	1	154	G	2.2
1	AS	219	G	2.2
1	AS	2936	G	2.2

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Mol	Chain	Res	Type	RSRZ
46	B	1115	G	2.2
5	k	74	GLU	2.2
22	2	94	GLU	2.2
8	n	7	LYS	2.2
42	AO	19	LYS	2.2
6	AY	233	HIS	2.2
24	6	35	TYR	2.2
64	DE	42	GLN	2.2
20	z	87	ALA	2.2
22	2	48	ILE	2.2
49	CP	87	ALA	2.2
66	DG	62	ALA	2.2
13	s	51	ARG	2.2
56	L	44	ARG	2.2
56	CW	3	ARG	2.2
16	BI	152	VAL	2.2
17	w	48	PHE	2.2
53	I	144	PHE	2.2
63	S	128	PHE	2.2
71	a	72	PHE	2.2
78	h	156	VAL	2.2
9	BB	107	THR	2.2
1	1	155	A	2.2
1	1	2308	C	2.2
3	AU	21	C	2.2
19	y	52	LEU	2.2
52	CS	194	LEU	2.2
60	P	117	LEU	2.2
65	U	140	THR	2.2
46	B	379	C	2.2
16	v	195	ASN	2.2
55	K	17	LYS	2.1
71	a	135	ASP	2.2
16	v	8	GLU	2.1
4	AW	232	GLY	2.1
9	o	125	ILE	2.1
22	BO	75	ILE	2.1
71	a	25	ILE	2.1
71	DL	88	ALA	2.1
54	CU	67	ARG	2.1
9	BB	232	PHE	2.1
11	BD	27	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
14	t	63	VAL	2.1
32	BY	92	VAL	2.1
36	AI	57	VAL	2.1
39	CF	25	VAL	2.1
1	1	1427	G	2.1
1	AS	1440	G	2.1
24	BQ	46	LEU	2.1
32	AE	19	LEU	2.1
54	CU	95	LEU	2.1
79	AR	32	LEU	2.1
67	W	66	THR	2.1
52	H	79	SER	2.1
1	AS	2322	U	2.1
46	B	1338	U	2.1
46	B	1400	U	2.1
40	CG	50	GLY	2.1
1	AS	3050	A	2.1
76	f	55	TYR	2.1
1	1	27	C	2.1
16	BI	26	ARG	2.1
18	BK	135	ARG	2.1
19	y	158	HIS	2.1
32	AE	31	ALA	2.1
60	DA	63	ALA	2.1
7	AZ	151	GLN	2.1
52	CS	170	GLN	2.1
27	BT	20	PHE	2.1
9	BB	104	LEU	2.1
19	BL	26	LEU	2.1
21	0	162	LEU	2.1
4	j	190	LYS	2.1
30	AC	24	PRO	2.1
65	U	2	PRO	2.1
66	DG	84	LYS	2.1
5	k	276	THR	2.1
55	K	62	THR	2.1
16	v	103	GLU	2.1
53	I	91	GLU	2.1
5	AX	369	ARG	2.1
10	BC	76	ILE	2.1
13	BF	145	ARG	2.1
20	z	97	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
35	CB	16	ARG	2.1
41	AN	37	ARG	2.1
55	CV	18	ARG	2.1
63	DD	132	GLY	2.1
1	AS	215	G	2.1
1	AS	419	G	2.1
1	AS	1489	G	2.1
1	AS	2099	G	2.1
1	AS	2430	G	2.1
33	AF	30	ALA	2.1
9	BB	222	GLN	2.1
15	u	119	GLN	2.1
7	m	131	LEU	2.1
16	BI	121	VAL	2.1
17	w	9	VAL	2.1
35	AH	34	HIS	2.1
27	9	30	LEU	2.1
32	BY	19	LEU	2.1
50	CQ	17	VAL	2.1
51	G	56	LEU	2.1
52	H	108	LEU	2.1
62	R	94	VAL	2.1
46	B	297	A	2.1
46	B	1136	A	2.1
51	G	43	PRO	2.1
1	AS	2942	C	2.1
4	AW	249	THR	2.1
46	B	1182	C	2.1
46	B	1726	C	2.1
52	H	147	THR	2.1
65	DF	47	CYS	2.1
5	AX	52	GLY	2.1
7	m	60	ILE	2.1
20	BM	15	ILE	2.1
20	BM	68	GLU	2.1
34	AG	100	ILE	2.1
59	O	49	SER	2.1
79	DT	78	GLY	2.1
8	n	163	PHE	2.1
47	C	14	ALA	2.1
8	BA	4	VAL	2.1
22	BO	89	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
27	9	95	VAL	2.1
50	CQ	73	LEU	2.1
75	e	48	VAL	2.1
9	o	88	LYS	2.1
48	CO	46	THR	2.1
64	T	55	THR	2.1
1	1	109	G	2.1
9	BB	93	ILE	2.1
46	B	750	G	2.1
46	B	1134	G	2.1
80	BE	149	ILE	2.1
63	DD	124	GLU	2.1
6	AY	329	ASN	2.1
10	p	200	ALA	2.1
12	r	199	PHE	2.1
16	BI	90	ASN	2.1
17	BJ	82	TYR	2.1
34	CA	50	ALA	2.1
46	B	1297	A	2.1
70	Z	4	GLY	2.1
76	DQ	43	PHE	2.1
4	AW	179	LEU	2.1
1	1	240	C	2.1
1	AS	1852	C	2.1
5	k	120	LYS	2.1
7	AZ	52	VAL	2.1
7	AZ	236	VAL	2.1
13	BF	80	LEU	2.1
15	u	126	LYS	2.1
17	w	8	VAL	2.1
17	BJ	54	LYS	2.1
36	AI	54	VAL	2.1
46	B	1621	C	2.1
48	CO	215	VAL	2.1
50	CQ	40	VAL	2.1
58	N	5	LEU	2.1
81	P0	15	LEU	2.1
14	t	19	GLN	2.1
43	AP	53	GLN	2.1
18	BK	128	ARG	2.1
39	AL	3	ARG	2.1
52	H	83	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
6	l	281	ILE	2.1
6	l	58	GLY	2.1
6	AY	195	LEU	2.1
6	AY	243	ALA	2.1
33	AF	14	TYR	2.1
38	AK	52	LYS	2.1
51	CR	38	LEU	2.1
59	O	101	ALA	2.1
70	Z	25	ALA	2.1
77	g	40	TYR	2.1
33	BZ	77	VAL	2.1
45	CL	36	SER	2.1
52	H	111	VAL	2.1
59	O	111	ASN	2.1
63	DD	68	VAL	2.1
12	r	59	GLN	2.0
50	CQ	175	HIS	2.0
53	CT	140	HIS	2.0
1	1	1139	A	2.0
1	AS	1487	A	2.0
1	AS	1782	G	2.0
46	B	1339	G	2.0
46	B	1779	G	2.0
16	BI	172	ARG	2.0
69	Y	28	ARG	2.0
1	1	2745	C	2.0
1	AS	944	C	2.0
1	AS	1185	C	2.0
78	h	133	ILE	2.0
56	L	147	THR	2.0
4	j	16	PHE	2.0
5	k	236	LYS	2.0
20	BM	128	LYS	2.0
34	AG	86	LYS	2.0
44	CK	14	PHE	2.0
9	BB	131	TYR	2.0
20	z	45	TYR	2.0
9	BB	132	VAL	2.0
11	BD	33	GLU	2.0
16	v	58	GLY	2.0
35	CB	62	TYR	2.0
63	DD	43	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
16	v	79	ALA	2.0
55	K	204	ALA	2.0
67	W	74	GLY	2.0
73	DN	14	GLY	2.0
49	CP	191	VAL	2.0
58	N	139	VAL	2.0
4	j	115	ASN	2.0
79	AR	35	SER	2.0
30	BW	7	HIS	2.0
52	CS	190	ILE	2.0
61	Q	14	ILE	2.0
7	m	20	PHE	2.0
30	BW	23	LYS	2.0
50	F	149	LYS	2.0
54	J	88	PHE	2.0
1	1	2350	A	2.0
5	AX	253	GLY	2.0
6	AY	287	VAL	2.0
24	BQ	53	ALA	2.0
33	AF	31	GLU	2.0
35	CB	65	VAL	2.0
38	AK	41	ALA	2.0
46	CM	1178	A	2.0
56	CW	4	ALA	2.0
62	R	97	TYR	2.0
1	AS	169	G	2.0
3	AU	150	G	2.0
1	1	26	C	2.0
1	1	965	C	2.0
46	B	695	C	2.0
73	DN	29	CYS	2.0
5	AX	243	HIS	2.0
6	AY	59	HIS	2.0
7	m	59	ASP	2.0
17	BJ	50	ARG	2.0
54	J	146	GLN	2.0
19	y	67	ILE	2.0
61	Q	76	ILE	2.0
33	AF	9	LYS	2.0
45	i	100	LYS	2.0
77	g	30	PRO	2.0
17	BJ	100	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
51	G	23	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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
84	MG	AS	3650	1/1	0.10	0.10	115,115,115,115	0
84	MG	BL	202	1/1	0.11	0.23	107,107,107,107	0
84	MG	1	3751	1/1	0.15	0.27	111,111,111,111	0
84	MG	AS	3713	1/1	0.22	0.26	95,95,95,95	0
84	MG	AS	3715	1/1	0.29	0.31	158,158,158,158	0
84	MG	1	3570	1/1	0.30	0.21	112,112,112,112	0
84	MG	1	3595	1/1	0.32	0.28	89,89,89,89	0
84	MG	1	3837	1/1	0.36	0.23	82,82,82,82	0
84	MG	AS	3756	1/1	0.36	0.20	69,69,69,69	0
84	MG	BC	301	1/1	0.36	0.32	125,125,125,125	0
84	MG	B	1886	1/1	0.36	0.12	66,66,66,66	0
84	MG	AS	3692	1/1	0.37	0.19	86,86,86,86	0
84	MG	1	3761	1/1	0.37	0.32	106,106,106,106	0
84	MG	CM	1830	1/1	0.37	0.23	96,96,96,96	0
84	MG	1	3726	1/1	0.38	0.13	96,96,96,96	0
84	MG	AS	3517	1/1	0.38	0.25	106,106,106,106	0
84	MG	AS	3576	1/1	0.39	0.20	97,97,97,97	0
84	MG	AS	3641	1/1	0.39	1.15	81,81,81,81	0
84	MG	1	3800	1/1	0.40	0.12	70,70,70,70	0
84	MG	AS	3649	1/1	0.40	0.18	101,101,101,101	0
84	MG	AS	3536	1/1	0.42	0.35	110,110,110,110	0
84	MG	1	3778	1/1	0.44	0.25	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	DK	201	1/1	0.44	0.15	91,91,91,91	0
84	MG	1	3741	1/1	0.45	0.25	98,98,98,98	0
84	MG	AS	3489	1/1	0.45	0.34	57,57,57,57	0
84	MG	AS	3529	1/1	0.46	0.14	88,88,88,88	0
84	MG	AS	3678	1/1	0.46	0.18	108,108,108,108	0
84	MG	AS	3735	1/1	0.47	0.24	89,89,89,89	0
84	MG	AS	3765	1/1	0.47	0.23	96,96,96,96	0
84	MG	1	3481	1/1	0.48	0.39	113,113,113,113	0
84	MG	AS	3560	1/1	0.49	0.31	96,96,96,96	0
84	MG	1	3756	1/1	0.49	0.16	79,79,79,79	0
84	MG	o	304	1/1	0.50	0.17	75,75,75,75	0
84	MG	1	3576	1/1	0.50	0.16	58,58,58,58	0
84	MG	1	3747	1/1	0.51	0.28	82,82,82,82	0
84	MG	AS	3752	1/1	0.51	0.22	115,115,115,115	0
84	MG	1	3870	1/1	0.52	0.44	87,87,87,87	0
84	MG	1	3408	1/1	0.52	0.17	71,71,71,71	0
84	MG	1	3711	1/1	0.52	0.19	64,64,64,64	0
84	MG	CM	1878	1/1	0.52	0.11	58,58,58,58	0
84	MG	1	3770	1/1	0.52	0.23	85,85,85,85	0
84	MG	AS	3580	1/1	0.53	0.14	80,80,80,80	0
84	MG	B	1803	1/1	0.53	0.26	113,113,113,113	0
84	MG	AY	402	1/1	0.53	0.19	120,120,120,120	0
84	MG	AS	3651	1/1	0.53	0.17	122,122,122,122	0
84	MG	AS	3518	1/1	0.54	0.24	88,88,88,88	0
84	MG	C	301	1/1	0.54	0.12	89,89,89,89	0
84	MG	AS	3710	1/1	0.54	0.20	69,69,69,69	0
84	MG	1	3505	1/1	0.55	0.16	77,77,77,77	0
84	MG	1	3605	1/1	0.55	0.16	60,60,60,60	0
84	MG	AS	3673	1/1	0.55	0.14	79,79,79,79	0
84	MG	1	3492	1/1	0.56	0.31	72,72,72,72	0
84	MG	AS	3481	1/1	0.56	0.28	76,76,76,76	0
84	MG	1	3441	1/1	0.56	0.31	71,71,71,71	0
84	MG	1	3678	1/1	0.56	0.21	75,75,75,75	0
84	MG	AS	3716	1/1	0.56	0.18	86,86,86,86	0
84	MG	AS	3717	1/1	0.56	0.30	79,79,79,79	0
84	MG	1	3744	1/1	0.56	0.17	84,84,84,84	0
84	MG	AS	3601	1/1	0.56	0.22	78,78,78,78	0
84	MG	AS	3789	1/1	0.57	0.15	94,94,94,94	0
84	MG	AS	3755	1/1	0.57	0.15	64,64,64,64	0
84	MG	CL	301	1/1	0.57	0.50	85,85,85,85	0
84	MG	B	1850	1/1	0.58	0.26	198,198,198,198	0
84	MG	AS	3569	1/1	0.58	0.28	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3723	1/1	0.58	0.28	72,72,72,72	0
84	MG	B	1900	1/1	0.58	0.19	101,101,101,101	0
84	MG	1	3662	1/1	0.58	0.12	88,88,88,88	0
84	MG	1	3675	1/1	0.58	0.25	77,77,77,77	0
84	MG	B	1802	1/1	0.59	0.25	67,67,67,67	0
84	MG	1	3476	1/1	0.59	0.24	80,80,80,80	0
84	MG	AS	3585	1/1	0.59	0.29	78,78,78,78	0
84	MG	AS	3588	1/1	0.59	0.28	72,72,72,72	0
84	MG	1	3415	1/1	0.59	0.15	69,69,69,69	0
84	MG	AS	3703	1/1	0.59	0.14	77,77,77,77	0
84	MG	B	1859	1/1	0.59	0.23	85,85,85,85	0
84	MG	1	3731	1/1	0.59	0.44	82,82,82,82	0
84	MG	1	3470	1/1	0.60	0.25	77,77,77,77	0
84	MG	AS	3790	1/1	0.60	0.24	98,98,98,98	0
84	MG	1	3508	1/1	0.60	0.59	123,123,123,123	0
84	MG	1	3776	1/1	0.60	0.28	66,66,66,66	0
84	MG	1	3754	1/1	0.60	0.17	108,108,108,108	0
84	MG	AS	3539	1/1	0.60	0.22	95,95,95,95	0
84	MG	AS	3618	1/1	0.60	0.17	73,73,73,73	0
84	MG	1	3730	1/1	0.60	0.38	70,70,70,70	0
84	MG	1	3824	1/1	0.60	0.20	80,80,80,80	0
84	MG	AS	3568	1/1	0.61	0.20	81,81,81,81	0
84	MG	B	1821	1/1	0.61	0.24	80,80,80,80	0
84	MG	AS	3584	1/1	0.61	0.19	99,99,99,99	0
84	MG	AS	3614	1/1	0.61	0.12	74,74,74,74	0
84	MG	1	3665	1/1	0.62	0.19	70,70,70,70	0
84	MG	AS	3511	1/1	0.62	0.23	75,75,75,75	0
84	MG	1	3794	1/1	0.62	0.13	71,71,71,71	0
84	MG	CG	101	1/1	0.63	0.13	101,101,101,101	0
84	MG	1	3742	1/1	0.63	0.15	69,69,69,69	0
84	MG	AS	3592	1/1	0.63	0.22	66,66,66,66	0
84	MG	1	3417	1/1	0.63	0.25	82,82,82,82	0
84	MG	AS	3426	1/1	0.63	0.22	56,56,56,56	0
84	MG	1	3799	1/1	0.64	0.10	78,78,78,78	0
84	MG	1	3490	1/1	0.64	0.24	47,47,47,47	0
84	MG	1	3823	1/1	0.64	0.15	99,99,99,99	0
84	MG	AS	3512	1/1	0.64	0.27	78,78,78,78	0
84	MG	1	3763	1/1	0.64	0.11	61,61,61,61	0
84	MG	1	3567	1/1	0.64	0.25	87,87,87,87	0
84	MG	B	1834	1/1	0.64	0.23	63,63,63,63	0
84	MG	1	3672	1/1	0.65	0.24	68,68,68,68	0
84	MG	1	3405	1/1	0.65	0.23	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3783	1/1	0.65	0.20	84,84,84,84	0
84	MG	1	3535	1/1	0.65	0.27	86,86,86,86	0
84	MG	1	3788	1/1	0.65	0.23	78,78,78,78	0
84	MG	1	3733	1/1	0.65	0.37	83,83,83,83	0
84	MG	AS	3532	1/1	0.65	0.31	65,65,65,65	0
84	MG	AS	3729	1/1	0.65	0.13	71,71,71,71	0
84	MG	1	3740	1/1	0.65	0.22	79,79,79,79	0
84	MG	AS	3739	1/1	0.65	0.35	93,93,93,93	0
84	MG	AS	3751	1/1	0.65	0.13	81,81,81,81	0
84	MG	1	3543	1/1	0.65	0.21	58,58,58,58	0
84	MG	1	3585	1/1	0.65	0.18	98,98,98,98	0
84	MG	1	3691	1/1	0.66	0.10	73,73,73,73	0
84	MG	1	3697	1/1	0.66	0.16	74,74,74,74	0
84	MG	AS	3709	1/1	0.66	0.06	90,90,90,90	0
84	MG	AS	3759	1/1	0.66	0.29	81,81,81,81	0
84	MG	1	3599	1/1	0.66	0.13	72,72,72,72	0
84	MG	CM	1816	1/1	0.66	0.24	67,67,67,67	0
84	MG	AS	3674	1/1	0.66	0.10	94,94,94,94	0
84	MG	CM	1847	1/1	0.66	0.16	85,85,85,85	0
84	MG	AS	3744	1/1	0.66	0.28	71,71,71,71	0
84	MG	1	3689	1/1	0.66	0.23	78,78,78,78	0
84	MG	3	206	1/1	0.67	0.20	83,83,83,83	0
84	MG	1	3565	1/1	0.67	0.10	49,49,49,49	0
84	MG	AS	3433	1/1	0.67	0.23	60,60,60,60	0
84	MG	AX	401	1/1	0.67	0.09	76,76,76,76	0
84	MG	CM	1846	1/1	0.67	0.23	69,69,69,69	0
84	MG	B	1831	1/1	0.67	0.20	79,79,79,79	0
84	MG	AS	3764	1/1	0.67	0.12	86,86,86,86	0
84	MG	DG	201	1/1	0.67	0.16	121,121,121,121	0
84	MG	1	3593	1/1	0.67	0.22	83,83,83,83	0
84	MG	1	3717	1/1	0.68	0.25	54,54,54,54	0
84	MG	1	3681	1/1	0.68	0.14	63,63,63,63	0
84	MG	1	3847	1/1	0.68	0.13	68,68,68,68	0
84	MG	1	3451	1/1	0.68	0.14	50,50,50,50	0
84	MG	1	3411	1/1	0.68	0.16	90,90,90,90	0
84	MG	AS	3714	1/1	0.68	0.21	54,54,54,54	0
84	MG	CM	1826	1/1	0.68	0.15	69,69,69,69	0
84	MG	1	3609	1/1	0.68	0.14	82,82,82,82	0
84	MG	AS	3525	1/1	0.68	0.16	46,46,46,46	0
84	MG	1	3817	1/1	0.68	0.22	101,101,101,101	0
84	MG	1	3821	1/1	0.68	0.17	64,64,64,64	0
84	MG	1	3528	1/1	0.68	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3681	1/1	0.68	0.23	82,82,82,82	0
84	MG	AS	3704	1/1	0.69	0.12	75,75,75,75	0
84	MG	1	3787	1/1	0.69	0.13	76,76,76,76	0
84	MG	1	3698	1/1	0.69	0.21	79,79,79,79	0
84	MG	B	1885	1/1	0.69	0.15	100,100,100,100	0
84	MG	AS	3656	1/1	0.69	0.17	70,70,70,70	0
84	MG	AS	3663	1/1	0.69	0.19	103,103,103,103	0
84	MG	1	3732	1/1	0.69	0.28	65,65,65,65	0
84	MG	CM	1838	1/1	0.69	0.20	101,101,101,101	0
84	MG	1	3825	1/1	0.69	0.18	104,104,104,104	0
84	MG	1	3547	1/1	0.69	0.19	72,72,72,72	0
84	MG	CM	1871	1/1	0.69	0.20	76,76,76,76	0
84	MG	1	3482	1/1	0.69	0.13	99,99,99,99	0
84	MG	AS	3625	1/1	0.69	0.09	66,66,66,66	0
84	MG	1	3785	1/1	0.69	0.23	35,35,35,35	0
84	MG	1	3692	1/1	0.70	0.21	56,56,56,56	0
84	MG	AS	3428	1/1	0.70	0.17	71,71,71,71	0
84	MG	1	3856	1/1	0.70	0.24	91,91,91,91	0
84	MG	AS	3633	1/1	0.70	0.27	43,43,43,43	0
84	MG	AS	3472	1/1	0.70	0.25	64,64,64,64	0
84	MG	AS	3563	1/1	0.70	0.18	75,75,75,75	0
84	MG	1	3606	1/1	0.70	0.30	67,67,67,67	0
84	MG	CM	1850	1/1	0.70	0.16	63,63,63,63	0
84	MG	1	3807	1/1	0.70	0.27	65,65,65,65	0
84	MG	AS	3757	1/1	0.70	0.24	65,65,65,65	0
84	MG	BZ	201	1/1	0.70	0.12	70,70,70,70	0
84	MG	AS	3725	1/1	0.70	0.06	89,89,89,89	0
84	MG	1	3845	1/1	0.71	0.26	60,60,60,60	0
84	MG	1	3546	1/1	0.71	0.15	82,82,82,82	0
84	MG	1	3709	1/1	0.71	0.12	53,53,53,53	0
84	MG	AZ	301	1/1	0.71	0.18	82,82,82,82	0
84	MG	AS	3570	1/1	0.71	0.18	87,87,87,87	0
84	MG	B	1868	1/1	0.71	0.16	64,64,64,64	0
84	MG	1	3748	1/1	0.71	0.22	86,86,86,86	0
84	MG	1	3572	1/1	0.71	0.28	45,45,45,45	0
84	MG	AS	3741	1/1	0.71	0.15	85,85,85,85	0
84	MG	1	3412	1/1	0.71	0.14	66,66,66,66	0
84	MG	1	3722	1/1	0.71	0.13	82,82,82,82	0
84	MG	E	301	1/1	0.71	0.11	54,54,54,54	0
84	MG	AS	3697	1/1	0.71	0.20	65,65,65,65	0
84	MG	CM	1843	1/1	0.71	0.16	80,80,80,80	0
84	MG	1	3506	1/1	0.71	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3832	1/1	0.71	0.22	62,62,62,62	0
84	MG	AS	3705	1/1	0.71	0.24	78,78,78,78	0
84	MG	1	3418	1/1	0.71	0.09	64,64,64,64	0
84	MG	AS	3542	1/1	0.71	0.28	61,61,61,61	0
84	MG	AS	3545	1/1	0.71	0.24	84,84,84,84	0
84	MG	AS	3443	1/1	0.71	0.24	62,62,62,62	0
84	MG	AS	3737	1/1	0.72	0.34	107,107,107,107	0
84	MG	1	3461	1/1	0.72	0.26	59,59,59,59	0
84	MG	1	3806	1/1	0.72	0.18	44,44,44,44	0
84	MG	B	1844	1/1	0.72	0.12	45,45,45,45	0
84	MG	AS	3745	1/1	0.72	0.14	104,104,104,104	0
84	MG	Y	202	1/1	0.72	0.17	108,108,108,108	0
84	MG	CM	1805	1/1	0.72	0.33	63,63,63,63	0
84	MG	AS	3552	1/1	0.72	0.22	77,77,77,77	0
84	MG	AS	3667	1/1	0.72	0.07	70,70,70,70	0
84	MG	AS	3516	1/1	0.72	0.12	90,90,90,90	0
84	MG	1	3830	1/1	0.72	0.14	49,49,49,49	0
84	MG	1	3587	1/1	0.72	0.16	96,96,96,96	0
84	MG	1	3661	1/1	0.72	0.15	102,102,102,102	0
84	MG	AS	3718	1/1	0.72	0.12	60,60,60,60	0
84	MG	AS	3720	1/1	0.72	0.19	60,60,60,60	0
84	MG	AS	3721	1/1	0.72	0.11	83,83,83,83	0
84	MG	AS	3686	1/1	0.72	0.18	75,75,75,75	0
84	MG	1	3516	1/1	0.72	0.09	86,86,86,86	0
84	MG	1	3745	1/1	0.72	0.24	80,80,80,80	0
84	MG	B	1806	1/1	0.73	0.23	99,99,99,99	0
84	MG	AS	3484	1/1	0.73	0.15	64,64,64,64	0
84	MG	1	3850	1/1	0.73	0.07	57,57,57,57	0
84	MG	1	3693	1/1	0.73	0.16	53,53,53,53	0
84	MG	1	3624	1/1	0.73	0.09	63,63,63,63	0
84	MG	1	3804	1/1	0.73	0.19	85,85,85,85	0
84	MG	AS	3567	1/1	0.73	0.14	82,82,82,82	0
84	MG	a	201	1/1	0.73	0.13	78,78,78,78	0
84	MG	1	3841	1/1	0.73	0.15	71,71,71,71	0
84	MG	CM	1845	1/1	0.73	0.13	57,57,57,57	0
84	MG	AS	3642	1/1	0.73	0.10	62,62,62,62	0
84	MG	AD	201	1/1	0.73	0.26	58,58,58,58	0
84	MG	AX	402	1/1	0.73	0.12	81,81,81,81	0
84	MG	AS	3572	1/1	0.73	0.22	94,94,94,94	0
84	MG	CM	1877	1/1	0.73	0.13	97,97,97,97	0
84	MG	1	3625	1/1	0.73	0.31	86,86,86,86	0
84	MG	B	1872	1/1	0.73	0.21	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3530	1/1	0.73	0.10	61,61,61,61	0
84	MG	B	1810	1/1	0.74	0.23	78,78,78,78	0
84	MG	AS	3575	1/1	0.74	0.14	38,38,38,38	0
84	MG	CM	1823	1/1	0.74	0.28	44,44,44,44	0
84	MG	AS	3509	1/1	0.74	0.13	62,62,62,62	0
84	MG	B	1815	1/1	0.74	0.10	64,64,64,64	0
84	MG	B	1820	1/1	0.74	0.10	66,66,66,66	0
84	MG	AS	3515	1/1	0.74	0.24	66,66,66,66	0
84	MG	1	3647	1/1	0.74	0.22	49,49,49,49	0
84	MG	1	3534	1/1	0.74	0.28	54,54,54,54	0
84	MG	B	1897	1/1	0.74	0.20	94,94,94,94	0
84	MG	AS	3749	1/1	0.74	0.25	73,73,73,73	0
84	MG	AS	3611	1/1	0.74	0.23	56,56,56,56	0
84	MG	AS	3612	1/1	0.74	0.21	77,77,77,77	0
84	MG	1	3752	1/1	0.74	0.20	77,77,77,77	0
84	MG	1	3571	1/1	0.74	0.08	94,94,94,94	0
84	MG	1	3828	1/1	0.74	0.28	81,81,81,81	0
84	MG	1	3654	1/1	0.75	0.23	102,102,102,102	0
84	MG	B	1892	1/1	0.75	0.23	81,81,81,81	0
84	MG	CM	1831	1/1	0.75	0.26	58,58,58,58	0
84	MG	1	3558	1/1	0.75	0.13	69,69,69,69	0
84	MG	1	3685	1/1	0.75	0.09	96,96,96,96	0
84	MG	CM	1844	1/1	0.75	0.20	78,78,78,78	0
84	MG	AS	3435	1/1	0.75	0.22	72,72,72,72	0
84	MG	1	3820	1/1	0.75	0.35	88,88,88,88	0
84	MG	AS	3724	1/1	0.75	0.12	87,87,87,87	0
84	MG	1	3538	1/1	0.75	0.18	59,59,59,59	0
84	MG	AS	3662	1/1	0.75	0.18	78,78,78,78	0
84	MG	G	301	1/1	0.75	0.11	68,68,68,68	0
84	MG	AS	3620	1/1	0.75	0.14	62,62,62,62	0
84	MG	1	3768	1/1	0.75	0.10	62,62,62,62	0
84	MG	AS	3631	1/1	0.75	0.23	53,53,53,53	0
84	MG	B	1857	1/1	0.76	0.22	50,50,50,50	0
84	MG	AS	3596	1/1	0.76	0.11	70,70,70,70	0
84	MG	1	3834	1/1	0.76	0.15	90,90,90,90	0
84	MG	AS	3528	1/1	0.76	0.20	83,83,83,83	0
84	MG	1	3427	1/1	0.76	0.18	64,64,64,64	0
84	MG	1	3545	1/1	0.76	0.11	50,50,50,50	0
84	MG	AS	3534	1/1	0.76	0.15	113,113,113,113	0
84	MG	1	3423	1/1	0.76	0.19	103,103,103,103	0
84	MG	1	3674	1/1	0.76	0.17	67,67,67,67	0
84	MG	1	3495	1/1	0.76	0.20	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	CM	1857	1/1	0.76	0.10	83,83,83,83	0
84	MG	CM	1869	1/1	0.76	0.25	64,64,64,64	0
84	MG	B	1804	1/1	0.76	0.15	77,77,77,77	0
84	MG	AS	3634	1/1	0.76	0.17	58,58,58,58	0
84	MG	AS	3638	1/1	0.76	0.16	76,76,76,76	0
84	MG	B	1899	1/1	0.76	0.12	83,83,83,83	0
84	MG	1	3758	1/1	0.76	0.17	67,67,67,67	0
85	ZN	d	101	1/1	0.76	0.09	314,314,314,314	0
84	MG	AS	3630	1/1	0.77	0.16	74,74,74,74	0
84	MG	1	3575	1/1	0.77	0.13	59,59,59,59	0
84	MG	1	3402	1/1	0.77	0.30	69,69,69,69	0
84	MG	1	3641	1/1	0.77	0.15	71,71,71,71	0
84	MG	AS	3635	1/1	0.77	0.24	76,76,76,76	0
84	MG	1	3582	1/1	0.77	0.16	49,49,49,49	0
84	MG	AS	3573	1/1	0.77	0.18	68,68,68,68	0
84	MG	1	3650	1/1	0.77	0.24	59,59,59,59	0
84	MG	AS	3412	1/1	0.77	0.25	84,84,84,84	0
84	MG	AS	3579	1/1	0.77	0.18	45,45,45,45	0
84	MG	B	1856	1/1	0.77	0.15	148,148,148,148	0
84	MG	0	201	1/1	0.77	0.14	87,87,87,87	0
84	MG	AS	3530	1/1	0.77	0.26	68,68,68,68	0
84	MG	AS	3586	1/1	0.77	0.28	61,61,61,61	0
84	MG	AS	3665	1/1	0.77	0.12	75,75,75,75	0
84	MG	1	3700	1/1	0.77	0.23	77,77,77,77	0
84	MG	1	3704	1/1	0.77	0.17	60,60,60,60	0
84	MG	CM	1841	1/1	0.77	0.09	42,42,42,42	0
84	MG	1	3489	1/1	0.77	0.35	67,67,67,67	0
84	MG	AS	3460	1/1	0.77	0.16	48,48,48,48	0
84	MG	1	3803	1/1	0.77	0.10	63,63,63,63	0
84	MG	AS	3682	1/1	0.77	0.24	67,67,67,67	0
84	MG	1	3762	1/1	0.77	0.21	82,82,82,82	0
84	MG	B	1809	1/1	0.77	0.18	71,71,71,71	0
84	MG	AS	3695	1/1	0.77	0.15	67,67,67,67	0
84	MG	AS	3696	1/1	0.77	0.27	78,78,78,78	0
84	MG	AS	3758	1/1	0.77	0.23	77,77,77,77	0
84	MG	AS	3615	1/1	0.77	0.12	102,102,102,102	0
84	MG	1	3683	1/1	0.77	0.19	74,74,74,74	0
84	MG	1	3431	1/1	0.77	0.23	41,41,41,41	0
84	MG	1	3591	1/1	0.77	0.11	45,45,45,45	0
84	MG	AS	3707	1/1	0.77	0.16	42,42,42,42	0
84	MG	1	3703	1/1	0.78	0.17	59,59,59,59	0
84	MG	1	3687	1/1	0.78	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	B	1812	1/1	0.78	0.19	52,52,52,52	0
84	MG	AS	3712	1/1	0.78	0.11	94,94,94,94	0
84	MG	1	3568	1/1	0.78	0.26	67,67,67,67	0
84	MG	o	301	1/1	0.78	0.29	67,67,67,67	0
84	MG	1	3463	1/1	0.78	0.26	32,32,32,32	0
84	MG	1	3578	1/1	0.78	0.30	72,72,72,72	0
84	MG	AS	3622	1/1	0.78	0.15	74,74,74,74	0
84	MG	AS	3623	1/1	0.78	0.12	70,70,70,70	0
84	MG	1	3618	1/1	0.78	0.18	63,63,63,63	0
84	MG	B	1835	1/1	0.78	0.14	67,67,67,67	0
84	MG	AS	3535	1/1	0.78	0.39	111,111,111,111	0
84	MG	1	3548	1/1	0.78	0.25	48,48,48,48	0
84	MG	B	1845	1/1	0.78	0.12	89,89,89,89	0
84	MG	AY	401	1/1	0.78	0.19	82,82,82,82	0
84	MG	1	3791	1/1	0.78	0.09	51,51,51,51	0
84	MG	R	201	1/1	0.78	0.28	61,61,61,61	0
84	MG	BB	302	1/1	0.78	0.18	83,83,83,83	0
84	MG	AS	3547	1/1	0.78	0.13	98,98,98,98	0
84	MG	1	3553	1/1	0.78	0.08	66,66,66,66	0
84	MG	AS	3645	1/1	0.78	0.24	72,72,72,72	0
84	MG	1	3630	1/1	0.78	0.12	39,39,39,39	0
84	MG	AS	3659	1/1	0.79	0.15	63,63,63,63	0
84	MG	1	3485	1/1	0.79	0.10	69,69,69,69	0
84	MG	AS	3503	1/1	0.79	0.16	83,83,83,83	0
84	MG	1	3478	1/1	0.79	0.18	53,53,53,53	0
84	MG	AS	3666	1/1	0.79	0.13	74,74,74,74	0
84	MG	1	3802	1/1	0.79	0.14	54,54,54,54	0
84	MG	AS	3668	1/1	0.79	0.18	68,68,68,68	0
84	MG	1	3480	1/1	0.79	0.10	57,57,57,57	0
84	MG	1	3670	1/1	0.79	0.20	77,77,77,77	0
84	MG	1	3515	1/1	0.79	0.17	70,70,70,70	0
84	MG	AS	3587	1/1	0.79	0.18	83,83,83,83	0
84	MG	B	1893	1/1	0.79	0.18	87,87,87,87	0
84	MG	1	3573	1/1	0.79	0.14	76,76,76,76	0
84	MG	AS	3519	1/1	0.79	0.16	110,110,110,110	0
84	MG	1	3449	1/1	0.79	0.34	54,54,54,54	0
84	MG	AS	3602	1/1	0.79	0.16	76,76,76,76	0
84	MG	AS	3606	1/1	0.79	0.19	83,83,83,83	0
84	MG	AS	3699	1/1	0.79	0.23	79,79,79,79	0
84	MG	AS	3700	1/1	0.79	0.16	95,95,95,95	0
84	MG	BL	201	1/1	0.79	0.16	66,66,66,66	0
84	MG	AS	3527	1/1	0.79	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3610	1/1	0.79	0.14	67,67,67,67	0
84	MG	AS	3613	1/1	0.79	0.23	71,71,71,71	0
84	MG	1	3680	1/1	0.79	0.20	70,70,70,70	0
84	MG	1	3614	1/1	0.79	0.13	83,83,83,83	0
84	MG	1	3493	1/1	0.79	0.23	65,65,65,65	0
84	MG	1	3425	1/1	0.79	0.28	36,36,36,36	0
84	MG	1	3827	1/1	0.79	0.21	50,50,50,50	0
84	MG	1	3579	1/1	0.79	0.24	93,93,93,93	0
84	MG	AS	3406	1/1	0.79	0.12	122,122,122,122	0
84	MG	1	3496	1/1	0.79	0.30	69,69,69,69	0
84	MG	AS	3413	1/1	0.79	0.38	71,71,71,71	0
84	MG	B	1828	1/1	0.79	0.18	70,70,70,70	0
84	MG	1	3583	1/1	0.79	0.10	81,81,81,81	0
84	MG	AS	3556	1/1	0.79	0.10	76,76,76,76	0
84	MG	1	3559	1/1	0.79	0.09	23,23,23,23	0
84	MG	1	3504	1/1	0.79	0.17	65,65,65,65	0
84	MG	1	3789	1/1	0.79	0.09	67,67,67,67	0
84	MG	AS	3446	1/1	0.79	0.13	55,55,55,55	0
84	MG	1	3790	1/1	0.79	0.18	56,56,56,56	0
84	MG	1	3694	1/1	0.79	0.14	84,84,84,84	0
84	MG	1	3536	1/1	0.79	0.27	73,73,73,73	0
84	MG	AS	3743	1/1	0.79	0.21	73,73,73,73	0
84	MG	AS	3654	1/1	0.79	0.42	87,87,87,87	0
84	MG	AS	3655	1/1	0.79	0.21	99,99,99,99	0
84	MG	1	3795	1/1	0.79	0.10	68,68,68,68	0
84	MG	AS	3684	1/1	0.80	0.19	63,63,63,63	0
84	MG	AS	3422	1/1	0.80	0.45	36,36,36,36	0
84	MG	v	302	1/1	0.80	0.14	77,77,77,77	0
84	MG	1	3519	1/1	0.80	0.26	80,80,80,80	0
84	MG	AS	3776	1/1	0.80	0.18	88,88,88,88	0
84	MG	1	3414	1/1	0.80	0.29	72,72,72,72	0
84	MG	AS	3788	1/1	0.80	0.12	63,63,63,63	0
84	MG	AS	3616	1/1	0.80	0.22	61,61,61,61	0
84	MG	1	3783	1/1	0.80	0.09	66,66,66,66	0
84	MG	AT	203	1/1	0.80	0.18	70,70,70,70	0
84	MG	AS	3437	1/1	0.80	0.17	68,68,68,68	0
84	MG	AS	3621	1/1	0.80	0.08	61,61,61,61	0
84	MG	AS	3439	1/1	0.80	0.27	67,67,67,67	0
84	MG	B	1860	1/1	0.80	0.18	73,73,73,73	0
84	MG	AS	3555	1/1	0.80	0.10	80,80,80,80	0
84	MG	AS	3444	1/1	0.80	0.18	52,52,52,52	0
84	MG	B	1861	1/1	0.80	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3644	1/1	0.80	0.13	62,62,62,62	0
84	MG	AS	3564	1/1	0.80	0.11	60,60,60,60	0
84	MG	1	3542	1/1	0.80	0.26	55,55,55,55	0
84	MG	AS	3475	1/1	0.80	0.10	62,62,62,62	0
84	MG	B	1884	1/1	0.80	0.18	58,58,58,58	0
84	MG	1	3592	1/1	0.80	0.18	73,73,73,73	0
84	MG	AS	3571	1/1	0.80	0.15	84,84,84,84	0
84	MG	1	3514	1/1	0.80	0.22	87,87,87,87	0
84	MG	AS	3498	1/1	0.80	0.21	48,48,48,48	0
84	MG	1	3849	1/1	0.80	0.09	70,70,70,70	0
84	MG	1	3426	1/1	0.80	0.27	51,51,51,51	0
84	MG	1	3725	1/1	0.80	0.17	90,90,90,90	0
84	MG	AS	3731	1/1	0.80	0.22	77,77,77,77	0
84	MG	B	1818	1/1	0.80	0.20	57,57,57,57	0
84	MG	AS	3583	1/1	0.80	0.34	60,60,60,60	0
84	MG	1	3765	1/1	0.80	0.26	98,98,98,98	0
84	MG	1	3497	1/1	0.80	0.33	78,78,78,78	0
84	MG	j	301	1/1	0.80	0.15	65,65,65,65	0
84	MG	B	1829	1/1	0.80	0.15	56,56,56,56	0
84	MG	CM	1856	1/1	0.80	0.21	88,88,88,88	0
84	MG	1	3769	1/1	0.80	0.12	51,51,51,51	0
84	MG	AS	3748	1/1	0.80	0.15	67,67,67,67	0
84	MG	Y	201	1/1	0.80	0.22	85,85,85,85	0
84	MG	o	303	1/1	0.80	0.28	56,56,56,56	0
84	MG	1	3603	1/1	0.80	0.26	54,54,54,54	0
84	MG	B	1841	1/1	0.80	0.35	73,73,73,73	0
84	MG	u	201	1/1	0.80	0.13	83,83,83,83	0
84	MG	v	301	1/1	0.80	0.14	56,56,56,56	0
84	MG	AT	201	1/1	0.81	0.12	59,59,59,59	0
84	MG	1	3560	1/1	0.81	0.09	66,66,66,66	0
84	MG	B	1895	1/1	0.81	0.16	78,78,78,78	0
84	MG	B	1896	1/1	0.81	0.10	78,78,78,78	0
84	MG	AS	3653	1/1	0.81	0.16	54,54,54,54	0
84	MG	1	3779	1/1	0.81	0.12	60,60,60,60	0
84	MG	1	3637	1/1	0.81	0.21	65,65,65,65	0
84	MG	BB	301	1/1	0.81	0.22	60,60,60,60	0
84	MG	1	3638	1/1	0.81	0.15	89,89,89,89	0
84	MG	AS	3478	1/1	0.81	0.09	74,74,74,74	0
84	MG	1	3639	1/1	0.81	0.11	61,61,61,61	0
84	MG	AS	3609	1/1	0.81	0.20	98,98,98,98	0
84	MG	AS	3610	1/1	0.81	0.14	83,83,83,83	0
84	MG	B	1839	1/1	0.81	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AB	201	1/1	0.81	0.11	55,55,55,55	0
84	MG	AC	101	1/1	0.81	0.08	59,59,59,59	0
84	MG	1	3466	1/1	0.81	0.12	79,79,79,79	0
84	MG	AS	3562	1/1	0.81	0.24	61,61,61,61	0
84	MG	CM	1825	1/1	0.81	0.21	51,51,51,51	0
84	MG	AS	3504	1/1	0.81	0.11	74,74,74,74	0
84	MG	1	3479	1/1	0.81	0.32	49,49,49,49	0
84	MG	1	3809	1/1	0.81	0.11	179,179,179,179	0
84	MG	AS	3683	1/1	0.81	0.19	61,61,61,61	0
84	MG	1	3810	1/1	0.81	0.18	144,144,144,144	0
84	MG	1	3813	1/1	0.81	0.08	69,69,69,69	0
84	MG	1	3749	1/1	0.81	0.16	77,77,77,77	0
84	MG	1	3819	1/1	0.81	0.18	84,84,84,84	0
84	MG	AS	3627	1/1	0.81	0.30	72,72,72,72	0
84	MG	1	3646	1/1	0.81	0.17	86,86,86,86	0
84	MG	B	1814	1/1	0.81	0.27	40,40,40,40	0
84	MG	AS	3632	1/1	0.81	0.12	85,85,85,85	0
84	MG	AS	3523	1/1	0.81	0.13	103,103,103,103	0
84	MG	1	3793	1/1	0.81	0.09	46,46,46,46	0
84	MG	AS	3770	1/1	0.81	0.08	61,61,61,61	0
84	MG	AS	3526	1/1	0.81	0.16	80,80,80,80	0
84	MG	AS	3434	1/1	0.81	0.31	64,64,64,64	0
84	MG	1	3454	1/1	0.81	0.24	59,59,59,59	0
84	MG	1	3457	1/1	0.81	0.24	43,43,43,43	0
84	MG	1	3796	1/1	0.81	0.10	105,105,105,105	0
84	MG	AS	3784	1/1	0.82	0.07	57,57,57,57	0
84	MG	y	201	1/1	0.82	0.12	63,63,63,63	0
84	MG	1	3510	1/1	0.82	0.18	56,56,56,56	0
84	MG	B	1832	1/1	0.82	0.12	92,92,92,92	0
84	MG	1	3805	1/1	0.82	0.10	84,84,84,84	0
84	MG	AS	3440	1/1	0.82	0.21	42,42,42,42	0
84	MG	AS	3646	1/1	0.82	0.23	74,74,74,74	0
84	MG	AS	3711	1/1	0.82	0.20	78,78,78,78	0
84	MG	1	3771	1/1	0.82	0.16	64,64,64,64	0
84	MG	B	1838	1/1	0.82	0.17	38,38,38,38	0
84	MG	1	3853	1/1	0.82	0.09	106,106,106,106	0
84	MG	AS	3459	1/1	0.82	0.12	66,66,66,66	0
84	MG	1	3555	1/1	0.82	0.25	70,70,70,70	0
84	MG	1	3863	1/1	0.82	0.19	83,83,83,83	0
84	MG	AS	3603	1/1	0.82	0.23	38,38,38,38	0
84	MG	AS	3658	1/1	0.82	0.21	59,59,59,59	0
84	MG	1	3869	1/1	0.82	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	CB	202	1/1	0.82	0.14	65,65,65,65	0
84	MG	1	3533	1/1	0.82	0.26	37,37,37,37	0
84	MG	3	201	1/1	0.82	0.22	63,63,63,63	0
84	MG	AS	3551	1/1	0.82	0.10	74,74,74,74	0
84	MG	R	204	1/1	0.82	0.24	55,55,55,55	0
84	MG	CM	1821	1/1	0.82	0.30	77,77,77,77	0
84	MG	AS	3485	1/1	0.82	0.14	91,91,91,91	0
84	MG	1	3597	1/1	0.82	0.21	97,97,97,97	1
84	MG	AS	3670	1/1	0.82	0.13	98,98,98,98	0
84	MG	AS	3740	1/1	0.82	0.10	40,40,40,40	0
84	MG	1	3734	1/1	0.82	0.10	73,73,73,73	0
84	MG	CM	1832	1/1	0.82	0.19	99,99,99,99	0
84	MG	AS	3500	1/1	0.82	0.20	80,80,80,80	0
84	MG	AS	3676	1/1	0.82	0.12	61,61,61,61	0
84	MG	1	3735	1/1	0.82	0.10	87,87,87,87	0
84	MG	AS	3680	1/1	0.82	0.06	108,108,108,108	0
84	MG	1	3499	1/1	0.82	0.36	50,50,50,50	0
84	MG	AS	3408	1/1	0.82	0.09	87,87,87,87	0
84	MG	B	1867	1/1	0.82	0.17	62,62,62,62	0
84	MG	1	3580	1/1	0.82	0.27	60,60,60,60	0
84	MG	AS	3685	1/1	0.82	0.24	67,67,67,67	0
84	MG	AS	3420	1/1	0.82	0.15	50,50,50,50	0
84	MG	CM	1868	1/1	0.82	0.25	74,74,74,74	0
84	MG	AS	3691	1/1	0.82	0.10	59,59,59,59	0
84	MG	1	3842	1/1	0.82	0.14	88,88,88,88	0
84	MG	B	1878	1/1	0.82	0.19	102,102,102,102	0
84	MG	1	3753	1/1	0.82	0.42	79,79,79,79	0
84	MG	CM	1879	1/1	0.82	0.15	61,61,61,61	0
84	MG	AS	3431	1/1	0.82	0.14	60,60,60,60	0
84	MG	1	3846	1/1	0.82	0.15	99,99,99,99	0
84	MG	AS	3524	1/1	0.82	0.11	83,83,83,83	0
84	MG	AS	3787	1/1	0.83	0.16	96,96,96,96	0
84	MG	1	3767	1/1	0.83	0.08	58,58,58,58	0
84	MG	B	1858	1/1	0.83	0.13	48,48,48,48	0
84	MG	1	3458	1/1	0.83	0.21	65,65,65,65	0
84	MG	1	3859	1/1	0.83	0.24	59,59,59,59	0
84	MG	AS	3708	1/1	0.83	0.10	71,71,71,71	0
84	MG	1	3860	1/1	0.83	0.12	54,54,54,54	0
84	MG	AS	3423	1/1	0.83	0.20	61,61,61,61	0
84	MG	AX	403	1/1	0.83	0.27	45,45,45,45	0
84	MG	B	1862	1/1	0.83	0.21	76,76,76,76	0
84	MG	1	3701	1/1	0.83	0.06	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3727	1/1	0.83	0.31	61,61,61,61	0
84	MG	1	3797	1/1	0.83	0.14	48,48,48,48	0
84	MG	1	3651	1/1	0.83	0.26	55,55,55,55	0
84	MG	1	3640	1/1	0.83	0.16	48,48,48,48	0
84	MG	AS	3597	1/1	0.83	0.15	70,70,70,70	0
84	MG	1	3801	1/1	0.83	0.17	55,55,55,55	0
84	MG	AS	3719	1/1	0.83	0.16	95,95,95,95	0
84	MG	AS	3660	1/1	0.83	0.11	95,95,95,95	0
84	MG	k	401	1/1	0.83	0.09	71,71,71,71	0
84	MG	B	1888	1/1	0.83	0.10	59,59,59,59	0
84	MG	B	1826	1/1	0.83	0.11	76,76,76,76	0
84	MG	1	3705	1/1	0.83	0.15	68,68,68,68	0
84	MG	1	3707	1/1	0.83	0.18	44,44,44,44	0
84	MG	AS	3453	1/1	0.83	0.08	54,54,54,54	0
84	MG	AS	3458	1/1	0.83	0.12	83,83,83,83	0
84	MG	1	3782	1/1	0.83	0.12	76,76,76,76	0
84	MG	1	3835	1/1	0.83	0.14	65,65,65,65	0
84	MG	1	3628	1/1	0.83	0.12	99,99,99,99	0
84	MG	AS	3677	1/1	0.83	0.21	49,49,49,49	0
84	MG	CM	1834	1/1	0.83	0.22	130,130,130,130	0
84	MG	1	3550	1/1	0.83	0.32	56,56,56,56	0
84	MG	x	201	1/1	0.83	0.17	53,53,53,53	0
84	MG	AS	3746	1/1	0.83	0.24	79,79,79,79	0
84	MG	1	3737	1/1	0.83	0.15	57,57,57,57	0
84	MG	1	3714	1/1	0.83	0.14	77,77,77,77	0
84	MG	1	3598	1/1	0.83	0.25	78,78,78,78	0
84	MG	R	202	1/1	0.83	0.16	61,61,61,61	0
84	MG	AS	3491	1/1	0.83	0.08	39,39,39,39	0
84	MG	AS	3626	1/1	0.83	0.23	52,52,52,52	0
84	MG	AS	3688	1/1	0.83	0.06	120,120,120,120	0
84	MG	CM	1861	1/1	0.83	0.09	92,92,92,92	0
84	MG	1	3669	1/1	0.83	0.19	83,83,83,83	0
84	MG	B	1846	1/1	0.83	0.19	64,64,64,64	0
84	MG	1	3552	1/1	0.83	0.14	64,64,64,64	0
84	MG	CM	1875	1/1	0.83	0.07	57,57,57,57	0
84	MG	CM	1876	1/1	0.83	0.05	76,76,76,76	0
84	MG	B	1855	1/1	0.83	0.14	67,67,67,67	0
84	MG	AS	3508	1/1	0.83	0.15	71,71,71,71	0
84	MG	AS	3698	1/1	0.83	0.13	51,51,51,51	0
84	MG	AS	3780	1/1	0.83	0.07	35,35,35,35	0
84	MG	AS	3403	1/1	0.83	0.08	84,84,84,84	0
84	MG	1	3818	1/1	0.83	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3410	1/1	0.84	0.37	50,50,50,50	0
84	MG	1	3619	1/1	0.84	0.07	5,5,5,5	0
84	MG	B	1811	1/1	0.84	0.17	54,54,54,54	0
84	MG	AS	3417	1/1	0.84	0.21	47,47,47,47	0
84	MG	1	3623	1/1	0.84	0.13	66,66,66,66	0
84	MG	1	3444	1/1	0.84	0.22	50,50,50,50	0
84	MG	B	1854	1/1	0.84	0.18	64,64,64,64	0
84	MG	AS	3581	1/1	0.84	0.17	61,61,61,61	0
84	MG	1	3858	1/1	0.84	0.08	81,81,81,81	0
84	MG	AS	3497	1/1	0.84	0.15	51,51,51,51	0
84	MG	AS	3767	1/1	0.84	0.17	54,54,54,54	0
84	MG	1	3642	1/1	0.84	0.11	51,51,51,51	0
84	MG	1	3517	1/1	0.84	0.10	50,50,50,50	0
84	MG	AS	3778	1/1	0.84	0.14	60,60,60,60	0
84	MG	1	3586	1/1	0.84	0.26	71,71,71,71	0
84	MG	AS	3543	1/1	0.84	0.12	66,66,66,66	0
84	MG	B	1823	1/1	0.84	0.20	60,60,60,60	0
84	MG	AS	3505	1/1	0.84	0.14	90,90,90,90	0
84	MG	1	3865	1/1	0.84	0.16	60,60,60,60	0
84	MG	AS	3599	1/1	0.84	0.12	50,50,50,50	0
84	MG	AS	3726	1/1	0.84	0.13	80,80,80,80	0
84	MG	Q	202	1/1	0.84	0.17	57,57,57,57	0
84	MG	1	3839	1/1	0.84	0.32	80,80,80,80	0
84	MG	1	3562	1/1	0.84	0.07	66,66,66,66	0
84	MG	1	3750	1/1	0.84	0.10	91,91,91,91	0
84	MG	AS	3738	1/1	0.84	0.23	43,43,43,43	0
84	MG	AS	3607	1/1	0.84	0.23	56,56,56,56	0
84	MG	AP	203	1/1	0.84	0.15	86,86,86,86	0
84	MG	1	3636	1/1	0.84	0.19	43,43,43,43	0
84	MG	AS	3742	1/1	0.84	0.22	93,93,93,93	0
84	MG	1	3581	1/1	0.84	0.15	70,70,70,70	0
84	MG	1	3434	1/1	0.84	0.45	47,47,47,47	0
84	MG	CW	201	1/1	0.84	0.16	81,81,81,81	0
84	MG	AS	3520	1/1	0.84	0.16	66,66,66,66	0
84	MG	1	3659	1/1	0.84	0.10	69,69,69,69	0
84	MG	o	302	1/1	0.84	0.14	46,46,46,46	0
85	ZN	CB	201	1/1	0.84	0.07	296,296,296,296	0
84	MG	AS	3643	1/1	0.85	0.10	47,47,47,47	0
84	MG	1	3584	1/1	0.85	0.17	81,81,81,81	0
84	MG	AS	3429	1/1	0.85	0.22	83,83,83,83	0
84	MG	AS	3648	1/1	0.85	0.16	55,55,55,55	0
84	MG	1	3617	1/1	0.85	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3553	1/1	0.85	0.11	96,96,96,96	0
84	MG	1	3764	1/1	0.85	0.29	74,74,74,74	0
84	MG	1	3743	1/1	0.85	0.08	81,81,81,81	0
84	MG	1	3511	1/1	0.85	0.26	38,38,38,38	0
84	MG	AS	3754	1/1	0.85	0.10	106,106,106,106	0
84	MG	1	3494	1/1	0.85	0.18	48,48,48,48	0
84	MG	1	3563	1/1	0.85	0.21	129,129,129,129	0
84	MG	CM	1829	1/1	0.85	0.09	52,52,52,52	0
84	MG	1	3673	1/1	0.85	0.29	68,68,68,68	0
84	MG	1	3602	1/1	0.85	0.09	57,57,57,57	0
84	MG	1	3589	1/1	0.85	0.11	75,75,75,75	0
84	MG	1	3864	1/1	0.85	0.08	46,46,46,46	0
84	MG	CM	1836	1/1	0.85	0.14	57,57,57,57	0
84	MG	1	3677	1/1	0.85	0.11	68,68,68,68	0
84	MG	AS	3454	1/1	0.85	0.14	71,71,71,71	0
84	MG	AS	3402	1/1	0.85	0.14	75,75,75,75	0
84	MG	B	1880	1/1	0.85	0.10	88,88,88,88	0
84	MG	1	3648	1/1	0.85	0.09	63,63,63,63	0
84	MG	1	3780	1/1	0.85	0.07	103,103,103,103	0
84	MG	AS	3671	1/1	0.85	0.11	48,48,48,48	0
84	MG	AS	3577	1/1	0.85	0.11	63,63,63,63	0
84	MG	1	3532	1/1	0.85	0.18	44,44,44,44	0
84	MG	AS	3411	1/1	0.85	0.17	69,69,69,69	0
84	MG	AS	3722	1/1	0.85	0.07	90,90,90,90	0
84	MG	1	3424	1/1	0.85	0.09	74,74,74,74	0
84	MG	AS	3628	1/1	0.85	0.17	67,67,67,67	0
84	MG	AT	202	1/1	0.85	0.06	64,64,64,64	0
84	MG	CM	1873	1/1	0.85	0.14	81,81,81,81	0
84	MG	B	1807	1/1	0.85	0.26	48,48,48,48	0
84	MG	1	3607	1/1	0.85	0.19	72,72,72,72	0
84	MG	1	3523	1/1	0.85	0.14	84,84,84,84	0
84	MG	AS	3734	1/1	0.85	0.15	80,80,80,80	0
84	MG	AS	3421	1/1	0.85	0.25	54,54,54,54	0
84	MG	AS	3496	1/1	0.85	0.20	52,52,52,52	0
84	MG	DA	201	1/1	0.85	0.18	86,86,86,86	0
84	MG	1	3759	1/1	0.85	0.16	74,74,74,74	0
84	MG	AS	3591	1/1	0.85	0.26	68,68,68,68	0
84	MG	1	3594	1/1	0.85	0.07	76,76,76,76	0
84	MG	B	1898	1/1	0.85	0.11	67,67,67,67	0
84	MG	B	1840	1/1	0.86	0.24	47,47,47,47	0
84	MG	BO	201	1/1	0.86	0.10	91,91,91,91	0
84	MG	AS	3693	1/1	0.86	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	CA	201	1/1	0.86	0.11	58,58,58,58	0
84	MG	1	3867	1/1	0.86	0.11	48,48,48,48	0
84	MG	1	3833	1/1	0.86	0.13	47,47,47,47	0
84	MG	1	3786	1/1	0.86	0.06	45,45,45,45	0
84	MG	AS	3538	1/1	0.86	0.14	98,98,98,98	0
84	MG	AS	3486	1/1	0.86	0.21	46,46,46,46	0
84	MG	AS	3487	1/1	0.86	0.17	62,62,62,62	0
84	MG	1	3702	1/1	0.86	0.11	76,76,76,76	0
84	MG	AS	3600	1/1	0.86	0.09	76,76,76,76	0
84	MG	3	202	1/1	0.86	0.10	45,45,45,45	0
84	MG	1	3686	1/1	0.86	0.09	103,103,103,103	0
84	MG	AS	3550	1/1	0.86	0.20	71,71,71,71	0
84	MG	1	3838	1/1	0.86	0.10	53,53,53,53	0
84	MG	AS	3657	1/1	0.86	0.15	78,78,78,78	0
84	MG	1	3746	1/1	0.86	0.06	71,71,71,71	0
84	MG	1	3521	1/1	0.86	0.20	57,57,57,57	0
84	MG	AS	3554	1/1	0.86	0.20	85,85,85,85	0
84	MG	CM	1840	1/1	0.86	0.11	60,60,60,60	0
84	MG	1	3410	1/1	0.86	0.21	77,77,77,77	0
84	MG	1	3815	1/1	0.86	0.17	44,44,44,44	0
84	MG	1	3420	1/1	0.86	0.15	21,21,21,21	0
84	MG	1	3498	1/1	0.86	0.11	58,58,58,58	0
84	MG	1	3406	1/1	0.86	0.17	46,46,46,46	0
84	MG	AS	3785	1/1	0.86	0.17	59,59,59,59	0
84	MG	1	3544	1/1	0.86	0.12	58,58,58,58	0
84	MG	B	1827	1/1	0.86	0.17	61,61,61,61	0
84	MG	1	3715	1/1	0.86	0.16	47,47,47,47	0
84	MG	AS	3447	1/1	0.86	0.17	55,55,55,55	0
84	MG	CM	1866	1/1	0.86	0.17	83,83,83,83	0
84	MG	AS	3451	1/1	0.86	0.25	72,72,72,72	0
84	MG	1	3798	1/1	0.86	0.06	44,44,44,44	0
84	MG	1	3738	1/1	0.86	0.20	67,67,67,67	0
84	MG	AT	204	1/1	0.86	0.23	54,54,54,54	0
84	MG	1	3755	1/1	0.86	0.10	55,55,55,55	0
84	MG	AS	3521	1/1	0.86	0.17	54,54,54,54	0
84	MG	1	3509	1/1	0.86	0.07	11,11,11,11	0
84	MG	1	3601	1/1	0.86	0.18	57,57,57,57	0
84	MG	AS	3462	1/1	0.86	0.14	60,60,60,60	0
84	MG	AS	3469	1/1	0.86	0.12	42,42,42,42	0
84	MG	1	3684	1/1	0.86	0.11	86,86,86,86	0
84	MG	AS	3474	1/1	0.86	0.10	72,72,72,72	0
84	MG	1	3500	1/1	0.86	0.44	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	ZN	AH	201	1/1	0.86	0.08	232,232,232,232	0
84	MG	BK	201	1/1	0.86	0.11	73,73,73,73	0
84	MG	AS	3477	1/1	0.86	0.09	50,50,50,50	0
84	MG	AS	3652	1/1	0.87	0.21	105,105,105,105	0
84	MG	AS	3608	1/1	0.87	0.25	46,46,46,46	0
84	MG	AS	3753	1/1	0.87	0.30	74,74,74,74	0
84	MG	CM	1802	1/1	0.87	0.22	53,53,53,53	0
84	MG	AS	3701	1/1	0.87	0.20	75,75,75,75	0
84	MG	CM	1807	1/1	0.87	0.12	72,72,72,72	0
84	MG	1	3814	1/1	0.87	0.26	56,56,56,56	0
84	MG	1	3667	1/1	0.87	0.15	37,37,37,37	0
84	MG	1	3816	1/1	0.87	0.26	59,59,59,59	0
84	MG	AS	3466	1/1	0.87	0.07	44,44,44,44	0
84	MG	1	3455	1/1	0.87	0.20	45,45,45,45	0
84	MG	1	3760	1/1	0.87	0.13	83,83,83,83	0
84	MG	1	3781	1/1	0.87	0.16	54,54,54,54	0
84	MG	1	3682	1/1	0.87	0.19	44,44,44,44	0
84	MG	k	402	1/1	0.87	0.27	98,98,98,98	0
84	MG	AS	3775	1/1	0.87	0.08	43,43,43,43	0
84	MG	1	3440	1/1	0.87	0.13	67,67,67,67	0
84	MG	1	3712	1/1	0.87	0.12	50,50,50,50	0
84	MG	1	3403	1/1	0.87	0.27	56,56,56,56	0
84	MG	1	3699	1/1	0.87	0.14	44,44,44,44	0
84	MG	1	3468	1/1	0.87	0.14	40,40,40,40	0
84	MG	1	3718	1/1	0.87	0.12	42,42,42,42	0
84	MG	AS	3786	1/1	0.87	0.09	70,70,70,70	0
84	MG	1	3629	1/1	0.87	0.12	49,49,49,49	0
84	MG	AS	3436	1/1	0.87	0.20	65,65,65,65	0
84	MG	B	1822	1/1	0.87	0.16	105,105,105,105	0
84	MG	1	3459	1/1	0.87	0.21	43,43,43,43	0
84	MG	1	3862	1/1	0.87	0.23	77,77,77,77	0
84	MG	AS	3679	1/1	0.87	0.15	61,61,61,61	0
84	MG	CM	1862	1/1	0.87	0.07	66,66,66,66	0
84	MG	AS	3540	1/1	0.87	0.17	108,108,108,108	0
84	MG	AS	3441	1/1	0.87	0.18	39,39,39,39	0
84	MG	AS	3502	1/1	0.87	0.15	74,74,74,74	0
84	MG	AS	3636	1/1	0.87	0.13	60,60,60,60	0
84	MG	1	3792	1/1	0.87	0.11	150,150,150,150	0
84	MG	CM	1874	1/1	0.87	0.10	68,68,68,68	0
84	MG	AS	3640	1/1	0.87	0.11	76,76,76,76	0
84	MG	0	202	1/1	0.87	0.20	54,54,54,54	0
84	MG	B	1870	1/1	0.87	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3690	1/1	0.87	0.07	46,46,46,46	0
84	MG	AS	3507	1/1	0.87	0.14	80,80,80,80	0
84	MG	1	3539	1/1	0.87	0.15	53,53,53,53	0
84	MG	AB	202	1/1	0.87	0.11	70,70,70,70	0
84	MG	AS	3694	1/1	0.87	0.18	45,45,45,45	0
84	MG	B	1879	1/1	0.87	0.16	58,58,58,58	0
84	MG	1	3541	1/1	0.87	0.13	26,26,26,26	0
84	MG	AS	3514	1/1	0.87	0.23	53,53,53,53	0
84	MG	1	3836	1/1	0.87	0.24	77,77,77,77	0
85	ZN	DS	201	1/1	0.87	0.06	353,353,353,353	0
84	MG	AS	3558	1/1	0.88	0.11	58,58,58,58	0
84	MG	AS	3629	1/1	0.88	0.27	43,43,43,43	0
84	MG	1	3524	1/1	0.88	0.14	93,93,93,93	0
84	MG	1	3526	1/1	0.88	0.09	103,103,103,103	0
84	MG	B	1869	1/1	0.88	0.12	65,65,65,65	0
84	MG	1	3695	1/1	0.88	0.10	44,44,44,44	0
84	MG	1	3728	1/1	0.88	0.13	59,59,59,59	0
84	MG	1	3649	1/1	0.88	0.07	85,85,85,85	0
84	MG	AU	203	1/1	0.88	0.08	61,61,61,61	0
84	MG	CM	1842	1/1	0.88	0.16	67,67,67,67	0
84	MG	AS	3747	1/1	0.88	0.17	47,47,47,47	0
84	MG	AS	3506	1/1	0.88	0.11	74,74,74,74	0
84	MG	AS	3637	1/1	0.88	0.10	46,46,46,46	0
84	MG	1	3518	1/1	0.88	0.20	69,69,69,69	0
84	MG	1	3474	1/1	0.88	0.10	58,58,58,58	0
84	MG	CM	1848	1/1	0.88	0.11	104,104,104,104	0
84	MG	B	1882	1/1	0.88	0.21	76,76,76,76	0
84	MG	CM	1853	1/1	0.88	0.13	80,80,80,80	0
84	MG	B	1883	1/1	0.88	0.08	47,47,47,47	0
84	MG	1	3432	1/1	0.88	0.20	78,78,78,78	0
84	MG	1	3716	1/1	0.88	0.14	46,46,46,46	0
84	MG	1	3604	1/1	0.88	0.07	49,49,49,49	0
84	MG	AS	3647	1/1	0.88	0.28	54,54,54,54	0
84	MG	AS	3544	1/1	0.88	0.28	52,52,52,52	0
84	MG	B	1830	1/1	0.88	0.08	79,79,79,79	0
84	MG	B	1889	1/1	0.88	0.11	44,44,44,44	0
84	MG	AS	3766	1/1	0.88	0.17	63,63,63,63	0
84	MG	AS	3548	1/1	0.88	0.12	91,91,91,91	0
84	MG	AS	3768	1/1	0.88	0.10	62,62,62,62	0
84	MG	AS	3619	1/1	0.88	0.12	60,60,60,60	0
84	MG	CM	1801	1/1	0.88	0.23	41,41,41,41	0
84	MG	B	1891	1/1	0.88	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
84	MG	1	3829	1/1	0.88	0.11	42,42,42,42	0
84	MG	AS	3409	1/1	0.88	0.17	86,86,86,86	0
84	MG	1	3447	1/1	0.88	0.07	81,81,81,81	0
84	MG	AS	3624	1/1	0.88	0.10	85,85,85,85	0
84	MG	DH	201	1/1	0.88	0.08	53,53,53,53	0
84	MG	1	3632	1/1	0.88	0.11	51,51,51,51	0
84	MG	CM	1824	1/1	0.88	0.19	62,62,62,62	0
84	MG	1	3635	1/1	0.88	0.23	45,45,45,45	0
84	MG	6	201	1/1	0.88	0.17	53,53,53,53	0
84	MG	CM	1828	1/1	0.88	0.16	69,69,69,69	0
84	MG	AS	3546	1/1	0.89	0.16	38,38,38,38	0
84	MG	1	3435	1/1	0.89	0.13	44,44,44,44	0
84	MG	AS	3450	1/1	0.89	0.18	47,47,47,47	0
84	MG	AS	3733	1/1	0.89	0.13	102,102,102,102	0
84	MG	B	1843	1/1	0.89	0.13	75,75,75,75	0
84	MG	AS	3407	1/1	0.89	0.09	83,83,83,83	0
84	MG	1	3868	1/1	0.89	0.34	70,70,70,70	0
84	MG	AS	3456	1/1	0.89	0.11	31,31,31,31	0
84	MG	1	3439	1/1	0.89	0.19	43,43,43,43	0
84	MG	B	1817	1/1	0.89	0.25	56,56,56,56	0
84	MG	B	1847	1/1	0.89	0.14	60,60,60,60	0
84	MG	1	3633	1/1	0.89	0.24	27,27,27,27	0
84	MG	AU	205	1/1	0.89	0.10	54,54,54,54	0
84	MG	B	1819	1/1	0.89	0.12	50,50,50,50	0
84	MG	1	3588	1/1	0.89	0.12	71,71,71,71	0
83	3K5	1	3401	57/57	0.89	0.19	72,107,146,164	0
84	MG	AS	3473	1/1	0.89	0.21	60,60,60,60	0
84	MG	CM	1849	1/1	0.89	0.14	67,67,67,67	0
84	MG	B	1894	1/1	0.89	0.07	98,98,98,98	0
84	MG	1	3569	1/1	0.89	0.14	54,54,54,54	0
84	MG	3	207	1/1	0.89	0.12	48,48,48,48	0
84	MG	4	201	1/1	0.89	0.07	43,43,43,43	0
84	MG	1	3855	1/1	0.89	0.09	43,43,43,43	0
84	MG	AJ	101	1/1	0.89	0.22	100,100,100,100	0
84	MG	1	3766	1/1	0.89	0.13	47,47,47,47	0
84	MG	CM	1867	1/1	0.89	0.17	60,60,60,60	0
84	MG	AS	3432	1/1	0.89	0.21	92,92,92,92	0
84	MG	B	1863	1/1	0.89	0.17	53,53,53,53	0
84	MG	AS	3533	1/1	0.89	0.14	64,64,64,64	0
84	MG	1	3484	1/1	0.89	0.08	27,27,27,27	0
84	MG	m	301	1/1	0.89	0.14	61,61,61,61	0
84	MG	1	3527	1/1	0.89	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3537	1/1	0.89	0.19	72,72,72,72	0
84	MG	CL	302	1/1	0.89	0.14	88,88,88,88	0
84	MG	1	3658	1/1	0.89	0.12	62,62,62,62	0
84	MG	B	1871	1/1	0.89	0.09	40,40,40,40	0
84	MG	1	3706	1/1	0.89	0.10	60,60,60,60	0
84	MG	B	1877	1/1	0.89	0.14	47,47,47,47	0
84	MG	CM	1809	1/1	0.89	0.19	60,60,60,60	0
84	MG	AS	3771	1/1	0.89	0.33	69,69,69,69	0
84	MG	1	3471	1/1	0.89	0.09	40,40,40,40	0
84	MG	DK	202	1/1	0.89	0.11	51,51,51,51	0
84	MG	AS	3590	1/1	0.89	0.07	58,58,58,58	0
85	ZN	AP	201	1/1	0.89	0.06	294,294,294,294	0
84	MG	1	3529	1/1	0.89	0.27	57,57,57,57	0
85	ZN	h	201	1/1	0.89	0.09	285,285,285,285	0
84	MG	1	3487	1/1	0.89	0.14	43,43,43,43	0
85	ZN	CJ	201	1/1	0.89	0.06	300,300,300,300	0
84	MG	AS	3595	1/1	0.89	0.12	72,72,72,72	0
84	MG	1	3848	1/1	0.90	0.08	69,69,69,69	0
84	MG	1	3554	1/1	0.90	0.04	65,65,65,65	0
84	MG	1	3537	1/1	0.90	0.16	27,27,27,27	0
84	MG	B	1813	1/1	0.90	0.15	74,74,74,74	0
84	MG	AS	3557	1/1	0.90	0.08	60,60,60,60	0
84	MG	AS	3669	1/1	0.90	0.12	71,71,71,71	0
84	MG	AS	3488	1/1	0.90	0.26	32,32,32,32	0
84	MG	1	3557	1/1	0.90	0.09	70,70,70,70	0
84	MG	AS	3445	1/1	0.90	0.13	75,75,75,75	0
84	MG	1	3643	1/1	0.90	0.25	51,51,51,51	0
84	MG	1	3713	1/1	0.90	0.10	62,62,62,62	0
84	MG	AS	3565	1/1	0.90	0.23	68,68,68,68	0
84	MG	AS	3605	1/1	0.90	0.16	91,91,91,91	0
84	MG	B	1842	1/1	0.90	0.15	67,67,67,67	0
84	MG	AS	3760	1/1	0.90	0.14	67,67,67,67	0
84	MG	AS	3763	1/1	0.90	0.19	65,65,65,65	0
83	3K5	AS	3401	57/57	0.90	0.15	82,121,151,184	0
84	MG	1	3453	1/1	0.90	0.26	67,67,67,67	0
84	MG	CM	1865	1/1	0.90	0.06	119,119,119,119	0
84	MG	AS	3419	1/1	0.90	0.18	82,82,82,82	0
84	MG	B	1875	1/1	0.90	0.07	48,48,48,48	0
84	MG	1	3462	1/1	0.90	0.15	49,49,49,49	0
84	MG	k	403	1/1	0.90	0.09	58,58,58,58	0
84	MG	CM	1870	1/1	0.90	0.17	94,94,94,94	0
84	MG	AS	3574	1/1	0.90	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	1	3549	1/1	0.90	0.18	66,66,66,66	0
84	MG	CM	1803	1/1	0.90	0.06	192,192,192,192	0
84	MG	AS	3727	1/1	0.90	0.06	50,50,50,50	0
84	MG	AS	3689	1/1	0.90	0.05	59,59,59,59	0
84	MG	CM	1808	1/1	0.90	0.06	61,61,61,61	0
84	MG	AS	3779	1/1	0.90	0.07	66,66,66,66	0
84	MG	CM	1810	1/1	0.90	0.27	52,52,52,52	0
84	MG	K	301	1/1	0.90	0.07	63,63,63,63	0
84	MG	Q	201	1/1	0.90	0.20	110,110,110,110	0
84	MG	AS	3617	1/1	0.90	0.18	62,62,62,62	0
84	MG	1	3404	1/1	0.90	0.13	22,22,22,22	0
84	MG	1	3577	1/1	0.90	0.08	48,48,48,48	0
84	MG	1	3472	1/1	0.90	0.11	60,60,60,60	0
84	MG	CM	1827	1/1	0.90	0.10	35,35,35,35	0
84	MG	1	3522	1/1	0.90	0.07	38,38,38,38	0
84	MG	r	301	1/1	0.90	0.10	48,48,48,48	0
84	MG	1	3775	1/1	0.90	0.09	55,55,55,55	0
84	MG	B	1887	1/1	0.90	0.09	81,81,81,81	0
84	MG	AS	3480	1/1	0.90	0.13	77,77,77,77	0
84	MG	1	3676	1/1	0.90	0.16	65,65,65,65	0
86	GET	B	1851	34/34	0.90	0.09	105,127,149,167	0
84	MG	B	1873	1/1	0.91	0.21	61,61,61,61	0
84	MG	CM	1837	1/1	0.91	0.16	62,62,62,62	0
84	MG	B	1874	1/1	0.91	0.12	44,44,44,44	0
84	MG	D	301	1/1	0.91	0.12	24,24,24,24	0
84	MG	AS	3582	1/1	0.91	0.07	44,44,44,44	0
84	MG	1	3452	1/1	0.91	0.15	63,63,63,63	0
84	MG	AS	3461	1/1	0.91	0.18	74,74,74,74	0
84	MG	AS	3425	1/1	0.91	0.09	68,68,68,68	0
84	MG	AS	3465	1/1	0.91	0.12	52,52,52,52	0
84	MG	AS	3510	1/1	0.91	0.13	70,70,70,70	0
84	MG	1	3520	1/1	0.91	0.14	95,95,95,95	0
84	MG	AS	3467	1/1	0.91	0.14	79,79,79,79	0
84	MG	AS	3513	1/1	0.91	0.09	47,47,47,47	0
84	MG	1	3627	1/1	0.91	0.35	46,46,46,46	0
84	MG	AS	3675	1/1	0.91	0.15	60,60,60,60	0
84	MG	AS	3594	1/1	0.91	0.11	104,104,104,104	0
84	MG	AS	3471	1/1	0.91	0.21	41,41,41,41	0
84	MG	CM	1858	1/1	0.91	0.09	111,111,111,111	0
84	MG	CM	1860	1/1	0.91	0.18	69,69,69,69	0
84	MG	1	3491	1/1	0.91	0.29	52,52,52,52	0
84	MG	1	3724	1/1	0.91	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	B	1852	1/1	0.91	0.16	57,57,57,57	0
84	MG	1	3421	1/1	0.91	0.14	48,48,48,48	0
84	MG	1	3668	1/1	0.91	0.07	23,23,23,23	0
84	MG	1	3428	1/1	0.91	0.28	43,43,43,43	0
84	MG	AS	3772	1/1	0.91	0.08	59,59,59,59	0
84	MG	1	3502	1/1	0.91	0.20	53,53,53,53	0
84	MG	1	3729	1/1	0.91	0.05	56,56,56,56	0
84	MG	CM	1872	1/1	0.91	0.07	85,85,85,85	0
84	MG	AS	3482	1/1	0.91	0.09	69,69,69,69	0
84	MG	1	3671	1/1	0.91	0.12	75,75,75,75	0
84	MG	AS	3732	1/1	0.91	0.11	85,85,85,85	0
84	MG	AS	3782	1/1	0.91	0.17	72,72,72,72	0
84	MG	CM	1815	1/1	0.91	0.18	43,43,43,43	0
84	MG	1	3612	1/1	0.91	0.12	74,74,74,74	0
84	MG	CM	1817	1/1	0.91	0.07	190,190,190,190	0
84	MG	CM	1818	1/1	0.91	0.22	46,46,46,46	0
84	MG	CM	1820	1/1	0.91	0.15	68,68,68,68	0
84	MG	B	1890	1/1	0.91	0.12	54,54,54,54	0
84	MG	B	1833	1/1	0.91	0.09	72,72,72,72	0
84	MG	1	3503	1/1	0.91	0.16	70,70,70,70	0
84	MG	1	3773	1/1	0.91	0.12	62,62,62,62	0
84	MG	1	3433	1/1	0.91	0.18	34,34,34,34	0
84	MG	1	3488	1/1	0.91	0.09	51,51,51,51	0
84	MG	1	3844	1/1	0.91	0.19	74,74,74,74	0
84	MG	1	3475	1/1	0.91	0.21	16,16,16,16	0
84	MG	1	3656	1/1	0.91	0.18	52,52,52,52	0
84	MG	1	3566	1/1	0.91	0.08	32,32,32,32	0
84	MG	AS	3578	1/1	0.91	0.14	52,52,52,52	0
84	MG	AT	205	1/1	0.91	0.16	75,75,75,75	0
84	MG	1	3551	1/1	0.92	0.12	52,52,52,52	0
84	MG	1	3450	1/1	0.92	0.20	54,54,54,54	0
84	MG	1	3507	1/1	0.92	0.10	50,50,50,50	0
84	MG	1	3442	1/1	0.92	0.15	45,45,45,45	0
84	MG	1	3590	1/1	0.92	0.24	57,57,57,57	0
84	MG	CM	1835	1/1	0.92	0.09	68,68,68,68	0
84	MG	1	3611	1/1	0.92	0.15	81,81,81,81	0
84	MG	1	3443	1/1	0.92	0.20	35,35,35,35	0
84	MG	1	3486	1/1	0.92	0.19	62,62,62,62	0
84	MG	1	3615	1/1	0.92	0.13	40,40,40,40	0
84	MG	1	3422	1/1	0.92	0.15	45,45,45,45	0
84	MG	AU	201	1/1	0.92	0.07	64,64,64,64	0
84	MG	AS	3490	1/1	0.92	0.05	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3639	1/1	0.92	0.05	60,60,60,60	0
84	MG	AW	301	1/1	0.92	0.10	82,82,82,82	0
84	MG	1	3512	1/1	0.92	0.16	53,53,53,53	0
84	MG	AS	3492	1/1	0.92	0.16	97,97,97,97	0
84	MG	1	3513	1/1	0.92	0.23	64,64,64,64	0
84	MG	B	1816	1/1	0.92	0.07	34,34,34,34	0
84	MG	AS	3644	1/1	0.92	0.18	86,86,86,86	0
84	MG	CM	1852	1/1	0.92	0.15	37,37,37,37	0
84	MG	1	3620	1/1	0.92	0.10	49,49,49,49	0
84	MG	1	3708	1/1	0.92	0.12	103,103,103,103	0
84	MG	AS	3442	1/1	0.92	0.23	22,22,22,22	0
84	MG	1	3596	1/1	0.92	0.05	51,51,51,51	0
84	MG	BI	301	1/1	0.92	0.05	48,48,48,48	0
84	MG	B	1864	1/1	0.92	0.18	67,67,67,67	0
84	MG	B	1866	1/1	0.92	0.11	47,47,47,47	0
84	MG	CM	1863	1/1	0.92	0.14	70,70,70,70	0
84	MG	1	3561	1/1	0.92	0.11	63,63,63,63	0
84	MG	1	3407	1/1	0.92	0.12	50,50,50,50	0
84	MG	1	3626	1/1	0.92	0.12	65,65,65,65	0
84	MG	1	3811	1/1	0.92	0.07	90,90,90,90	0
84	MG	B	1824	1/1	0.92	0.14	49,49,49,49	0
84	MG	1	3812	1/1	0.92	0.16	45,45,45,45	0
84	MG	AS	3761	1/1	0.92	0.14	89,89,89,89	0
84	MG	AS	3455	1/1	0.92	0.11	64,64,64,64	0
84	MG	1	3655	1/1	0.92	0.07	58,58,58,58	0
84	MG	w	301	1/1	0.92	0.11	49,49,49,49	0
84	MG	1	3477	1/1	0.92	0.17	41,41,41,41	0
84	MG	1	3600	1/1	0.92	0.19	55,55,55,55	0
84	MG	y	202	1/1	0.92	0.09	54,54,54,54	0
84	MG	y	203	1/1	0.92	0.19	82,82,82,82	0
84	MG	1	3688	1/1	0.92	0.09	106,106,106,106	0
84	MG	1	3448	1/1	0.92	0.15	54,54,54,54	0
84	MG	CM	1812	1/1	0.92	0.08	152,152,152,152	0
84	MG	AS	3773	1/1	0.92	0.13	96,96,96,96	0
84	MG	AS	3774	1/1	0.92	0.11	37,37,37,37	0
84	MG	1	3719	1/1	0.92	0.10	74,74,74,74	0
84	MG	1	3721	1/1	0.92	0.09	86,86,86,86	0
84	MG	AS	3777	1/1	0.92	0.15	98,98,98,98	0
84	MG	AS	3416	1/1	0.92	0.15	41,41,41,41	0
84	MG	1	3690	1/1	0.92	0.11	61,61,61,61	0
84	MG	AS	3672	1/1	0.92	0.11	63,63,63,63	0
84	MG	1	3467	1/1	0.92	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
84	MG	1	3456	1/1	0.92	0.19	47,47,47,47	0
84	MG	1	3416	1/1	0.92	0.15	89,89,89,89	0
84	MG	1	3757	1/1	0.92	0.07	44,44,44,44	0
84	MG	1	3540	1/1	0.93	0.11	72,72,72,72	0
84	MG	1	3663	1/1	0.93	0.07	69,69,69,69	0
84	MG	1	3679	1/1	0.93	0.15	56,56,56,56	0
84	MG	AS	3664	1/1	0.93	0.13	61,61,61,61	0
84	MG	AS	3781	1/1	0.93	0.03	58,58,58,58	0
84	MG	AS	3522	1/1	0.93	0.09	82,82,82,82	0
84	MG	1	3822	1/1	0.93	0.09	51,51,51,51	0
84	MG	1	3664	1/1	0.93	0.25	40,40,40,40	0
84	MG	AS	3559	1/1	0.93	0.19	71,71,71,71	0
84	MG	1	3556	1/1	0.93	0.17	43,43,43,43	0
84	MG	AS	3561	1/1	0.93	0.07	78,78,78,78	0
84	MG	1	3666	1/1	0.93	0.11	50,50,50,50	0
84	MG	CM	1811	1/1	0.93	0.09	59,59,59,59	0
84	MG	2	201	1/1	0.93	0.12	44,44,44,44	0
84	MG	AS	3750	1/1	0.93	0.20	62,62,62,62	0
84	MG	1	3460	1/1	0.93	0.16	45,45,45,45	0
84	MG	B	1848	1/1	0.93	0.10	46,46,46,46	0
84	MG	1	3564	1/1	0.93	0.15	46,46,46,46	0
84	MG	CM	1819	1/1	0.93	0.09	54,54,54,54	0
84	MG	L	201	1/1	0.93	0.26	55,55,55,55	0
84	MG	AS	3501	1/1	0.93	0.07	52,52,52,52	0
84	MG	1	3851	1/1	0.93	0.21	76,76,76,76	0
84	MG	1	3445	1/1	0.93	0.11	32,32,32,32	0
84	MG	AU	204	1/1	0.93	0.11	82,82,82,82	0
84	MG	1	3854	1/1	0.93	0.07	81,81,81,81	0
84	MG	AS	3430	1/1	0.93	0.17	51,51,51,51	0
84	MG	1	3446	1/1	0.93	0.12	77,77,77,77	0
84	MG	AP	202	1/1	0.93	0.16	49,49,49,49	0
84	MG	T	201	1/1	0.93	0.12	121,121,121,121	0
84	MG	AS	3723	1/1	0.93	0.10	60,60,60,60	0
84	MG	AS	3541	1/1	0.93	0.10	55,55,55,55	0
84	MG	CM	1833	1/1	0.93	0.10	40,40,40,40	0
84	MG	1	3772	1/1	0.93	0.09	61,61,61,61	0
84	MG	1	3616	1/1	0.93	0.09	65,65,65,65	0
84	MG	1	3774	1/1	0.93	0.09	43,43,43,43	0
84	MG	P0	401	1/1	0.93	0.08	200,200,200,200	0
84	MG	AS	3769	1/1	0.93	0.07	61,61,61,61	0
84	MG	1	3574	1/1	0.93	0.05	41,41,41,41	0
84	MG	1	3436	1/1	0.93	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3405	1/1	0.93	0.22	57,57,57,57	0
84	MG	1	3631	1/1	0.93	0.08	48,48,48,48	0
84	MG	1	3608	1/1	0.93	0.11	53,53,53,53	0
84	MG	1	3645	1/1	0.93	0.17	68,68,68,68	0
84	MG	1	3866	1/1	0.93	0.15	86,86,86,86	0
84	MG	0	204	1/1	0.94	0.10	77,77,77,77	0
84	MG	1	3710	1/1	0.94	0.13	42,42,42,42	1
84	MG	1	3857	1/1	0.94	0.13	92,92,92,92	0
84	MG	AS	3702	1/1	0.94	0.08	66,66,66,66	0
84	MG	CM	1855	1/1	0.94	0.07	45,45,45,45	0
84	MG	AS	3483	1/1	0.94	0.08	103,103,103,103	0
84	MG	AS	3589	1/1	0.94	0.19	65,65,65,65	0
84	MG	1	3469	1/1	0.94	0.09	31,31,31,31	0
84	MG	1	3657	1/1	0.94	0.09	69,69,69,69	0
84	MG	1	3840	1/1	0.94	0.09	67,67,67,67	0
84	MG	AS	3593	1/1	0.94	0.11	68,68,68,68	0
84	MG	1	3464	1/1	0.94	0.10	8,8,8,8	0
84	MG	CM	1864	1/1	0.94	0.06	34,34,34,34	0
84	MG	1	3429	1/1	0.94	0.14	59,59,59,59	0
84	MG	1	3843	1/1	0.94	0.12	71,71,71,71	0
84	MG	B	1876	1/1	0.94	0.12	56,56,56,56	0
84	MG	B	1849	1/1	0.94	0.08	91,91,91,91	0
84	MG	AU	202	1/1	0.94	0.05	60,60,60,60	0
84	MG	1	3622	1/1	0.94	0.05	72,72,72,72	0
84	MG	AS	3495	1/1	0.94	0.25	41,41,41,41	0
84	MG	B	1825	1/1	0.94	0.08	68,68,68,68	0
84	MG	AS	3457	1/1	0.94	0.17	44,44,44,44	0
84	MG	AS	3604	1/1	0.94	0.13	62,62,62,62	0
84	MG	B	1801	1/1	0.94	0.26	46,46,46,46	0
84	MG	AS	3499	1/1	0.94	0.04	70,70,70,70	0
84	MG	1	3826	1/1	0.94	0.07	38,38,38,38	0
84	MG	1	3634	1/1	0.94	0.22	41,41,41,41	0
84	MG	1	3501	1/1	0.94	0.14	64,64,64,64	0
84	MG	R	203	1/1	0.94	0.14	59,59,59,59	0
84	MG	1	3531	1/1	0.94	0.12	84,84,84,84	0
84	MG	1	3613	1/1	0.94	0.13	51,51,51,51	0
84	MG	AS	3728	1/1	0.94	0.06	55,55,55,55	0
84	MG	1	3720	1/1	0.94	0.16	58,58,58,58	0
84	MG	1	3483	1/1	0.94	0.08	112,112,112,112	0
84	MG	3	205	1/1	0.94	0.18	32,32,32,32	0
84	MG	1	3430	1/1	0.94	0.13	43,43,43,43	0
84	MG	1	3525	1/1	0.94	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	AS	3404	1/1	0.94	0.04	41,41,41,41	0
84	MG	AS	3736	1/1	0.94	0.21	47,47,47,47	0
84	MG	AS	3438	1/1	0.94	0.08	46,46,46,46	0
84	MG	B	1865	1/1	0.94	0.20	65,65,65,65	0
84	MG	1	3409	1/1	0.94	0.06	52,52,52,52	0
84	MG	AS	3549	1/1	0.94	0.09	60,60,60,60	0
86	GET	CM	1822	34/34	0.94	0.12	107,119,148,157	0
84	MG	1	3473	1/1	0.95	0.10	59,59,59,59	0
84	MG	AS	3463	1/1	0.95	0.08	41,41,41,41	0
84	MG	B	1881	1/1	0.95	0.08	52,52,52,52	0
84	MG	AS	3449	1/1	0.95	0.05	39,39,39,39	0
84	MG	1	3808	1/1	0.95	0.09	144,144,144,144	0
84	MG	AS	3566	1/1	0.95	0.05	55,55,55,55	0
84	MG	B	1836	1/1	0.95	0.12	51,51,51,51	0
84	MG	AS	3452	1/1	0.95	0.07	24,24,24,24	0
84	MG	B	1837	1/1	0.95	0.08	57,57,57,57	0
84	MG	1	3438	1/1	0.95	0.14	75,75,75,75	0
84	MG	0	203	1/1	0.95	0.04	33,33,33,33	0
84	MG	AS	3494	1/1	0.95	0.07	105,105,105,105	0
84	MG	1	3652	1/1	0.95	0.09	44,44,44,44	0
84	MG	AS	3476	1/1	0.95	0.16	49,49,49,49	0
84	MG	1	3465	1/1	0.95	0.13	44,44,44,44	0
84	MG	CM	1814	1/1	0.95	0.08	127,127,127,127	0
84	MG	1	3413	1/1	0.95	0.15	44,44,44,44	0
84	MG	AS	3479	1/1	0.95	0.17	42,42,42,42	0
84	MG	AS	3598	1/1	0.95	0.11	42,42,42,42	0
84	MG	1	3831	1/1	0.95	0.10	51,51,51,51	0
84	MG	1	3861	1/1	0.95	0.08	54,54,54,54	0
84	MG	BQ	201	1/1	0.95	0.19	54,54,54,54	0
84	MG	F	301	1/1	0.95	0.13	77,77,77,77	0
84	MG	1	3777	1/1	0.96	0.18	29,29,29,29	0
84	MG	AS	3661	1/1	0.96	0.10	66,66,66,66	0
84	MG	AS	3424	1/1	0.96	0.10	57,57,57,57	0
84	MG	B	1805	1/1	0.96	0.11	38,38,38,38	0
84	MG	AS	3468	1/1	0.96	0.14	42,42,42,42	0
84	MG	AS	3414	1/1	0.96	0.14	54,54,54,54	0
84	MG	AS	3427	1/1	0.96	0.11	39,39,39,39	0
84	MG	AS	3415	1/1	0.96	0.16	81,81,81,81	0
84	MG	CM	1851	1/1	0.96	0.05	49,49,49,49	0
84	MG	1	3852	1/1	0.96	0.09	71,71,71,71	0
84	MG	1	3653	1/1	0.96	0.15	30,30,30,30	0
84	MG	AS	3687	1/1	0.96	0.07	85,85,85,85	0

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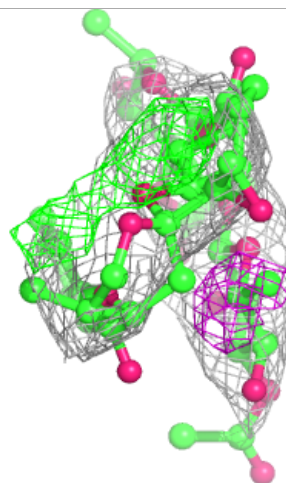
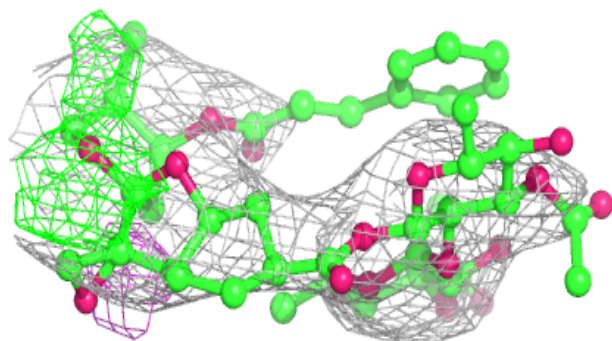
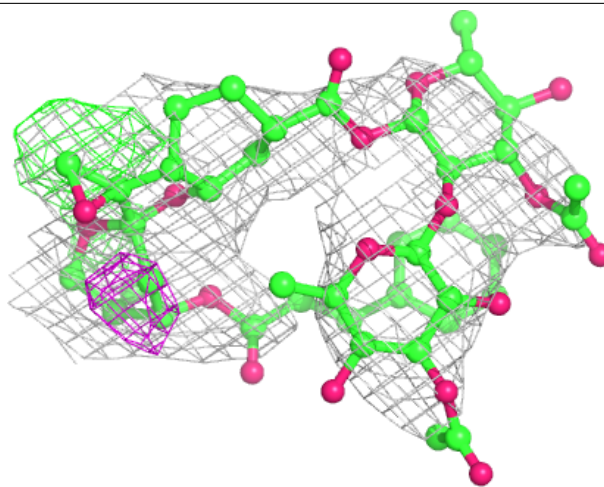
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
84	MG	CM	1804	1/1	0.96	0.05	48,48,48,48	0
84	MG	AS	3706	1/1	0.96	0.07	51,51,51,51	0
84	MG	CM	1806	1/1	0.96	0.06	38,38,38,38	0
84	MG	CM	1859	1/1	0.96	0.15	46,46,46,46	0
84	MG	AS	3418	1/1	0.96	0.22	39,39,39,39	0
84	MG	1	3739	1/1	0.96	0.10	98,98,98,98	0
84	MG	B	1853	1/1	0.96	0.13	47,47,47,47	0
84	MG	1	3784	1/1	0.96	0.11	67,67,67,67	0
84	MG	BE	301	1/1	0.96	0.11	59,59,59,59	0
84	MG	AS	3730	1/1	0.96	0.13	46,46,46,46	0
84	MG	CM	1813	1/1	0.96	0.07	168,168,168,168	0
85	ZN	DN	201	1/1	0.96	0.05	125,125,125,125	0
84	MG	AS	3448	1/1	0.96	0.09	73,73,73,73	0
84	MG	1	3419	1/1	0.96	0.04	49,49,49,49	0
84	MG	AS	3464	1/1	0.96	0.07	43,43,43,43	0
84	MG	B	1808	1/1	0.97	0.04	57,57,57,57	0
84	MG	AS	3470	1/1	0.97	0.08	48,48,48,48	0
84	MG	1	3660	1/1	0.97	0.14	35,35,35,35	0
85	ZN	AK	101	1/1	0.97	0.06	115,115,115,115	0
84	MG	CM	1839	1/1	0.97	0.06	50,50,50,50	0
84	MG	1	3437	1/1	0.97	0.07	49,49,49,49	0
85	ZN	f	101	1/1	0.97	0.09	125,125,125,125	0
84	MG	AS	3531	1/1	0.97	0.14	86,86,86,86	1
84	MG	1	3621	1/1	0.97	0.08	56,56,56,56	0
85	ZN	CE	101	1/1	0.97	0.05	128,128,128,128	0
84	MG	1	3736	1/1	0.97	0.09	40,40,40,40	0
84	MG	AS	3493	1/1	0.97	0.14	36,36,36,36	0
85	ZN	DQ	101	1/1	0.97	0.08	121,121,121,121	0
84	MG	1	3696	1/1	0.97	0.09	39,39,39,39	0
84	MG	3	203	1/1	0.97	0.20	54,54,54,54	0
84	MG	3	204	1/1	0.97	0.16	30,30,30,30	0
85	ZN	c	201	1/1	0.98	0.04	132,132,132,132	0
84	MG	CM	1854	1/1	0.98	0.16	41,41,41,41	0
85	ZN	AN	101	1/1	0.98	0.05	110,110,110,110	0
84	MG	AS	3762	1/1	0.98	0.08	41,41,41,41	0
85	ZN	CK	101	1/1	0.99	0.03	151,151,151,151	0
85	ZN	CH	101	1/1	0.99	0.09	117,117,117,117	0
85	ZN	AQ	101	1/1	0.99	0.08	128,128,128,128	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

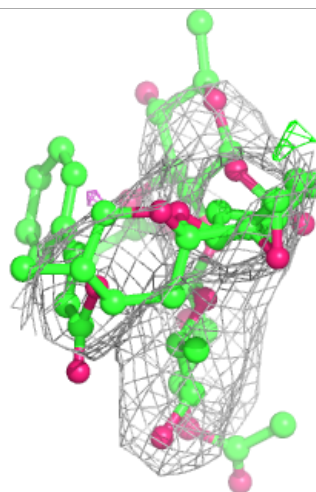
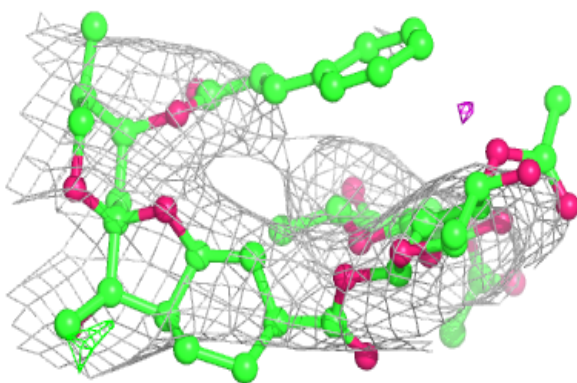
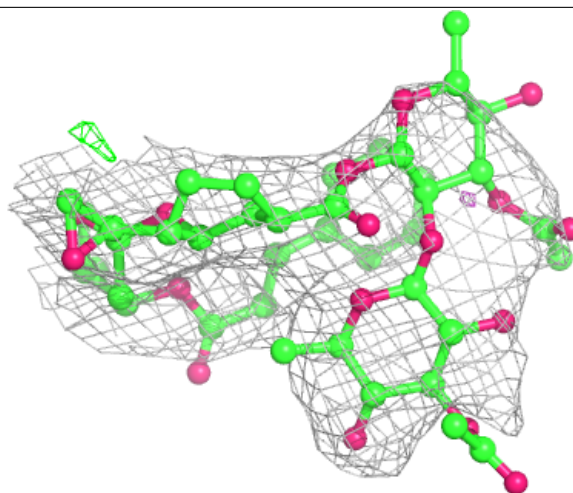
Electron density around 3K5 1 3401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



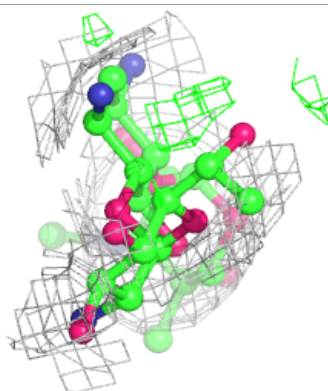
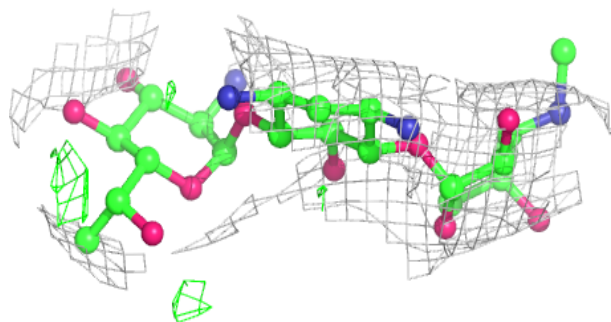
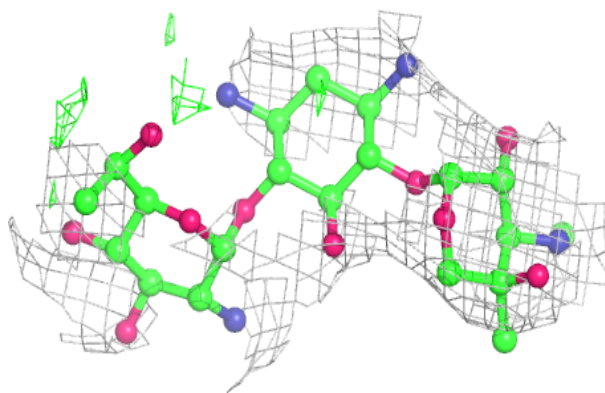
Electron density around 3K5 AS 3401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

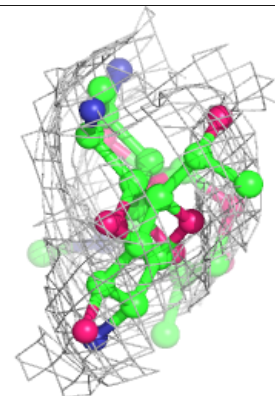
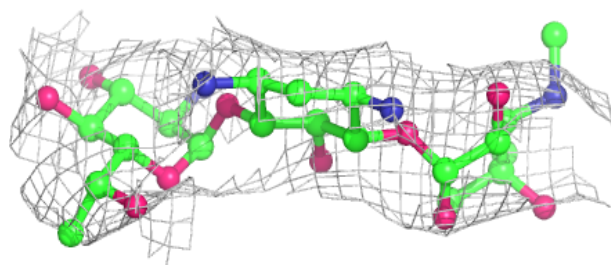
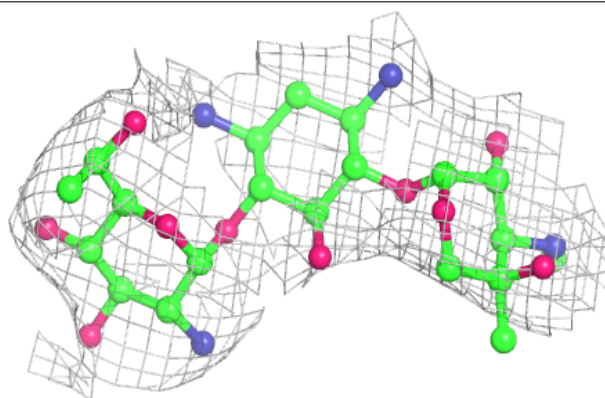


Electron density around GET B 1851:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GET CM 1822:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.