Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 09:57 AM EDT

PDB ID	:	4W29
Title	:	70S ribosome translocation intermediate containing elongation factor EFG/GDP/fusidic acid, mRNA, and tRNAs trapped in the AP/AP pe/E chimeric hybrid state.
Authors	:	Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on	:	2014-07-02
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

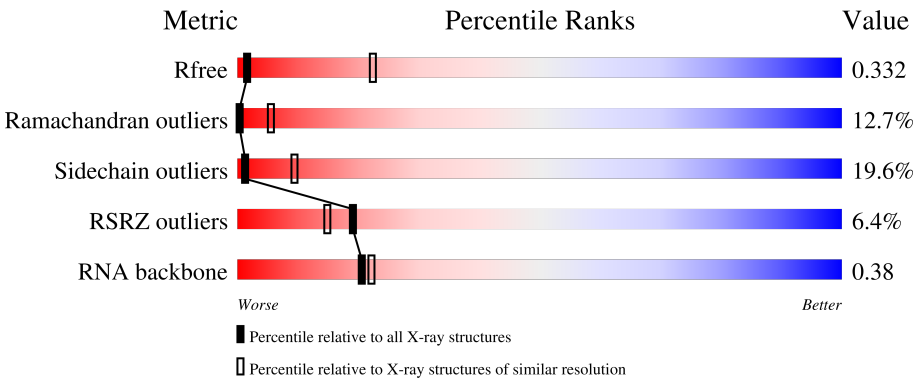
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 <=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	AB	235	2%, 76%, 22%, •
1	CB	235	%, 75%, 23%, •
2	AC	207	43%, 72%, 27%, •
2	CC	207	39%, 75%, 24%, •

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Mol	Chain	Length	Quality of chain
3	AD	208	%, 71%, 27%
3	CD	208	75%, 24%
4	AE	151	10%, 80%, 19%
4	CE	151	6%, 78%, 19%
5	AF	101	76%, 23%
5	CF	101	79%, 20%
6	AG	155	5%, 86%, 14%
6	CG	155	4%, 83%, 15%
7	AH	138	78%, 22%
7	CH	138	76%, 22%
8	AI	127	2%, 83%, 17%
8	CI	127	%, 81%, 17%
9	AJ	99	37%, 72%, 27%
9	CJ	99	35%, 73%, 26%
10	AK	119	8%, 82%, 17%
10	CK	119	3%, 77%, 21%
11	AL	125	3%, 58%, 35%, 6%
11	CL	125	5%, 58%, 36%, 5%
12	AM	125	5%, 80%, 19%
12	CM	125	6%, 76%, 22%
13	AN	60	22%, 82%, 17%
13	CN	60	17%, 72%, 23%, 5%
14	AO	88	%, 80%, 18%
14	CO	88	85%, 13%
15	AP	84	8%, 85%, 15%

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Mol	Chain	Length	Quality of chain
15	CP	84	12% 76% 24%
16	AQ	100	80% 18%
16	CQ	100	2% 82% 16%
17	AR	70	6% 73% 24%
17	CR	70	4% 84% 16%
18	AS	79	% 70% 25% 5%
18	CS	79	6% 76% 24%
19	AT	99	5% 82% 16%
19	CT	99	16% 79% 19%
20	AY	687	3% 71% 23%
20	CY	687	3% 70% 24%
21	AA	1511	% 74% 24%
21	CA	1511	2% 71% 26%
22	AW	77	12% 42% 51% 8%
22	CW	77	9% 38% 52% 10%
23	AV	36	22% 19% 72% 8%
23	CV	36	44% 19% 64% 17%
24	AX	78	4% 50% 42% 8%
24	CX	78	3% 49% 42% 9%
25	BC	228	29% 58% 33% 8%
25	DC	228	21% 62% 32% 6%
26	BD	275	8% 74% 24%
26	DD	275	5% 74% 23%
27	BE	205	5% 74% 23%
27	DE	205	4% 69% 29%

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Mol	Chain	Length	Quality of chain
28	BF	208	11% 74% 21%
28	DF	208	15% 71% 27%
29	BG	181	12% 86% 14%
29	DG	181	14% 80% 18%
30	BH	167	4% 75% 25%
30	DH	167	5% 78% 22%
31	BJ	170	99%
31	DJ	170	98%
32	BK	140	5% 71% 26%
32	DK	140	5% 74% 22%
33	BN	139	40% 42% 40% 14%
33	DN	139	41% 43% 40% 12% 6%
34	BO	122	37% 75% 23%
34	DO	122	46% 77% 20%
35	BP	146	3% 66% 32%
35	DP	146	2% 71% 27%
36	BQ	141	3% 67% 28% 5%
36	DQ	141	6% 79% 21%
37	BR	117	74% 24%
37	DR	117	% 73% 25%
38	BS	99	20% 72% 23% 5%
38	DS	99	11% 66% 30%
39	BT	138	31% 66% 28% 5%
39	DT	138	25% 64% 30% 5%
40	BU	117	% 79% 21%

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Mol	Chain	Length	Quality of chain
40	DU	117	%, 80%, 18%
41	BV	101	5%, 68%, 24%, 8%
41	DV	101	5%, 74%, 23%
42	BW	113	3%, 78%, 21%
42	DW	113	4%, 73%, 23%
43	BX	93	4%, 75%, 23%
43	DX	93	2%, 70%, 27%
44	BY	107	9%, 64%, 31%, 5%
44	DY	107	6%, 71%, 25%
45	BZ	185	72%, 26%
45	DZ	185	2%, 72%, 25%
46	B0	84	18%, 87%, 12%
46	D0	84	5%, 79%, 21%
47	B1	93	22%, 63%, 26%, 6%
47	D1	93	29%, 61%, 30%, 8%
48	B2	71	79%, 20%
48	D2	71	3%, 83%, 15%
49	B3	60	2%, 85%, 13%
49	D3	60	83%, 17%
50	B4	35	31%, 66%, 31%
50	D4	35	23%, 63%, 34%
51	B5	59	69%, 27%
51	D5	59	3%, 69%, 29%
52	B6	50	28%, 60%, 30%, 8%
52	D6	50	26%, 50%, 42%, 8%

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Mol	Chain	Length	Quality of chain
53	B7	49	33% 80% 16%
53	D7	49	20% 76% 22%
54	B8	64	16% 70% 27%
54	D8	64	11% 66% 28% 6%
55	B9	37	3% 76% 24%
55	D9	37	84% 16%
56	Be	103	12% 86% 12%
56	De	103	9% 80% 19%
57	Bf	31	100%
57	Bg	31	100%
57	Df	31	100%
57	Dg	31	100%
58	Bh	30	100%
58	Dh	30	100%
59	BA	2879	% 71% 27%
59	DA	2879	% 71% 26%
60	BB	119	5% 67% 31%
60	DB	119	61% 38%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 312066 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AB	235	1910	1218	342	345	5	0	0	0
1	CB	235	1910	1218	342	345	5	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AC	207	1621	1022	315	283	1	0	0	0
2	CC	207	1621	1022	315	283	1	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AE	151	1156	729	218	205	4	0	0	0
4	CE	151	1156	729	218	205	4	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	AI	127	1010	639	197	174	0	0	0
8	CI	127	1010	639	197	174	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AJ	99	802	504	157	140	1	0	0	0
9	CJ	99	802	504	157	140	1	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AL	125	976	614	196	165	1	0	0	0
11	CL	125	976	614	196	165	1	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AM	125	997	617	207	171	2	0	0	0
12	CM	125	997	617	207	171	2	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AP	84	706	446	140	119	1	0	0	0
15	CP	84	706	446	140	119	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AQ	100	835	534	155	144	2	0	0	0
16	CQ	100	835	534	155	144	2	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	AS	79	634	405	115	112	2	0	0	0
18	CS	79	634	405	115	112	2	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AY	661	5173	3288	884	983	18	0	0	0
20	CY	661	5173	3288	884	983	18	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	40	THR	HIS	conflict	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	40	THR	HIS	conflict	UNP Q72I01
CY	129	LYS	HIS	conflict	UNP Q72I01
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 21 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
21	AA	1511	32474	14455	6015	10494	1510	0	0	0
21	CA	1511	32474	14455	6015	10494	1510	0	0	0

- Molecule 22 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AW	77	1635	732	291	536	76	0	0	0
22	CW	77	1635	732	291	536	76	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AV	36	783	351	159	237	36	0	0	0
23	CV	36	781	352	159	235	35	0	0	0

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	AX	78	1629	730	293	531	75	0	0	0
24	CX	78	1629	730	293	531	75	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	77	VAL	-	expression tag	GB 1154835240

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Chain	Residue	Modelled	Actual	Comment	Reference
AX	78	ACE	-	expression tag	GB 1154835240
CX	77	VAL	-	expression tag	GB 1154835240
CX	78	ACE	-	expression tag	GB 1154835240

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	BC	228	1742	1101	319	319	3	0	0	0
25	DC	228	1742	1101	319	319	3	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	BD	275	2145	1353	428	361	3	0	0	0
26	DD	275	2145	1353	428	361	3	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BE	205	1569	991	300	272	6	0	0	0
27	DE	205	1569	991	300	272	6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BF	208	1628	1037	304	284	3	0	0	0
28	DF	208	1628	1037	304	284	3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BH	167	1274	806	238	229	1	0	0	0
30	DH	167	1274	806	238	229	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein l10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
31	BJ	170	851	510	170	171	0	0	0
31	DJ	170	851	510	170	171	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BK	140	1035	659	183	188	5	0	0	0
32	DK	140	1035	659	183	188	5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BN	139	1114	717	207	186	4	0	0	0
33	DN	139	1114	717	207	186	4	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	conflict	UNP Q72I11
DQ	32	TYR	PHE	conflict	UNP Q72I11

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
38	BS	99	775	488	155	132	0	0	0
38	DS	99	775	488	155	132	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BT	138	1147	713	235	198	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	DT	138	1147	713	235	198	1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BU	117	964	610	202	151	1	0	0	0
			Total	C	N	O	S			
40	DU	117	964	610	202	151	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BW	113	900	566	177	155	2	0	0	0
			Total	C	N	O	S			
42	DW	113	900	566	177	155	2	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BX	93	734	477	132	125	0	0	0
			Total	C	N	O			
43	DX	93	734	477	132	125	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BY	107	818	524	155	134	5	0	0	0
			Total	C	N	O	S			
44	DY	107	818	524	155	134	5	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BZ	185	1473	939	262	270	2	0	0	0
45	DZ	185	1473	939	262	270	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	B1	93	732	460	145	126	1	0	0	0
47	D1	93	732	460	145	126	1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	B3	60	477	303	91	82	1	0	0	0
49	D3	60	477	303	91	82	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B4	35	271	174	44	50	3	0	0	0
50	D4	35	271	174	44	50	3	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B6	50	433	270	88	71	4	0	0	0
52	D6	50	433	270	88	71	4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	B7	49	430	263	108	57	2	0	0	0
53	D7	49	430	263	108	57	2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	B8	64	517	331	102	82	2	0	0	0
54	D8	64	517	331	102	82	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B9	37	307	188	68	47	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	D9	37	307	188	68	47	4	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	Be	102	686	430	119	137	0	0	0
56	De	102	686	430	119	137	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	1	UNK	-	expression tag	UNP Q72GS2
Be	2	UNK	-	expression tag	UNP Q72GS2
Be	3	UNK	-	expression tag	UNP Q72GS2
Be	4	UNK	-	expression tag	UNP Q72GS2
Be	5	UNK	-	expression tag	UNP Q72GS2
Be	6	UNK	-	expression tag	UNP Q72GS2
Be	7	UNK	-	expression tag	UNP Q72GS2
Be	8	UNK	-	expression tag	UNP Q72GS2
Be	9	UNK	-	expression tag	UNP Q72GS2
Be	10	UNK	-	expression tag	UNP Q72GS2
Be	11	UNK	-	expression tag	UNP Q72GS2
Be	12	UNK	-	expression tag	UNP Q72GS2
Be	13	UNK	-	expression tag	UNP Q72GS2
Be	14	UNK	-	expression tag	UNP Q72GS2
Be	15	UNK	-	expression tag	UNP Q72GS2
Be	16	UNK	-	expression tag	UNP Q72GS2
Be	17	UNK	-	expression tag	UNP Q72GS2
Be	18	UNK	-	expression tag	UNP Q72GS2
Be	19	UNK	-	expression tag	UNP Q72GS2
Be	20	UNK	-	expression tag	UNP Q72GS2
Be	21	UNK	-	expression tag	UNP Q72GS2
Be	22	UNK	-	expression tag	UNP Q72GS2
Be	23	UNK	-	expression tag	UNP Q72GS2
Be	24	UNK	-	expression tag	UNP Q72GS2
Be	25	UNK	-	expression tag	UNP Q72GS2
Be	26	UNK	-	expression tag	UNP Q72GS2
Be	27	UNK	-	expression tag	UNP Q72GS2
Be	28	UNK	-	expression tag	UNP Q72GS2

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Chain	Residue	Modelled	Actual	Comment	Reference
Be	29	UNK	-	expression tag	UNP Q72GS2
Be	30	UNK	-	expression tag	UNP Q72GS2
Be	31	UNK	-	expression tag	UNP Q72GS2
De	1	UNK	-	expression tag	UNP Q72GS2
De	2	UNK	-	expression tag	UNP Q72GS2
De	3	UNK	-	expression tag	UNP Q72GS2
De	4	UNK	-	expression tag	UNP Q72GS2
De	5	UNK	-	expression tag	UNP Q72GS2
De	6	UNK	-	expression tag	UNP Q72GS2
De	7	UNK	-	expression tag	UNP Q72GS2
De	8	UNK	-	expression tag	UNP Q72GS2
De	9	UNK	-	expression tag	UNP Q72GS2
De	10	UNK	-	expression tag	UNP Q72GS2
De	11	UNK	-	expression tag	UNP Q72GS2
De	12	UNK	-	expression tag	UNP Q72GS2
De	13	UNK	-	expression tag	UNP Q72GS2
De	14	UNK	-	expression tag	UNP Q72GS2
De	15	UNK	-	expression tag	UNP Q72GS2
De	16	UNK	-	expression tag	UNP Q72GS2
De	17	UNK	-	expression tag	UNP Q72GS2
De	18	UNK	-	expression tag	UNP Q72GS2
De	19	UNK	-	expression tag	UNP Q72GS2
De	20	UNK	-	expression tag	UNP Q72GS2
De	21	UNK	-	expression tag	UNP Q72GS2
De	22	UNK	-	expression tag	UNP Q72GS2
De	23	UNK	-	expression tag	UNP Q72GS2
De	24	UNK	-	expression tag	UNP Q72GS2
De	25	UNK	-	expression tag	UNP Q72GS2
De	26	UNK	-	expression tag	UNP Q72GS2
De	27	UNK	-	expression tag	UNP Q72GS2
De	28	UNK	-	expression tag	UNP Q72GS2
De	29	UNK	-	expression tag	UNP Q72GS2
De	30	UNK	-	expression tag	UNP Q72GS2
De	31	UNK	-	expression tag	UNP Q72GS2

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	Bf	31	156	93	31	32	0	0	0
			Total	C	N	O			
57	Bg	31	156	93	31	32	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	Df	31	156	93	31	32	0	0	0
57	Dg	31	156	93	31	32	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	Bh	30	151	90	30	31	0	0	0
58	Dh	30	151	90	30	31	0	0	0

- Molecule 59 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
59	BA	2879	61997	27594	11582	19943	2878	0	0	0
59	DA	2879	61997	27594	11582	19943	2878	0	0	0

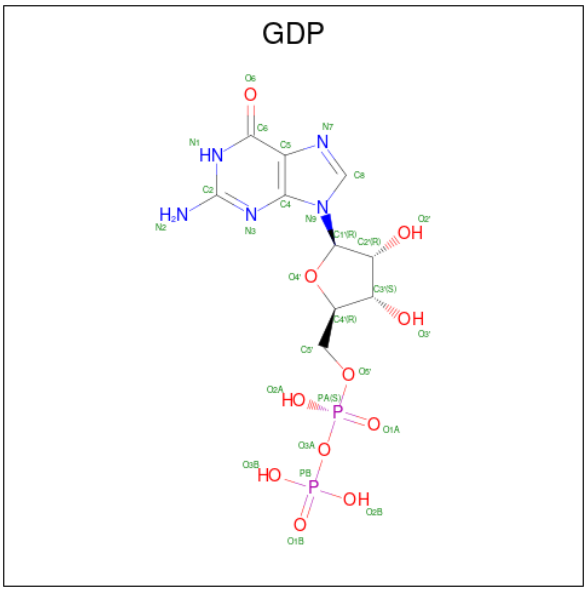
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1141A	U	C	conflict	GB 46197919
BA	2825	U	G	conflict	GB 46197919
DA	1141A	U	C	conflict	GB 46197919
DA	2825	U	G	conflict	GB 46197919

- Molecule 60 is a RNA chain called 5S Ribosomal RNA.

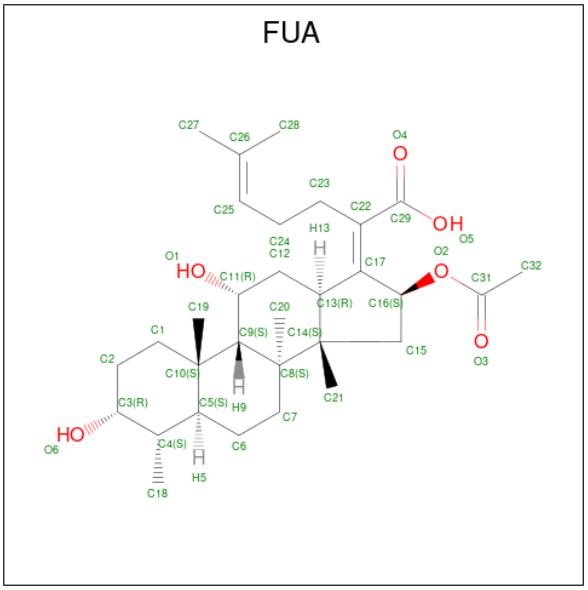
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
60	BB	119	2551	1136	471	826	118	0	0	0
60	DB	119	2551	1136	471	826	118	0	0	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



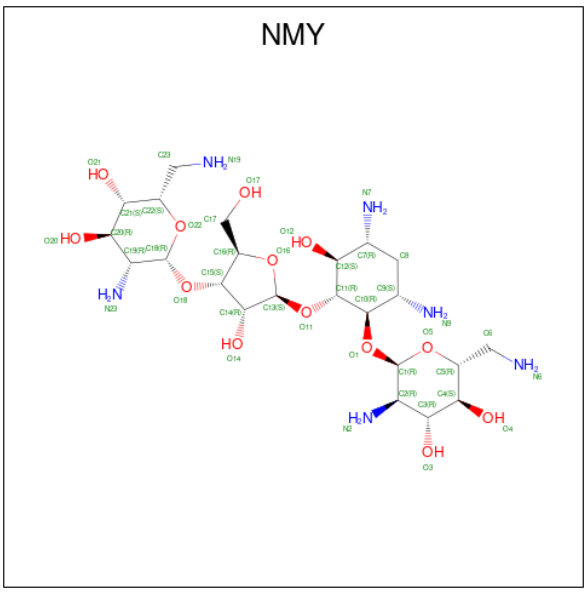
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
61	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 62 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	AY	1	Total	C	O	0	0
			37	31	6		
62	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 63 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
63	AA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	CA	1	42	23	6	13	0	0
			Total	C	N	O		
63	DA	1	42	23	6	13	0	0

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

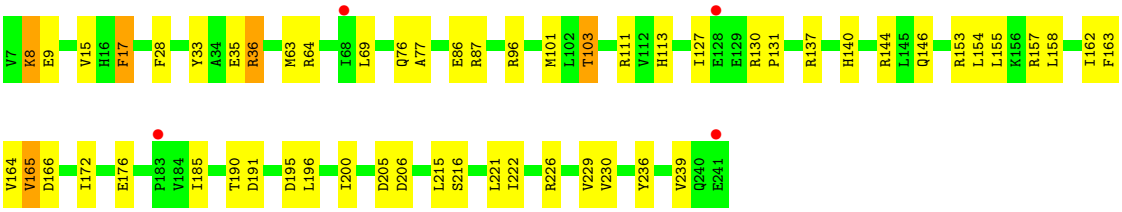
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
64	BA	1	1	1	0	0
			Total	Mg		
64	CY	1	1	1	0	0

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.

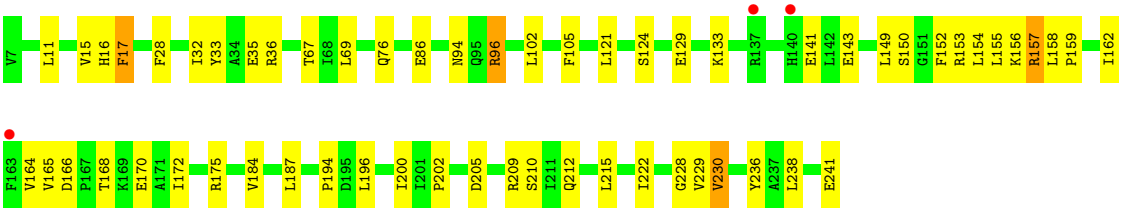
• Molecule 1: 30S ribosomal protein S2

Chain AB:



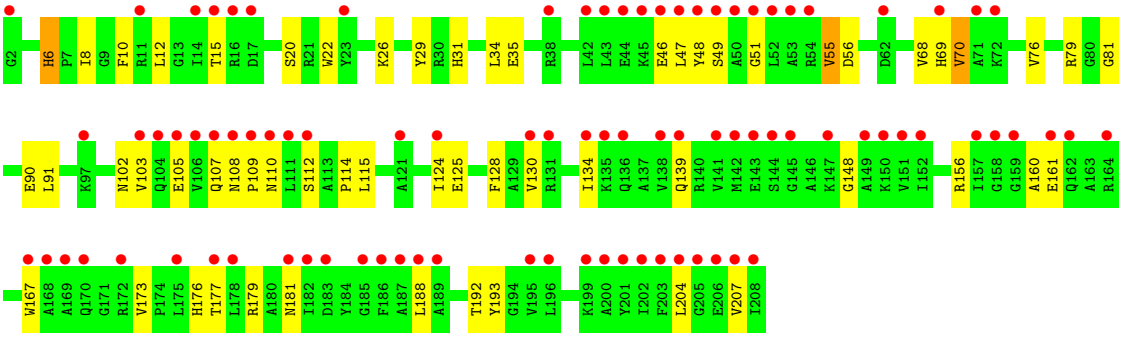
• Molecule 1: 30S ribosomal protein S2

Chain CB:



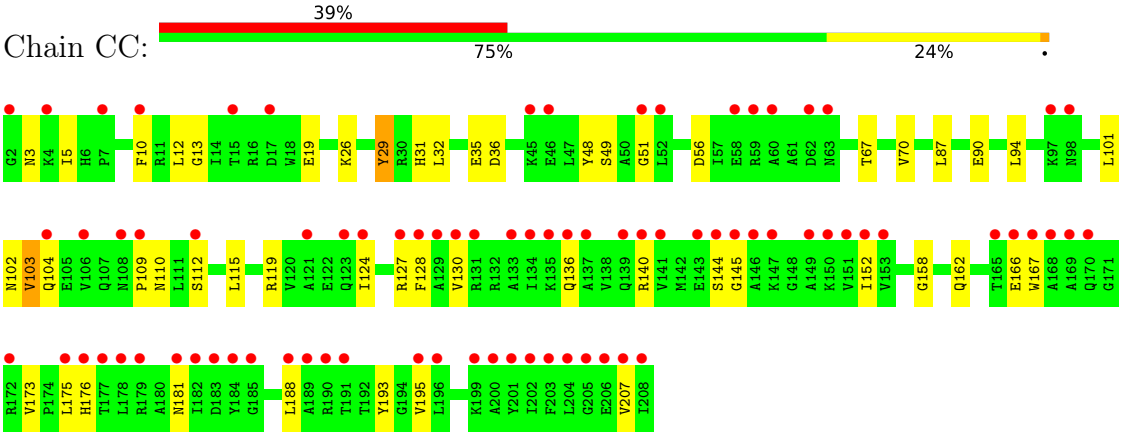
• Molecule 2: 30S ribosomal protein S3

Chain AC:



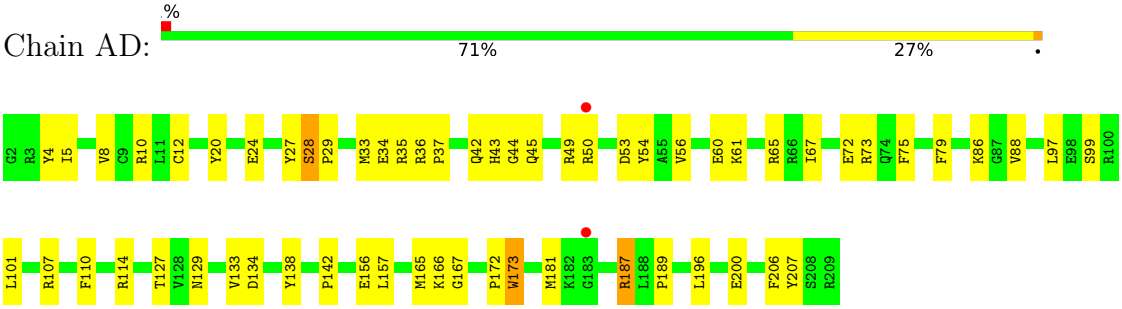
• Molecule 2: 30S ribosomal protein S3

Chain CC:



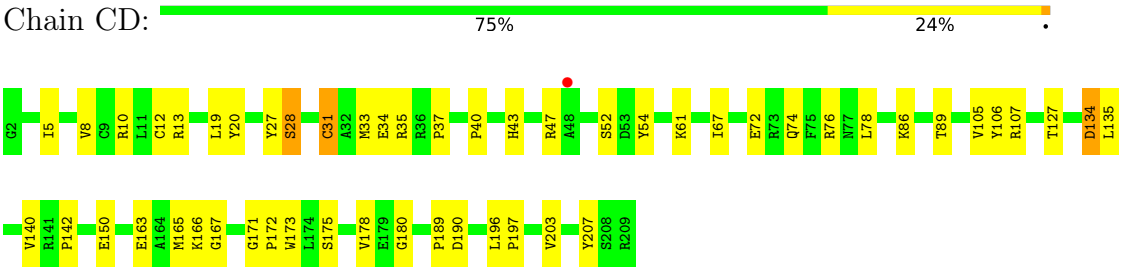
- Molecule 3: 30S ribosomal protein S4

Chain AD:



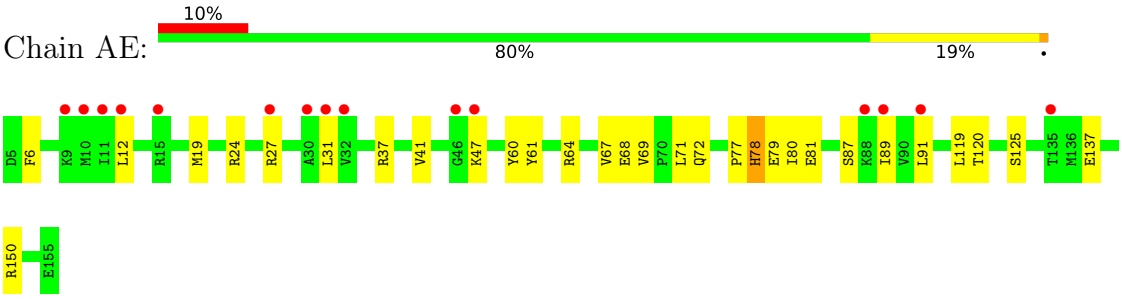
- Molecule 3: 30S ribosomal protein S4

Chain CD:



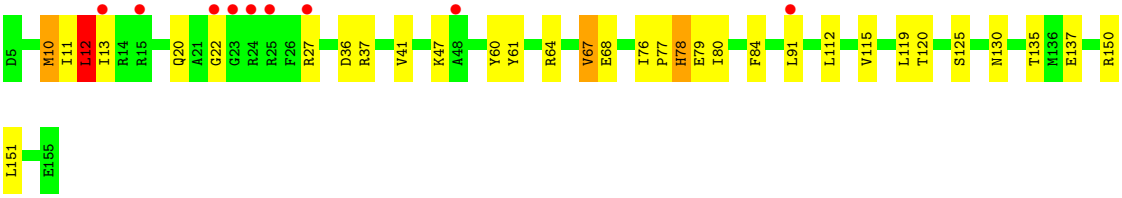
- Molecule 4: 30S ribosomal protein S5

Chain AE:



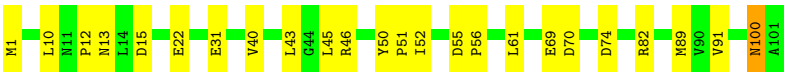
- Molecule 4: 30S ribosomal protein S5

Chain CE:



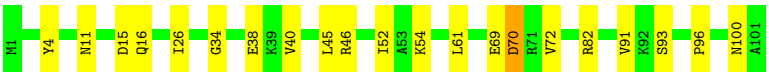
• Molecule 5: 30S ribosomal protein S6

Chain AF:



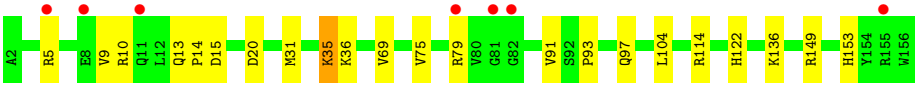
• Molecule 5: 30S ribosomal protein S6

Chain CF:



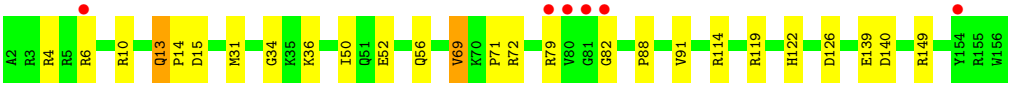
• Molecule 6: 30S ribosomal protein S7

Chain AG:



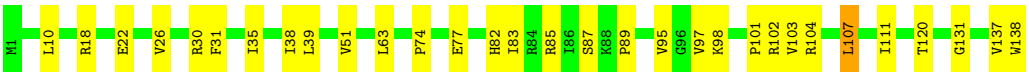
• Molecule 6: 30S ribosomal protein S7

Chain CG:



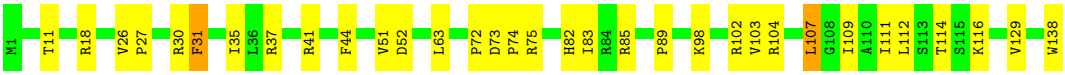
• Molecule 7: 30S ribosomal protein S8

Chain AH:



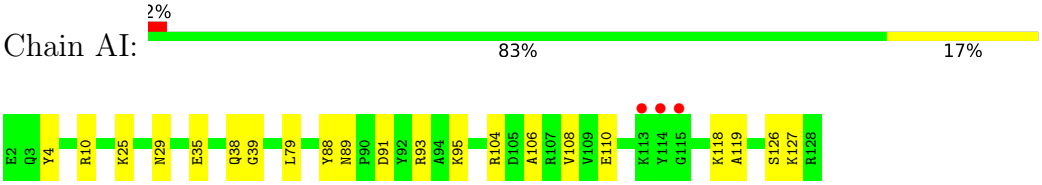
• Molecule 7: 30S ribosomal protein S8

Chain CH:



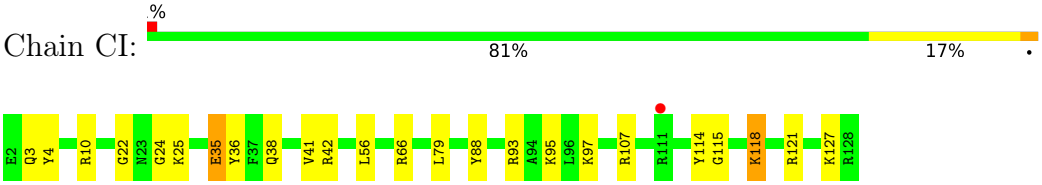
• Molecule 8: 30S ribosomal protein S9

Chain AI:



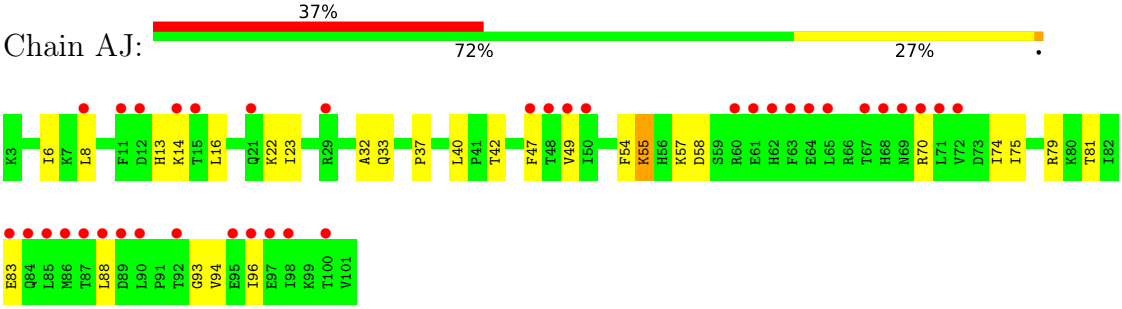
• Molecule 8: 30S ribosomal protein S9

Chain CI:



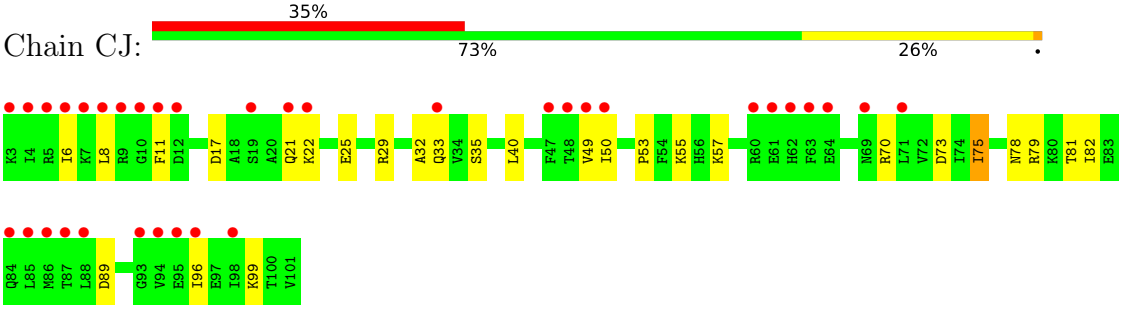
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



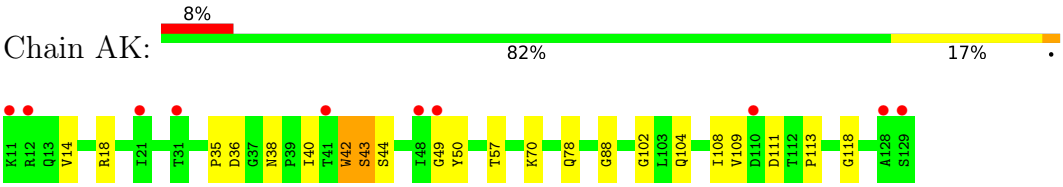
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



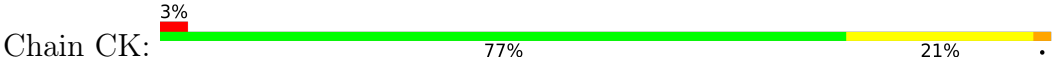
• Molecule 10: 30S ribosomal protein S11

Chain AK:



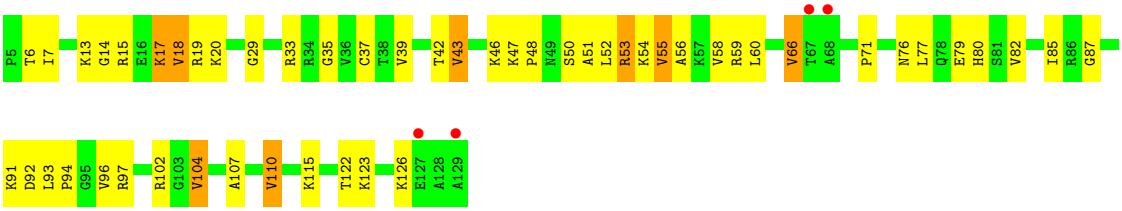
• Molecule 10: 30S ribosomal protein S11

Chain CK:



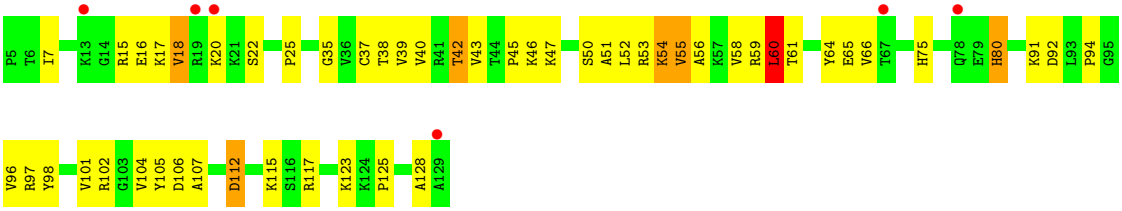
• Molecule 11: 30S ribosomal protein S12

Chain AL:



• Molecule 11: 30S ribosomal protein S12

Chain CL:



• Molecule 12: 30S ribosomal protein S13

Chain AM:

• Molecule 12: 30S ribosomal protein S13

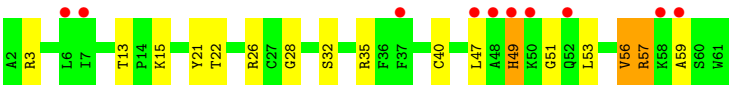
Chain CM:

• Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:

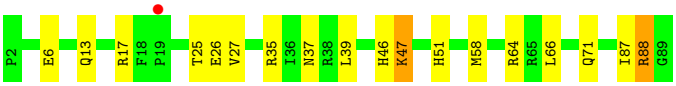
• Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:



• Molecule 14: 30S ribosomal protein S15

Chain AO:

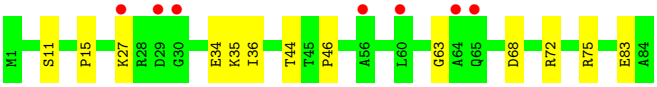


• Molecule 14: 30S ribosomal protein S15

Chain CO:

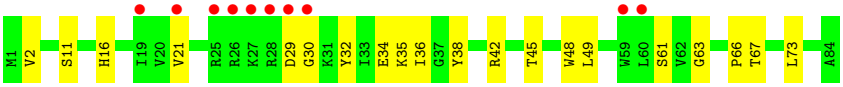
• Molecule 15: 30S ribosomal protein S16

Chain AP:



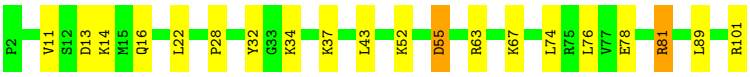
• Molecule 15: 30S ribosomal protein S16

Chain CP:



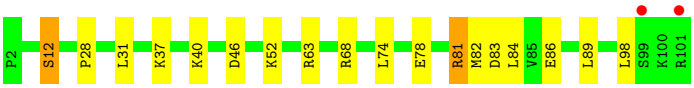
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



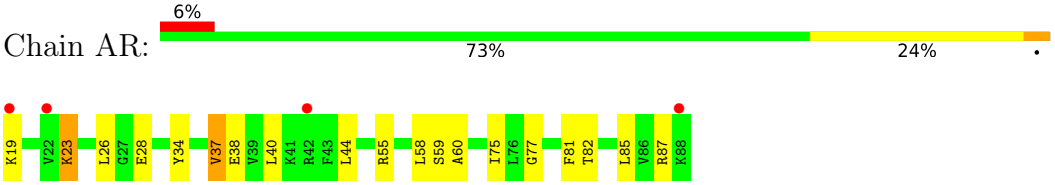
• Molecule 16: 30S ribosomal protein S17

Chain CQ:



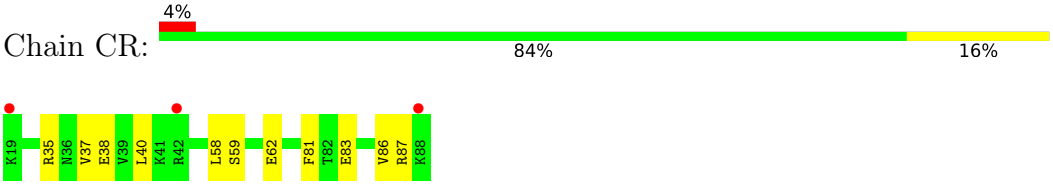
• Molecule 17: 30S ribosomal protein S18

Chain AR:



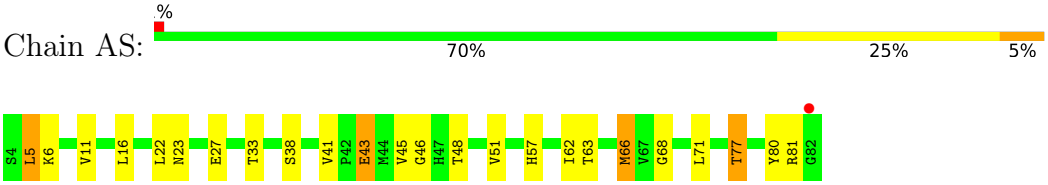
• Molecule 17: 30S ribosomal protein S18

Chain CR:



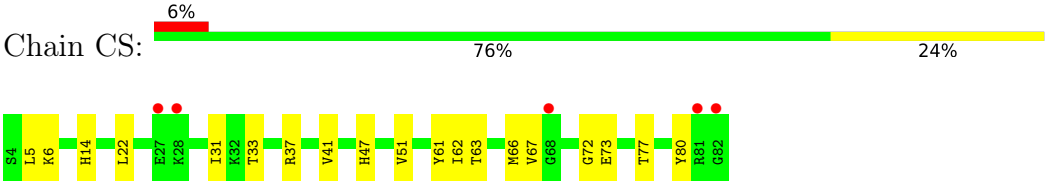
• Molecule 18: 30S ribosomal protein S19

Chain AS:



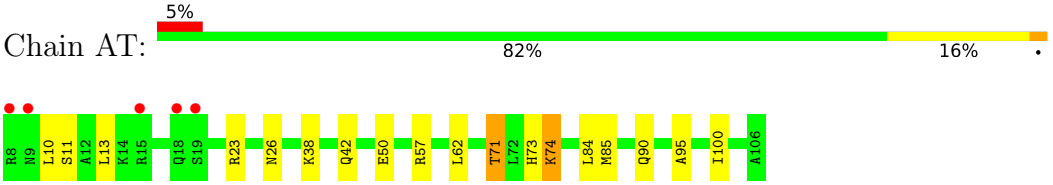
• Molecule 18: 30S ribosomal protein S19

Chain CS:



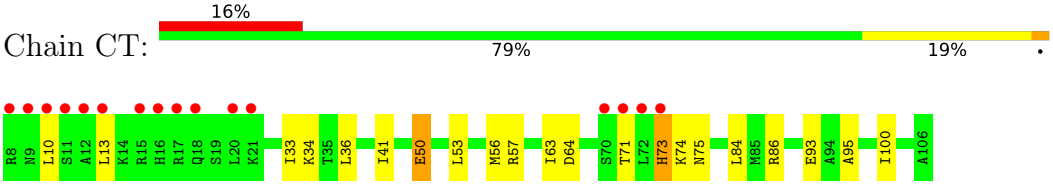
• Molecule 19: 30S ribosomal protein S20

Chain AT:



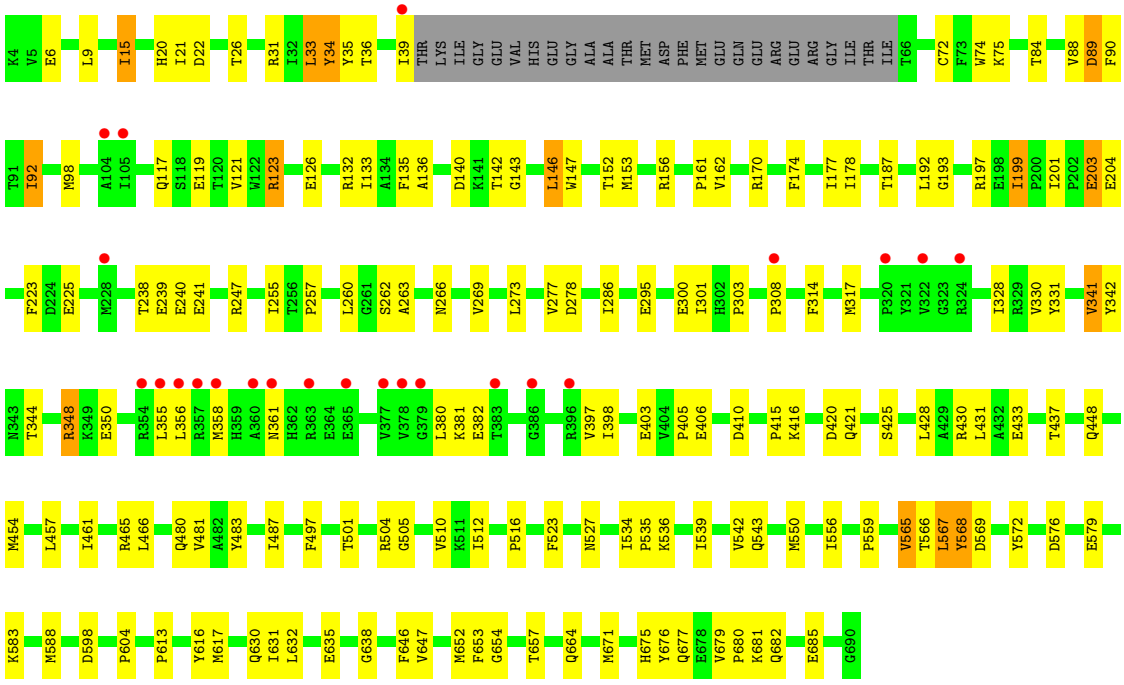
• Molecule 19: 30S ribosomal protein S20

Chain CT:



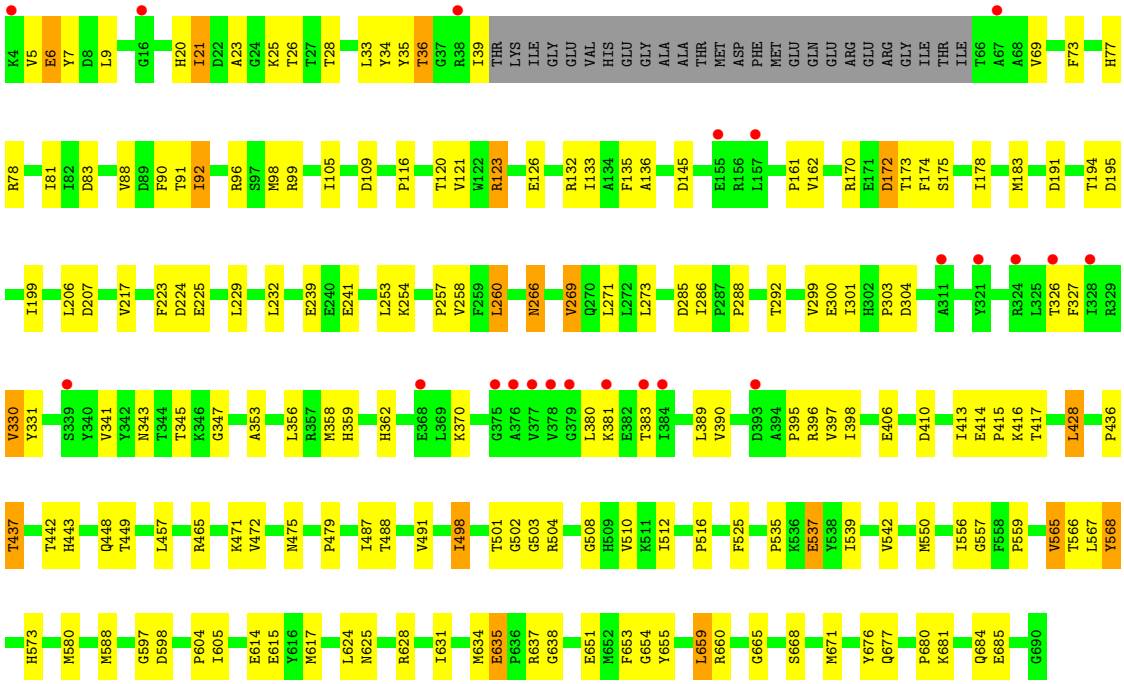
• Molecule 20: Elongation factor G

Chain AY:



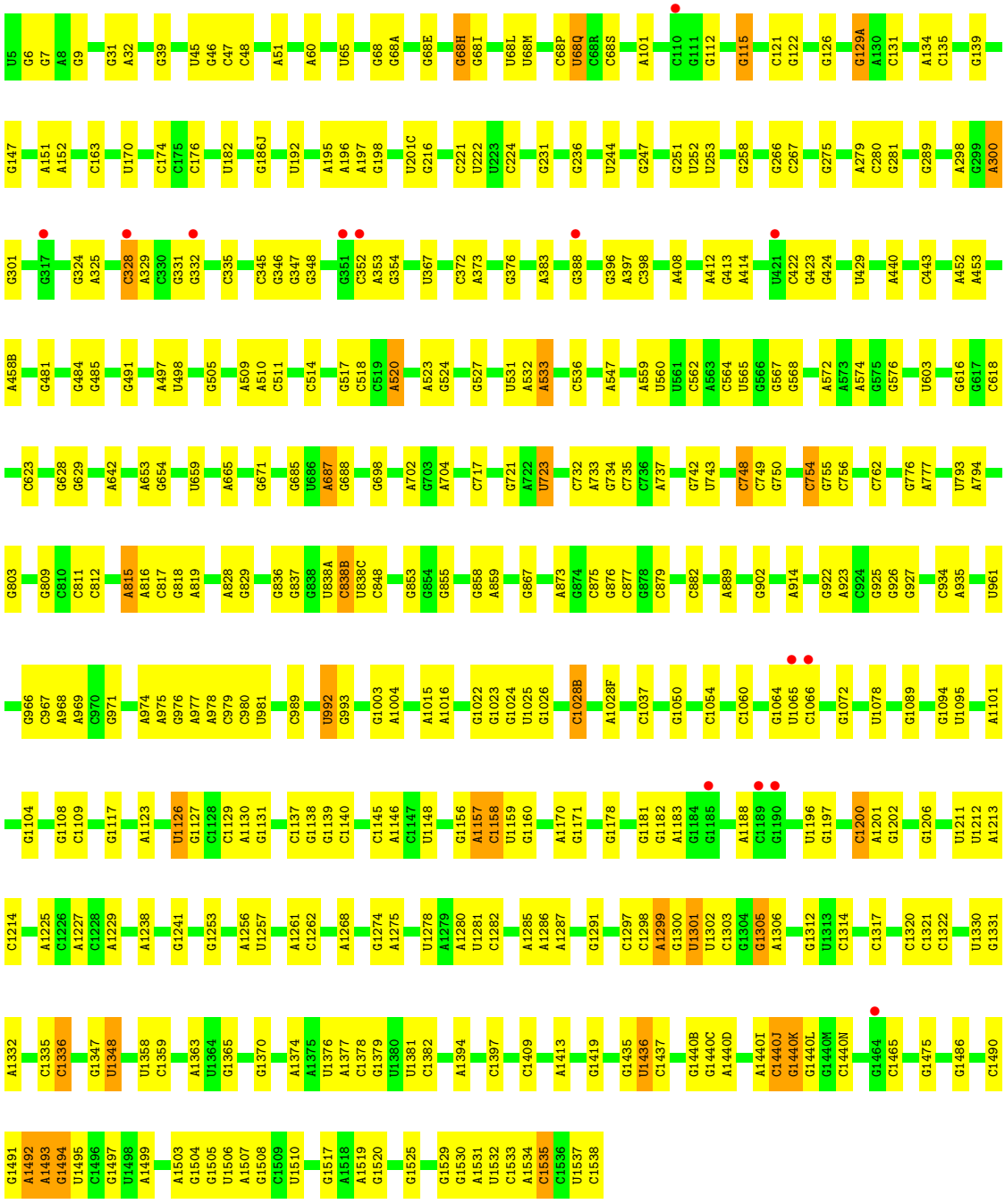
- Molecule 20: Elongation factor G

Chain CY:



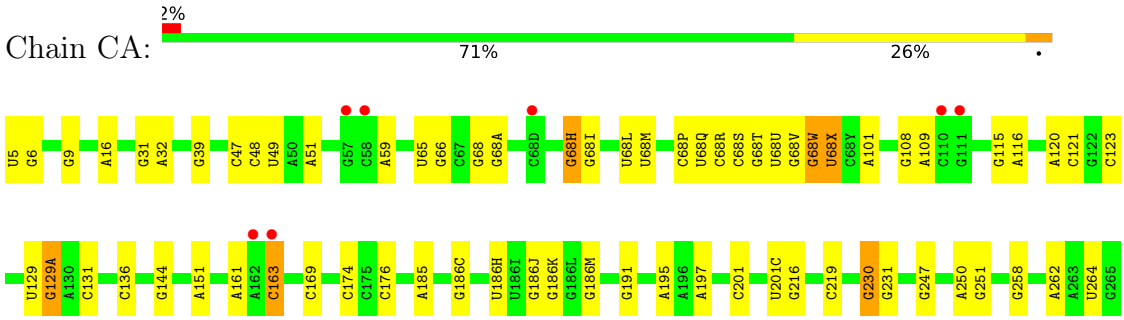
- Molecule 21: 16S Ribosomal RNA

Chain AA:



- Molecule 21: 16S Ribosomal RNA

Chain CA:



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A533 U534 A535 C536 A547 C555 A559 C562 G567 G568 A572 A573 A574 G575 G576 G585 C590 U591 C596 G597 U598 C599 C600 U603 A607 G616 G617 C618 U619 C620 G629 G638 U641 U652 A653 G661 A665 U669 G670 G671

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- Molecule 22: tRNA

Chain AW:

G1 G2 C3 U4 A5 C6 G7 U8 A9 G10 A14 G15 U16 U17 G18 G19 U20 U20A A21 G22 A23 G24 C25 A26 C27 A28 U29 C30 A37 A38 U42 G43 G44 G45 G46 U47 C48 A49 C50 A51 G52 G53 U54 U55 C56 G57 A58 A59 U60 C61 C62 C63 G64 U68 A69 G70

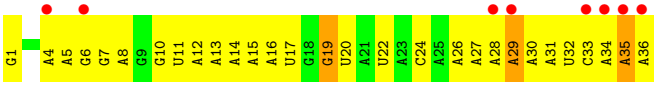
C71 C72 A73 C74 C75 A76

- Molecule 22: tRNA

Chain CW:

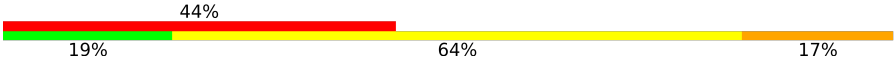
• Molecule 23: mRNA

Chain AV:



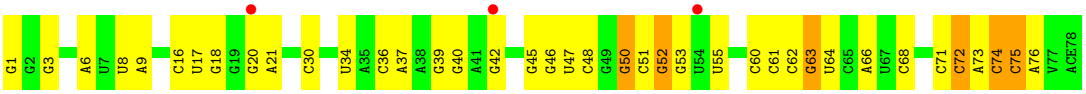
• Molecule 23: mRNA

Chain CV:



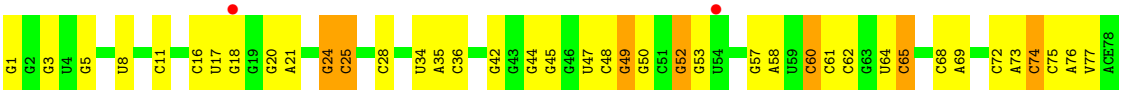
• Molecule 24: tRNA

Chain AX:



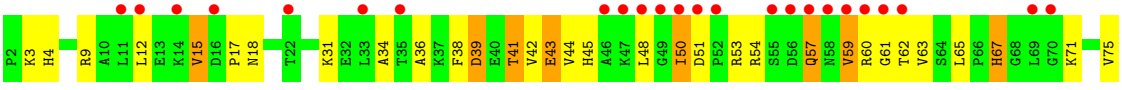
• Molecule 24: tRNA

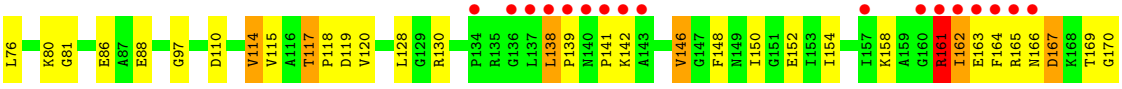
Chain CX:

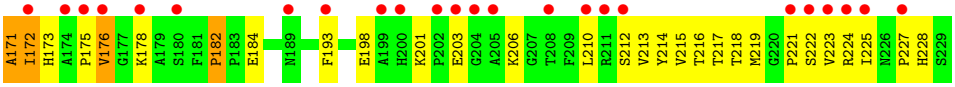


• Molecule 25: 50S ribosomal protein L1

Chain BC:

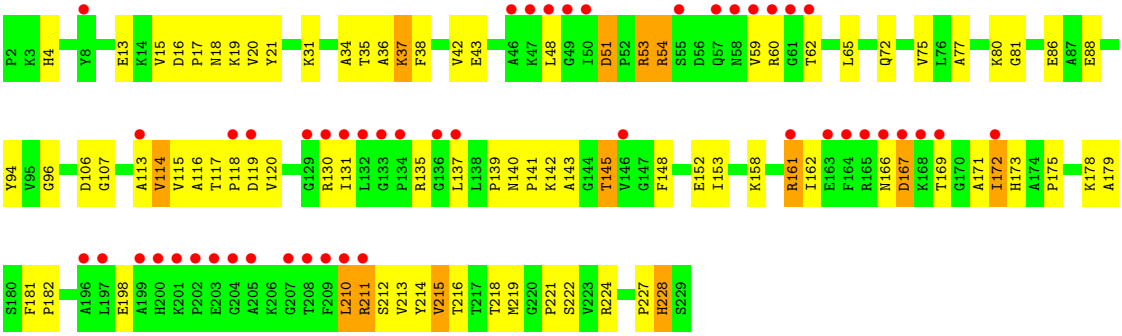






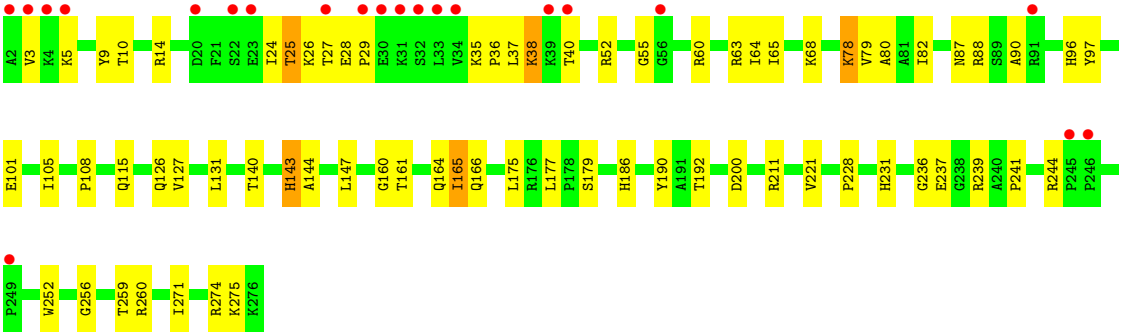
• Molecule 25: 50S ribosomal protein L1

Chain DC:



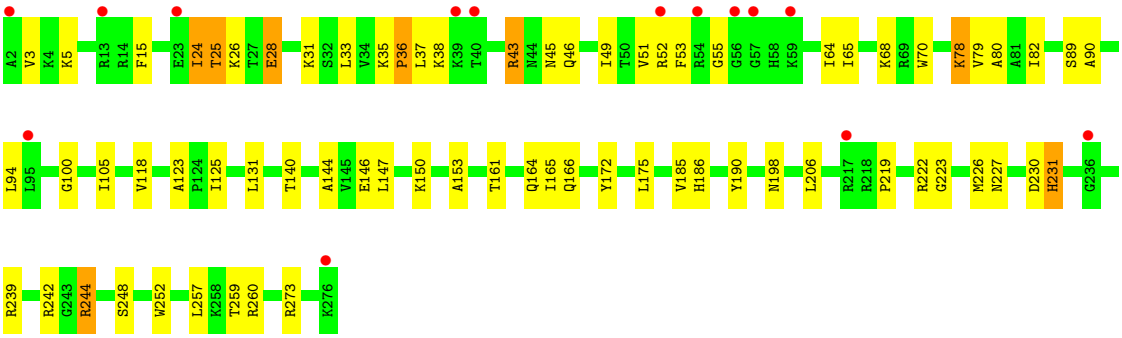
• Molecule 26: 50S ribosomal protein L2

Chain BD:



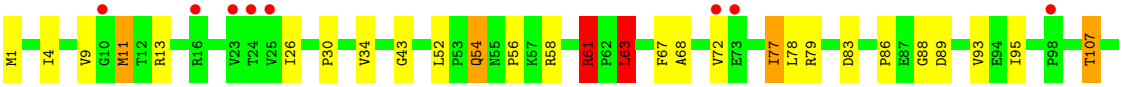
• Molecule 26: 50S ribosomal protein L2

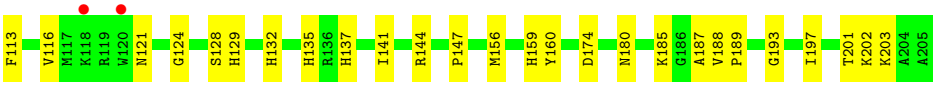
Chain DD:



• Molecule 27: 50S ribosomal protein L3

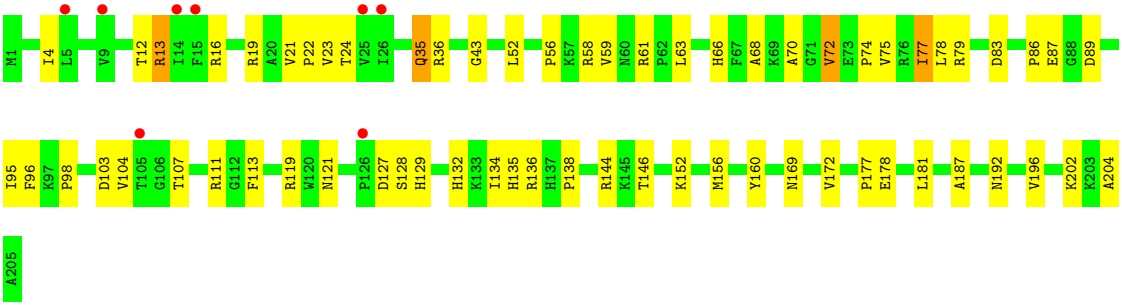
Chain BE:





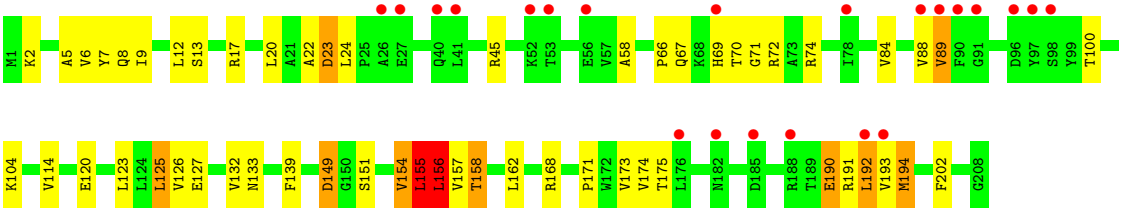
• Molecule 27: 50S ribosomal protein L3

Chain DE:



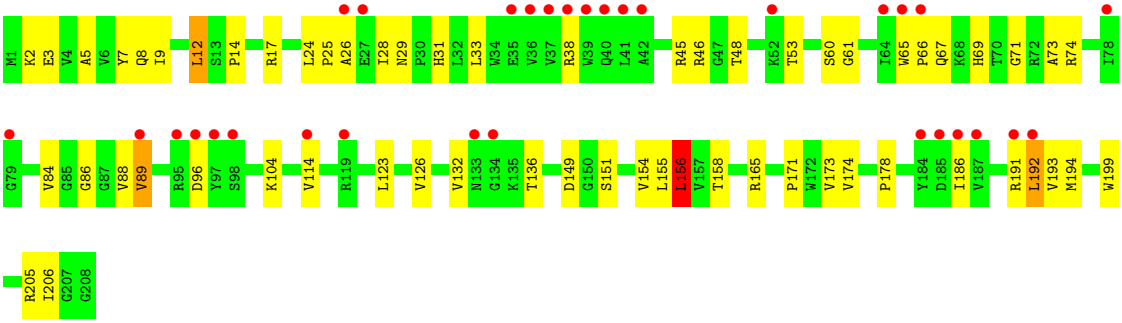
• Molecule 28: 50S ribosomal protein L4

Chain BF:



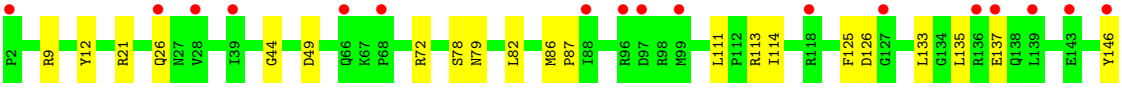
• Molecule 28: 50S ribosomal protein L4

Chain DF:



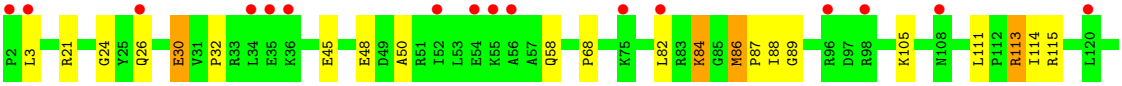
• Molecule 29: 50S ribosomal protein L5

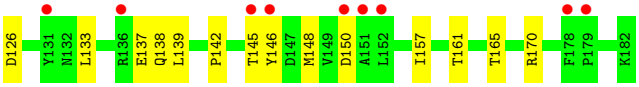
Chain BG:



• Molecule 29: 50S ribosomal protein L5

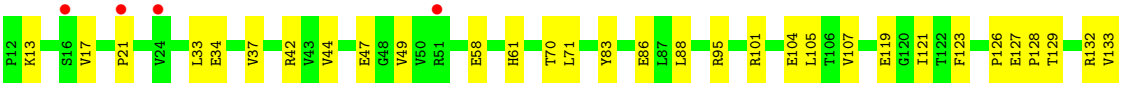
Chain DG:

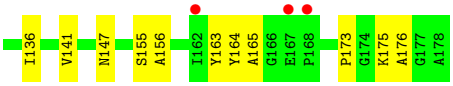




• Molecule 30: 50S ribosomal protein L6

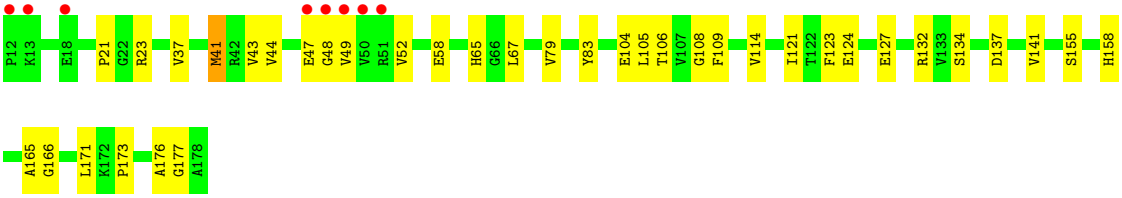
Chain BH:





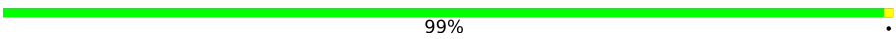
• Molecule 30: 50S ribosomal protein L6

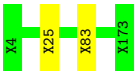
Chain DH:



• Molecule 31: 50S ribosomal protein l10

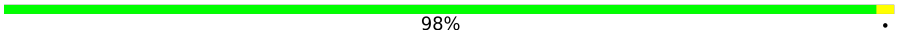
Chain BJ:

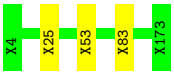




• Molecule 31: 50S ribosomal protein l10

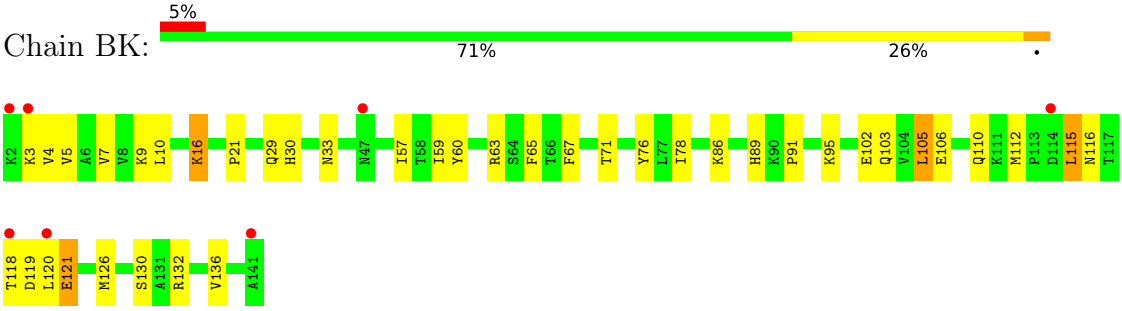
Chain DJ:





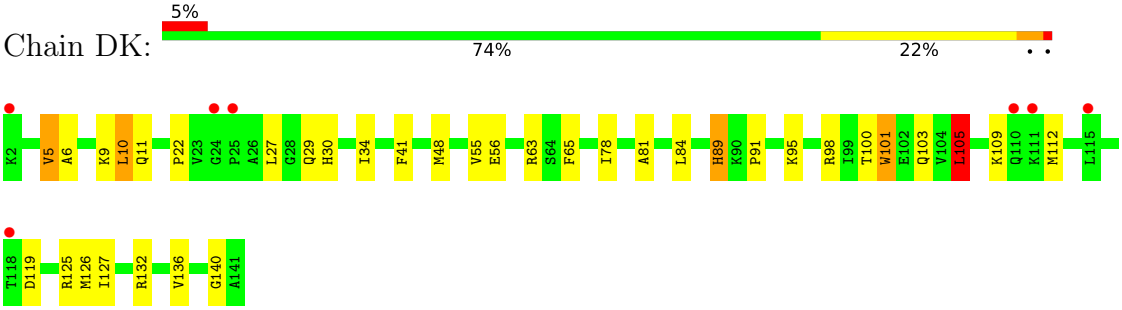
• Molecule 32: 50S ribosomal protein L11

Chain BK:



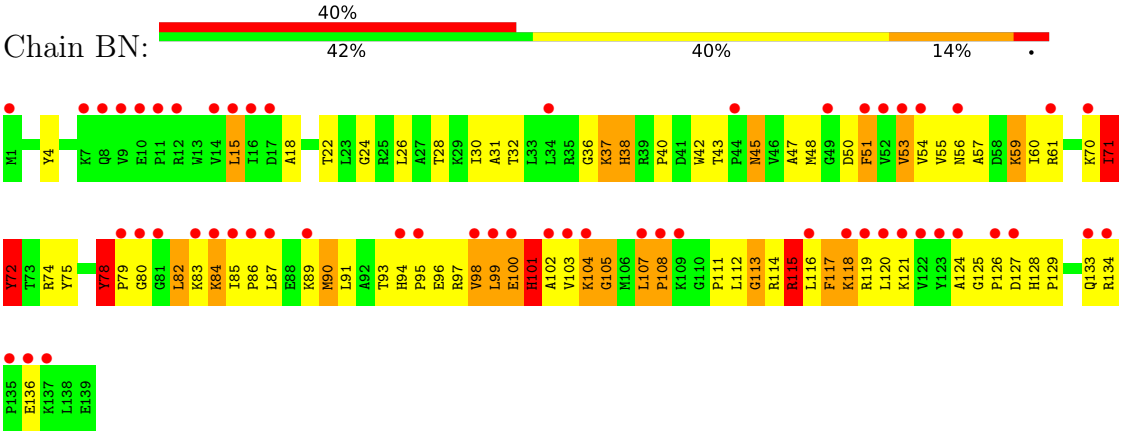
• Molecule 32: 50S ribosomal protein L11

Chain DK:



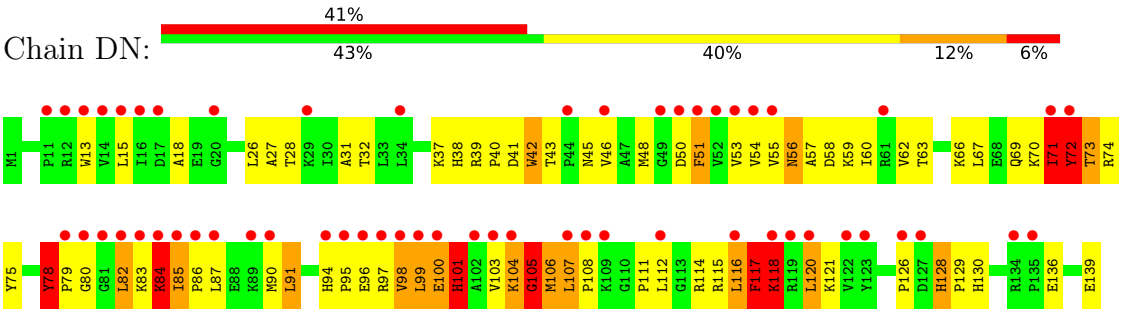
• Molecule 33: 50S ribosomal protein L13

Chain BN:



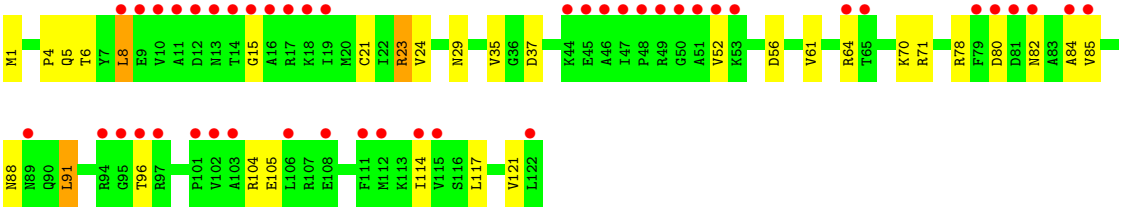
• Molecule 33: 50S ribosomal protein L13

Chain DN:



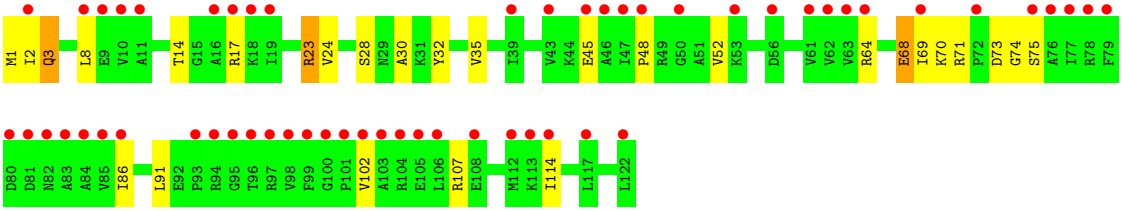
• Molecule 34: 50S ribosomal protein L14

Chain BO:



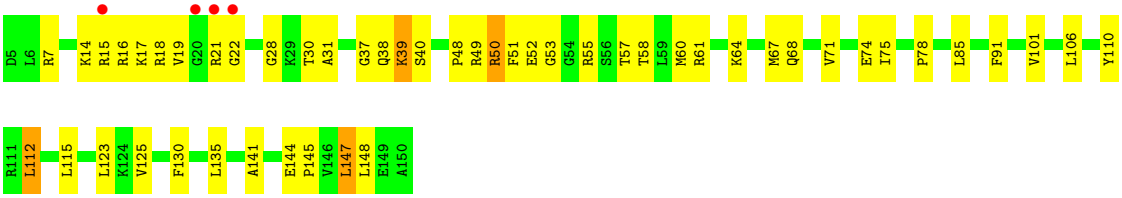
• Molecule 34: 50S ribosomal protein L14

Chain DO:



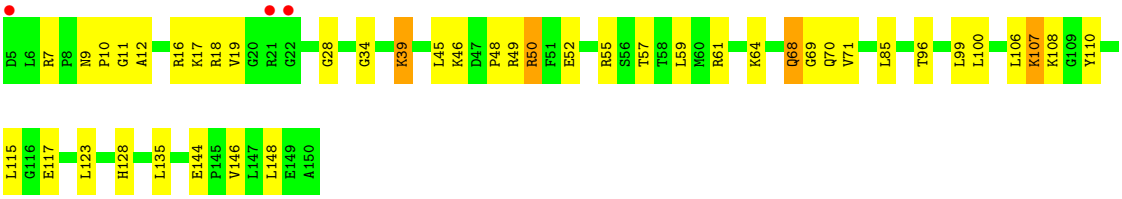
• Molecule 35: 50S ribosomal protein L15

Chain BP:



• Molecule 35: 50S ribosomal protein L15

Chain DP:



• Molecule 36: 50S ribosomal protein L16

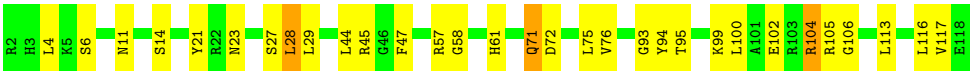
Chain BQ:

• Molecule 36: 50S ribosomal protein L16

Chain DQ:

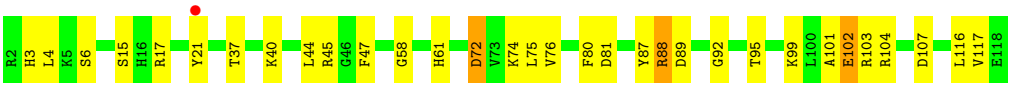
• Molecule 37: 50S ribosomal protein L17

Chain BR:



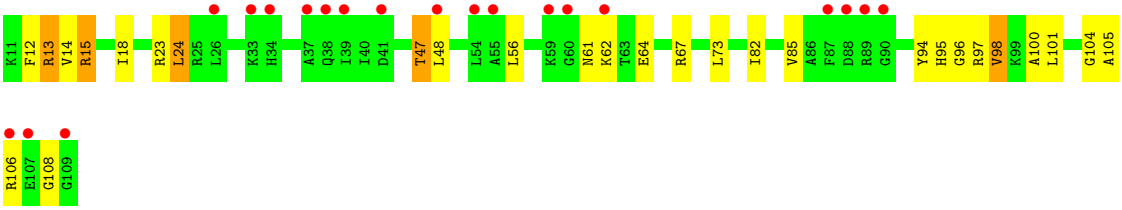
• Molecule 37: 50S ribosomal protein L17

Chain DR:



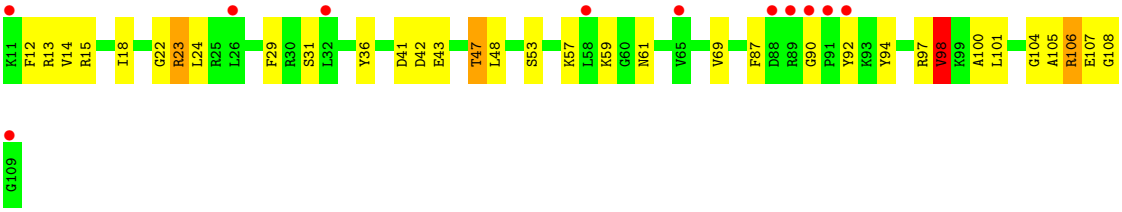
• Molecule 38: 50S ribosomal protein L18

Chain BS:



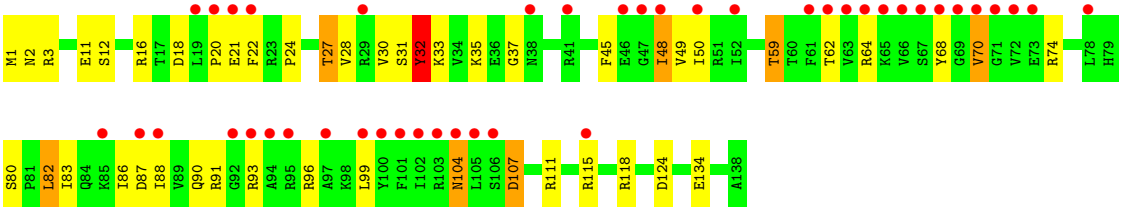
• Molecule 38: 50S ribosomal protein L18

Chain DS:



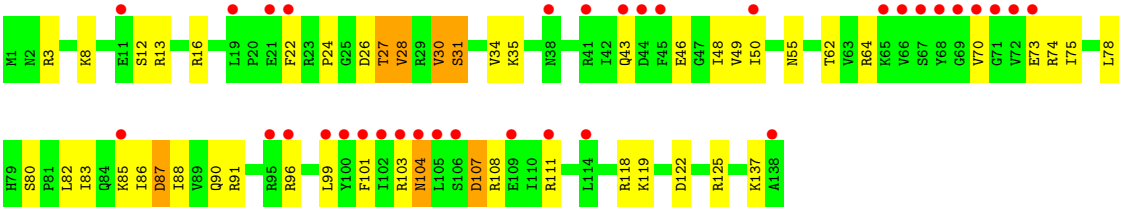
• Molecule 39: 50S ribosomal protein L19

Chain BT:



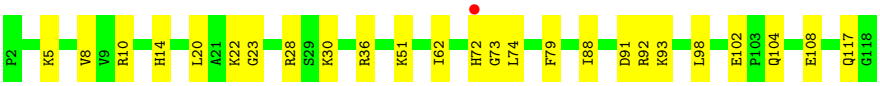
- Molecule 39: 50S ribosomal protein L19

Chain DT:



- Molecule 40: 50S ribosomal protein L20

Chain BU:

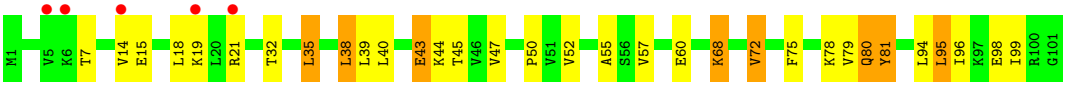


- Molecule 40: 50S ribosomal protein L20

Chain DU:

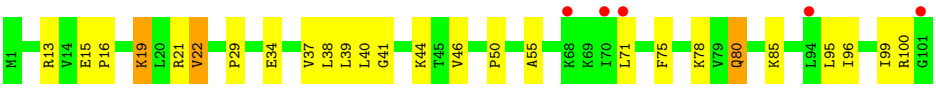
- Molecule 41: 50S ribosomal protein L21

Chain BV:



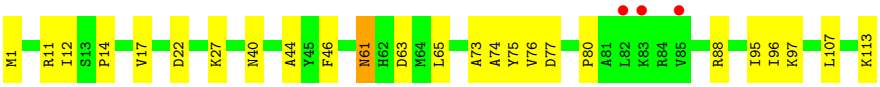
- Molecule 41: 50S ribosomal protein L21

Chain DV:



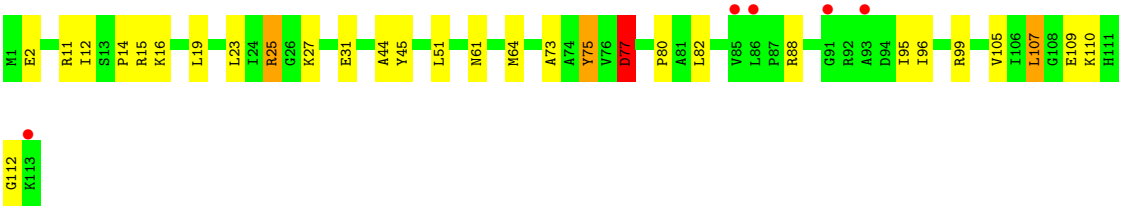
- Molecule 42: 50S ribosomal protein L22

Chain BW: 3% 78% 21%



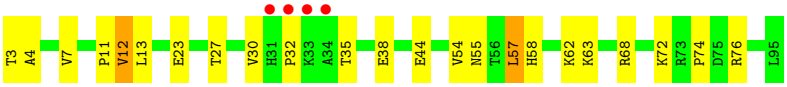
• Molecule 42: 50S ribosomal protein L22

Chain DW: 4% 73% 23%



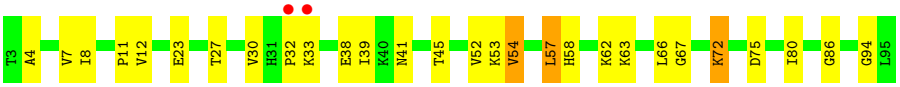
• Molecule 43: 50S ribosomal protein L23

Chain BX: 4% 75% 23%



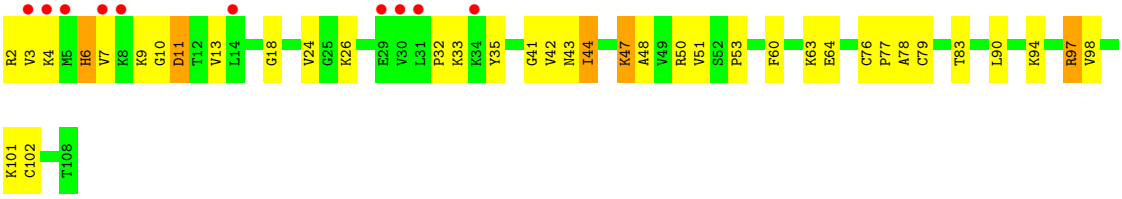
• Molecule 43: 50S ribosomal protein L23

Chain DX: 2% 70% 27%



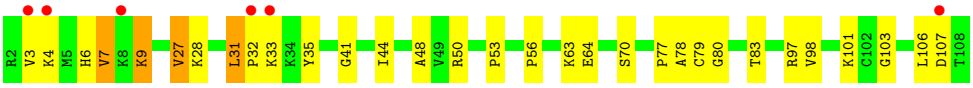
• Molecule 44: 50S ribosomal protein L24

Chain BY: 9% 64% 31% 5%



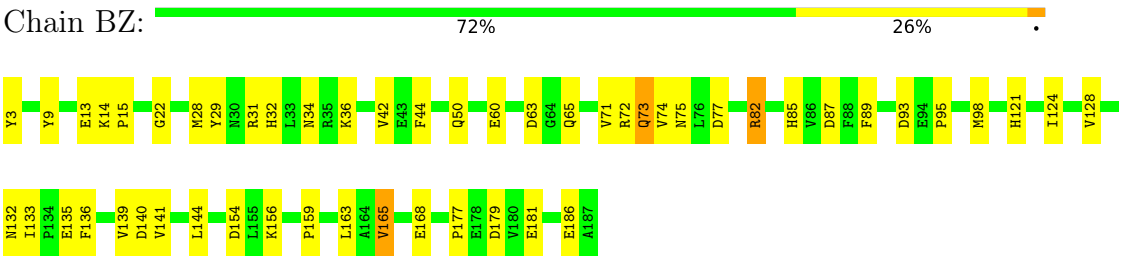
• Molecule 44: 50S ribosomal protein L24

Chain DY: 6% 71% 25%



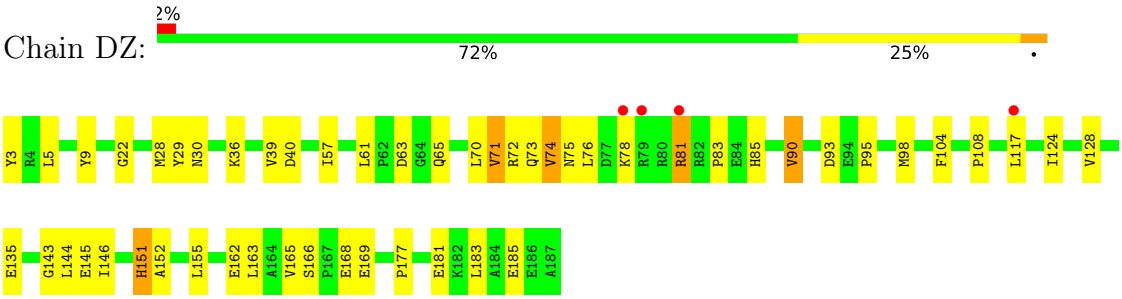
• Molecule 45: 50S ribosomal protein L25

Chain BZ:



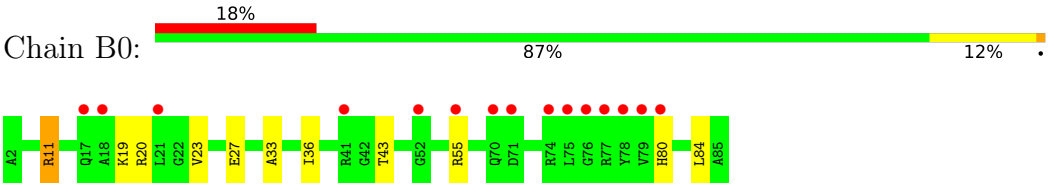
• Molecule 45: 50S ribosomal protein L25

Chain DZ:



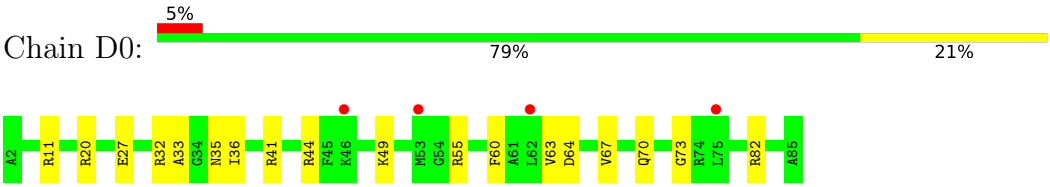
• Molecule 46: 50S ribosomal protein L27

Chain B0:



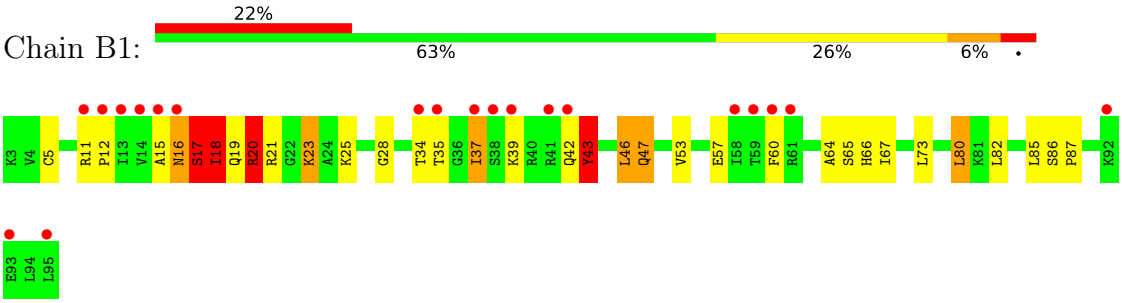
• Molecule 46: 50S ribosomal protein L27

Chain D0:



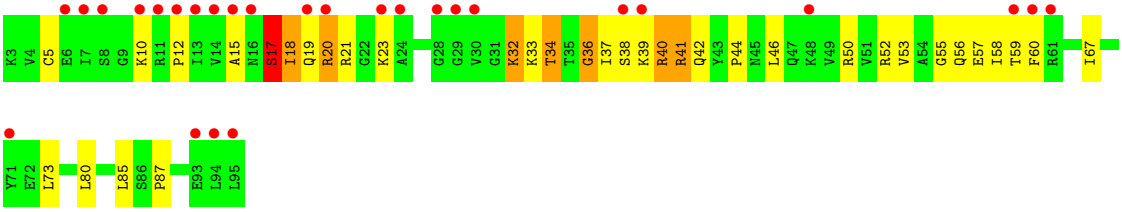
• Molecule 47: 50S ribosomal protein L28

Chain B1:



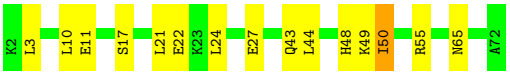
• Molecule 47: 50S ribosomal protein L28

Chain D1:



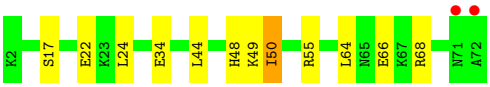
• Molecule 48: 50S ribosomal protein L29

Chain B2:



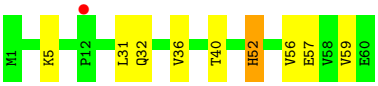
• Molecule 48: 50S ribosomal protein L29

Chain D2:



• Molecule 49: 50S ribosomal protein L30

Chain B3:

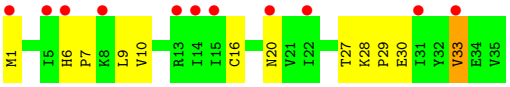


• Molecule 49: 50S ribosomal protein L30

Chain D3:

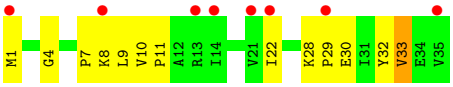
• Molecule 50: 50S ribosomal protein L31

Chain B4:



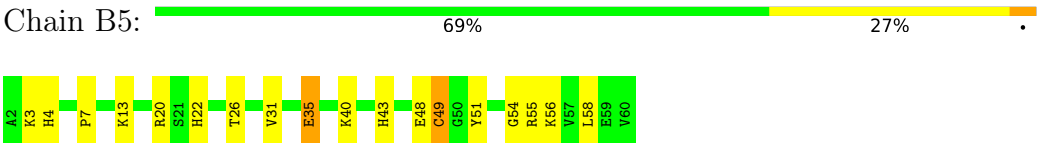
• Molecule 50: 50S ribosomal protein L31

Chain D4:



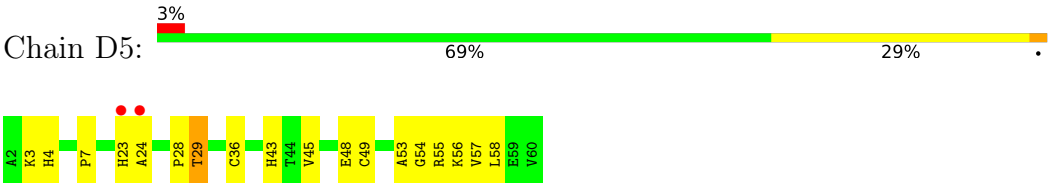
• Molecule 51: 50S ribosomal protein L32

Chain B5:



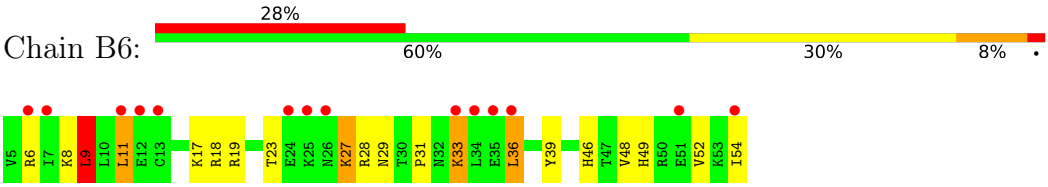
• Molecule 51: 50S ribosomal protein L32

Chain D5:



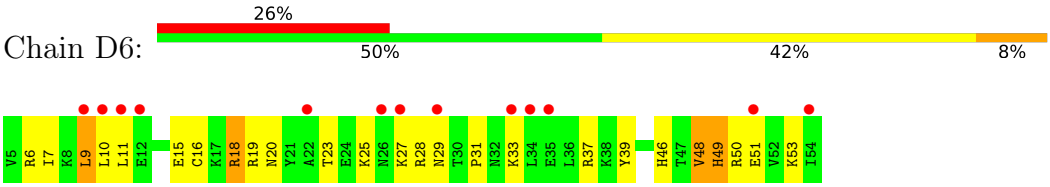
• Molecule 52: 50S ribosomal protein L33

Chain B6:



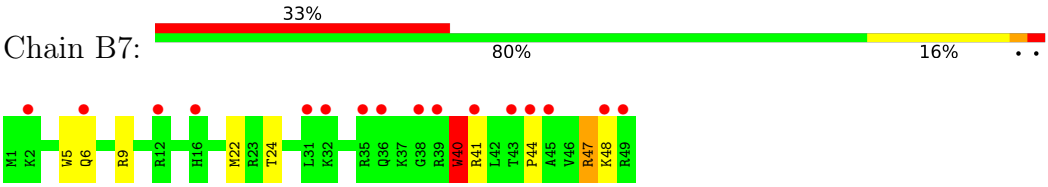
• Molecule 52: 50S ribosomal protein L33

Chain D6:



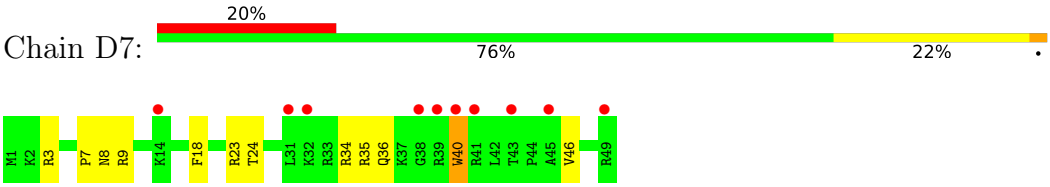
• Molecule 53: 50S ribosomal protein L34

Chain B7:



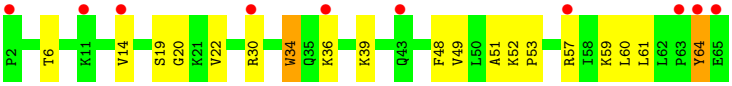
• Molecule 53: 50S ribosomal protein L34

Chain D7:



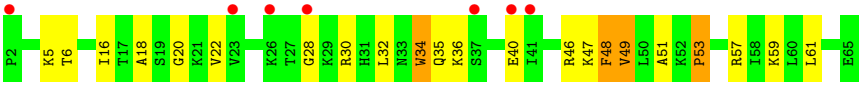
• Molecule 54: 50S ribosomal protein L35

Chain B8:



• Molecule 54: 50S ribosomal protein L35

Chain D8:

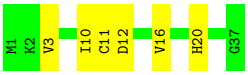


• Molecule 55: 50S ribosomal protein L36

Chain B9:

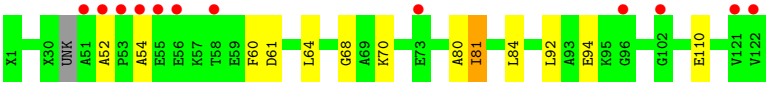
• Molecule 55: 50S ribosomal protein L36

Chain D9:



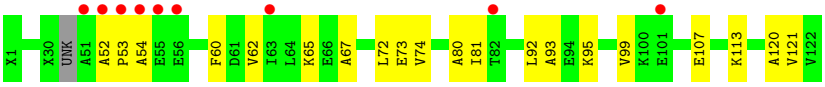
• Molecule 56: 50S ribosomal protein L7/L12

Chain Be:



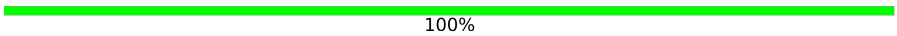
• Molecule 56: 50S ribosomal protein L7/L12

Chain De:



• Molecule 57: 50S ribosomal protein L7/L12

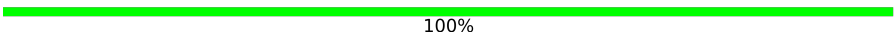
Chain Bf:



There are no outlier residues recorded for this chain.

• Molecule 57: 50S ribosomal protein L7/L12

Chain Bg:



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df: 100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg: 100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh: 100%

There are no outlier residues recorded for this chain.

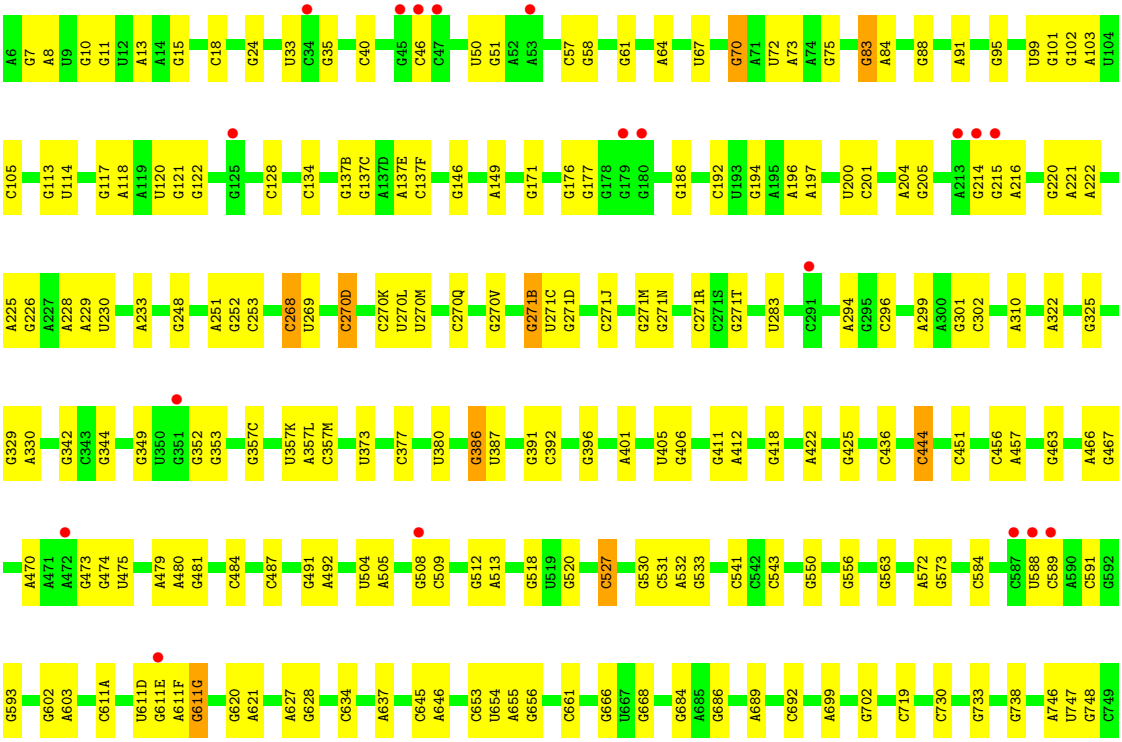
- Molecule 58: 50S ribosomal protein L7/L12

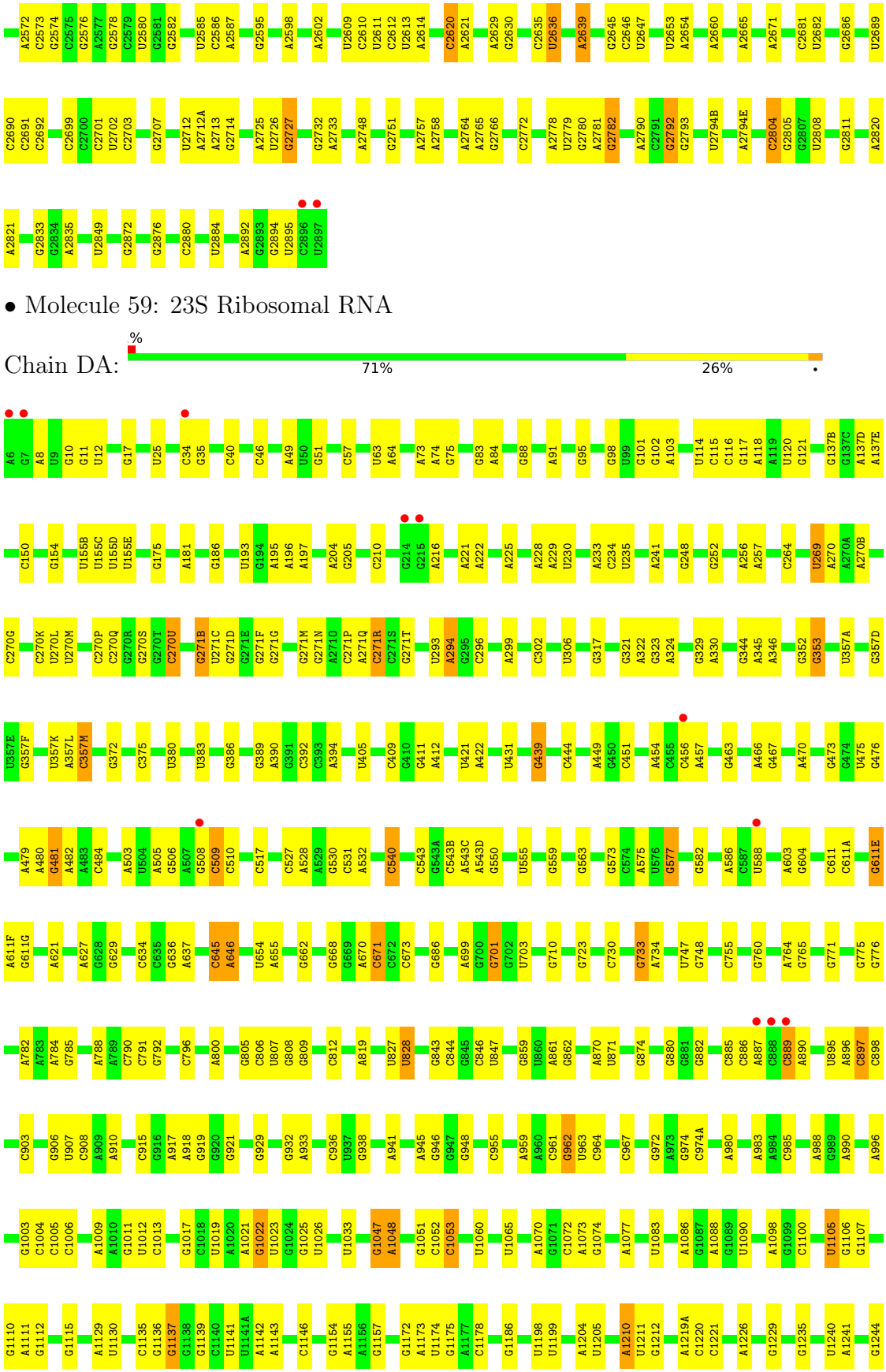
Chain Dh: 100%

There are no outlier residues recorded for this chain.

- Molecule 59: 23S Ribosomal RNA

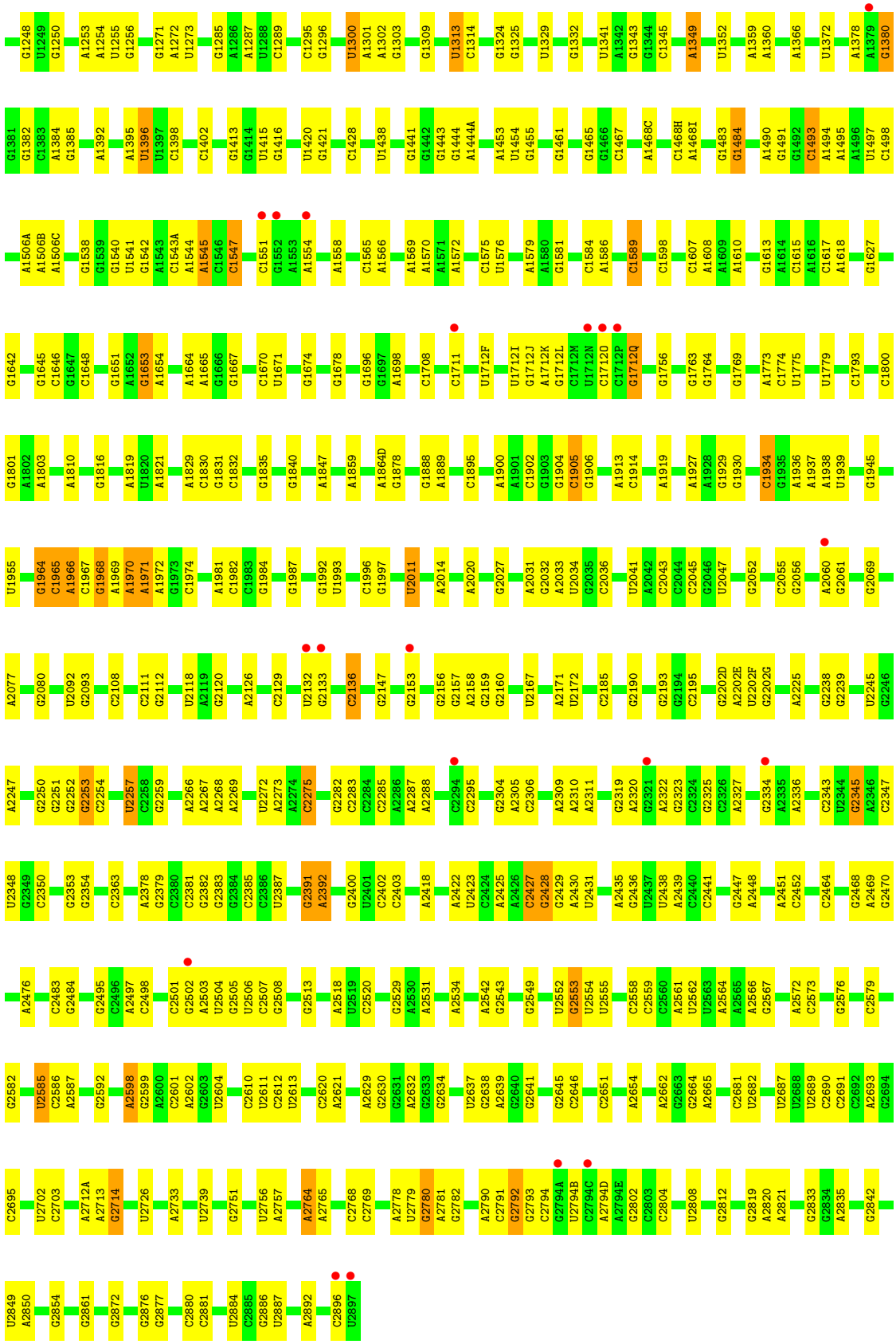
Chain BA: % 71% 27%





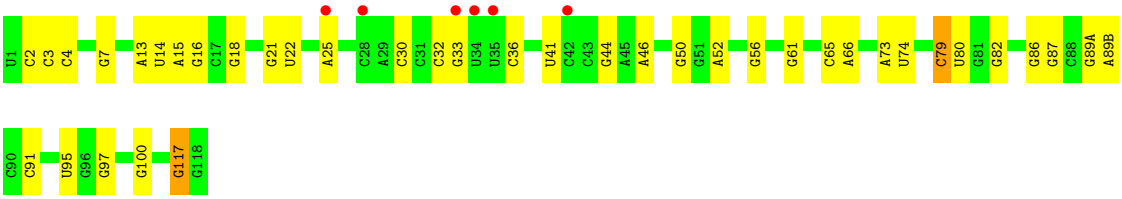
• Molecule 59: 23S Ribosomal RNA

Chain DA: % 71% 26% •



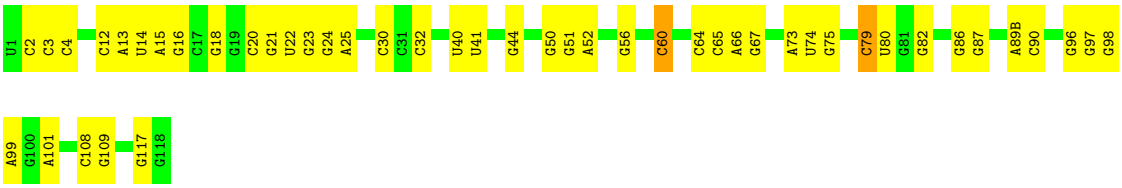
- Molecule 60: 5S Ribosomal RNA

Chain BB:



- Molecule 60: 5S Ribosomal RNA

Chain DB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	306.92Å 677.00Å 356.78Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	49.98 – 3.80 127.40 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.98-3.80) 60.2 (127.40-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.331 0.302 , 0.332	Depositor DCC
R_{free} test set	8467 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , -101.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.17$, $< L^2 > = 0.05$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	312066	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, FUA, NMY, ACE, GDP

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	AB	0.41	0/1945	0.69	0/2621
1	CB	0.41	0/1945	0.69	1/2621 (0.0%)
2	AC	0.27	0/1645	0.55	0/2216
2	CC	0.29	0/1645	0.56	0/2216
3	AD	0.31	0/1733	0.59	0/2318
3	CD	0.29	0/1733	0.61	1/2318 (0.0%)
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.61	1/1576 (0.1%)
5	AF	0.28	0/856	0.56	0/1154
5	CF	0.30	0/856	0.59	0/1154
6	AG	0.27	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.51	0/1709
7	AH	0.29	0/1136	0.60	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.27	0/1029	0.56	0/1379
8	CI	0.27	0/1029	0.50	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.56	0/1095
10	AK	0.38	0/900	0.62	0/1213
10	CK	0.39	0/900	0.61	0/1213
11	AL	0.43	0/992	0.80	0/1327
11	CL	0.45	0/992	0.81	1/1327 (0.1%)
12	AM	0.27	0/1008	0.53	0/1347
12	CM	0.27	0/1008	0.58	0/1347
13	AN	0.29	0/501	0.51	0/664
13	CN	0.34	0/501	0.57	0/664
14	AO	0.34	0/745	0.61	0/992
14	CO	0.33	0/745	0.57	1/992 (0.1%)
15	AP	0.32	0/722	0.61	0/970
15	CP	0.32	0/722	0.60	0/970
16	AQ	0.35	0/848	0.67	1/1131 (0.1%)
16	CQ	0.36	0/848	0.68	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AR	0.29	0/579	0.58	0/768
17	CR	0.29	0/579	0.57	0/768
18	AS	0.29	0/647	0.56	0/870
18	CS	0.26	0/647	0.53	0/870
19	AT	0.30	0/765	0.54	0/1007
19	CT	0.31	0/765	0.51	0/1007
20	AY	0.37	0/5270	0.66	1/7135 (0.0%)
20	CY	0.36	0/5270	0.67	3/7135 (0.0%)
21	AA	0.39	9/36351 (0.0%)	1.12	149/56736 (0.3%)
21	CA	0.42	6/36351 (0.0%)	1.17	239/56736 (0.4%)
22	AW	0.52	0/1827	1.42	41/2845 (1.4%)
22	CW	0.48	0/1827	1.36	23/2845 (0.8%)
23	AV	1.27	1/881 (0.1%)	1.42	12/1372 (0.9%)
23	CV	0.82	7/880 (0.8%)	2.11	42/1372 (3.1%)
24	AX	0.62	1/1815 (0.1%)	1.56	47/2826 (1.7%)
24	CX	0.60	3/1815 (0.2%)	1.54	43/2826 (1.5%)
25	BC	0.51	1/1774 (0.1%)	0.86	2/2391 (0.1%)
25	DC	0.51	0/1774	0.80	0/2391
26	BD	0.40	2/2195 (0.1%)	0.62	1/2955 (0.0%)
26	DD	0.31	0/2195	0.60	0/2955
27	BE	0.35	0/1602	0.69	2/2160 (0.1%)
27	DE	0.33	0/1602	0.67	0/2160
28	BF	0.39	0/1663	0.81	6/2249 (0.3%)
28	DF	0.38	0/1663	0.78	4/2249 (0.2%)
29	BG	0.27	0/1499	0.54	0/2016
29	DG	0.29	0/1499	0.58	0/2016
30	BH	0.28	0/1298	0.58	0/1751
30	DH	0.28	0/1298	0.55	0/1751
32	BK	0.28	0/1054	0.55	1/1427 (0.1%)
32	DK	0.31	0/1054	0.58	1/1427 (0.1%)
33	BN	0.81	3/1141 (0.3%)	1.39	16/1537 (1.0%)
33	DN	0.81	2/1141 (0.2%)	1.28	13/1537 (0.8%)
34	BO	0.32	0/943	0.63	2/1269 (0.2%)
34	DO	0.32	0/943	0.65	0/1269
35	BP	0.28	0/1131	0.64	2/1504 (0.1%)
35	DP	0.29	0/1131	0.63	0/1504
36	BQ	0.36	0/1143	0.67	0/1527
36	DQ	0.33	0/1143	0.63	0/1527
37	BR	0.33	0/974	0.64	1/1302 (0.1%)
37	DR	0.32	0/974	0.59	0/1302
38	BS	0.35	0/783	0.69	0/1041
38	DS	0.36	0/783	0.71	0/1041
39	BT	0.30	0/1161	0.63	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	DT	0.30	0/1161	0.64	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.33	0/982	0.57	0/1306
41	BV	0.34	0/790	0.76	2/1057 (0.2%)
41	DV	0.31	0/790	0.65	1/1057 (0.1%)
42	BW	0.32	0/911	0.64	0/1220
42	DW	0.38	0/911	0.69	1/1220 (0.1%)
43	BX	0.28	0/748	0.56	1/1004 (0.1%)
43	DX	0.28	0/748	0.56	1/1004 (0.1%)
44	BY	0.28	0/831	0.54	0/1108
44	DY	0.27	0/831	0.57	1/1108 (0.1%)
45	BZ	0.28	0/1505	0.58	0/2042
45	DZ	0.29	0/1505	0.58	0/2042
46	B0	0.25	0/671	0.54	0/892
46	D0	0.25	0/671	0.50	0/892
47	B1	0.51	0/739	1.01	5/981 (0.5%)
47	D1	0.48	0/739	0.92	2/981 (0.2%)
48	B2	0.37	0/600	0.63	0/793
48	D2	0.34	0/600	0.65	0/793
49	B3	0.29	0/482	0.58	0/646
49	D3	0.26	0/482	0.58	0/646
50	B4	0.38	0/276	0.67	0/372
50	D4	0.37	0/276	0.68	0/372
51	B5	0.28	0/473	0.57	0/639
51	D5	0.32	0/473	0.62	0/639
52	B6	0.30	0/440	0.82	3/586 (0.5%)
52	D6	0.31	0/440	0.68	0/586
53	B7	1.14	6/438 (1.4%)	1.51	7/575 (1.2%)
53	D7	0.29	0/438	0.55	0/575
54	B8	0.31	0/525	0.58	0/691
54	D8	0.30	0/525	0.61	0/691
55	B9	0.28	0/310	0.55	0/407
55	D9	0.32	0/310	0.57	0/407
56	Be	0.25	0/538	0.53	0/715
56	De	0.27	0/538	0.51	0/715
59	BA	0.38	1/69437 (0.0%)	1.11	247/108401 (0.2%)
59	DA	0.40	2/69437 (0.0%)	1.14	333/108401 (0.3%)
60	BB	0.43	0/2853	1.28	29/4451 (0.7%)
60	DB	0.48	0/2853	1.34	49/4451 (1.1%)
All	All	0.40	44/334735 (0.0%)	1.04	1339/498724 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
3	CD	0	1
10	AK	0	1
10	CK	0	1
15	AP	0	1
15	CP	0	1
20	AY	0	2
25	BC	0	6
25	DC	0	5
26	BD	0	1
26	DD	0	1
27	BE	0	1
28	BF	0	4
28	DF	0	2
29	DG	0	1
31	BJ	0	2
31	DJ	0	3
33	BN	0	17
33	DN	0	15
34	BO	0	1
34	DO	0	1
36	BQ	0	1
38	BS	0	1
38	DS	0	1
39	BT	0	1
39	DT	0	1
42	BW	0	1
42	DW	0	2
45	BZ	0	1
45	DZ	0	1
47	B1	0	4
47	D1	0	3
53	B7	0	1
All	All	0	86

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AV	1	G	P-O5'	35.77	1.95	1.59
53	B7	40	TRP	CD2-CE2	-12.82	1.25	1.41
21	AA	1126	U	C2-O2	-9.80	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	CA	1126	U	C2-O2	-9.32	1.14	1.22
53	B7	40	TRP	CE3-CZ3	8.92	1.53	1.38
53	B7	40	TRP	CZ2-CH2	-8.40	1.21	1.37
23	CV	10	G	N1-C2	-8.30	1.31	1.37
21	CA	1374	A	N7-C5	-7.69	1.34	1.39
26	BD	143	HIS	CG-ND1	-7.55	1.22	1.38
53	B7	40	TRP	CZ3-CH2	7.38	1.51	1.40
33	BN	115	ARG	C-O	7.34	1.37	1.23
21	AA	1374	A	N3-C4	-7.05	1.30	1.34
24	CX	75	C	C4-C5	-6.80	1.37	1.43
24	CX	75	C	C4-N4	-6.71	1.27	1.33
33	BN	101	HIS	CA-C	-6.61	1.35	1.52
24	AX	36	C	C5-C6	-6.54	1.29	1.34
21	CA	1126	U	N1-C6	-6.53	1.32	1.38
33	DN	117	PHE	CA-C	-6.50	1.36	1.52
33	BN	85	ILE	CB-CG2	-6.47	1.32	1.52
26	BD	143	HIS	CE1-NE2	-6.42	1.17	1.32
53	B7	40	TRP	CD2-CE3	6.35	1.49	1.40
23	CV	7	G	N3-C4	-6.19	1.31	1.35
21	AA	1374	A	C6-N1	-6.12	1.31	1.35
59	DA	1971	A	N9-C4	5.99	1.41	1.37
23	CV	7	G	C2-N3	-5.94	1.27	1.32
21	AA	1126	U	N1-C6	-5.88	1.32	1.38
59	DA	2592	G	N9-C4	5.84	1.42	1.38
33	DN	101	HIS	CA-C	-5.81	1.37	1.52
21	AA	1126	U	N3-C4	-5.78	1.33	1.38
23	CV	10	G	C6-O6	-5.73	1.19	1.24
21	CA	1126	U	N3-C4	-5.63	1.33	1.38
21	CA	520	A	N3-C4	-5.40	1.31	1.34
21	CA	1374	A	C5-C6	-5.29	1.36	1.41
59	BA	2553	G	N9-C4	5.23	1.42	1.38
23	CV	10	G	C6-N1	-5.22	1.35	1.39
53	B7	41	ARG	CB-CG	5.20	1.66	1.52
21	AA	520	A	N3-C4	-5.15	1.31	1.34
23	CV	8	A	N3-C4	-5.12	1.31	1.34
23	CV	10	G	N9-C4	5.12	1.42	1.38
24	CX	75	C	C5-C6	-5.10	1.30	1.34
25	BC	43	GLU	C-O	5.09	1.33	1.23
21	AA	1374	A	C5-C6	-5.07	1.36	1.41
21	AA	1148	U	C2-N3	5.06	1.41	1.37
21	AA	1374	A	N7-C5	-5.04	1.36	1.39

All (1339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AV	1	G	O5'-P-OP2	24.05	139.56	110.70
23	CV	10	G	N1-C6-O6	-22.12	106.63	119.90
21	AA	1126	U	N1-C2-N3	18.77	126.16	114.90
53	B7	40	TRP	CE2-CD2-CG	18.75	122.30	107.30
21	CA	1126	U	N1-C2-N3	18.50	126.00	114.90
53	B7	40	TRP	CD1-CG-CD2	-16.51	93.09	106.30
23	CV	7	G	N9-C4-C5	16.31	111.93	105.40
21	CA	1126	U	C4-C5-C6	16.25	129.45	119.70
59	BA	2553	G	N3-C4-N9	15.91	135.55	126.00
23	CV	7	G	N3-C4-N9	-15.90	116.46	126.00
23	CV	10	G	C5-C6-N1	15.27	119.14	111.50
24	CX	75	C	C5-C4-N4	-15.19	109.57	120.20
21	AA	1126	U	C4-C5-C6	14.95	128.67	119.70
23	CV	10	G	N3-C2-N2	14.76	130.23	119.90
59	BA	2553	G	C6-C5-N7	-14.73	121.56	130.40
21	AA	1491	G	C8-N9-C4	-14.54	100.58	106.40
59	BA	2553	G	C4-N9-C1'	14.43	145.26	126.50
21	AA	1126	U	C6-N1-C2	-14.38	112.37	121.00
59	BA	2553	G	C8-N9-C1'	-14.38	108.31	127.00
21	AA	1374	A	C2-N3-C4	-14.25	103.48	110.60
59	DA	2553	G	N1-C6-O6	14.18	128.41	119.90
23	CV	10	G	N3-C4-C5	-13.70	121.75	128.60
21	AA	1374	A	N1-C2-N3	13.37	135.98	129.30
59	BA	2553	G	C5-C6-O6	-13.17	120.70	128.60
24	AX	37	A	N1-C2-N3	-13.03	122.79	129.30
23	CV	7	G	N3-C2-N2	-12.90	110.87	119.90
21	AA	815	A	N1-C6-N6	-12.83	110.90	118.60
21	CA	1535	C	N3-C2-O2	-12.81	112.94	121.90
59	BA	2553	G	N1-C6-O6	12.77	127.56	119.90
59	DA	2553	G	C6-C5-N7	-12.61	122.84	130.40
21	CA	1538	C	C2-N3-C4	12.42	126.11	119.90
24	AX	75	C	N1-C2-O2	12.29	126.27	118.90
23	AV	1	G	P-O5'-C5'	-12.05	101.62	120.90
23	CV	10	G	N1-C2-N2	-12.00	105.40	116.20
59	DA	2553	G	N9-C4-C5	-11.99	100.61	105.40
23	CV	7	G	C5-C6-O6	11.92	135.75	128.60
24	AX	37	A	C4-C5-C6	-11.89	111.06	117.00
23	CV	7	G	C4-C5-N7	-11.85	106.06	110.80
21	CA	1538	C	N3-C2-O2	11.76	130.13	121.90
21	AA	1148	U	C2-N3-C4	-11.66	120.00	127.00
24	CX	75	C	N1-C2-O2	11.61	125.86	118.90
59	BA	962	G	N3-C4-N9	11.53	132.92	126.00
24	CX	75	C	N3-C4-C5	11.50	126.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CV	10	G	C2-N3-C4	11.48	117.64	111.90
59	BA	2553	G	N9-C4-C5	-11.45	100.82	105.40
21	AA	1374	A	C5-C6-N1	-11.44	111.98	117.70
59	BA	2553	G	C4-C5-N7	11.43	115.37	110.80
59	DA	2592	G	N3-C4-N9	11.36	132.81	126.00
59	DA	2553	G	C4-C5-N7	11.29	115.32	110.80
21	CA	1126	U	C6-N1-C2	-11.28	114.23	121.00
21	CA	1535	C	N3-C4-N4	-11.21	110.15	118.00
21	CA	1538	C	N3-C4-C5	-11.19	117.42	121.90
53	B7	40	TRP	CE2-CD2-CE3	-11.17	105.30	118.70
21	AA	815	A	C5-C6-N6	11.13	132.61	123.70
24	AX	75	C	N3-C2-O2	-11.06	114.16	121.90
21	AA	1126	U	N3-C4-C5	-10.95	108.03	114.60
59	DA	2601	C	N1-C2-O2	10.92	125.45	118.90
24	AX	75	C	N3-C4-C5	10.85	126.24	121.90
21	CA	1535	C	C6-N1-C2	-10.84	115.96	120.30
23	CV	7	G	C6-C5-N7	10.84	136.91	130.40
21	AA	1492	A	OP1-P-O3'	-10.83	81.37	105.20
21	AA	1126	U	N3-C2-O2	-10.79	114.64	122.20
21	CA	1538	C	C5-C4-N4	10.79	127.75	120.20
21	CA	815	A	N1-C6-N6	-10.78	112.14	118.60
23	CV	8	A	N9-C4-C5	10.62	110.05	105.80
59	DA	2553	G	C8-N9-C1'	-10.55	113.28	127.00
21	AA	1374	A	C4-C5-C6	10.46	122.23	117.00
21	CA	815	A	C5-C6-N6	10.42	132.04	123.70
21	CA	1299	A	N1-C6-N6	-10.34	112.39	118.60
24	CX	24	G	N3-C4-N9	10.34	132.20	126.00
24	CX	34	U	N3-C4-O4	-10.30	112.19	119.40
24	CX	74	C	N1-C2-O2	-10.18	112.79	118.90
21	CA	1148	U	C2-N3-C4	-10.10	120.94	127.00
59	BA	955	C	C5-C6-N1	10.05	126.03	121.00
23	CV	7	G	N1-C6-O6	-10.05	113.87	119.90
60	DB	89(B)	A	N1-C6-N6	10.05	124.63	118.60
24	AX	50	G	N1-C6-O6	-10.01	113.90	119.90
59	BA	1970	A	O4'-C1'-N9	-10.01	100.19	108.20
21	CA	1538	C	C2-N1-C1'	-10.01	107.79	118.80
23	CV	7	G	C8-N9-C1'	10.00	140.00	127.00
59	BA	2553	G	N3-C4-C5	-9.96	123.62	128.60
33	BN	91	LEU	CA-CB-CG	9.93	138.14	115.30
21	CA	1126	U	N3-C4-C5	-9.92	108.65	114.60
59	DA	2601	C	C2-N1-C1'	9.91	129.70	118.80
23	CV	10	G	N3-C4-N9	9.87	131.92	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	1535	C	C5-C4-N4	9.85	127.10	120.20
21	AA	1299	A	N1-C6-N6	-9.83	112.70	118.60
59	DA	906	G	C5-C6-O6	9.81	134.49	128.60
59	BA	962	G	N3-C2-N2	9.78	126.74	119.90
59	BA	1967	C	C6-N1-C2	-9.76	116.40	120.30
21	CA	1126	U	N3-C2-O2	-9.76	115.37	122.20
53	B7	40	TRP	CE3-CZ3-CH2	-9.74	110.48	121.20
21	AA	1492	A	OP2-P-O3'	-9.74	83.77	105.20
59	BA	962	G	N9-C4-C5	-9.70	101.52	105.40
21	CA	1536	C	C5-C4-N4	9.65	126.96	120.20
21	CA	1535	C	C2-N1-C1'	9.64	129.41	118.80
21	CA	1348	U	C2-N3-C4	-9.61	121.23	127.00
21	CA	1538	C	N1-C2-O2	-9.61	113.13	118.90
21	AA	815	A	N9-C4-C5	9.58	109.63	105.80
59	DA	2553	G	C4-N9-C1'	9.58	138.96	126.50
21	AA	1491	G	N7-C8-N9	9.57	117.88	113.10
59	DA	2592	G	N3-C4-C5	-9.54	123.83	128.60
23	CV	8	A	N1-C6-N6	-9.52	112.89	118.60
21	CA	815	A	N9-C4-C5	9.50	109.60	105.80
24	CX	34	U	C5-C4-O4	9.50	131.60	125.90
24	AX	3	G	N3-C4-N9	9.49	131.70	126.00
59	BA	527	C	C2-N1-C1'	9.43	129.18	118.80
59	BA	955	C	N3-C4-N4	9.43	124.60	118.00
23	CV	19	G	N9-C4-C5	9.36	109.14	105.40
22	CW	61	C	C2-N1-C1'	9.31	129.04	118.80
21	CA	1535	C	N1-C2-O2	9.27	124.46	118.90
23	CV	10	G	C5-C6-O6	9.24	134.15	128.60
21	CA	1538	C	C6-N1-C1'	9.24	131.89	120.80
59	BA	955	C	N1-C2-O2	9.23	124.44	118.90
59	DA	103	A	N1-C6-N6	9.22	124.13	118.60
21	CA	1440(N)	C	N1-C2-O2	9.21	124.42	118.90
59	DA	962	G	N3-C4-N9	9.13	131.47	126.00
23	AV	19	G	C2-N3-C4	9.06	116.43	111.90
60	BB	2	C	C2-N1-C1'	9.06	128.76	118.80
59	DA	1966	A	C8-N9-C4	-9.02	102.19	105.80
21	CA	1052	U	N1-C2-O2	9.01	129.11	122.80
59	DA	2553	G	C5-C6-O6	-8.92	123.25	128.60
60	DB	3	C	C6-N1-C2	-8.89	116.74	120.30
59	DA	962	G	N9-C4-C5	-8.87	101.85	105.40
21	CA	1440(E)	G	N3-C4-N9	8.87	131.32	126.00
53	B7	40	TRP	CH2-CZ2-CE2	8.86	126.26	117.40
21	AA	1491	G	N9-C4-C5	8.86	108.94	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	B7	40	TRP	NE1-CE2-CD2	-8.84	98.46	107.30
21	AA	1374	A	N1-C6-N6	8.79	123.87	118.60
59	BA	962	G	C4-C5-N7	8.79	114.32	110.80
4	CE	12	LEU	CA-CB-CG	8.74	135.40	115.30
33	DN	117	PHE	N-CA-C	-8.72	87.44	111.00
28	DF	193	VAL	N-CA-C	-8.69	87.53	111.00
60	BB	3	C	C6-N1-C2	-8.68	116.83	120.30
59	DA	2553	G	N3-C4-N9	8.68	131.21	126.00
23	CV	10	G	C4-N9-C1'	8.67	137.78	126.50
28	BF	193	VAL	N-CA-C	-8.67	87.60	111.00
59	DA	357(D)	G	N3-C4-N9	-8.62	120.83	126.00
59	BA	955	C	C2-N3-C4	8.60	124.20	119.90
21	CA	1301	U	C2-N1-C1'	8.60	128.01	117.70
60	DB	3	C	N3-C4-C5	-8.54	118.48	121.90
23	CV	10	G	C6-N1-C2	-8.51	120.00	125.10
21	CA	1374	A	N1-C6-N6	8.49	123.69	118.60
24	CX	75	C	N3-C4-N4	8.47	123.93	118.00
59	BA	1048	A	N1-C6-N6	8.46	123.67	118.60
21	AA	723	U	C2-N1-C1'	8.42	127.81	117.70
22	AW	50	C	N1-C2-O2	8.41	123.95	118.90
28	BF	156	LEU	N-CA-C	-8.34	88.48	111.00
59	BA	527	C	C6-N1-C2	-8.33	116.97	120.30
21	CA	1127	G	N9-C4-C5	8.30	108.72	105.40
59	DA	271(R)	C	N1-C2-O2	-8.28	113.93	118.90
59	DA	294	A	N1-C6-N6	8.27	123.56	118.60
59	DA	906	G	N3-C4-N9	-8.26	121.05	126.00
21	CA	735	C	C2-N1-C1'	8.25	127.88	118.80
21	AA	1157	A	O4'-C1'-N9	8.24	114.79	108.20
24	CX	11	C	N1-C2-O2	8.24	123.84	118.90
21	CA	1306	A	N1-C6-N6	8.23	123.54	118.60
59	DA	2601	C	N3-C2-O2	-8.22	116.15	121.90
59	BA	2249	U	N1-C2-O2	8.21	128.54	122.80
21	CA	1494	G	N3-C4-C5	-8.19	124.50	128.60
22	AW	14	A	N1-C6-N6	8.18	123.51	118.60
24	CX	11	C	C2-N1-C1'	8.16	127.77	118.80
24	CX	75	C	N3-C2-O2	-8.15	116.19	121.90
23	CV	19	G	N3-C4-N9	-8.12	121.12	126.00
28	DF	156	LEU	N-CA-C	-8.12	89.07	111.00
59	DA	357(D)	G	N9-C4-C5	8.10	108.64	105.40
24	AX	72	C	N1-C2-O2	8.10	123.76	118.90
24	AX	75	C	O4'-C1'-N1	-8.09	101.73	108.20
22	CW	61	C	C6-N1-C1'	-8.07	111.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B1	17	SER	N-CA-C	8.05	132.75	111.00
59	BA	1493	C	C2-N1-C1'	8.03	127.63	118.80
21	AA	1301	U	C2-N1-C1'	8.03	127.33	117.70
59	DA	2585	U	C2-N1-C1'	8.02	127.33	117.70
60	DB	18	G	N3-C4-N9	8.01	130.80	126.00
60	DB	4	C	C2-N1-C1'	7.99	127.59	118.80
59	BA	1945	G	N9-C4-C5	-7.99	102.20	105.40
22	AW	61	C	C2-N1-C1'	7.97	127.57	118.80
59	DA	1107	G	N9-C4-C5	7.95	108.58	105.40
24	AX	37	A	C6-N1-C2	7.95	123.37	118.60
21	AA	68(Q)	U	N1-C2-O2	7.94	128.36	122.80
21	CA	1494	G	C4-N9-C1'	7.94	136.82	126.50
24	CX	36	C	C2-N3-C4	7.93	123.87	119.90
60	BB	3	C	C2-N3-C4	7.92	123.86	119.90
59	BA	527	C	N1-C2-O2	7.92	123.65	118.90
21	AA	1409	C	C4-C5-C6	7.91	121.35	117.40
59	BA	2560	C	C6-N1-C2	-7.88	117.15	120.30
21	CA	1440(N)	C	N3-C2-O2	-7.87	116.39	121.90
24	AX	3	G	N9-C4-C5	-7.86	102.25	105.40
33	BN	118	LYS	C-N-CA	-7.86	102.05	121.70
59	DA	2681	C	C5-C4-N4	7.85	125.70	120.20
21	CA	68(H)	G	N9-C4-C5	7.84	108.54	105.40
59	DA	503	A	N9-C4-C5	7.83	108.93	105.80
59	DA	1107	G	N3-C2-N2	-7.83	114.42	119.90
59	DA	2592	G	C6-C5-N7	-7.83	125.70	130.40
21	CA	1052	U	N3-C2-O2	-7.80	116.74	122.20
59	DA	466	A	N1-C6-N6	7.79	123.28	118.60
21	AA	1302	U	C2-N1-C1'	7.75	127.00	117.70
59	BA	962	G	C5-C6-O6	-7.73	123.96	128.60
60	DB	89(B)	A	C5-C6-N6	-7.73	117.52	123.70
22	CW	14	A	N1-C6-N6	7.72	123.23	118.60
21	CA	1465	C	C5-C4-N4	-7.72	114.79	120.20
59	BA	1945	G	C4-C5-N7	7.72	113.89	110.80
59	DA	1970	A	O4'-C1'-N9	-7.70	102.04	108.20
24	AX	30	C	C2-N1-C1'	7.68	127.25	118.80
24	CX	75	C	O4'-C1'-N1	-7.67	102.06	108.20
59	DA	1396	U	C2-N1-C1'	7.67	126.90	117.70
21	CA	421	U	C2-N1-C1'	7.67	126.90	117.70
24	AX	74	C	C2-N1-C1'	7.65	127.21	118.80
59	BA	1493	C	N1-C2-O2	7.64	123.48	118.90
21	AA	1301	U	N1-C2-O2	7.62	128.13	122.80
21	AA	520	A	N1-C2-N3	7.62	133.11	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BC	45	HIS	N-CA-C	-7.62	90.44	111.00
28	BF	156	LEU	CA-CB-CG	7.61	132.80	115.30
23	CV	7	G	C4-N9-C1'	-7.61	116.61	126.50
21	AA	1332	A	N1-C6-N6	7.61	123.16	118.60
33	BN	115	ARG	CA-C-N	-7.60	100.49	117.20
59	DA	121	G	N3-C4-N9	7.59	130.56	126.00
21	CA	815	A	N3-C4-N9	-7.59	121.33	127.40
23	CV	7	G	C8-N9-C4	-7.56	103.38	106.40
60	DB	65	C	N1-C2-O2	7.56	123.44	118.90
24	CX	74	C	N3-C2-O2	7.55	127.18	121.90
60	DB	101	A	C6-N1-C2	-7.54	114.08	118.60
24	AX	50	G	C5-C6-O6	7.53	133.12	128.60
21	AA	1374	A	C6-C5-N7	-7.53	127.03	132.30
21	CA	300	A	N1-C6-N6	7.52	123.11	118.60
24	CX	36	C	C5-C6-N1	7.52	124.76	121.00
59	DA	357(D)	G	C8-N9-C1'	7.51	136.77	127.00
24	AX	72	C	N3-C2-O2	-7.51	116.65	121.90
59	DA	294	A	C4-C5-C6	7.50	120.75	117.00
59	BA	962	G	C5-C6-N1	7.49	115.25	111.50
24	AX	3	G	C8-N9-C1'	-7.48	117.27	127.00
60	BB	2	C	C6-N1-C1'	-7.48	111.83	120.80
21	CA	1126	U	C2-N3-C4	-7.47	122.52	127.00
11	CL	60	LEU	CA-CB-CG	7.46	132.46	115.30
23	CV	19	G	N3-C2-N2	-7.45	114.69	119.90
22	AW	8	U	N1-C2-O2	7.44	128.01	122.80
33	BN	120	LEU	CA-CB-CG	7.43	132.39	115.30
59	BA	2249	U	N3-C2-O2	-7.43	117.00	122.20
22	CW	8	U	N1-C2-O2	7.43	128.00	122.80
60	DB	75	G	C6-N1-C2	-7.42	120.65	125.10
59	DA	2391	G	C4-N9-C1'	-7.42	116.86	126.50
52	B6	9	LEU	CA-CB-CG	7.42	132.36	115.30
59	DA	2391	G	N3-C4-N9	-7.41	121.55	126.00
21	CA	1103	C	C5-C6-N1	7.41	124.70	121.00
59	DA	962	G	C5-C6-N1	7.41	115.20	111.50
59	BA	466	A	N1-C6-N6	7.41	123.04	118.60
21	CA	815	A	C6-C5-N7	7.41	137.48	132.30
21	CA	1440(N)	C	C2-N1-C1'	7.39	126.93	118.80
21	AA	1126	U	C5-C4-O4	7.39	130.33	125.90
21	CA	1348	U	C5-C4-O4	-7.38	121.47	125.90
59	BA	1313	U	N1-C2-O2	7.36	127.95	122.80
60	DB	117	G	N9-C4-C5	7.36	108.34	105.40
59	DA	271(R)	C	C6-N1-C1'	7.36	129.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	1126	U	C5-C6-N1	-7.35	119.02	122.70
59	BA	1414	G	N3-C4-N9	-7.35	121.59	126.00
24	AX	30	C	N1-C2-O2	7.34	123.31	118.90
59	BA	1048	A	C4-C5-C6	7.34	120.67	117.00
23	CV	8	A	C6-C5-N7	7.34	137.44	132.30
21	CA	500	G	N3-C4-N9	7.33	130.40	126.00
59	DA	1022	G	P-O3'-C3'	7.33	128.49	119.70
60	DB	65	C	C2-N1-C1'	7.32	126.86	118.80
59	DA	2681	C	C6-N1-C2	-7.31	117.38	120.30
22	AW	71	C	N1-C2-O2	7.30	123.28	118.90
23	AV	19	G	N1-C2-N2	7.30	122.78	116.20
59	DA	1048	A	N1-C6-N6	7.30	122.98	118.60
21	CA	68(H)	G	O4'-C1'-N9	7.29	114.04	108.20
21	CA	1362(A)	C	C2-N1-C1'	-7.29	110.78	118.80
59	BA	1961	C	C2-N1-C1'	7.26	126.79	118.80
21	AA	1148	U	N3-C4-C5	7.26	118.95	114.60
59	BA	194	G	N3-C4-N9	-7.26	121.65	126.00
59	DA	271(R)	C	C2-N1-C1'	-7.25	110.82	118.80
22	AW	14	A	C6-C5-N7	-7.25	127.23	132.30
21	CA	943	U	C5-C6-N1	7.24	126.32	122.70
59	DA	103	A	C4-C5-C6	7.24	120.62	117.00
59	DA	871	U	N1-C2-N3	7.23	119.24	114.90
59	DA	1107	G	N3-C4-N9	-7.23	121.66	126.00
21	AA	328	C	C2-N1-C1'	7.23	126.75	118.80
22	AW	61	C	N1-C2-O2	7.22	123.23	118.90
21	CA	1332	A	N1-C6-N6	7.22	122.93	118.60
21	CA	1336	C	C2-N1-C1'	7.22	126.74	118.80
59	DA	962	G	C8-N9-C1'	-7.21	117.63	127.00
21	AA	68(H)	G	O4'-C1'-N9	7.21	113.97	108.20
21	CA	1127	G	N3-C4-N9	-7.21	121.68	126.00
59	BA	2250	G	C4-N9-C1'	7.19	135.85	126.50
21	AA	520	A	N9-C4-C5	7.18	108.67	105.80
22	AW	68	U	C2-N1-C1'	-7.18	109.08	117.70
47	D1	17	SER	N-CA-C	7.17	130.37	111.00
24	AX	53	G	N3-C4-N9	-7.17	121.70	126.00
23	CV	8	A	N3-C4-N9	-7.17	121.67	127.40
60	DB	117	G	N3-C4-N9	-7.16	121.70	126.00
21	CA	1494	G	N3-C4-N9	7.16	130.29	126.00
22	CW	20	U	C2-N1-C1'	7.16	126.29	117.70
59	DA	2391	G	C8-N9-C1'	7.15	136.30	127.00
21	CA	1537	U	N3-C4-C5	-7.14	110.31	114.60
59	DA	543	C	C2-N1-C1'	7.14	126.66	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	673	C	C2-N3-C4	-7.14	116.33	119.90
59	DA	503	A	C8-N9-C4	-7.13	102.95	105.80
21	CA	1494	G	N7-C8-N9	7.12	116.66	113.10
59	DA	271(B)	G	N3-C4-C5	-7.12	125.04	128.60
21	CA	1374	A	C4-C5-C6	7.12	120.56	117.00
59	DA	2601	C	C6-N1-C1'	-7.11	112.26	120.80
22	CW	61	C	N1-C2-O2	7.11	123.17	118.90
21	AA	533	A	N1-C2-N3	7.11	132.85	129.30
33	DN	101	HIS	CA-C-N	-7.09	101.59	117.20
21	AA	1302	U	N1-C2-O2	7.09	127.76	122.80
24	AX	74	C	C5-C6-N1	7.08	124.54	121.00
21	AA	1465	C	C5-C4-N4	-7.08	115.25	120.20
59	BA	1396	U	C2-N1-C1'	7.06	126.17	117.70
21	CA	1037	C	O4'-C1'-N1	7.05	113.84	108.20
60	BB	61	G	C5-C6-O6	-7.04	124.38	128.60
59	BA	1967	C	P-O3'-C3'	-7.03	111.26	119.70
33	BN	101	HIS	CA-C-N	-7.03	101.75	117.20
21	CA	1028(G)	G	C6-C5-N7	-7.02	126.19	130.40
23	CV	8	A	O4'-C1'-N9	7.02	113.81	108.20
59	BA	251	A	C6-N1-C2	-7.02	114.39	118.60
21	CA	68(H)	G	C8-N9-C1'	7.01	136.12	127.00
59	DA	2592	G	C4-N9-C1'	7.01	135.62	126.50
21	AA	328	C	N1-C2-O2	7.01	123.11	118.90
59	BA	270(V)	G	N3-C4-N9	-7.00	121.80	126.00
24	AX	3	G	C4-N9-C1'	7.00	135.60	126.50
59	BA	2553	G	C4-C5-C6	7.00	123.00	118.80
24	AX	36	C	C4-C5-C6	-6.99	113.90	117.40
22	AW	53	G	N3-C4-N9	6.99	130.19	126.00
59	DA	271(B)	G	N3-C4-N9	6.98	130.19	126.00
59	DA	383	U	N1-C2-O2	6.97	127.68	122.80
59	DA	83	G	C2-N3-C4	-6.96	108.42	111.90
59	BA	1313	U	C2-N1-C1'	6.95	126.04	117.70
59	BA	1945	G	N3-C4-N9	6.95	130.17	126.00
59	DA	1053	C	N1-C2-O2	6.95	123.07	118.90
59	DA	1971	A	C2-N3-C4	6.94	114.07	110.60
33	BN	115	ARG	CA-C-O	6.93	134.66	120.10
21	CA	500	G	N9-C4-C5	-6.93	102.63	105.40
59	BA	527	C	N3-C2-O2	-6.92	117.05	121.90
60	BB	2	C	N1-C2-O2	6.91	123.04	118.90
24	CX	24	G	N3-C4-C5	-6.89	125.15	128.60
24	CX	24	G	N9-C4-C5	-6.89	102.64	105.40
21	CA	1299	A	C5-C6-N6	6.89	129.21	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BB	3	C	N1-C2-O2	6.88	123.03	118.90
23	AV	19	G	C8-N9-C4	-6.88	103.65	106.40
21	CA	1060	C	C5-C6-N1	6.88	124.44	121.00
21	CA	1037	C	N3-C4-C5	-6.87	119.15	121.90
21	CA	68(Q)	U	C5-C6-N1	6.87	126.14	122.70
23	CV	10	G	C8-N9-C1'	-6.87	118.07	127.00
59	DA	344	G	C2-N3-C4	-6.87	108.46	111.90
59	BA	906	G	N3-C4-N9	-6.87	121.88	126.00
21	AA	815	A	C8-N9-C4	-6.86	103.06	105.80
21	CA	1465	C	C2-N3-C4	-6.86	116.47	119.90
22	CW	20	U	N1-C2-O2	6.86	127.60	122.80
21	CA	1536	C	N3-C4-N4	-6.84	113.21	118.00
59	DA	1779	U	C2-N1-C1'	6.84	125.91	117.70
28	BF	156	LEU	C-N-CA	-6.84	104.60	121.70
59	BA	1961	C	C5-C6-N1	6.84	124.42	121.00
59	DA	1589	C	C2-N1-C1'	-6.83	111.29	118.80
59	BA	2727	G	N7-C8-N9	6.82	116.51	113.10
21	CA	1059	C	O4'-C1'-N1	6.82	113.65	108.20
24	AX	74	C	C6-N1-C1'	-6.82	112.62	120.80
60	DB	89(B)	A	C6-C5-N7	-6.80	127.54	132.30
1	CB	187	LEU	CA-CB-CG	6.80	130.94	115.30
23	AV	19	G	N9-C4-C5	6.79	108.12	105.40
20	CY	659	LEU	CA-CB-CG	6.78	130.90	115.30
59	DA	1589	C	C6-N1-C1'	6.77	128.92	120.80
21	AA	224	C	C2-N1-C1'	-6.76	111.37	118.80
22	AW	64	G	N3-C4-N9	6.75	130.05	126.00
21	CA	1374	A	C6-C5-N7	-6.75	127.57	132.30
24	AX	37	A	N3-C4-C5	6.75	131.52	126.80
21	CA	1440(E)	G	N3-C4-C5	-6.75	125.22	128.60
23	CV	8	A	C5-C6-N6	6.74	129.09	123.70
59	DA	270(U)	C	C2-N1-C1'	-6.74	111.39	118.80
59	BA	906	G	C5-C6-O6	6.73	132.64	128.60
59	DA	880	G	N3-C4-N9	6.73	130.04	126.00
21	CA	169	C	C2-N3-C4	6.72	123.26	119.90
22	AW	61	C	C6-N1-C1'	-6.72	112.74	120.80
21	CA	1059	C	C6-N1-C1'	6.72	128.86	120.80
33	DN	105	GLY	N-CA-C	-6.72	96.31	113.10
59	DA	2714	G	N3-C4-N9	6.72	130.03	126.00
21	CA	1272	G	C4-N9-C1'	6.71	135.22	126.50
21	CA	1537	U	N1-C2-O2	-6.70	118.11	122.80
59	DA	906	G	N1-C6-O6	-6.70	115.88	119.90
35	BP	112	LEU	CA-CB-CG	6.69	130.68	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1336	C	C2-N1-C1'	6.68	126.15	118.80
22	AW	71	C	N3-C2-O2	-6.68	117.22	121.90
59	BA	2249	U	C2-N1-C1'	6.68	125.72	117.70
21	CA	735	C	C6-N1-C1'	-6.68	112.79	120.80
60	BB	18	G	N3-C4-N9	6.68	130.01	126.00
21	CA	68(Q)	U	N1-C2-O2	6.68	127.47	122.80
59	DA	357(M)	C	C2-N1-C1'	6.66	126.12	118.80
59	DA	1545	A	C5-N7-C8	-6.66	100.57	103.90
21	CA	129(A)	G	N3-C2-N2	6.64	124.55	119.90
22	CW	53	G	N3-C4-N9	6.64	129.98	126.00
21	CA	1508	G	N3-C4-N9	6.63	129.98	126.00
21	CA	1037	C	C2-N3-C4	6.63	123.22	119.90
32	DK	105	LEU	CA-CB-CG	6.63	130.55	115.30
59	DA	962	G	C2-N3-C4	6.63	115.22	111.90
21	AA	68(E)	G	C5-C6-O6	6.63	132.58	128.60
59	DA	1313	U	C2-N1-C1'	6.62	125.65	117.70
59	BA	294	A	N1-C6-N6	6.62	122.57	118.60
21	CA	1157	A	O4'-C1'-N9	6.61	113.49	108.20
21	CA	1028(G)	G	N1-C6-O6	6.60	123.86	119.90
59	BA	1019	U	N3-C2-O2	-6.59	117.58	122.20
59	DA	1712(I)	U	C2-N1-C1'	6.59	125.61	117.70
21	CA	1227	A	N1-C6-N6	6.59	122.56	118.60
59	BA	422	A	C8-N9-C4	-6.59	103.16	105.80
21	CA	1336	C	N1-C2-O2	6.58	122.85	118.90
22	AW	14	A	C4-N9-C1'	6.58	138.14	126.30
47	B1	19	GLN	N-CA-C	-6.58	93.25	111.00
21	CA	1148	U	N3-C4-C5	6.58	118.55	114.60
59	BA	962	G	C6-C5-N7	-6.57	126.46	130.40
59	BA	2181	G	N3-C4-N9	-6.57	122.06	126.00
59	DA	103	A	C6-C5-N7	-6.57	127.70	132.30
21	AA	754	C	C2-N1-C1'	6.56	126.01	118.80
59	BA	1048	A	C6-C5-N7	-6.55	127.72	132.30
21	CA	838(A)	U	C2-N1-C1'	6.53	125.54	117.70
21	CA	1272	G	N3-C4-N9	6.53	129.92	126.00
59	BA	962	G	N1-C2-N2	-6.53	110.33	116.20
59	DA	1966	A	N9-C4-C5	6.53	108.41	105.80
33	DN	91	LEU	CA-CB-CG	6.52	130.30	115.30
60	BB	3	C	C5-C6-N1	6.52	124.26	121.00
21	CA	1305	G	N3-C2-N2	6.52	124.46	119.90
22	AW	14	A	C4-C5-C6	6.52	120.26	117.00
21	AA	1305	G	C2-N3-C4	-6.51	108.64	111.90
21	CA	1374	A	C5-C6-N1	-6.51	114.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	1137	G	N3-C4-C5	-6.50	125.35	128.60
21	AA	1148	U	N1-C2-N3	6.50	118.80	114.90
24	AX	40	G	N3-C4-N9	6.50	129.90	126.00
59	BA	95	G	N3-C4-N9	-6.50	122.10	126.00
21	CA	1362(A)	C	O4'-C1'-N1	6.49	113.39	108.20
21	CA	1494	G	C8-N9-C4	-6.48	103.81	106.40
21	AA	1440(J)	C	O4'-C1'-N1	6.48	113.38	108.20
21	AA	1003	G	C5-C6-O6	6.48	132.49	128.60
21	CA	1305	G	N1-C2-N2	-6.47	110.38	116.20
59	DA	2780	G	O4'-C1'-N9	6.47	113.38	108.20
21	AA	815	A	C4-C5-N7	-6.47	107.47	110.70
21	CA	669	U	C5-C6-N1	6.46	125.93	122.70
21	CA	1440(N)	C	C6-N1-C2	-6.46	117.72	120.30
59	DA	807	U	C2-N3-C4	-6.45	123.13	127.00
59	BA	955	C	C2-N1-C1'	6.45	125.90	118.80
59	BA	2598	A	N1-C6-N6	6.45	122.47	118.60
59	DA	1139	G	N7-C8-N9	6.45	116.32	113.10
59	DA	2553	G	C5-C6-N1	-6.44	108.28	111.50
59	DA	1106	G	N3-C4-N9	6.44	129.86	126.00
21	AA	1409	C	C5-C6-N1	-6.43	117.78	121.00
21	CA	1145	C	C2-N1-C1'	-6.43	111.72	118.80
21	CA	68(I)	G	C5-C6-O6	-6.43	124.74	128.60
59	DA	2592	G	C8-N9-C1'	-6.43	118.64	127.00
22	AW	72	C	C5-C4-N4	-6.42	115.70	120.20
33	DN	116	LEU	N-CA-C	-6.42	93.66	111.00
23	CV	19	G	C8-N9-C4	-6.42	103.83	106.40
24	AX	62	C	N1-C2-O2	-6.42	115.05	118.90
59	BA	192	C	O4'-C1'-N1	6.42	113.33	108.20
59	DA	1484	G	N3-C4-N9	-6.42	122.15	126.00
60	DB	51	G	N3-C4-N9	6.42	129.85	126.00
21	AA	376	G	C5-C6-O6	6.42	132.45	128.60
59	BA	1945	G	C8-N9-C1'	-6.42	118.66	127.00
59	DA	481	G	O5'-P-OP1	6.41	118.39	110.70
33	BN	119	ARG	N-CA-C	6.41	128.30	111.00
21	CA	1362(A)	C	C6-N1-C1'	6.41	128.49	120.80
59	DA	2804	C	C6-N1-C1'	6.40	128.48	120.80
59	BA	702	G	N3-C4-N9	-6.40	122.16	126.00
21	CA	1003	G	N9-C4-C5	6.40	107.96	105.40
21	AA	1170	A	N1-C6-N6	6.39	122.44	118.60
21	CA	1037	C	C6-N1-C1'	6.39	128.47	120.80
23	CV	8	A	C8-N9-C1'	6.38	139.19	127.70
59	BA	422	A	N1-C6-N6	-6.38	114.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	906	G	C6-C5-N7	6.38	134.23	130.40
59	BA	955	C	C6-N1-C2	-6.38	117.75	120.30
21	AA	1409	C	N1-C2-O2	-6.38	115.08	118.90
21	CA	1491	G	C8-N9-C4	-6.37	103.85	106.40
21	CA	500	G	C8-N9-C1'	-6.36	118.74	127.00
24	AX	61	C	C5-C6-N1	6.35	124.18	121.00
21	CA	929	G	N3-C4-N9	6.35	129.81	126.00
21	CA	1127	G	C6-C5-N7	6.34	134.21	130.40
59	BA	1961	C	N1-C2-O2	6.34	122.70	118.90
21	CA	68(H)	G	N3-C4-N9	-6.33	122.20	126.00
21	CA	421	U	N1-C2-O2	6.33	127.23	122.80
59	DA	962	G	C4-C5-N7	6.33	113.33	110.80
59	DA	1996	C	C2-N3-C4	6.32	123.06	119.90
60	BB	22	U	C2-N1-C1'	-6.31	110.12	117.70
59	DA	908	C	N1-C2-O2	-6.31	115.12	118.90
21	AA	1490	C	C6-N1-C2	-6.30	117.78	120.30
21	CA	1003	G	C5-C6-O6	6.30	132.38	128.60
59	BA	2712	U	C2-N1-C1'	6.29	125.25	117.70
21	AA	1348	U	C2-N3-C4	-6.29	123.23	127.00
21	CA	810	C	O4'-C1'-N1	6.29	113.23	108.20
24	CX	11	C	C6-N1-C1'	-6.28	113.26	120.80
59	BA	1945	G	C5-C6-O6	-6.28	124.83	128.60
21	CA	815	A	C4-C5-N7	-6.28	107.56	110.70
24	CX	24	G	C8-N9-C1'	-6.28	118.84	127.00
59	DA	1589	C	N1-C2-O2	-6.28	115.14	118.90
22	AW	14	A	C8-N9-C1'	-6.27	116.41	127.70
60	BB	117	G	C5-C6-O6	6.27	132.36	128.60
22	CW	72	C	C5-C4-N4	-6.27	115.81	120.20
33	DN	120	LEU	CB-CG-CD2	-6.27	100.34	111.00
59	DA	270(U)	C	O4'-C1'-N1	6.27	113.21	108.20
24	AX	3	G	C4-C5-N7	6.27	113.31	110.80
59	BA	2250	G	N3-C4-N9	6.26	129.76	126.00
59	BA	270(V)	G	N9-C4-C5	6.26	107.90	105.40
59	BA	955	C	C5-C4-N4	-6.25	115.82	120.20
60	DB	79	C	C2-N1-C1'	6.25	125.68	118.80
59	BA	422	A	N9-C4-C5	6.25	108.30	105.80
21	CA	1527	C	N3-C2-O2	-6.25	117.53	121.90
21	CA	1272	G	C8-N9-C1'	-6.24	118.89	127.00
24	CX	49	G	N3-C4-N9	-6.24	122.26	126.00
21	CA	1301	U	C6-N1-C1'	-6.23	112.47	121.20
60	DB	117	G	C5-C6-O6	6.22	132.34	128.60
23	CV	7	G	N1-C2-N3	6.22	127.63	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	2804	C	C2-N1-C1'	-6.22	111.96	118.80
22	AW	72	C	N3-C4-C5	6.22	124.39	121.90
59	BA	1937	A	N1-C6-N6	-6.22	114.87	118.60
59	BA	1226	A	N1-C6-N6	6.21	122.32	118.60
59	BA	2024	G	N9-C4-C5	6.20	107.88	105.40
34	BO	91	LEU	CA-CB-CG	6.20	129.56	115.30
21	CA	1059	C	C2-N1-C1'	-6.20	111.98	118.80
21	CA	1200	C	P-O3'-C3'	6.20	127.14	119.70
59	BA	906	G	C6-N1-C2	6.20	128.82	125.10
21	CA	754	C	C2-N1-C1'	6.19	125.61	118.80
59	DA	955	C	N3-C4-N4	6.19	122.33	118.00
59	DA	1544	A	C8-N9-C4	-6.19	103.32	105.80
59	BA	807	U	C5-C4-O4	-6.19	122.19	125.90
59	BA	2111	C	C2-N1-C1'	6.19	125.61	118.80
24	CX	65	C	C2-N3-C4	6.18	122.99	119.90
24	AX	75	C	C5-C4-N4	-6.18	115.87	120.20
59	BA	2554	U	C2-N1-C1'	6.18	125.11	117.70
21	CA	500	G	C5-C6-O6	-6.18	124.89	128.60
33	BN	72	TYR	CA-CB-CG	6.17	125.13	113.40
21	CA	1145	C	C6-N1-C1'	6.17	128.21	120.80
59	BA	1967	C	C4'-C3'-O3'	6.17	125.34	113.00
21	AA	1494	G	N3-C4-N9	6.17	129.70	126.00
42	DW	107	LEU	CA-CB-CG	6.17	129.48	115.30
21	CA	520	A	N1-C2-N3	6.16	132.38	129.30
59	DA	809	G	C6-C5-N7	-6.16	126.70	130.40
59	BA	962	G	N3-C4-C5	-6.16	125.52	128.60
21	CA	68(R)	C	C6-N1-C2	-6.16	117.84	120.30
59	DA	962	G	C4-N9-C1'	6.15	134.50	126.50
24	AX	61	C	C2-N3-C4	6.15	122.98	119.90
22	AW	53	G	N9-C4-C5	-6.15	102.94	105.40
28	BF	125	LEU	CA-CB-CG	6.14	129.43	115.30
32	BK	105	LEU	CA-CB-CG	6.14	129.43	115.30
59	DA	828	U	C2-N1-C1'	6.14	125.07	117.70
59	DA	2585	U	N1-C2-O2	6.14	127.10	122.80
59	BA	392	C	C2-N1-C1'	6.14	125.55	118.80
21	AA	224	C	N1-C2-O2	-6.13	115.22	118.90
21	AA	1493	A	O5'-P-OP2	6.12	118.05	110.70
59	DA	809	G	N3-C4-N9	6.12	129.68	126.00
22	AW	30	C	C2-N1-C1'	6.12	125.53	118.80
21	CA	1126	U	N1-C2-O2	-6.12	118.52	122.80
59	DA	906	G	C8-N9-C1'	6.11	134.95	127.00
21	AA	1440(K)	G	C4-N9-C1'	6.11	134.44	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	357(D)	G	C4-N9-C1'	-6.10	118.57	126.50
59	DA	2382	G	N3-C4-N9	6.09	129.66	126.00
22	AW	64	G	N9-C4-C5	-6.09	102.96	105.40
20	AY	33	LEU	CA-CB-CG	6.09	129.30	115.30
21	CA	1037	C	C6-N1-C2	-6.09	117.87	120.30
21	CA	500	G	C4-C5-N7	6.08	113.23	110.80
21	AA	809	G	O4'-C1'-N9	6.08	113.07	108.20
21	AA	762	C	C6-N1-C2	-6.08	117.87	120.30
33	BN	101	HIS	N-CA-C	-6.08	94.58	111.00
59	DA	1864(D)	A	N1-C6-N6	6.08	122.25	118.60
59	BA	401	A	N1-C6-N6	-6.08	114.95	118.60
59	BA	1653	G	O4'-C1'-N9	6.08	113.06	108.20
24	CX	3	G	N3-C4-N9	6.08	129.65	126.00
60	DB	51	G	N9-C4-C5	-6.07	102.97	105.40
21	CA	68(Q)	U	C2-N1-C1'	6.07	124.98	117.70
21	CA	68(W)	G	N3-C4-N9	-6.07	122.36	126.00
59	DA	2553	G	C6-N1-C2	6.07	128.74	125.10
24	AX	63	G	N3-C4-N9	-6.06	122.36	126.00
24	AX	3	G	N3-C2-N2	6.06	124.14	119.90
59	BA	1347	G	N3-C4-N9	-6.06	122.36	126.00
60	DB	75	G	C5-C6-N1	6.06	114.53	111.50
21	CA	169	C	N3-C4-C5	-6.05	119.48	121.90
21	AA	68(Q)	U	C2-N1-C1'	6.05	124.96	117.70
59	BA	1864(D)	A	N1-C6-N6	6.05	122.23	118.60
21	AA	1535	C	C5-C6-N1	6.05	124.02	121.00
24	CX	36	C	C4-C5-C6	-6.04	114.38	117.40
59	DA	2391	G	N3-C4-C5	6.04	131.62	128.60
21	AA	68(I)	G	C5-C6-O6	-6.04	124.98	128.60
59	BA	1563	G	N3-C4-N9	6.04	129.62	126.00
60	BB	3	C	N3-C4-C5	-6.04	119.49	121.90
21	CA	1158	C	N3-C2-O2	-6.04	117.68	121.90
21	CA	1127	G	C4-C5-N7	-6.03	108.39	110.80
59	BA	70	G	N3-C4-N9	6.03	129.62	126.00
23	CV	7	G	N3-C4-C5	6.03	131.61	128.60
21	CA	1052	U	C2-N1-C1'	6.03	124.93	117.70
21	AA	1508	G	N3-C4-N9	6.02	129.61	126.00
21	CA	1508	G	N1-C2-N3	6.01	127.51	123.90
33	DN	72	TYR	CA-CB-CG	6.01	124.82	113.40
59	DA	353	G	N3-C4-N9	6.01	129.61	126.00
59	DA	1017	G	N3-C4-N9	6.00	129.60	126.00
59	DA	1544	A	N7-C8-N9	6.00	116.80	113.80
41	BV	35	LEU	CA-CB-CG	6.00	129.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	543(D)	A	C8-N9-C4	-6.00	103.40	105.80
59	DA	906	G	C6-N1-C2	6.00	128.70	125.10
24	CX	24	G	C4-N9-C1'	6.00	134.29	126.50
59	BA	1492	G	N3-C4-N9	5.99	129.59	126.00
59	DA	294	A	C6-C5-N7	-5.99	128.11	132.30
60	DB	4	C	C6-N1-C1'	-5.99	113.61	120.80
59	DA	1545	A	N7-C8-N9	5.99	116.79	113.80
59	DA	2585	U	C6-N1-C1'	-5.98	112.82	121.20
21	AA	1332	A	C4-C5-C6	5.98	119.99	117.00
33	BN	85	ILE	CB-CA-C	5.98	123.56	111.60
59	BA	1945	G	C6-C5-N7	-5.98	126.81	130.40
28	DF	156	LEU	CA-CB-CG	5.98	129.06	115.30
59	DA	1396	U	N1-C2-O2	5.98	126.99	122.80
21	AA	1486	G	C5-C6-O6	-5.98	125.01	128.60
59	BA	1416	G	N3-C4-N9	-5.98	122.41	126.00
59	DA	466	A	C4-C5-C6	5.98	119.99	117.00
59	BA	2250	G	C8-N9-C1'	-5.98	119.23	127.00
33	BN	102	ALA	C-N-CA	-5.98	106.76	121.70
59	BA	828	U	C2-N1-C1'	5.98	124.87	117.70
21	CA	1306	A	C5-C6-N6	-5.97	118.92	123.70
59	BA	836	G	C6-N1-C2	5.97	128.68	125.10
59	DA	306	U	C2-N1-C1'	5.97	124.86	117.70
22	AW	68	U	C6-N1-C1'	5.97	129.55	121.20
22	AW	8	U	C2-N1-C1'	5.96	124.86	117.70
59	BA	114	U	C2-N1-C1'	5.96	124.86	117.70
59	BA	2553	G	C2-N3-C4	5.96	114.88	111.90
21	CA	1332	A	C4-C5-C6	5.96	119.98	117.00
59	BA	702	G	N1-C2-N2	5.96	121.57	116.20
21	AA	1299	A	C5-C6-N6	5.96	128.47	123.70
59	DA	555	U	N1-C2-O2	-5.96	118.63	122.80
21	AA	1508	G	N9-C4-C5	-5.96	103.02	105.40
33	DN	85	ILE	CB-CA-C	5.96	123.51	111.60
59	DA	870	A	N9-C4-C5	5.95	108.18	105.80
59	BA	2804	C	C2-N1-C1'	-5.95	112.26	118.80
21	CA	1301	U	C5-C6-N1	5.95	125.67	122.70
22	CW	14	A	C6-C5-N7	-5.95	128.14	132.30
26	BD	143	HIS	CG-CD2-NE2	-5.95	97.91	109.20
59	DA	880	G	C4-N9-C1'	5.95	134.23	126.50
59	BA	1430	C	C5-C6-N1	5.94	123.97	121.00
24	AX	62	C	C2-N1-C1'	-5.94	112.26	118.80
59	BA	2250	G	N3-C4-C5	-5.94	125.63	128.60
43	BX	57	LEU	CA-CB-CG	5.94	128.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	2171	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	383	A	N1-C6-N6	5.94	122.16	118.60
60	BB	95	U	O4'-C1'-N1	5.93	112.95	108.20
21	CA	514	C	C2-N1-C1'	5.93	125.33	118.80
22	CW	66	C	N1-C2-O2	5.93	122.46	118.90
59	BA	2553	G	N3-C2-N2	5.93	124.05	119.90
59	DA	2553	G	N3-C2-N2	5.92	124.05	119.90
59	DA	270(U)	C	C6-N1-C1'	5.92	127.90	120.80
59	DA	1402	C	C6-N1-C1'	5.92	127.90	120.80
24	AX	30	C	C6-N1-C1'	-5.92	113.70	120.80
21	CA	1494	G	C8-N9-C1'	-5.92	119.31	127.00
59	DA	234	C	N1-C2-O2	5.92	122.45	118.90
59	DA	2592	G	N3-C2-N2	5.91	124.04	119.90
22	AW	64	G	C6-C5-N7	-5.91	126.85	130.40
59	DA	392	C	C2-N1-C1'	5.91	125.30	118.80
33	BN	85	ILE	CG1-CB-CG2	-5.91	98.41	111.40
59	BA	269	U	C2-N1-C1'	5.91	124.79	117.70
22	AW	64	G	C8-N9-C1'	-5.90	119.33	127.00
59	BA	2598	A	C4-C5-C6	5.90	119.95	117.00
59	DA	2601	C	C5-C6-N1	5.90	123.95	121.00
21	AA	129(A)	G	N3-C2-N2	5.90	124.03	119.90
22	AW	50	C	C2-N1-C1'	5.90	125.29	118.80
59	DA	2167	U	N1-C2-N3	5.90	118.44	114.90
59	BA	2501	C	O4'-C1'-N1	5.90	112.92	108.20
21	CA	230	G	N3-C4-N9	5.89	129.54	126.00
59	BA	1110	G	C2-N3-C4	-5.89	108.95	111.90
22	CW	20	U	N3-C2-O2	-5.89	118.08	122.20
59	DA	1934	C	C2-N1-C1'	5.88	125.27	118.80
21	AA	1301	U	C5-C6-N1	5.88	125.64	122.70
22	AW	8	U	C5-C6-N1	5.88	125.64	122.70
21	CA	1158	C	C6-N1-C2	-5.88	117.95	120.30
24	AX	36	C	N3-C4-C5	5.88	124.25	121.90
21	CA	838(A)	U	N1-C2-O2	5.88	126.91	122.80
21	CA	1440(E)	G	C4-N9-C1'	5.88	134.14	126.50
24	AX	62	C	C6-N1-C1'	5.87	127.85	120.80
59	DA	1137	G	C2-N3-C4	5.87	114.84	111.90
59	DA	2392	A	O4'-C1'-N9	5.87	112.90	108.20
59	DA	1544	A	C4-C5-C6	5.87	119.94	117.00
59	BA	1493	C	C6-N1-C1'	-5.87	113.76	120.80
21	CA	1343	G	N3-C4-N9	5.87	129.52	126.00
59	BA	1967	C	N3-C4-C5	-5.87	119.55	121.90
21	CA	500	G	C4-N9-C1'	5.87	134.13	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	463	G	C2-N3-C4	-5.87	108.97	111.90
59	BA	1961	C	C6-N1-C1'	-5.87	113.76	120.80
21	CA	1257	U	C2-N1-C1'	5.86	124.73	117.70
59	DA	503	A	N1-C6-N6	-5.86	115.08	118.60
21	CA	68(R)	C	C5-C6-N1	5.86	123.93	121.00
23	CV	7	G	N1-C2-N2	5.86	121.47	116.20
60	DB	75	G	N3-C4-C5	-5.86	125.67	128.60
21	AA	1170	A	C4-C5-C6	5.85	119.93	117.00
21	CA	735	C	N1-C2-O2	5.85	122.41	118.90
33	DN	98	VAL	N-CA-C	5.85	126.79	111.00
21	CA	638	G	N3-C4-N9	-5.85	122.49	126.00
21	CA	1301	U	N1-C2-O2	5.85	126.89	122.80
60	DB	75	G	C5-C6-O6	-5.85	125.09	128.60
59	BA	466	A	C4-C5-C6	5.85	119.92	117.00
47	D1	36	GLY	N-CA-C	5.84	127.71	113.10
60	BB	22	U	N1-C2-O2	-5.84	118.71	122.80
59	BA	974(A)	C	C2-N1-C1'	5.84	125.22	118.80
59	BA	2804	C	C6-N1-C1'	5.84	127.80	120.80
21	CA	1216	G	N3-C4-N9	-5.83	122.50	126.00
59	BA	270(V)	G	N3-C2-N2	-5.83	115.82	119.90
22	CW	30	C	N1-C2-O2	5.83	122.40	118.90
21	CA	1537	U	N3-C2-O2	5.83	126.28	122.20
60	BB	50	G	N3-C4-N9	-5.82	122.51	126.00
21	CA	1497	G	N3-C4-N9	5.82	129.49	126.00
60	DB	98	G	N3-C4-N9	-5.82	122.51	126.00
21	CA	1003	G	N3-C4-N9	-5.82	122.51	126.00
59	DA	2641	G	O4'-C1'-N9	5.82	112.86	108.20
21	AA	1465	C	N3-C4-N4	5.82	122.07	118.00
24	AX	3	G	C6-C5-N7	-5.82	126.91	130.40
59	BA	955	C	N3-C4-C5	-5.81	119.57	121.90
23	CV	10	G	C8-N9-C4	-5.81	104.07	106.40
59	DA	1052	C	N3-C4-C5	-5.81	119.57	121.90
59	DA	2601	C	C6-N1-C2	-5.81	117.97	120.30
21	CA	1227	A	C5-C6-N6	-5.81	119.05	123.70
59	BA	1346	G	N3-C4-N9	-5.81	122.51	126.00
59	DA	862	G	N3-C4-N9	5.81	129.49	126.00
59	DA	1774	C	C2-N1-C1'	5.81	125.19	118.80
59	BA	1421	G	N3-C4-N9	5.81	129.49	126.00
59	DA	2275	C	N3-C2-O2	-5.81	117.84	121.90
28	BF	155	LEU	N-CA-C	-5.80	95.33	111.00
59	DA	1444	G	N3-C4-C5	-5.80	125.70	128.60
59	DA	2598	A	N1-C6-N6	5.80	122.08	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AW	23	A	N9-C4-C5	-5.79	103.48	105.80
59	BA	2149	G	N3-C4-N9	-5.79	122.52	126.00
59	BA	513	A	N1-C6-N6	5.79	122.08	118.60
59	BA	527	C	C6-N1-C1'	-5.79	113.85	120.80
21	CA	1440(E)	G	C6-C5-N7	-5.79	126.93	130.40
24	CX	75	C	C2-N1-C1'	5.79	125.17	118.80
21	AA	139	G	N3-C4-N9	-5.78	122.53	126.00
59	BA	2595	G	C2-N3-C4	-5.78	109.01	111.90
59	DA	1172	G	O4'-C1'-N9	5.77	112.82	108.20
24	AX	75	C	C2-N3-C4	-5.77	117.01	119.90
59	BA	527	C	C5-C6-N1	5.77	123.89	121.00
21	AA	1508	G	C6-C5-N7	-5.76	126.94	130.40
59	DA	2363	C	O4'-C1'-N1	5.76	112.81	108.20
60	BB	95	U	C2-N1-C1'	-5.76	110.79	117.70
21	CA	407	G	N3-C4-N9	-5.76	122.54	126.00
21	CA	1158	C	N1-C2-O2	5.76	122.36	118.90
59	BA	1326	U	N1-C2-O2	5.76	126.83	122.80
21	CA	1148	U	N1-C2-N3	5.76	118.35	114.90
21	CA	1527	C	C2-N1-C1'	5.75	125.12	118.80
59	DA	271(B)	G	C4-N9-C1'	5.75	133.97	126.50
21	CA	1494	G	C6-C5-N7	-5.75	126.95	130.40
59	DA	1413	G	N9-C4-C5	5.75	107.70	105.40
59	BA	270(D)	C	C6-N1-C1'	5.74	127.69	120.80
60	BB	95	U	C5-C4-O4	5.74	129.35	125.90
21	CA	1263	C	C2-N1-C1'	5.74	125.12	118.80
21	AA	1494	G	C8-N9-C1'	-5.74	119.54	127.00
60	BB	89(B)	A	N1-C6-N6	5.74	122.04	118.60
59	DA	2129	C	N1-C2-O2	5.74	122.34	118.90
59	BA	1558	A	P-O3'-C3'	5.74	126.58	119.70
23	CV	8	A	C4-C5-N7	-5.73	107.83	110.70
59	DA	2382	G	N3-C4-C5	-5.73	125.73	128.60
23	AV	19	G	N3-C2-N2	-5.73	115.89	119.90
60	DB	89(B)	A	N9-C4-C5	-5.73	103.51	105.80
59	BA	1326	U	C2-N1-C1'	5.72	124.57	117.70
60	BB	36	C	C2-N1-C1'	5.72	125.09	118.80
59	BA	2580	U	N1-C2-O2	5.72	126.80	122.80
21	CA	421	U	N3-C2-O2	-5.72	118.20	122.20
59	DA	962	G	N3-C2-N2	5.72	123.90	119.90
59	DA	2275	C	N1-C2-O2	5.72	122.33	118.90
21	AA	1200	C	P-O3'-C3'	5.72	126.56	119.70
22	AW	64	G	C4-N9-C1'	5.71	133.93	126.50
59	DA	1052	C	C2-N3-C4	5.71	122.76	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	1493	C	N1-C2-O2	5.71	122.33	118.90
59	DA	114	U	C2-N1-C1'	5.71	124.56	117.70
21	CA	1145	C	C5-C4-N4	5.71	124.20	120.20
59	BA	2111	C	N1-C2-O2	5.71	122.33	118.90
22	CW	74	C	O4'-C1'-N1	5.71	112.77	108.20
59	DA	1413	G	C5-C6-O6	5.71	132.03	128.60
23	AV	35	A	P-O3'-C3'	5.70	126.55	119.70
59	BA	194	G	N9-C4-C5	5.70	107.68	105.40
47	B1	43	TYR	C-N-CD	5.70	140.37	128.40
59	BA	2061	G	O4'-C1'-N9	5.70	112.76	108.20
59	DA	2275	C	C2-N1-C1'	5.70	125.07	118.80
59	DA	2378	A	N7-C8-N9	5.70	116.65	113.80
21	AA	1465	C	C2-N3-C4	-5.70	117.05	119.90
59	BA	270(D)	C	C2-N1-C1'	-5.69	112.54	118.80
21	AA	1494	G	C4-N9-C1'	5.69	133.90	126.50
59	BA	702	G	N3-C2-N2	-5.69	115.92	119.90
59	BA	611(G)	G	N3-C4-N9	5.69	129.41	126.00
59	BA	1414	G	N9-C4-C5	5.69	107.67	105.40
21	AA	723	U	C6-N1-C1'	-5.68	113.24	121.20
59	DA	2592	G	C5-C6-O6	-5.68	125.19	128.60
59	DA	2804	C	O4'-C1'-N1	5.68	112.74	108.20
59	BA	271(B)	G	P-O3'-C3'	5.68	126.51	119.70
59	DA	1139	G	N1-C6-O6	5.68	123.31	119.90
60	DB	79	C	C5-C6-N1	5.68	123.84	121.00
59	DA	2391	G	C6-C5-N7	5.67	133.80	130.40
33	BN	36	GLY	N-CA-C	-5.67	98.93	113.10
59	BA	386	G	C6-N1-C2	-5.67	121.70	125.10
21	AA	252	U	N1-C2-O2	5.66	126.77	122.80
21	CA	1075	C	C5-C6-N1	5.66	123.83	121.00
59	DA	906	G	C4-N9-C1'	-5.66	119.14	126.50
59	DA	2592	G	C4-C5-C6	5.66	122.20	118.80
59	DA	871	U	C2-N3-C4	-5.66	123.60	127.00
59	BA	83	G	C2-N3-C4	-5.66	109.07	111.90
59	BA	906	G	C8-N9-C1'	5.66	134.36	127.00
60	BB	33	G	N3-C4-N9	-5.66	122.61	126.00
59	DA	889	C	N3-C4-C5	5.66	124.16	121.90
59	DA	1106	G	N3-C4-C5	-5.66	125.77	128.60
27	BE	61	ARG	NE-CZ-NH1	5.66	123.13	120.30
21	CA	1003	G	N1-C6-O6	-5.66	116.51	119.90
60	BB	3	C	N3-C2-O2	-5.65	117.94	121.90
21	CA	1127	G	C8-N9-C1'	5.65	134.35	127.00
21	AA	723	U	N1-C2-O2	5.65	126.76	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	2792	G	N9-C4-C5	5.65	107.66	105.40
21	AA	1301	U	C6-N1-C1'	-5.65	113.29	121.20
24	CX	75	C	C6-N1-C1'	-5.65	114.02	120.80
21	CA	520	A	C6-N1-C2	-5.65	115.21	118.60
59	BA	906	G	C4-N9-C1'	-5.64	119.16	126.50
59	DA	880	G	C8-N9-C1'	-5.64	119.66	127.00
59	DA	2167	U	C2-N3-C4	-5.64	123.61	127.00
22	AW	44	G	C4-C5-N7	5.64	113.06	110.80
21	CA	1037	C	C5-C4-N4	5.64	124.15	120.20
59	BA	2681	C	C5-C4-N4	5.64	124.15	120.20
59	BA	2181	G	N9-C4-C5	5.64	107.66	105.40
21	AA	328	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1302	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	723	U	C5-C6-N1	5.63	125.52	122.70
21	CA	1072	G	N3-C2-N2	-5.63	115.96	119.90
59	DA	353	G	C4-N9-C1'	5.63	133.82	126.50
21	CA	68(H)	G	C4-N9-C1'	-5.63	119.18	126.50
60	DB	117	G	C4-C5-N7	-5.63	108.55	110.80
24	CX	1	G	C6-N1-C2	5.63	128.48	125.10
59	DA	2896	C	C5-C6-N1	5.63	123.82	121.00
22	CW	53	G	N9-C4-C5	-5.63	103.15	105.40
59	DA	1053	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	1200	C	OP2-P-O3'	5.62	117.57	105.20
21	CA	1440(E)	G	C8-N9-C1'	-5.62	119.69	127.00
59	DA	439	G	N3-C4-N9	5.62	129.37	126.00
60	DB	22	U	C2-N1-C1'	-5.62	110.96	117.70
16	AQ	43	LEU	CA-CB-CG	-5.62	102.38	115.30
21	AA	224	C	C6-N1-C1'	5.62	127.54	120.80
21	CA	1028(F)	A	N1-C6-N6	5.62	121.97	118.60
28	DF	156	LEU	C-N-CA	-5.61	107.67	121.70
59	BA	301	G	N3-C4-N9	-5.61	122.63	126.00
59	BA	1810	A	N1-C6-N6	5.61	121.97	118.60
22	AW	30	C	N1-C2-O2	5.61	122.27	118.90
21	CA	930	C	C2-N1-C1'	5.61	124.97	118.80
24	CX	25	C	C2-N1-C1'	5.60	124.96	118.80
59	DA	1021	A	C5-N7-C8	-5.60	101.10	103.90
41	DV	39	LEU	CA-CB-CG	5.60	128.18	115.30
59	DA	543	C	C6-N1-C1'	-5.60	114.08	120.80
21	CA	1537	U	N3-C4-O4	5.60	123.32	119.40
59	DA	2253	G	C6-N1-C2	-5.60	121.74	125.10
60	DB	51	G	N3-C2-N2	5.60	123.82	119.90
59	DA	543(D)	A	N7-C8-N9	5.59	116.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	DB	32	C	C6-N1-C1'	5.59	127.51	120.80
59	DA	392	C	N1-C2-O2	5.59	122.25	118.90
21	CA	129(A)	G	N9-C4-C5	-5.59	103.17	105.40
21	CA	1332	A	C6-C5-N7	-5.59	128.39	132.30
59	BA	1019	U	N1-C2-O2	5.58	126.71	122.80
59	BA	1297	C	O5'-P-OP1	-5.58	100.67	105.70
59	BA	1961	C	C2-N3-C4	5.58	122.69	119.90
59	DA	645	C	C2-N1-C1'	5.58	124.94	118.80
21	AA	748	C	P-O3'-C3'	5.58	126.39	119.70
3	CD	28	SER	C-N-CD	5.58	140.11	128.40
59	DA	422	A	C8-N9-C4	-5.57	103.57	105.80
21	AA	1302	U	C5-C6-N1	5.57	125.49	122.70
59	DA	809	G	N1-C6-O6	5.57	123.24	119.90
59	DA	906	G	N3-C4-C5	5.57	131.38	128.60
21	AA	989	C	C6-N1-C1'	5.56	127.48	120.80
21	AA	1492	A	C6-C5-N7	5.56	136.19	132.30
60	DB	101	A	C5-C6-N1	5.56	120.48	117.70
59	DA	611(E)	G	O4'-C1'-N9	5.56	112.65	108.20
60	DB	65	C	C6-N1-C1'	-5.56	114.13	120.80
59	BA	1025	G	N1-C6-O6	5.56	123.23	119.90
59	DA	2559	C	C6-N1-C1'	5.56	127.47	120.80
60	BB	3	C	C5-C4-N4	5.55	124.09	120.20
20	CY	428	LEU	CA-CB-CG	5.55	128.07	115.30
21	CA	191	G	N3-C4-N9	5.55	129.33	126.00
59	BA	771	G	N3-C4-N9	-5.55	122.67	126.00
21	CA	1440(E)	G	N3-C2-N2	5.55	123.78	119.90
21	AA	1126	U	C2-N3-C4	-5.55	123.67	127.00
21	AA	989	C	O4'-C1'-N1	5.55	112.64	108.20
59	DA	1402	C	C2-N1-C1'	-5.55	112.70	118.80
60	DB	18	G	N3-C4-C5	-5.55	125.83	128.60
59	BA	543	C	C2-N1-C1'	5.54	124.90	118.80
21	CA	1028(G)	G	C5-C6-O6	-5.54	125.27	128.60
21	AA	1016	A	N1-C6-N6	5.54	121.93	118.60
59	DA	1396	U	N3-C2-O2	-5.54	118.32	122.20
60	DB	117	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	1148	U	N3-C4-O4	-5.54	115.52	119.40
59	BA	1430	C	C2-N1-C1'	5.54	124.89	118.80
59	BA	463	G	N1-C2-N2	-5.54	111.22	116.20
59	BA	1945	G	C4-N9-C1'	5.53	133.69	126.50
60	DB	3	C	C2-N3-C4	5.53	122.67	119.90
59	BA	251	A	N1-C2-N3	5.53	132.06	129.30
59	BA	444	C	C2-N1-C1'	-5.53	112.72	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	1072	G	N3-C4-N9	-5.52	122.69	126.00
59	DA	294	A	N3-C4-N9	5.52	131.81	127.40
21	CA	591	U	O4'-C1'-N1	5.52	112.61	108.20
59	DA	1810	A	C5-N7-C8	-5.52	101.14	103.90
21	CA	68(I)	G	N3-C4-N9	5.51	129.31	126.00
59	DA	1053	C	C2-N1-C1'	5.51	124.87	118.80
22	CW	50	C	N1-C2-O2	5.51	122.21	118.90
59	DA	306	U	N1-C2-O2	5.51	126.66	122.80
59	DA	1810	A	N7-C8-N9	5.51	116.55	113.80
21	AA	992	U	P-O3'-C3'	5.50	126.31	119.70
21	AA	1332	A	C6-C5-N7	-5.50	128.45	132.30
21	AA	300	A	N1-C6-N6	5.50	121.90	118.60
33	DN	117	PHE	CA-C-N	-5.50	105.10	117.20
60	DB	24	G	C5-C6-O6	-5.50	125.30	128.60
59	BA	2782	G	C4-C5-N7	5.50	113.00	110.80
21	AA	252	U	N3-C2-O2	-5.50	118.35	122.20
23	AV	24	C	O4'-C1'-N1	5.50	112.60	108.20
59	BA	906	G	N3-C4-C5	5.50	131.35	128.60
21	CA	526	C	C6-N1-C2	-5.50	118.10	120.30
59	BA	95	G	C4-N9-C1'	-5.49	119.36	126.50
23	CV	34	A	P-O3'-C3'	5.49	126.29	119.70
21	CA	68(W)	G	N1-C2-N2	5.49	121.14	116.20
59	BA	2522	U	N1-C2-O2	5.49	126.64	122.80
21	CA	600	C	C5-C6-N1	5.48	123.74	121.00
59	DA	1831	G	N3-C4-N9	5.48	129.29	126.00
21	AA	1037	C	N3-C4-C5	-5.47	119.71	121.90
21	AA	520	A	C4-C5-C6	5.47	119.74	117.00
21	CA	1404	C	N1-C2-O2	5.47	122.18	118.90
59	BA	2478	A	N1-C6-N6	5.47	121.88	118.60
21	CA	68(H)	G	C6-C5-N7	5.47	133.68	130.40
59	DA	2171	A	N1-C6-N6	-5.47	115.32	118.60
59	DA	1226	A	N1-C6-N6	5.47	121.88	118.60
59	DA	915	C	N1-C2-O2	5.47	122.18	118.90
59	DA	1107	G	C8-N9-C4	-5.47	104.21	106.40
59	DA	1547	C	C6-N1-C2	-5.46	118.11	120.30
59	BA	270(V)	G	C8-N9-C1'	5.46	134.09	127.00
21	CA	1103	C	C2-N3-C4	5.46	122.63	119.90
22	CW	14	A	C4-C5-C6	5.45	119.72	117.00
59	DA	2553	G	O4'-C1'-N9	-5.45	103.84	108.20
21	CA	1387	G	N3-C4-N9	5.44	129.27	126.00
22	CW	43	G	N3-C4-N9	5.44	129.27	126.00
59	DA	1139	G	C5-N7-C8	-5.44	101.58	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	871	U	N1-C2-O2	-5.44	118.99	122.80
59	DA	895	U	N1-C2-O2	5.44	126.61	122.80
59	DA	2714	G	C4-N9-C1'	5.44	133.57	126.50
24	AX	53	G	N3-C4-C5	5.44	131.32	128.60
21	CA	68(I)	G	C6-C5-N7	-5.43	127.14	130.40
59	DA	809	G	C5-C6-O6	-5.43	125.34	128.60
21	CA	1535	C	C6-N1-C1'	-5.43	114.28	120.80
21	CA	1529	G	N3-C4-N9	5.43	129.26	126.00
24	CX	24	G	C5-C6-N1	5.43	114.21	111.50
59	DA	1964	G	C8-N9-C4	-5.43	104.23	106.40
21	AA	1494	G	N9-C4-C5	-5.43	103.23	105.40
59	BA	342	G	N3-C4-N9	-5.43	122.74	126.00
60	BB	95	U	C6-N1-C1'	5.43	128.80	121.20
59	BA	301	G	C4-N9-C1'	-5.43	119.44	126.50
59	DA	353	G	C8-N9-C1'	-5.42	119.95	127.00
59	BA	270(D)	C	N1-C2-O2	-5.42	115.65	118.90
21	CA	575	G	C4-N9-C1'	-5.42	119.45	126.50
59	DA	1968	G	O4'-C1'-N9	5.42	112.54	108.20
59	BA	1048	A	N3-C4-N9	5.42	131.73	127.40
59	DA	506	G	C2-N3-C4	-5.42	109.19	111.90
59	DA	870	A	N3-C4-N9	-5.42	123.06	127.40
59	DA	1905	C	N1-C2-O2	5.42	122.15	118.90
21	CA	1537	U	C5-C6-N1	5.42	125.41	122.70
20	CY	260	LEU	CA-CB-CG	5.42	127.76	115.30
59	DA	906	G	N9-C4-C5	5.41	107.56	105.40
60	DB	117	G	C8-N9-C1'	5.41	134.03	127.00
21	AA	520	A	C6-N1-C2	-5.41	115.35	118.60
59	BA	103	A	N1-C6-N6	5.41	121.84	118.60
59	DA	121	G	C8-N9-C1'	-5.41	119.97	127.00
59	DA	936	C	C6-N1-C2	-5.41	118.14	120.30
24	AX	1	G	N3-C4-N9	5.41	129.24	126.00
59	BA	1049	C	C6-N1-C2	-5.40	118.14	120.30
59	DA	121	G	C4-N9-C1'	5.40	133.52	126.50
21	AA	1378	C	C2-N1-C1'	5.40	124.74	118.80
59	BA	611(A)	C	N1-C2-O2	5.40	122.14	118.90
59	DA	915	C	N3-C2-O2	-5.40	118.12	121.90
59	DA	908	C	C2-N1-C1'	-5.40	112.86	118.80
33	DN	118	LYS	C-N-CA	-5.39	108.22	121.70
59	DA	897	C	C2-N1-C1'	5.39	124.73	118.80
21	CA	1155	G	N3-C4-N9	5.39	129.24	126.00
59	BA	2620	C	O4'-C1'-N1	5.39	112.51	108.20
24	CX	35	A	N7-C8-N9	5.39	116.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	CW	7	G	N3-C4-N9	5.39	129.23	126.00
59	DA	1945	G	C8-N9-C1'	-5.39	120.00	127.00
59	BA	1961	C	N3-C4-N4	5.39	121.77	118.00
23	CV	8	A	C4-N9-C1'	-5.39	116.60	126.30
59	DA	155(E)	U	N1-C2-O2	5.39	126.57	122.80
59	DA	577	G	N3-C4-N9	5.39	129.23	126.00
59	DA	2391	G	N1-C2-N2	5.39	121.05	116.20
59	DA	2483	C	C2-N1-C1'	5.39	124.73	118.80
59	DA	1019	U	C5-C4-O4	5.38	129.13	125.90
59	DA	646	A	N1-C6-N6	-5.38	115.37	118.60
59	BA	1223	G	C2-N3-C4	-5.38	109.21	111.90
21	CA	68(I)	G	C4-N9-C1'	5.38	133.50	126.50
22	CW	66	C	C2-N1-C1'	5.38	124.72	118.80
59	BA	1570	A	N1-C6-N6	5.38	121.83	118.60
21	CA	300	A	C6-C5-N7	-5.38	128.53	132.30
21	CA	1440(K)	G	C4-N9-C1'	5.38	133.49	126.50
21	AA	112	G	N3-C4-N9	-5.37	122.78	126.00
21	AA	1348	U	C2-N1-C1'	-5.37	111.25	117.70
59	BA	2529	G	N3-C2-N2	-5.37	116.14	119.90
60	BB	65	C	N1-C2-O2	5.37	122.12	118.90
59	DA	540	C	C6-N1-C1'	5.37	127.25	120.80
59	BA	520	G	N3-C4-N9	5.37	129.22	126.00
59	BA	2149	G	N9-C4-C5	5.37	107.55	105.40
21	AA	1126	U	N1-C2-O2	-5.37	119.04	122.80
59	BA	194	G	C8-N9-C1'	5.37	133.97	127.00
60	BB	79	C	C2-N1-C1'	5.37	124.70	118.80
24	CX	49	G	N9-C4-C5	5.37	107.55	105.40
59	DA	357(D)	G	N3-C2-N2	-5.37	116.14	119.90
21	AA	838(B)	C	O4'-C1'-N1	5.36	112.49	108.20
60	DB	22	U	O4'-C1'-N1	5.36	112.49	108.20
59	DA	1022	G	OP2-P-O3'	5.36	116.99	105.20
24	CX	24	G	C5-C6-O6	-5.36	125.39	128.60
59	DA	1774	C	C5-C6-N1	5.36	123.68	121.00
59	DA	1712(I)	U	N1-C2-O2	5.36	126.55	122.80
59	DA	1570	A	N7-C8-N9	5.35	116.48	113.80
59	DA	2295	C	C2-N1-C1'	5.35	124.69	118.80
22	AW	50	C	C6-N1-C1'	-5.35	114.38	120.80
59	DA	2171	A	C5-N7-C8	-5.35	101.23	103.90
24	AX	30	C	C5-C6-N1	5.35	123.67	121.00
47	B1	46	LEU	CA-CB-CG	5.35	127.60	115.30
59	BA	2250	G	O4'-C1'-N9	5.35	112.48	108.20
24	AX	72	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	68(Q)	U	N3-C2-O2	-5.34	118.46	122.20
23	AV	1	G	O5'-P-OP1	-5.34	100.89	105.70
52	B6	36	LEU	CA-CB-CG	5.34	127.59	115.30
59	BA	2792	G	C8-N9-C4	-5.34	104.26	106.40
24	CX	11	C	N3-C2-O2	-5.34	118.16	121.90
59	BA	1493	C	N3-C2-O2	-5.34	118.16	121.90
59	DA	870	A	C5-C6-N6	5.34	127.97	123.70
24	AX	74	C	C4-C5-C6	-5.34	114.73	117.40
21	AA	1336	C	N1-C2-O2	5.33	122.10	118.90
59	DA	1945	G	N3-C4-N9	5.33	129.20	126.00
59	BA	1396	U	N1-C2-O2	5.33	126.53	122.80
21	CA	735	C	C5-C6-N1	5.33	123.67	121.00
24	CX	36	C	N3-C2-O2	5.33	125.63	121.90
59	BA	1964	G	N9-C4-C5	-5.33	103.27	105.40
60	DB	101	A	N3-C4-N9	5.33	131.66	127.40
59	BA	2257	U	C5-C6-N1	5.33	125.36	122.70
59	DA	357(M)	C	N1-C2-O2	5.33	122.09	118.90
59	DA	1965	C	OP1-P-OP2	-5.32	111.61	119.60
59	BA	194	G	N3-C2-N2	-5.32	116.17	119.90
21	CA	1407	C	N1-C2-O2	5.32	122.09	118.90
59	DA	671	C	N1-C2-O2	5.32	122.09	118.90
59	DA	2764	A	C4-C5-C6	-5.32	114.34	117.00
59	BA	2111	C	N3-C2-O2	-5.32	118.18	121.90
33	BN	101	HIS	O-C-N	5.32	131.21	122.70
59	DA	809	G	C4-N9-C1'	5.32	133.41	126.50
60	DB	87	G	C2-N3-C4	-5.32	109.24	111.90
59	DA	155(E)	U	C2-N1-C1'	5.32	124.08	117.70
21	CA	638	G	N3-C2-N2	-5.31	116.18	119.90
35	BP	53	GLY	N-CA-C	-5.31	99.82	113.10
59	DA	1380	G	N3-C4-N9	5.31	129.19	126.00
41	BV	39	LEU	CA-CB-CG	5.31	127.51	115.30
59	BA	1313	U	C6-N1-C1'	-5.31	113.77	121.20
21	CA	365	U	O4'-C1'-N1	5.31	112.44	108.20
59	DA	1945	G	C4-C5-N7	5.31	112.92	110.80
21	AA	1145	C	C5-C4-N4	5.31	123.91	120.20
59	BA	2077	A	N1-C6-N6	5.31	121.78	118.60
59	DA	1139	G	C4-C5-N7	5.30	112.92	110.80
60	DB	98	G	C4-N9-C1'	-5.30	119.60	126.50
59	DA	121	G	N3-C2-N2	5.30	123.61	119.90
59	BA	24	G	N3-C2-N2	-5.30	116.19	119.90
59	DA	1642	G	N3-C4-N9	5.30	129.18	126.00
21	AA	1314	C	C2-N1-C1'	5.30	124.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1440(K)	G	C8-N9-C1'	-5.30	120.12	127.00
59	DA	733	G	C5-C6-O6	-5.30	125.42	128.60
59	DA	1349	A	O4'-C1'-N9	5.30	112.44	108.20
21	CA	1508	G	N9-C4-C5	-5.29	103.28	105.40
24	CX	60	C	C6-N1-C2	-5.29	118.18	120.30
59	DA	121	G	N9-C4-C5	-5.29	103.28	105.40
59	BA	1414	G	C5-C6-O6	5.29	131.77	128.60
59	DA	509	C	C5-C6-N1	5.29	123.64	121.00
59	BA	1346	G	C8-N9-C1'	5.29	133.87	127.00
59	DA	1413	G	N3-C4-N9	-5.29	122.83	126.00
21	AA	221	C	N1-C2-O2	5.29	122.07	118.90
21	AA	1493	A	P-O3'-C3'	5.29	126.04	119.70
59	BA	146	G	N3-C4-N9	-5.29	122.83	126.00
59	DA	897	C	N1-C2-O2	5.29	122.07	118.90
59	BA	1313	U	N3-C2-O2	-5.28	118.50	122.20
24	CX	62	C	N1-C2-O2	-5.28	115.73	118.90
59	DA	1019	U	C6-N1-C2	-5.28	117.83	121.00
59	DA	1047	G	O4'-C1'-N9	5.28	112.43	108.20
21	AA	1492	A	N1-C6-N6	-5.28	115.43	118.60
21	CA	500	G	C6-C5-N7	-5.28	127.23	130.40
22	AW	14	A	N3-C4-N9	5.28	131.62	127.40
23	AV	19	G	C8-N9-C1'	5.28	133.86	127.00
59	DA	466	A	C5-C6-N6	-5.28	119.48	123.70
59	DA	880	G	N3-C4-C5	-5.28	125.96	128.60
59	DA	2639	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	46	G	N3-C4-N9	-5.28	122.83	126.00
59	DA	1048	A	C6-C5-N7	-5.27	128.61	132.30
60	DB	117	G	C6-C5-N7	5.27	133.56	130.40
59	BA	1346	G	N9-C4-C5	5.27	107.51	105.40
14	CO	31	LEU	CA-CB-CG	5.27	127.42	115.30
25	BC	44	VAL	N-CA-C	-5.27	96.77	111.00
59	BA	1172	G	O4'-C1'-N9	5.27	112.42	108.20
59	DA	155(E)	U	N3-C2-O2	-5.27	118.51	122.20
59	DA	1139	G	C6-C5-N7	-5.27	127.24	130.40
59	DA	1945	G	N9-C4-C5	-5.27	103.29	105.40
59	DA	2681	C	N3-C4-N4	-5.27	114.31	118.00
60	DB	87	G	N1-C2-N2	-5.27	111.46	116.20
21	AA	989	C	C2-N1-C1'	-5.26	113.01	118.80
22	CW	41	A	O4'-C1'-N9	5.26	112.41	108.20
59	BA	2181	G	N3-C2-N2	-5.26	116.22	119.90
21	CA	1336	C	C6-N1-C1'	-5.26	114.48	120.80
21	CA	68(W)	G	N3-C2-N2	-5.26	116.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	BA	2111	C	C6-N1-C2	-5.26	118.20	120.30
21	CA	1529	G	C4-N9-C1'	5.26	133.34	126.50
59	DA	357(A)	U	C5-C6-N1	5.26	125.33	122.70
24	AX	72	C	C2-N1-C1'	5.25	124.58	118.80
59	DA	1712(Q)	G	C5-C6-O6	5.25	131.75	128.60
21	AA	328	C	P-O3'-C3'	5.25	126.00	119.70
21	CA	930	C	N1-C2-O2	5.25	122.05	118.90
44	DY	31	LEU	C-N-CD	-5.25	109.05	120.60
37	BR	28	LEU	CA-CB-CG	5.25	127.37	115.30
21	CA	1536	C	N3-C4-C5	-5.25	119.80	121.90
59	DA	908	C	C6-N1-C1'	5.25	127.10	120.80
59	DA	2092	U	C2-N1-C1'	5.25	124.00	117.70
59	DA	2582	G	C5-C6-O6	-5.25	125.45	128.60
21	AA	328	C	C6-N1-C1'	-5.25	114.51	120.80
21	AA	1493	A	O5'-P-OP1	5.24	116.99	110.70
59	BA	2639	A	O4'-C1'-N9	5.24	112.39	108.20
60	DB	98	G	C8-N9-C1'	5.24	133.81	127.00
59	BA	1598	C	C6-N1-C2	-5.24	118.20	120.30
59	DA	1971	A	C5-C6-N1	5.24	120.32	117.70
21	CA	1348	U	N3-C4-C5	5.24	117.74	114.60
59	BA	2580	U	N3-C2-O2	-5.24	118.54	122.20
59	DA	257	A	N1-C6-N6	5.24	121.74	118.60
59	DA	540	C	O4'-C1'-N1	5.24	112.39	108.20
21	CA	68(A)	G	C8-N9-C4	-5.23	104.31	106.40
22	AW	68	U	N1-C2-O2	-5.23	119.14	122.80
59	DA	1945	G	C4-N9-C1'	5.23	133.30	126.50
59	BA	2647	U	N1-C2-O2	5.23	126.46	122.80
59	BA	1396	U	N3-C2-O2	-5.23	118.54	122.20
59	DA	1141	U	C2-N3-C4	-5.23	123.86	127.00
59	DA	2887	U	C5-C6-N1	5.23	125.31	122.70
21	CA	1126	U	C5-C4-O4	5.22	129.03	125.90
59	DA	2582	G	N9-C4-C5	-5.22	103.31	105.40
21	CA	1336	C	C5-C6-N1	5.22	123.61	121.00
59	DA	383	U	N3-C2-O2	-5.22	118.54	122.20
21	CA	68(H)	G	C4-C5-N7	-5.22	108.71	110.80
21	CA	1537	U	C6-N1-C1'	5.22	128.51	121.20
60	DB	96	G	C5-C6-O6	5.22	131.73	128.60
59	BA	1832	C	C2-N1-C1'	5.22	124.54	118.80
21	AA	1436	U	N3-C4-O4	-5.22	115.75	119.40
59	BA	1937	A	C5-C6-N6	5.22	127.88	123.70
23	CV	19	G	C4-C5-N7	-5.22	108.71	110.80
33	DN	71	ILE	N-CA-C	5.22	125.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	703	U	N1-C2-O2	5.21	126.45	122.80
60	DB	18	G	N3-C2-N2	5.21	123.55	119.90
59	BA	57	C	C6-N1-C2	-5.21	118.22	120.30
59	DA	2428	G	OP1-P-O3'	5.21	116.66	105.20
21	CA	533	A	N1-C2-N3	5.21	131.90	129.30
43	DX	57	LEU	CA-CB-CG	5.21	127.28	115.30
59	DA	1048	A	C4-C5-C6	5.20	119.60	117.00
59	BA	807	U	C2-N3-C4	-5.20	123.88	127.00
59	DA	2011	U	C2-N1-C1'	-5.20	111.46	117.70
21	AA	762	C	C5-C6-N1	5.20	123.60	121.00
59	BA	95	G	C8-N9-C1'	5.20	133.76	127.00
59	DA	1712(O)	C	C2-N1-C1'	-5.20	113.08	118.80
21	AA	1158	C	C2-N1-C1'	5.20	124.52	118.80
22	AW	5	A	N1-C6-N6	-5.20	115.48	118.60
59	BA	466	A	C5-C6-N6	-5.20	119.54	123.70
59	BA	943	U	N1-C2-O2	-5.20	119.16	122.80
59	BA	1430	C	N1-C2-O2	5.19	122.02	118.90
60	DB	3	C	C5-C4-N4	5.19	123.84	120.20
59	BA	344	G	C2-N3-C4	-5.19	109.30	111.90
59	BA	353	G	N3-C4-N9	5.19	129.12	126.00
59	BA	1421	G	C6-C5-N7	-5.19	127.28	130.40
59	BA	2529	G	N3-C4-N9	-5.19	122.89	126.00
59	DA	1105	U	O4'-C1'-N1	5.19	112.35	108.20
59	BA	2636	U	N1-C2-O2	5.19	126.43	122.80
59	DA	269	U	C2-N1-C1'	5.18	123.92	117.70
59	DA	1300	U	P-O3'-C3'	5.18	125.92	119.70
59	DA	1141	U	N1-C2-N3	5.18	118.01	114.90
59	DA	1653	G	C5-C6-O6	-5.18	125.49	128.60
59	DA	1934	C	C6-N1-C2	-5.18	118.23	120.30
21	AA	1336	C	C6-N1-C1'	-5.18	114.59	120.80
59	BA	1022	G	P-O3'-C3'	5.17	125.91	119.70
59	DA	710	G	N3-C4-N9	5.17	129.10	126.00
59	BA	1430	C	C6-N1-C2	-5.17	118.23	120.30
59	BA	2136	C	N1-C2-O2	5.17	122.00	118.90
21	CA	1536	C	N1-C2-O2	-5.17	115.80	118.90
21	CA	712	A	C6-N1-C2	-5.17	115.50	118.60
21	CA	998	G	N9-C4-C5	5.17	107.47	105.40
33	BN	98	VAL	N-CA-C	5.17	124.95	111.00
59	BA	2792	G	N9-C4-C5	5.17	107.47	105.40
24	CX	24	G	C6-C5-N7	-5.17	127.30	130.40
24	AX	37	A	C6-C5-N7	5.16	135.91	132.30
59	DA	357(M)	C	C6-N1-C1'	-5.16	114.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	DA	2812	G	O4'-C1'-N9	5.16	112.33	108.20
23	CV	35	A	P-O3'-C3'	5.16	125.89	119.70
59	DA	271(G)	G	N1-C6-O6	5.16	123.00	119.90
21	AA	1028(F)	A	N1-C6-N6	5.16	121.69	118.60
21	CA	163	C	C6-N1-C1'	5.16	126.99	120.80
59	DA	2136	C	C5-C6-N1	5.16	123.58	121.00
59	DA	2739	U	N1-C2-N3	5.16	117.99	114.90
34	BO	8	LEU	CA-CB-CG	5.15	127.16	115.30
59	BA	2554	U	N1-C2-O2	5.15	126.41	122.80
59	DA	809	G	C8-N9-C1'	-5.15	120.30	127.00
23	AV	29	A	OP1-P-O3'	5.15	116.53	105.20
52	B6	11	LEU	CA-CB-CG	5.15	127.15	115.30
59	DA	2714	G	N3-C4-C5	-5.15	126.03	128.60
59	BA	121	G	C8-N9-C1'	-5.15	120.31	127.00
59	DA	40	C	C2-N1-C1'	5.15	124.46	118.80
59	BA	1569	A	O4'-C1'-N9	5.15	112.32	108.20
59	BA	733	G	C5-C6-O6	-5.14	125.51	128.60
59	DA	1210	A	P-O3'-C3'	5.14	125.87	119.70
53	B7	40	TRP	CZ3-CH2-CZ2	-5.14	115.43	121.60
24	CX	52	G	N3-C4-N9	-5.14	122.91	126.00
59	BA	1385	G	N3-C4-N9	-5.14	122.92	126.00
21	AA	1302	U	C6-N1-C1'	-5.14	114.00	121.20
59	BA	1047	G	O4'-C1'-N9	5.14	112.31	108.20
21	CA	68(X)	U	C2-N1-C1'	5.14	123.87	117.70
21	CA	1527	C	N1-C2-O2	5.14	121.98	118.90
59	DA	103	A	C5-C6-N6	-5.14	119.59	123.70
59	DA	306	U	C5-C6-N1	5.14	125.27	122.70
21	AA	687	A	P-O3'-C3'	5.14	125.86	119.70
33	DN	101	HIS	N-CA-C	-5.14	97.13	111.00
21	AA	1494	G	C6-C5-N7	-5.13	127.32	130.40
60	BB	50	G	N9-C4-C5	5.13	107.45	105.40
22	CW	61	C	C5-C6-N1	5.13	123.57	121.00
24	CX	69	A	C6-N1-C2	-5.13	115.52	118.60
59	BA	1653	G	C4-N9-C1'	-5.13	119.83	126.50
59	DA	2257	U	C5-C4-O4	-5.13	122.82	125.90
60	DB	32	C	O4'-C1'-N1	5.13	112.31	108.20
59	BA	2598	A	C6-C5-N7	-5.13	128.71	132.30
59	BA	1019	U	C6-N1-C2	-5.12	117.93	121.00
59	BA	1570	A	N7-C8-N9	5.12	116.36	113.80
21	CA	998	G	N3-C4-N9	-5.12	122.93	126.00
21	AA	1332	A	N3-C4-N9	5.12	131.50	127.40
59	BA	251	A	N3-C4-C5	-5.12	123.22	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	998	G	C8-N9-C1'	5.12	133.65	127.00
59	DA	1547	C	N3-C2-O2	-5.12	118.32	121.90
21	AA	1348	U	N1-C2-O2	-5.12	119.22	122.80
59	BA	1468(D)	A	N1-C6-N6	5.12	121.67	118.60
59	BA	176	G	N3-C4-N9	-5.12	122.93	126.00
60	BB	32	C	C5-C4-N4	5.12	123.78	120.20
24	CX	62	C	C6-N1-C1'	5.12	126.94	120.80
59	DA	2592	G	N9-C4-C5	-5.12	103.35	105.40
60	DB	65	C	N3-C2-O2	-5.12	118.32	121.90
22	AW	23	A	N3-C4-N9	5.11	131.49	127.40
21	CA	1494	G	C4-C5-C6	5.11	121.87	118.80
59	DA	1968	G	C4-N9-C1'	-5.11	119.86	126.50
59	DA	2157	G	N3-C2-N2	5.11	123.48	119.90
59	DA	955	C	N3-C4-C5	-5.11	119.86	121.90
59	DA	2391	G	O4'-C1'-N9	5.11	112.29	108.20
59	BA	268	C	N1-C2-O2	5.11	121.96	118.90
21	CA	300	A	C4-C5-C6	5.10	119.55	117.00
24	AX	3	G	N3-C4-C5	-5.10	126.05	128.60
21	CA	1436	U	C2-N3-C4	-5.10	123.94	127.00
59	DA	484	C	C5-C6-N1	5.10	123.55	121.00
59	DA	1966	A	N7-C8-N9	5.10	116.35	113.80
24	CX	60	C	C2-N1-C1'	5.10	124.41	118.80
59	BA	296	C	C6-N1-C1'	5.09	126.91	120.80
24	CX	24	G	C4-C5-N7	5.09	112.84	110.80
59	DA	2427	C	N1-C2-O2	-5.09	115.84	118.90
21	CA	1075	C	C2-N1-C1'	5.09	124.40	118.80
21	AA	1003	G	N9-C4-C5	5.09	107.44	105.40
59	DA	701	G	O4'-C1'-N9	5.09	112.27	108.20
59	DA	1969	A	C5-N7-C8	-5.09	101.36	103.90
60	BB	3	C	C2-N1-C1'	5.08	124.39	118.80
59	DA	1711	C	O4'-C1'-N1	5.08	112.27	108.20
22	AW	14	A	N9-C4-C5	-5.08	103.77	105.80
22	AW	71	C	C6-N1-C2	-5.08	118.27	120.30
59	BA	2620	C	C6-N1-C1'	5.08	126.90	120.80
21	CA	1043	C	C2-N1-C1'	-5.08	113.21	118.80
21	CA	1061	G	C4-N9-C1'	5.08	133.10	126.50
21	AA	1003	G	N1-C6-O6	-5.08	116.85	119.90
59	DA	2592	G	N1-C2-N2	-5.08	111.63	116.20
21	CA	978	A	N9-C4-C5	5.08	107.83	105.80
21	AA	1437	C	C6-N1-C2	-5.07	118.27	120.30
22	AW	53	G	C6-C5-N7	-5.07	127.36	130.40
59	BA	2699	C	N1-C2-O2	-5.07	115.86	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	810	C	C6-N1-C1'	5.07	126.89	120.80
24	CX	62	C	C2-N1-C1'	-5.07	113.22	118.80
60	DB	18	G	N9-C4-C5	-5.07	103.37	105.40
21	AA	1491	G	C5-N7-C8	-5.07	101.77	104.30
59	BA	836	G	C5-C6-O6	5.07	131.64	128.60
59	DA	344	G	N1-C2-N3	5.07	126.94	123.90
59	DA	2780	G	C4-N9-C1'	-5.07	119.91	126.50
21	AA	115	G	C4-N9-C1'	5.07	133.09	126.50
59	BA	296	C	C2-N1-C1'	-5.07	113.23	118.80
21	CA	1263	C	N1-C2-O2	5.07	121.94	118.90
59	DA	83	G	N9-C4-C5	-5.07	103.37	105.40
59	DA	454	A	N1-C6-N6	-5.07	115.56	118.60
59	BA	301	G	C8-N9-C1'	5.06	133.58	127.00
59	DA	103	A	N3-C4-N9	5.06	131.45	127.40
59	DA	1859	A	N1-C6-N6	5.06	121.64	118.60
59	BA	2792	G	N3-C2-N2	-5.05	116.36	119.90
59	DA	646	A	C5-C6-N6	5.05	127.74	123.70
59	DA	2780	G	N3-C4-N9	-5.05	122.97	126.00
22	AW	30	C	C5-C6-N1	5.05	123.53	121.00
59	BA	466	A	C6-C5-N7	-5.05	128.76	132.30
21	AA	815	A	C6-C5-N7	5.05	135.83	132.30
21	CA	1527	C	C6-N1-C2	-5.05	118.28	120.30
59	DA	2714	G	C8-N9-C1'	-5.05	120.44	127.00
21	CA	443	C	C2-N1-C1'	5.05	124.35	118.80
21	CA	1028(G)	G	C4-C5-N7	5.05	112.82	110.80
59	DA	271(B)	G	P-O3'-C3'	5.05	125.76	119.70
59	BA	1674	G	C6-C5-N7	-5.04	127.37	130.40
21	AA	115	G	C8-N9-C1'	-5.04	120.45	127.00
59	BA	2553	G	N7-C8-N9	5.04	115.62	113.10
21	AA	1028(B)	C	C5-C6-N1	5.04	123.52	121.00
24	AX	52	G	N3-C4-N9	-5.04	122.98	126.00
21	AA	45	U	N1-C2-O2	5.04	126.33	122.80
21	AA	1037	C	C5-C4-N4	5.04	123.72	120.20
59	DA	2345	G	N1-C6-O6	5.04	122.92	119.90
24	AX	37	A	N3-C4-N9	-5.03	123.37	127.40
21	CA	1158	C	C2-N1-C1'	5.03	124.33	118.80
59	DA	296	C	N1-C2-O2	-5.03	115.88	118.90
27	BE	63	LEU	CA-CB-CG	5.03	126.87	115.30
33	BN	15	LEU	CA-CB-CG	5.03	126.87	115.30
59	DA	1254	A	N1-C6-N6	-5.03	115.58	118.60
59	BA	2552	U	C2-N1-C1'	5.03	123.73	117.70
59	DA	1964	G	N3-C4-C5	-5.03	126.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	CA	1061	G	C8-N9-C1'	-5.03	120.47	127.00
21	CA	1285	A	P-O3'-C3'	5.03	125.73	119.70
59	DA	154	G	N3-C4-N9	5.03	129.02	126.00
59	DA	2641	G	C8-N9-C1'	5.03	133.53	127.00
21	AA	68(I)	G	N3-C4-N9	5.02	129.01	126.00
59	DA	506	G	N3-C4-C5	5.02	131.11	128.60
21	AA	1437	C	C5-C6-N1	5.02	123.51	121.00
22	AW	53	G	C8-N9-C1'	-5.02	120.47	127.00
21	AA	129(A)	G	N9-C4-C5	-5.02	103.39	105.40
21	AA	1440(N)	C	N1-C2-O2	5.02	121.91	118.90
60	DB	60	C	N1-C2-O2	5.02	121.91	118.90
59	BA	1982	C	N1-C2-O2	5.01	121.91	118.90
59	BA	2338	G	N3-C4-N9	-5.01	122.99	126.00
21	CA	1272	G	N3-C4-C5	-5.01	126.09	128.60
59	DA	1415	U	C2-N1-C1'	-5.01	111.68	117.70
21	AA	152	A	N1-C6-N6	-5.01	115.59	118.60
47	B1	17	SER	N-CA-CB	-5.01	102.98	110.50
59	BA	2136	C	C2-N1-C1'	5.01	124.31	118.80
59	BA	2553	G	O4'-C1'-N9	-5.01	104.19	108.20
59	DA	807	U	C5-C4-O4	-5.01	122.89	125.90
21	CA	328	C	P-O3'-C3'	5.01	125.71	119.70
59	DA	2695	C	C2-N1-C1'	5.01	124.31	118.80
21	AA	533	A	C4-C5-C6	5.01	119.50	117.00
59	DA	1484	G	N3-C4-C5	5.01	131.10	128.60
22	AW	64	G	C4-C5-N7	5.01	112.80	110.80
59	BA	2501	C	C2-N1-C1'	-5.01	113.29	118.80
21	CA	1508	G	C6-C5-N7	-5.01	127.40	130.40
22	CW	53	G	N3-C2-N2	5.01	123.40	119.90
59	DA	103	A	C8-N9-C1'	-5.01	118.69	127.70
59	BA	425	G	N3-C4-N9	5.00	129.00	126.00
60	BB	36	C	N1-C2-O2	5.00	121.90	118.90
21	CA	383	A	N1-C6-N6	5.00	121.60	118.60
59	DA	357(D)	G	C6-C5-N7	5.00	133.40	130.40
59	DA	540	C	C2-N1-C1'	-5.00	113.30	118.80
59	DA	1965	C	O5'-P-OP2	5.00	116.70	110.70
23	CV	26	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (86) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide

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Mol	Chain	Res	Type	Group
10	AK	43	SER	Peptide
15	AP	34	GLU	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	Peptide
47	B1	16	ASN	Peptide
47	B1	17	SER	Peptide
47	B1	18	ILE	Peptide
47	B1	20	ARG	Peptide
53	B7	40	TRP	Mainchain
25	BC	161	ARG	Peptide
25	BC	162	ILE	Peptide
25	BC	163	GLU	Peptide
25	BC	171	ALA	Peptide
25	BC	210	LEU	Peptide
25	BC	88	GLU	Peptide
26	BD	164	GLN	Peptide
27	BE	107	THR	Peptide
28	BF	154	VAL	Peptide
28	BF	156	LEU	Peptide
28	BF	173	VAL	Peptide
28	BF	194	MET	Peptide
31	BJ	25	UNK	Peptide
31	BJ	83	UNK	Peptide
33	BN	100	GLU	Peptide
33	BN	105	GLY	Peptide
33	BN	112	LEU	Peptide
33	BN	113	GLY	Peptide
33	BN	116	LEU	Peptide
33	BN	117	PHE	Peptide
33	BN	118	LYS	Peptide
33	BN	125	GLY	Peptide
33	BN	70	LYS	Peptide
33	BN	71	ILE	Peptide
33	BN	72	TYR	Peptide
33	BN	78	TYR	Peptide
33	BN	82	LEU	Peptide
33	BN	84	LYS	Peptide
33	BN	86	PRO	Peptide
33	BN	90	MET	Peptide
33	BN	99	LEU	Peptide
34	BO	23	ARG	Peptide
36	BQ	101	ARG	Peptide

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Mol	Chain	Res	Type	Group
38	BS	98	VAL	Peptide
39	BT	32	TYR	Peptide
42	BW	75	TYR	Peptide
45	BZ	73	GLN	Peptide
3	CD	31	CYS	Peptide
10	CK	43	SER	Peptide
15	CP	34	GLU	Peptide
47	D1	17	SER	Peptide
47	D1	18	ILE	Peptide
47	D1	19	GLN	Peptide
25	DC	161	ARG	Peptide
25	DC	171	ALA	Peptide
25	DC	210	LEU	Peptide
25	DC	211	ARG	Peptide
25	DC	88	GLU	Peptide
26	DD	164	GLN	Peptide
28	DF	154	VAL	Peptide
28	DF	156	LEU	Peptide
29	DG	111	LEU	Mainchain
31	DJ	25	UNK	Peptide
31	DJ	53	UNK	Peptide
31	DJ	83	UNK	Peptide
33	DN	100	GLU	Peptide
33	DN	105	GLY	Peptide
33	DN	116	LEU	Peptide
33	DN	117	PHE	Peptide
33	DN	118	LYS	Peptide
33	DN	128	HIS	Peptide
33	DN	70	LYS	Peptide
33	DN	71	ILE	Peptide
33	DN	72	TYR	Peptide
33	DN	73	THR	Peptide
33	DN	78	TYR	Peptide
33	DN	82	LEU	Peptide
33	DN	84	LYS	Peptide
33	DN	90	MET	Peptide
33	DN	99	LEU	Peptide
34	DO	23	ARG	Peptide
38	DS	98	VAL	Peptide
39	DT	28	VAL	Peptide
42	DW	75	TYR	Peptide
42	DW	77	ASP	Peptide

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Mol	Chain	Res	Type	Group
45	DZ	73	GLN	Peptide

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
1	AB	233/235 (99%)	168 (72%)	45 (19%)	20 (9%)	1 12
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1 16
2	AC	205/207 (99%)	137 (67%)	39 (19%)	29 (14%)	0 4
2	CC	205/207 (99%)	150 (73%)	35 (17%)	20 (10%)	0 10
3	AD	206/208 (99%)	140 (68%)	41 (20%)	25 (12%)	0 6
3	CD	206/208 (99%)	152 (74%)	33 (16%)	21 (10%)	0 9
4	AE	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	2 24
4	CE	149/151 (99%)	115 (77%)	24 (16%)	10 (7%)	1 19
5	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1 14
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1 12
6	AG	153/155 (99%)	123 (80%)	22 (14%)	8 (5%)	2 23
6	CG	153/155 (99%)	118 (77%)	23 (15%)	12 (8%)	1 15
7	AH	136/138 (99%)	102 (75%)	23 (17%)	11 (8%)	1 14
7	CH	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1 16
8	AI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2 24
8	CI	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2 24
9	AJ	97/99 (98%)	71 (73%)	15 (16%)	11 (11%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CJ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	17
10	AK	117/119 (98%)	83 (71%)	21 (18%)	13 (11%)	0	7
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	4
11	AL	123/125 (98%)	41 (33%)	44 (36%)	38 (31%)	0	0
11	CL	123/125 (98%)	49 (40%)	37 (30%)	37 (30%)	0	0
12	AM	123/125 (98%)	94 (76%)	19 (15%)	10 (8%)	1	14
12	CM	123/125 (98%)	95 (77%)	17 (14%)	11 (9%)	1	12
13	AN	58/60 (97%)	38 (66%)	17 (29%)	3 (5%)	2	23
13	CN	58/60 (97%)	35 (60%)	14 (24%)	9 (16%)	0	4
14	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	6	38
14	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	31
15	AP	82/84 (98%)	58 (71%)	16 (20%)	8 (10%)	0	10
15	CP	82/84 (98%)	62 (76%)	13 (16%)	7 (8%)	1	12
16	AQ	98/100 (98%)	70 (71%)	22 (22%)	6 (6%)	1	20
16	CQ	98/100 (98%)	76 (78%)	16 (16%)	6 (6%)	1	20
17	AR	68/70 (97%)	50 (74%)	9 (13%)	9 (13%)	0	5
17	CR	68/70 (97%)	56 (82%)	8 (12%)	4 (6%)	1	21
18	AS	77/79 (98%)	43 (56%)	23 (30%)	11 (14%)	0	4
18	CS	77/79 (98%)	47 (61%)	27 (35%)	3 (4%)	3	28
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	13
19	CT	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	23
20	AY	657/687 (96%)	407 (62%)	174 (26%)	76 (12%)	0	6
20	CY	657/687 (96%)	437 (66%)	135 (20%)	85 (13%)	0	5
25	BC	226/228 (99%)	107 (47%)	63 (28%)	56 (25%)	0	1
25	DC	226/228 (99%)	114 (50%)	52 (23%)	60 (26%)	0	0
26	BD	273/275 (99%)	174 (64%)	60 (22%)	39 (14%)	0	4
26	DD	273/275 (99%)	180 (66%)	59 (22%)	34 (12%)	0	6
27	BE	203/205 (99%)	134 (66%)	41 (20%)	28 (14%)	0	4
27	DE	203/205 (99%)	124 (61%)	49 (24%)	30 (15%)	0	4
28	BF	206/208 (99%)	139 (68%)	43 (21%)	24 (12%)	0	6
28	DF	206/208 (99%)	127 (62%)	51 (25%)	28 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BG	179/181 (99%)	131 (73%)	37 (21%)	11 (6%)	1	20
29	DG	179/181 (99%)	127 (71%)	37 (21%)	15 (8%)	1	13
30	BH	165/167 (99%)	117 (71%)	31 (19%)	17 (10%)	0	9
30	DH	165/167 (99%)	116 (70%)	30 (18%)	19 (12%)	0	7
32	BK	138/140 (99%)	91 (66%)	32 (23%)	15 (11%)	0	8
32	DK	138/140 (99%)	77 (56%)	44 (32%)	17 (12%)	0	6
33	BN	137/139 (99%)	52 (38%)	32 (23%)	53 (39%)	0	0
33	DN	137/139 (99%)	55 (40%)	28 (20%)	54 (39%)	0	0
34	BO	120/122 (98%)	89 (74%)	21 (18%)	10 (8%)	1	13
34	DO	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	9
35	BP	144/146 (99%)	84 (58%)	36 (25%)	24 (17%)	0	3
35	DP	144/146 (99%)	82 (57%)	39 (27%)	23 (16%)	0	3
36	BQ	139/141 (99%)	84 (60%)	35 (25%)	20 (14%)	0	4
36	DQ	139/141 (99%)	94 (68%)	34 (24%)	11 (8%)	1	14
37	BR	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	5
37	DR	115/117 (98%)	80 (70%)	22 (19%)	13 (11%)	0	7
38	BS	97/99 (98%)	52 (54%)	26 (27%)	19 (20%)	0	2
38	DS	97/99 (98%)	51 (53%)	27 (28%)	19 (20%)	0	2
39	BT	136/138 (99%)	81 (60%)	27 (20%)	28 (21%)	0	2
39	DT	136/138 (99%)	79 (58%)	31 (23%)	26 (19%)	0	2
40	BU	115/117 (98%)	88 (76%)	17 (15%)	10 (9%)	1	12
40	DU	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	17
41	BV	99/101 (98%)	56 (57%)	28 (28%)	15 (15%)	0	4
41	DV	99/101 (98%)	64 (65%)	21 (21%)	14 (14%)	0	4
42	BW	111/113 (98%)	74 (67%)	25 (22%)	12 (11%)	0	8
42	DW	111/113 (98%)	76 (68%)	23 (21%)	12 (11%)	0	8
43	BX	91/93 (98%)	71 (78%)	13 (14%)	7 (8%)	1	15
43	DX	91/93 (98%)	67 (74%)	10 (11%)	14 (15%)	0	4
44	BY	105/107 (98%)	54 (51%)	31 (30%)	20 (19%)	0	2
44	DY	105/107 (98%)	59 (56%)	26 (25%)	20 (19%)	0	2
45	BZ	183/185 (99%)	121 (66%)	43 (24%)	19 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DZ	183/185 (99%)	109 (60%)	45 (25%)	29 (16%)	0	3
46	B0	82/84 (98%)	63 (77%)	14 (17%)	5 (6%)	1	20
46	D0	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	20
47	B1	91/93 (98%)	48 (53%)	24 (26%)	19 (21%)	0	1
47	D1	91/93 (98%)	52 (57%)	20 (22%)	19 (21%)	0	1
48	B2	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	1	12
48	D2	69/71 (97%)	53 (77%)	12 (17%)	4 (6%)	1	21
49	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	31
49	D3	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	23
50	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	4
50	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	4
51	B5	57/59 (97%)	36 (63%)	14 (25%)	7 (12%)	0	6
51	D5	57/59 (97%)	38 (67%)	6 (10%)	13 (23%)	0	1
52	B6	48/50 (96%)	24 (50%)	15 (31%)	9 (19%)	0	2
52	D6	48/50 (96%)	20 (42%)	17 (35%)	11 (23%)	0	1
53	B7	47/49 (96%)	33 (70%)	11 (23%)	3 (6%)	1	20
53	D7	47/49 (96%)	26 (55%)	14 (30%)	7 (15%)	0	4
54	B8	62/64 (97%)	34 (55%)	16 (26%)	12 (19%)	0	2
54	D8	62/64 (97%)	35 (56%)	13 (21%)	14 (23%)	0	1
55	B9	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	4	34
55	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1	12
56	Be	70/103 (68%)	39 (56%)	23 (33%)	8 (11%)	0	7
56	De	70/103 (68%)	40 (57%)	17 (24%)	13 (19%)	0	2
All	All	13246/13568 (98%)	8764 (66%)	2800 (21%)	1682 (13%)	0	5

All (1682) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	190	THR
2	AC	12	LEU
2	AC	110	ASN
2	AC	130	VAL
2	AC	160	ALA

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Mol	Chain	Res	Type
2	AC	161	GLU
3	AD	20	TYR
3	AD	166	LYS
3	AD	172	PRO
3	AD	187	ARG
4	AE	27	ARG
4	AE	77	PRO
4	AE	78	HIS
4	AE	79	GLU
5	AF	69	GLU
5	AF	70	ASP
6	AG	10	ARG
6	AG	35	LYS
7	AH	22	GLU
7	AH	97	VAL
8	AI	110	GLU
9	AJ	75	ILE
10	AK	35	PRO
10	AK	109	VAL
11	AL	7	ILE
11	AL	15	ARG
11	AL	17	LYS
11	AL	39	VAL
11	AL	43	VAL
11	AL	55	VAL
11	AL	66	VAL
11	AL	71	PRO
11	AL	94	PRO
11	AL	97	ARG
11	AL	104	VAL
11	AL	122	THR
11	AL	123	LYS
11	AL	126	LYS
14	AO	88	ARG
15	AP	35	LYS
15	AP	36	ILE
16	AQ	28	PRO
16	AQ	34	LYS
17	AR	37	VAL
17	AR	55	ARG
17	AR	60	ALA
18	AS	5	LEU

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Mol	Chain	Res	Type
18	AS	27	GLU
19	AT	50	GLU
19	AT	74	LYS
20	AY	21	ILE
20	AY	22	ASP
20	AY	35	TYR
20	AY	92	ILE
20	AY	136	ALA
20	AY	142	THR
20	AY	146	LEU
20	AY	192	LEU
20	AY	204	GLU
20	AY	330	VAL
20	AY	331	TYR
20	AY	350	GLU
20	AY	382	GLU
20	AY	448	GLN
20	AY	480	GLN
20	AY	497	PHE
20	AY	501	THR
20	AY	559	PRO
20	AY	566	THR
20	AY	567	LEU
20	AY	613	PRO
20	AY	631	ILE
20	AY	680	PRO
25	BC	17	PRO
25	BC	36	ALA
25	BC	41	THR
25	BC	42	VAL
25	BC	43	GLU
25	BC	71	LYS
25	BC	80	LYS
25	BC	114	VAL
25	BC	115	VAL
25	BC	117	THR
25	BC	119	ASP
25	BC	141	PRO
25	BC	161	ARG
25	BC	162	ILE
25	BC	182	PRO
25	BC	212	SER

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Mol	Chain	Res	Type
25	BC	214	TYR
25	BC	221	PRO
25	BC	227	PRO
25	BC	228	HIS
26	BD	25	THR
26	BD	40	THR
26	BD	166	GLN
26	BD	256	GLY
27	BE	56	PRO
27	BE	61	ARG
27	BE	63	LEU
27	BE	68	ALA
27	BE	72	VAL
27	BE	77	ILE
27	BE	129	HIS
27	BE	135	HIS
27	BE	144	ARG
27	BE	180	ASN
27	BE	185	LYS
27	BE	188	VAL
28	BF	22	ALA
28	BF	66	PRO
28	BF	67	GLN
28	BF	69	HIS
28	BF	88	VAL
28	BF	158	THR
29	BG	78	SER
29	BG	87	PRO
29	BG	114	ILE
30	BH	21	PRO
30	BH	47	GLU
30	BH	126	PRO
30	BH	128	PRO
30	BH	176	ALA
32	BK	5	VAL
32	BK	115	LEU
33	BN	22	THR
33	BN	28	THR
33	BN	31	ALA
33	BN	32	THR
33	BN	38	HIS
33	BN	40	PRO

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Mol	Chain	Res	Type
33	BN	43	THR
33	BN	47	ALA
33	BN	50	ASP
33	BN	51	PHE
33	BN	59	LYS
33	BN	60	ILE
33	BN	72	TYR
33	BN	78	TYR
33	BN	80	GLY
33	BN	83	LYS
33	BN	93	THR
33	BN	94	HIS
33	BN	95	PRO
33	BN	98	VAL
33	BN	101	HIS
33	BN	107	LEU
33	BN	114	ARG
33	BN	115	ARG
33	BN	117	PHE
33	BN	121	LYS
33	BN	129	PRO
34	BO	52	VAL
34	BO	84	ALA
35	BP	14	LYS
35	BP	38	GLN
35	BP	57	THR
35	BP	60	MET
35	BP	68	GLN
35	BP	110	TYR
35	BP	148	LEU
36	BQ	8	LYS
36	BQ	75	THR
36	BQ	93	TYR
36	BQ	102	VAL
36	BQ	103	MET
36	BQ	127	ILE
37	BR	11	ASN
37	BR	14	SER
37	BR	57	ARG
37	BR	104	ARG
38	BS	13	ARG
38	BS	47	THR

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Mol	Chain	Res	Type
38	BS	48	LEU
38	BS	98	VAL
38	BS	100	ALA
38	BS	101	LEU
38	BS	106	ARG
39	BT	2	ASN
39	BT	30	VAL
39	BT	33	LYS
39	BT	37	GLY
39	BT	48	ILE
39	BT	68	TYR
39	BT	83	ILE
39	BT	107	ASP
40	BU	91	ASP
41	BV	14	VAL
41	BV	32	THR
41	BV	78	LYS
41	BV	81	TYR
41	BV	95	LEU
41	BV	96	ILE
42	BW	40	ASN
42	BW	74	ALA
42	BW	77	ASP
43	BX	12	VAL
44	BY	32	PRO
44	BY	53	PRO
44	BY	98	VAL
44	BY	101	LYS
45	BZ	71	VAL
45	BZ	85	HIS
45	BZ	135	GLU
46	B0	33	ALA
46	B0	55	ARG
47	B1	17	SER
47	B1	18	ILE
47	B1	20	ARG
47	B1	47	GLN
47	B1	53	VAL
48	B2	50	ILE
49	B3	52	HIS
50	B4	29	PRO
50	B4	33	VAL

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Mol	Chain	Res	Type
51	B5	35	GLU
51	B5	49	CYS
52	B6	8	LYS
52	B6	9	LEU
52	B6	17	LYS
52	B6	29	ASN
52	B6	33	LYS
53	B7	47	ARG
54	B8	34	TRP
1	CB	35	GLU
1	CB	76	GLN
1	CB	153	ARG
1	CB	202	PRO
1	CB	236	TYR
2	CC	49	SER
2	CC	127	ARG
2	CC	130	VAL
2	CC	207	VAL
3	CD	28	SER
3	CD	89	THR
3	CD	134	ASP
3	CD	166	LYS
3	CD	172	PRO
3	CD	175	SER
4	CE	77	PRO
4	CE	78	HIS
4	CE	115	VAL
5	CF	100	ASN
7	CH	107	LEU
8	CI	35	GLU
9	CJ	55	LYS
10	CK	41	THR
10	CK	43	SER
10	CK	109	VAL
11	CL	7	ILE
11	CL	17	LYS
11	CL	22	SER
11	CL	39	VAL
11	CL	43	VAL
11	CL	47	LYS
11	CL	51	ALA
11	CL	56	ALA

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Mol	Chain	Res	Type
11	CL	66	VAL
11	CL	94	PRO
11	CL	96	VAL
11	CL	104	VAL
11	CL	112	ASP
11	CL	123	LYS
12	CM	12	ASN
12	CM	21	TYR
13	CN	15	LYS
13	CN	49	HIS
13	CN	51	GLY
13	CN	56	VAL
13	CN	57	ARG
13	CN	59	ALA
15	CP	11	SER
15	CP	35	LYS
15	CP	36	ILE
16	CQ	28	PRO
16	CQ	83	ASP
17	CR	87	ARG
19	CT	50	GLU
19	CT	73	HIS
19	CT	100	ILE
20	CY	21	ILE
20	CY	23	ALA
20	CY	35	TYR
20	CY	36	THR
20	CY	88	VAL
20	CY	92	ILE
20	CY	136	ALA
20	CY	161	PRO
20	CY	206	LEU
20	CY	269	VAL
20	CY	303	PRO
20	CY	330	VAL
20	CY	331	TYR
20	CY	359	HIS
20	CY	395	PRO
20	CY	501	THR
20	CY	535	PRO
20	CY	566	THR
20	CY	567	LEU

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Mol	Chain	Res	Type
20	CY	631	ILE
20	CY	680	PRO
25	DC	17	PRO
25	DC	43	GLU
25	DC	53	ARG
25	DC	60	ARG
25	DC	80	LYS
25	DC	96	GLY
25	DC	116	ALA
25	DC	119	ASP
25	DC	141	PRO
25	DC	182	PRO
25	DC	211	ARG
25	DC	212	SER
25	DC	221	PRO
25	DC	227	PRO
25	DC	228	HIS
26	DD	3	VAL
26	DD	46	GLN
26	DD	52	ARG
26	DD	53	PHE
26	DD	90	ALA
26	DD	165	ILE
26	DD	166	GLN
26	DD	231	HIS
26	DD	273	ARG
27	DE	12	THR
27	DE	35	GLN
27	DE	56	PRO
27	DE	68	ALA
27	DE	72	VAL
27	DE	74	PRO
27	DE	75	VAL
27	DE	144	ARG
28	DF	3	GLU
28	DF	48	THR
28	DF	66	PRO
28	DF	69	HIS
28	DF	84	VAL
28	DF	89	VAL
28	DF	158	THR
28	DF	171	PRO

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Mol	Chain	Res	Type
28	DF	192	LEU
29	DG	30	GLU
29	DG	50	ALA
29	DG	113	ARG
29	DG	114	ILE
30	DH	109	PHE
30	DH	124	GLU
32	DK	5	VAL
32	DK	56	GLU
32	DK	89	HIS
33	DN	18	ALA
33	DN	28	THR
33	DN	31	ALA
33	DN	32	THR
33	DN	37	LYS
33	DN	38	HIS
33	DN	43	THR
33	DN	46	VAL
33	DN	50	ASP
33	DN	51	PHE
33	DN	54	VAL
33	DN	56	ASN
33	DN	57	ALA
33	DN	63	THR
33	DN	66	LYS
33	DN	72	TYR
33	DN	74	ARG
33	DN	78	TYR
33	DN	83	LYS
33	DN	84	LYS
33	DN	86	PRO
33	DN	94	HIS
33	DN	95	PRO
33	DN	96	GLU
33	DN	98	VAL
33	DN	101	HIS
33	DN	106	MET
33	DN	107	LEU
33	DN	108	PRO
33	DN	115	ARG
33	DN	118	LYS
33	DN	128	HIS

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Mol	Chain	Res	Type
33	DN	129	PRO
34	DO	24	VAL
34	DO	35	VAL
34	DO	68	GLU
35	DP	12	ALA
35	DP	50	ARG
35	DP	55	ARG
35	DP	57	THR
35	DP	68	GLN
35	DP	71	VAL
36	DQ	90	VAL
36	DQ	93	TYR
36	DQ	94	VAL
36	DQ	102	VAL
36	DQ	103	MET
38	DS	14	VAL
38	DS	23	ARG
38	DS	47	THR
38	DS	48	LEU
38	DS	53	SER
38	DS	94	TYR
38	DS	98	VAL
38	DS	101	LEU
38	DS	104	GLY
38	DS	105	ALA
38	DS	106	ARG
38	DS	108	GLY
39	DT	12	SER
39	DT	30	VAL
39	DT	78	LEU
39	DT	80	SER
39	DT	83	ILE
39	DT	88	ILE
39	DT	104	ASN
39	DT	119	LYS
40	DU	91	ASP
40	DU	92	ARG
40	DU	99	ALA
40	DU	102	GLU
41	DV	46	VAL
41	DV	96	ILE
42	DW	73	ALA

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Mol	Chain	Res	Type
42	DW	77	ASP
44	DY	6	HIS
44	DY	32	PRO
44	DY	53	PRO
44	DY	56	PRO
45	DZ	65	GLN
45	DZ	71	VAL
45	DZ	72	ARG
45	DZ	74	VAL
45	DZ	85	HIS
45	DZ	128	VAL
45	DZ	152	ALA
45	DZ	169	GLU
46	D0	35	ASN
46	D0	49	LYS
46	D0	55	ARG
47	D1	15	ALA
47	D1	34	THR
47	D1	36	GLY
47	D1	37	ILE
47	D1	40	ARG
48	D2	50	ILE
49	D3	27	GLY
50	D4	29	PRO
51	D5	28	PRO
51	D5	49	CYS
52	D6	7	ILE
52	D6	16	CYS
52	D6	29	ASN
52	D6	31	PRO
52	D6	49	HIS
53	D7	8	ASN
53	D7	46	VAL
54	D8	32	LEU
54	D8	34	TRP
54	D8	35	GLN
54	D8	46	ARG
54	D8	49	VAL
56	De	52	ALA
56	De	120	ALA
1	AB	17	PHE
1	AB	35	GLU

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Mol	Chain	Res	Type
1	AB	36	ARG
1	AB	103	THR
1	AB	157	ARG
1	AB	164	VAL
1	AB	165	VAL
1	AB	229	VAL
1	AB	236	TYR
2	AC	51	GLY
2	AC	55	VAL
2	AC	102	ASN
2	AC	207	VAL
3	AD	5	ILE
3	AD	73	ARG
3	AD	75	PHE
3	AD	99	SER
4	AE	6	PHE
4	AE	71	LEU
5	AF	13	ASN
5	AF	43	LEU
5	AF	100	ASN
6	AG	9	VAL
6	AG	114	ARG
7	AH	74	PRO
7	AH	107	LEU
8	AI	29	ASN
8	AI	106	ALA
9	AJ	54	PHE
10	AK	42	TRP
10	AK	49	GLY
10	AK	88	GLY
10	AK	108	ILE
10	AK	111	ASP
10	AK	113	PRO
11	AL	6	THR
11	AL	29	GLY
11	AL	46	LYS
11	AL	50	SER
11	AL	56	ALA
11	AL	58	VAL
11	AL	96	VAL
12	AM	12	ASN
12	AM	67	GLU

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Mol	Chain	Res	Type
12	AM	101	GLN
13	AN	14	PRO
13	AN	27	CYS
14	AO	47	LYS
15	AP	11	SER
15	AP	15	PRO
15	AP	68	ASP
16	AQ	55	ASP
17	AR	23	LYS
17	AR	59	SER
17	AR	87	ARG
18	AS	46	GLY
18	AS	48	THR
19	AT	11	SER
19	AT	71	THR
19	AT	100	ILE
20	AY	36	THR
20	AY	75	LYS
20	AY	89	ASP
20	AY	121	VAL
20	AY	123	ARG
20	AY	135	PHE
20	AY	161	PRO
20	AY	162	VAL
20	AY	203	GLU
20	AY	266	ASN
20	AY	341	VAL
20	AY	437	THR
20	AY	466	LEU
20	AY	505	GLY
20	AY	565	VAL
20	AY	568	TYR
20	AY	654	GLY
20	AY	664	GLN
20	AY	675	HIS
25	BC	15	VAL
25	BC	18	ASN
25	BC	34	ALA
25	BC	57	GLN
25	BC	59	VAL
25	BC	65	LEU
25	BC	67	HIS

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Mol	Chain	Res	Type
25	BC	81	GLY
25	BC	97	GLY
25	BC	118	PRO
25	BC	142	LYS
25	BC	213	VAL
25	BC	217	THR
25	BC	222	SER
25	BC	225	ILE
26	BD	38	LYS
26	BD	68	LYS
26	BD	78	LYS
26	BD	79	VAL
26	BD	90	ALA
26	BD	127	VAL
26	BD	165	ILE
26	BD	228	PRO
26	BD	237	GLU
26	BD	259	THR
27	BE	11	MET
27	BE	34	VAL
27	BE	124	GLY
27	BE	128	SER
27	BE	203	LYS
28	BF	5	ALA
28	BF	8	GLN
28	BF	23	ASP
28	BF	84	VAL
28	BF	104	LYS
28	BF	190	GLU
28	BF	192	LEU
29	BG	82	LEU
30	BH	71	LEU
30	BH	101	ARG
30	BH	165	ALA
30	BH	175	LYS
32	BK	3	LYS
32	BK	76	TYR
32	BK	121	GLU
33	BN	18	ALA
33	BN	37	LYS
33	BN	45	ASN
33	BN	54	VAL

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Mol	Chain	Res	Type
33	BN	57	ALA
33	BN	75	TYR
33	BN	79	PRO
33	BN	89	LYS
33	BN	96	GLU
33	BN	100	GLU
33	BN	104	LYS
33	BN	113	GLY
33	BN	126	PRO
33	BN	136	GLU
34	BO	5	GLN
34	BO	24	VAL
35	BP	17	LYS
35	BP	22	GLY
35	BP	28	GLY
35	BP	31	ALA
35	BP	50	ARG
35	BP	64	LYS
35	BP	71	VAL
36	BQ	27	VAL
36	BQ	54	MET
36	BQ	59	ARG
36	BQ	90	VAL
36	BQ	92	GLY
37	BR	6	SER
37	BR	102	GLU
37	BR	116	LEU
38	BS	14	VAL
38	BS	23	ARG
38	BS	96	GLY
38	BS	104	GLY
38	BS	105	ALA
39	BT	3	ARG
39	BT	28	VAL
39	BT	32	TYR
39	BT	35	LYS
39	BT	50	ILE
39	BT	59	THR
39	BT	86	ILE
39	BT	104	ASN
40	BU	92	ARG
41	BV	43	GLU

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Mol	Chain	Res	Type
41	BV	50	PRO
41	BV	55	ALA
41	BV	68	LYS
42	BW	12	ILE
44	BY	6	HIS
44	BY	41	GLY
44	BY	44	ILE
44	BY	77	PRO
44	BY	78	ALA
45	BZ	31	ARG
45	BZ	34	ASN
45	BZ	72	ARG
45	BZ	75	ASN
46	B0	84	LEU
47	B1	12	PRO
47	B1	15	ALA
47	B1	16	ASN
47	B1	21	ARG
47	B1	23	LYS
47	B1	64	ALA
47	B1	80	LEU
48	B2	43	GLN
48	B2	48	HIS
48	B2	49	LYS
51	B5	48	GLU
52	B6	49	HIS
54	B8	19	SER
54	B8	36	LYS
54	B8	49	VAL
56	Be	54	ALA
56	Be	80	ALA
56	Be	81	ILE
56	Be	92	LEU
1	CB	96	ARG
1	CB	230	VAL
2	CC	103	VAL
3	CD	20	TYR
3	CD	52	SER
3	CD	173	TRP
4	CE	27	ARG
5	CF	69	GLU
5	CF	70	ASP

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Mol	Chain	Res	Type
6	CG	114	ARG
7	CH	103	VAL
7	CH	109	ILE
8	CI	118	LYS
9	CJ	53	PRO
9	CJ	75	ILE
9	CJ	89	ASP
10	CK	88	GLY
10	CK	111	ASP
11	CL	35	GLY
11	CL	58	VAL
11	CL	91	LYS
11	CL	128	ALA
12	CM	10	PRO
12	CM	118	ALA
14	CO	47	LYS
15	CP	48	TRP
17	CR	37	VAL
17	CR	59	SER
18	CS	67	VAL
20	CY	5	VAL
20	CY	6	GLU
20	CY	90	PHE
20	CY	109	ASP
20	CY	123	ARG
20	CY	183	MET
20	CY	266	ASN
20	CY	271	LEU
20	CY	343	ASN
20	CY	347	GLY
20	CY	396	ARG
20	CY	416	LYS
20	CY	437	THR
20	CY	471	LYS
20	CY	502	GLY
20	CY	557	GLY
20	CY	565	VAL
20	CY	568	TYR
25	DC	35	THR
25	DC	37	LYS
25	DC	42	VAL
25	DC	72	GLN

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Mol	Chain	Res	Type
25	DC	75	VAL
25	DC	77	ALA
25	DC	81	GLY
25	DC	107	GLY
25	DC	115	VAL
25	DC	142	LYS
25	DC	162	ILE
25	DC	172	ILE
25	DC	222	SER
26	DD	24	ILE
26	DD	36	PRO
26	DD	43	ARG
26	DD	70	TRP
26	DD	79	VAL
26	DD	80	ALA
26	DD	125	ILE
26	DD	153	ALA
26	DD	222	ARG
27	DE	13	ARG
27	DE	61	ARG
27	DE	77	ILE
27	DE	86	PRO
27	DE	121	ASN
27	DE	128	SER
27	DE	129	HIS
27	DE	187	ALA
27	DE	204	ALA
28	DF	5	ALA
28	DF	8	GLN
28	DF	25	PRO
28	DF	46	ARG
29	DG	24	GLY
29	DG	87	PRO
30	DH	37	VAL
30	DH	41	MET
30	DH	67	LEU
30	DH	123	PHE
30	DH	155	SER
30	DH	165	ALA
30	DH	166	GLY
30	DH	176	ALA
32	DK	6	ALA

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Mol	Chain	Res	Type
32	DK	10	LEU
32	DK	30	HIS
32	DK	100	THR
32	DK	103	GLN
32	DK	105	LEU
33	DN	40	PRO
33	DN	42	TRP
33	DN	60	ILE
33	DN	71	ILE
33	DN	80	GLY
34	DO	14	THR
34	DO	69	ILE
35	DP	10	PRO
35	DP	11	GLY
35	DP	17	LYS
35	DP	45	LEU
35	DP	107	LYS
37	DR	72	ASP
37	DR	88	ARG
37	DR	101	ALA
38	DS	43	GLU
38	DS	100	ALA
39	DT	27	THR
39	DT	28	VAL
39	DT	31	SER
39	DT	50	ILE
39	DT	70	VAL
39	DT	107	ASP
40	DU	88	ILE
41	DV	19	LYS
41	DV	22	VAL
41	DV	44	LYS
41	DV	50	PRO
41	DV	78	LYS
41	DV	80	GLN
41	DV	100	ARG
42	DW	15	ARG
42	DW	44	ALA
42	DW	109	GLU
43	DX	4	ALA
43	DX	33	LYS
44	DY	41	GLY

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Mol	Chain	Res	Type
44	DY	63	LYS
44	DY	98	VAL
44	DY	107	ASP
45	DZ	5	LEU
45	DZ	76	LEU
45	DZ	81	ARG
45	DZ	90	VAL
45	DZ	95	PRO
45	DZ	151	HIS
47	D1	12	PRO
47	D1	20	ARG
47	D1	21	ARG
47	D1	23	LYS
47	D1	41	ARG
47	D1	52	ARG
47	D1	55	GLY
48	D2	48	HIS
49	D3	52	HIS
50	D4	7	PRO
50	D4	33	VAL
51	D5	48	GLU
51	D5	56	LYS
52	D6	9	LEU
52	D6	48	VAL
53	D7	3	ARG
53	D7	7	PRO
54	D8	6	THR
54	D8	28	GLY
54	D8	30	ARG
54	D8	48	PHE
56	De	62	VAL
56	De	65	LYS
56	De	80	ALA
56	De	81	ILE
1	AB	8	LYS
1	AB	77	ALA
1	AB	206	ASP
2	AC	6	HIS
2	AC	10	PHE
2	AC	56	ASP
2	AC	91	LEU
2	AC	109	PRO

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Mol	Chain	Res	Type
2	AC	112	SER
2	AC	181	ASN
3	AD	4	TYR
3	AD	27	TYR
3	AD	37	PRO
3	AD	110	PHE
3	AD	165	MET
3	AD	173	TRP
3	AD	181	MET
5	AF	51	PRO
8	AI	127	LYS
9	AJ	42	THR
9	AJ	55	LYS
9	AJ	83	GLU
9	AJ	94	VAL
10	AK	36	ASP
10	AK	102	GLY
11	AL	13	LYS
11	AL	14	GLY
11	AL	19	ARG
11	AL	35	GLY
11	AL	48	PRO
11	AL	51	ALA
11	AL	60	LEU
11	AL	107	ALA
11	AL	115	LYS
12	AM	39	ILE
15	AP	83	GLU
16	AQ	14	LYS
16	AQ	67	LYS
17	AR	58	LEU
18	AS	11	VAL
18	AS	66	MET
18	AS	68	GLY
18	AS	77	THR
19	AT	90	GLN
19	AT	95	ALA
20	AY	6	GLU
20	AY	147	TRP
20	AY	193	GLY
20	AY	405	PRO
20	AY	433	GLU

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Mol	Chain	Res	Type
20	AY	516	PRO
20	AY	535	PRO
20	AY	536	LYS
20	AY	539	ILE
20	AY	638	GLY
25	BC	39	ASP
25	BC	61	GLY
25	BC	167	ASP
25	BC	170	GLY
25	BC	175	PRO
25	BC	215	VAL
25	BC	224	ARG
26	BD	3	VAL
26	BD	9	TYR
26	BD	27	THR
26	BD	36	PRO
26	BD	52	ARG
26	BD	55	GLY
26	BD	80	ALA
26	BD	88	ARG
26	BD	144	ALA
26	BD	200	ASP
26	BD	239	ARG
26	BD	274	ARG
26	BD	275	LYS
27	BE	187	ALA
28	BF	72	ARG
28	BF	89	VAL
28	BF	151	SER
28	BF	171	PRO
29	BG	12	TYR
29	BG	146	TYR
29	BG	151	ALA
30	BH	155	SER
30	BH	156	ALA
32	BK	63	ARG
32	BK	89	HIS
33	BN	24	GLY
33	BN	26	LEU
33	BN	74	ARG
33	BN	87	LEU
33	BN	105	GLY

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Mol	Chain	Res	Type
33	BN	124	ALA
34	BO	6	THR
34	BO	64	ARG
35	BP	30	THR
35	BP	52	GLU
35	BP	67	MET
35	BP	141	ALA
36	BQ	4	PRO
36	BQ	14	ARG
36	BQ	82	ARG
36	BQ	135	ASP
37	BR	58	GLY
37	BR	105	ARG
38	BS	24	LEU
38	BS	56	LEU
38	BS	94	TYR
38	BS	108	GLY
39	BT	27	THR
39	BT	80	SER
40	BU	22	LYS
40	BU	36	ARG
41	BV	44	LYS
41	BV	80	GLN
42	BW	73	ALA
42	BW	80	PRO
43	BX	32	PRO
43	BX	62	LYS
44	BY	26	LYS
44	BY	48	ALA
44	BY	97	ARG
45	BZ	22	GLY
45	BZ	73	GLN
45	BZ	93	ASP
45	BZ	95	PRO
45	BZ	168	GLU
46	B0	19	LYS
47	B1	43	TYR
47	B1	87	PRO
48	B2	17	SER
50	B4	7	PRO
52	B6	31	PRO
54	B8	6	THR

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Mol	Chain	Res	Type
54	B8	51	ALA
54	B8	53	PRO
56	Be	52	ALA
56	Be	110	GLU
1	CB	17	PHE
1	CB	157	ARG
1	CB	164	VAL
1	CB	166	ASP
1	CB	210	SER
2	CC	10	PHE
2	CC	35	GLU
2	CC	102	ASN
2	CC	110	ASN
2	CC	112	SER
2	CC	158	GLY
2	CC	181	ASN
3	CD	47	ARG
3	CD	189	PRO
4	CE	10	MET
4	CE	12	LEU
5	CF	34	GLY
5	CF	54	LYS
5	CF	93	SER
6	CG	6	ARG
6	CG	14	PRO
6	CG	15	ASP
6	CG	82	GLY
7	CH	72	PRO
8	CI	24	GLY
8	CI	115	GLY
9	CJ	32	ALA
10	CK	15	ALA
10	CK	35	PRO
10	CK	42	TRP
10	CK	124	LYS
10	CK	126	ARG
11	CL	46	LYS
11	CL	55	VAL
11	CL	65	GLU
11	CL	92	ASP
11	CL	98	TYR
11	CL	107	ALA

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Mol	Chain	Res	Type
12	CM	101	GLN
12	CM	106	ASN
12	CM	121	LYS
14	CO	16	ALA
15	CP	66	PRO
16	CQ	12	SER
18	CS	80	TYR
20	CY	25	LYS
20	CY	91	THR
20	CY	116	PRO
20	CY	162	VAL
20	CY	175	SER
20	CY	257	PRO
20	CY	285	ASP
20	CY	345	THR
20	CY	353	ALA
20	CY	415	PRO
20	CY	436	PRO
20	CY	448	GLN
20	CY	539	ILE
20	CY	614	GLU
20	CY	628	ARG
20	CY	654	GLY
25	DC	18	ASN
25	DC	21	TYR
25	DC	38	PHE
25	DC	59	VAL
25	DC	117	THR
25	DC	145	THR
25	DC	161	ARG
25	DC	167	ASP
25	DC	175	PRO
25	DC	178	LYS
25	DC	179	ALA
25	DC	224	ARG
26	DD	25	THR
26	DD	28	GLU
26	DD	89	SER
26	DD	144	ALA
27	DE	22	PRO
27	DE	43	GLY
27	DE	138	PRO

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Mol	Chain	Res	Type
27	DE	177	PRO
27	DE	192	ASN
28	DF	12	LEU
28	DF	26	ALA
28	DF	60	SER
28	DF	73	ALA
28	DF	151	SER
28	DF	155	LEU
29	DG	32	PRO
29	DG	82	LEU
29	DG	84	LYS
29	DG	86	MET
30	DH	21	PRO
30	DH	47	GLU
30	DH	134	SER
30	DH	137	ASP
30	DH	173	PRO
32	DK	91	PRO
33	DN	41	ASP
33	DN	100	GLU
33	DN	111	PRO
33	DN	117	PHE
33	DN	121	LYS
33	DN	136	GLU
34	DO	28	SER
34	DO	52	VAL
35	DP	39	LYS
35	DP	64	LYS
35	DP	106	LEU
36	DQ	4	PRO
37	DR	6	SER
37	DR	40	LYS
37	DR	92	GLY
37	DR	103	ARG
37	DR	104	ARG
38	DS	57	LYS
38	DS	59	LYS
38	DS	61	ASN
39	DT	3	ARG
39	DT	48	ILE
39	DT	87	ASP
39	DT	137	LYS

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Mol	Chain	Res	Type
40	DU	30	LYS
42	DW	12	ILE
42	DW	14	PRO
42	DW	25	ARG
42	DW	61	ASN
42	DW	80	PRO
43	DX	32	PRO
43	DX	72	LYS
44	DY	27	VAL
44	DY	78	ALA
44	DY	80	GLY
45	DZ	30	ASN
45	DZ	75	ASN
45	DZ	78	LYS
45	DZ	135	GLU
45	DZ	168	GLU
45	DZ	177	PRO
46	D0	33	ALA
46	D0	73	GLY
47	D1	17	SER
48	D2	49	LYS
49	D3	16	PRO
50	D4	4	GLY
51	D5	58	LEU
52	D6	15	GLU
53	D7	23	ARG
54	D8	18	ALA
54	D8	47	LYS
55	D9	11	CYS
56	De	54	ALA
56	De	60	PHE
56	De	93	ALA
1	AB	86	GLU
1	AB	130	ARG
1	AB	153	ARG
2	AC	35	GLU
2	AC	47	LEU
2	AC	48	TYR
2	AC	49	SER
2	AC	108	ASN
3	AD	29	PRO
3	AD	34	GLU

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Mol	Chain	Res	Type
3	AD	134	ASP
5	AF	12	PRO
6	AG	69	VAL
7	AH	87	SER
7	AH	89	PRO
7	AH	103	VAL
8	AI	119	ALA
9	AJ	23	ILE
9	AJ	37	PRO
11	AL	47	LYS
11	AL	53	ARG
11	AL	91	LYS
12	AM	11	ARG
12	AM	118	ALA
12	AM	121	LYS
16	AQ	81	ARG
20	AY	74	TRP
20	AY	239	GLU
20	AY	262	SER
20	AY	380	LEU
20	AY	403	GLU
20	AY	416	LYS
20	AY	579	GLU
20	AY	604	PRO
20	AY	681	LYS
25	BC	51	ASP
25	BC	60	ARG
25	BC	171	ALA
25	BC	176	VAL
26	BD	101	GLU
26	BD	108	PRO
26	BD	126	GLN
26	BD	147	LEU
26	BD	231	HIS
26	BD	244	ARG
27	BE	54	GLN
27	BE	86	PRO
27	BE	88	GLY
27	BE	189	PRO
27	BE	193	GLY
28	BF	9	ILE
28	BF	58	ALA

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Mol	Chain	Res	Type
28	BF	149	ASP
28	BF	155	LEU
29	BG	111	LEU
30	BH	13	LYS
30	BH	37	VAL
30	BH	42	ARG
32	BK	16	LYS
32	BK	91	PRO
32	BK	102	GLU
34	BO	15	GLY
35	BP	39	LYS
35	BP	145	PRO
36	BQ	20	ALA
36	BQ	52	VAL
37	BR	28	LEU
37	BR	71	GLN
38	BS	15	ARG
38	BS	67	ARG
39	BT	24	PRO
39	BT	91	ARG
39	BT	93	ARG
40	BU	5	LYS
40	BU	93	LYS
41	BV	38	LEU
42	BW	44	ALA
42	BW	65	LEU
43	BX	4	ALA
44	BY	11	ASP
44	BY	47	LYS
44	BY	63	LYS
44	BY	102	CYS
47	B1	28	GLY
47	B1	65	SER
48	B2	10	LEU
50	B4	16	CYS
51	B5	56	LYS
54	B8	20	GLY
54	B8	39	LYS
54	B8	64	TYR
2	CC	5	ILE
2	CC	12	LEU
2	CC	13	GLY

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Mol	Chain	Res	Type
2	CC	29	TYR
2	CC	109	PRO
3	CD	34	GLU
3	CD	37	PRO
3	CD	167	GLY
3	CD	180	GLY
4	CE	11	ILE
4	CE	79	GLU
5	CF	96	PRO
6	CG	10	ARG
6	CG	69	VAL
6	CG	71	PRO
6	CG	72	ARG
7	CH	31	PHE
9	CJ	29	ARG
10	CK	44	SER
10	CK	113	PRO
11	CL	38	THR
11	CL	42	THR
11	CL	64	TYR
12	CM	39	ILE
12	CM	124	PRO
13	CN	3	ARG
16	CQ	68	ARG
16	CQ	81	ARG
19	CT	95	ALA
20	CY	78	ARG
20	CY	135	PHE
20	CY	191	ASP
20	CY	224	ASP
20	CY	273	LEU
20	CY	397	VAL
20	CY	479	PRO
20	CY	503	GLY
20	CY	508	GLY
20	CY	516	PRO
20	CY	573	HIS
20	CY	637	ARG
20	CY	653	PHE
25	DC	16	ASP
25	DC	34	ALA
25	DC	65	LEU

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Mol	Chain	Res	Type
25	DC	86	GLU
25	DC	113	ALA
25	DC	215	VAL
26	DD	68	LYS
26	DD	78	LYS
26	DD	198	ASN
26	DD	239	ARG
26	DD	244	ARG
27	DE	16	ARG
27	DE	70	ALA
27	DE	83	ASP
27	DE	98	PRO
27	DE	152	LYS
28	DF	67	GLN
28	DF	71	GLY
28	DF	165	ARG
29	DG	105	LYS
33	DN	53	VAL
33	DN	104	LYS
33	DN	120	LEU
34	DO	30	ALA
34	DO	64	ARG
34	DO	74	GLY
36	DQ	14	ARG
36	DQ	87	LYS
37	DR	15	SER
37	DR	102	GLU
37	DR	116	LEU
38	DS	22	GLY
39	DT	26	ASP
39	DT	35	LYS
42	DW	75	TYR
43	DX	41	ASN
43	DX	67	GLY
44	DY	3	VAL
44	DY	77	PRO
45	DZ	143	GLY
47	D1	10	LYS
47	D1	32	LYS
47	D1	44	PRO
47	D1	53	VAL
47	D1	87	PRO

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Mol	Chain	Res	Type
48	D2	17	SER
51	D5	4	HIS
51	D5	7	PRO
51	D5	23	HIS
51	D5	29	THR
51	D5	53	ALA
52	D6	18	ARG
52	D6	27	LYS
53	D7	9	ARG
55	D9	3	VAL
56	De	113	LYS
1	AB	131	PRO
2	AC	68	VAL
2	AC	103	VAL
2	AC	114	PRO
2	AC	192	THR
2	AC	193	TYR
3	AD	28	SER
3	AD	189	PRO
9	AJ	32	ALA
10	AK	43	SER
10	AK	118	GLY
11	AL	92	ASP
13	AN	13	THR
17	AR	28	GLU
17	AR	77	GLY
18	AS	43	GLU
18	AS	80	TYR
19	AT	10	LEU
20	AY	88	VAL
20	AY	199	ILE
20	AY	257	PRO
20	AY	263	ALA
20	AY	314	PHE
20	AY	342	TYR
20	AY	348	ARG
20	AY	598	ASP
25	BC	76	LEU
25	BC	130	ARG
25	BC	172	ILE
25	BC	184	GLU
26	BD	28	GLU

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Mol	Chain	Res	Type
26	BD	160	GLY
27	BE	141	ILE
28	BF	13	SER
28	BF	127	GLU
29	BG	44	GLY
29	BG	49	ASP
29	BG	167	GLU
30	BH	61	HIS
32	BK	30	HIS
32	BK	112	MET
32	BK	116	ASN
33	BN	108	PRO
33	BN	128	HIS
34	BO	96	THR
35	BP	78	PRO
35	BP	147	LEU
36	BQ	18	LYS
39	BT	82	LEU
39	BT	87	ASP
39	BT	88	ILE
40	BU	30	LYS
40	BU	88	ILE
42	BW	14	PRO
42	BW	61	ASN
42	BW	63	ASP
43	BX	11	PRO
44	BY	79	CYS
45	BZ	74	VAL
45	BZ	159	PRO
45	BZ	165	VAL
46	B0	11	ARG
47	B1	34	THR
47	B1	37	ILE
51	B5	4	HIS
51	B5	54	GLY
52	B6	19	ARG
53	B7	9	ARG
54	B8	30	ARG
54	B8	61	LEU
55	B9	3	VAL
56	Be	61	ASP
3	CD	5	ILE

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Mol	Chain	Res	Type
3	CD	40	PRO
3	CD	135	LEU
3	CD	197	PRO
4	CE	22	GLY
6	CG	34	GLY
7	CH	27	PRO
7	CH	35	ILE
7	CH	74	PRO
8	CI	127	LYS
10	CK	36	ASP
10	CK	55	LYS
11	CL	25	PRO
11	CL	50	SER
11	CL	54	LYS
11	CL	60	LEU
11	CL	115	LYS
12	CM	115	LYS
12	CM	116	THR
13	CN	13	THR
16	CQ	82	MET
17	CR	58	LEU
19	CT	34	LYS
20	CY	286	ILE
20	CY	301	ILE
20	CY	341	VAL
20	CY	390	VAL
20	CY	537	GLU
20	CY	597	GLY
20	CY	604	PRO
20	CY	635	GLU
20	CY	681	LYS
25	DC	20	VAL
25	DC	36	ALA
25	DC	51	ASP
25	DC	54	ARG
25	DC	94	TYR
25	DC	210	LEU
25	DC	214	TYR
26	DD	55	GLY
26	DD	100	GLY
26	DD	123	ALA
27	DE	119	ARG

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Mol	Chain	Res	Type
27	DE	135	HIS
29	DG	3	LEU
29	DG	142	PRO
30	DH	108	GLY
32	DK	55	VAL
32	DK	81	ALA
32	DK	101	TRP
32	DK	112	MET
33	DN	27	ALA
33	DN	58	ASP
33	DN	75	TYR
33	DN	126	PRO
35	DP	28	GLY
35	DP	34	GLY
35	DP	49	ARG
35	DP	52	GLU
35	DP	70	GLN
36	DQ	27	VAL
36	DQ	127	ILE
37	DR	117	VAL
39	DT	85	LYS
39	DT	86	ILE
40	DU	93	LYS
41	DV	16	PRO
41	DV	55	ALA
43	DX	7	VAL
43	DX	62	LYS
44	DY	7	VAL
44	DY	48	ALA
44	DY	70	SER
44	DY	79	CYS
44	DY	103	GLY
45	DZ	40	ASP
45	DZ	166	SER
51	D5	24	ALA
52	D6	33	LYS
53	D7	40	TRP
54	D8	51	ALA
56	De	67	ALA
1	AB	226	ARG
6	AG	15	ASP
10	AK	78	GLN

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Mol	Chain	Res	Type
11	AL	18	VAL
15	AP	63	GLY
18	AS	45	VAL
25	BC	75	VAL
25	BC	138	LEU
25	BC	139	PRO
26	BD	29	PRO
26	BD	241	PRO
27	BE	30	PRO
27	BE	83	ASP
28	BF	71	GLY
32	BK	86	LYS
33	BN	111	PRO
33	BN	134	ARG
37	BR	61	HIS
37	BR	93	GLY
39	BT	12	SER
39	BT	49	VAL
39	BT	70	VAL
43	BX	74	PRO
45	BZ	82	ARG
45	BZ	128	VAL
47	B1	66	HIS
49	B3	57	GLU
50	B4	10	VAL
51	B5	7	PRO
52	B6	27	LYS
53	B7	44	PRO
3	CD	171	GLY
6	CG	88	PRO
8	CI	22	GLY
9	CJ	82	ILE
10	CK	107	SER
11	CL	40	VAL
11	CL	80	HIS
20	CY	172	ASP
20	CY	288	PRO
20	CY	498	ILE
25	DC	114	VAL
25	DC	118	PRO
25	DC	140	ASN
25	DC	143	ALA

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Mol	Chain	Res	Type
25	DC	218	THR
26	DD	219	PRO
28	DF	61	GLY
30	DH	177	GLY
32	DK	63	ARG
33	DN	79	PRO
33	DN	105	GLY
34	DO	3	GLN
35	DP	148	LEU
39	DT	49	VAL
39	DT	91	ARG
40	DU	76	TYR
41	DV	29	PRO
41	DV	41	GLY
43	DX	39	ILE
44	DY	9	LYS
44	DY	101	LYS
45	DZ	93	ASP
45	DZ	146	ILE
47	D1	38	SER
55	D9	10	ILE
1	AB	127	ILE
2	AC	70	VAL
2	AC	148	GLY
3	AD	44	GLY
3	AD	88	VAL
3	AD	133	VAL
6	AG	14	PRO
11	AL	110	VAL
20	AY	15	ILE
20	AY	143	GLY
25	BC	146	VAL
25	BC	223	VAL
26	BD	271	ILE
30	BH	141	VAL
30	BH	173	PRO
34	BO	35	VAL
36	BQ	94	VAL
37	BR	117	VAL
38	BS	85	VAL
43	BX	7	VAL
44	BY	18	GLY

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Mol	Chain	Res	Type
45	BZ	15	PRO
56	Be	68	GLY
7	CH	73	ASP
10	CK	45	GLY
11	CL	45	PRO
11	CL	125	PRO
13	CN	28	GLY
20	CY	258	VAL
20	CY	638	GLY
20	CY	665	GLY
28	DF	178	PRO
29	DG	89	GLY
30	DH	141	VAL
43	DX	86	GLY
45	DZ	22	GLY
45	DZ	83	PRO
45	DZ	108	PRO
51	D5	57	VAL
56	De	53	PRO
2	AC	81	GLY
3	AD	167	GLY
4	AE	67	VAL
5	AF	56	PRO
9	AJ	49	VAL
12	AM	4	ILE
12	AM	10	PRO
20	AY	308	PRO
20	AY	397	VAL
25	BC	50	ILE
26	BD	236	GLY
32	BK	21	PRO
33	BN	53	VAL
34	BO	4	PRO
40	BU	73	GLY
41	BV	79	VAL
42	BW	76	VAL
1	CB	159	PRO
1	CB	194	PRO
2	CC	51	GLY
2	CC	70	VAL
10	CK	37	GLY
14	CO	23	GLY

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Mol	Chain	Res	Type
18	CS	72	GLY
25	DC	139	PRO
34	DO	48	PRO
41	DV	15	GLU
42	DW	112	GLY
43	DX	11	PRO
43	DX	54	VAL
54	D8	53	PRO
3	AD	142	PRO
6	AG	93	PRO
7	AH	51	VAL
8	AI	39	GLY
11	AL	82	VAL
15	AP	46	PRO
20	AY	303	PRO
27	BE	43	GLY
33	BN	71	ILE
35	BP	37	GLY
37	BR	106	GLY
40	BU	23	GLY
41	BV	72	VAL
44	BY	3	VAL
44	BY	10	GLY
45	BZ	177	PRO
1	CB	165	VAL
3	CD	142	PRO
4	CE	67	VAL
6	CG	13	GLN
11	CL	18	VAL
15	CP	30	GLY
15	CP	63	GLY
20	CY	398	ILE
25	DC	181	PHE
26	DD	51	VAL
26	DD	118	VAL
26	DD	223	GLY
28	DF	24	LEU
28	DF	173	VAL
30	DH	48	GLY
32	DK	140	GLY
33	DN	103	VAL
36	DQ	24	GLY

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Mol	Chain	Res	Type
37	DR	58	GLY
39	DT	24	PRO
43	DX	52	VAL
7	AH	131	GLY
11	AL	87	GLY
20	AY	269	VAL
36	BQ	132	VAL
39	BT	20	PRO
1	CB	229	VAL
2	CC	145	GLY
5	CF	26	ILE
27	DE	59	VAL
28	DF	86	GLY
29	DG	68	PRO
35	DP	69	GLY
39	DT	34	VAL
50	D4	11	PRO
54	D8	20	GLY
56	De	121	VAL
7	AH	35	ILE
7	AH	101	PRO
9	AJ	93	GLY
12	AM	117	VAL
20	AY	415	PRO
1	CB	228	GLY
5	CF	72	VAL
7	CH	89	PRO
20	CY	559	PRO
28	DF	14	PRO
35	DP	9	ASN
38	DS	90	GLY
43	DX	94	GLY
45	DZ	165	VAL
51	D5	54	GLY
35	DP	48	PRO
32	DK	22	PRO
27	BE	147	PRO
35	BP	48	PRO

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	
1	AB	203/203 (100%)	163 (80%)	40 (20%)	1	9
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1	6
2	AC	161/161 (100%)	129 (80%)	32 (20%)	1	9
2	CC	161/161 (100%)	128 (80%)	33 (20%)	1	8
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1	8
3	CD	180/180 (100%)	148 (82%)	32 (18%)	2	12
4	AE	116/116 (100%)	92 (79%)	24 (21%)	1	8
4	CE	116/116 (100%)	89 (77%)	27 (23%)	1	5
5	AF	90/90 (100%)	73 (81%)	17 (19%)	1	10
5	CF	90/90 (100%)	77 (86%)	13 (14%)	3	20
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5	26
6	CG	126/126 (100%)	110 (87%)	16 (13%)	4	23
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	13
7	CH	119/119 (100%)	94 (79%)	25 (21%)	1	8
8	AI	98/98 (100%)	83 (85%)	15 (15%)	2	17
8	CI	98/98 (100%)	78 (80%)	20 (20%)	1	8
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	9
9	CJ	89/89 (100%)	68 (76%)	21 (24%)	1	5
10	AK	90/90 (100%)	80 (89%)	10 (11%)	6	29
10	CK	90/90 (100%)	79 (88%)	11 (12%)	5	25
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	7
11	CL	104/104 (100%)	82 (79%)	22 (21%)	1	7
12	AM	100/100 (100%)	84 (84%)	16 (16%)	2	16
12	CM	100/100 (100%)	79 (79%)	21 (21%)	1	8
13	AN	49/49 (100%)	40 (82%)	9 (18%)	1	11
13	CN	49/49 (100%)	38 (78%)	11 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	61 (77%)	18 (23%)	1	6
14	CO	79/79 (100%)	68 (86%)	11 (14%)	3	21
15	AP	72/72 (100%)	68 (94%)	4 (6%)	21	52
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	15
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	2	17
16	CQ	95/95 (100%)	81 (85%)	14 (15%)	3	19
17	AR	61/61 (100%)	49 (80%)	12 (20%)	1	9
17	CR	61/61 (100%)	54 (88%)	7 (12%)	5	27
18	AS	69/69 (100%)	52 (75%)	17 (25%)	0	5
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	6
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	17
19	CT	76/76 (100%)	58 (76%)	18 (24%)	1	5
20	AY	558/579 (96%)	450 (81%)	108 (19%)	1	9
20	CY	558/579 (96%)	446 (80%)	112 (20%)	1	9
25	BC	180/180 (100%)	130 (72%)	50 (28%)	0	3
25	DC	180/180 (100%)	146 (81%)	34 (19%)	1	10
26	BD	217/217 (100%)	182 (84%)	35 (16%)	2	16
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	8
27	BE	165/165 (100%)	134 (81%)	31 (19%)	1	10
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	6
28	BF	165/165 (100%)	129 (78%)	36 (22%)	1	7
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	9
29	BG	155/155 (100%)	140 (90%)	15 (10%)	8	33
29	DG	155/155 (100%)	131 (84%)	24 (16%)	2	17
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	11
30	DH	136/136 (100%)	117 (86%)	19 (14%)	3	21
32	BK	105/105 (100%)	77 (73%)	28 (27%)	0	3
32	DK	105/105 (100%)	81 (77%)	24 (23%)	1	6
33	BN	118/118 (100%)	88 (75%)	30 (25%)	0	4
33	DN	118/118 (100%)	84 (71%)	34 (29%)	0	2
34	BO	100/100 (100%)	79 (79%)	21 (21%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	DO	100/100 (100%)	82 (82%)	18 (18%)	1 12
35	BP	112/112 (100%)	84 (75%)	28 (25%)	0 4
35	DP	112/112 (100%)	88 (79%)	24 (21%)	1 7
36	BQ	111/111 (100%)	78 (70%)	33 (30%)	0 2
36	DQ	111/111 (100%)	91 (82%)	20 (18%)	1 12
37	BR	100/100 (100%)	82 (82%)	18 (18%)	1 12
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1 7
38	BS	77/77 (100%)	64 (83%)	13 (17%)	2 14
38	DS	77/77 (100%)	58 (75%)	19 (25%)	0 5
39	BT	120/120 (100%)	93 (78%)	27 (22%)	1 6
39	DT	120/120 (100%)	91 (76%)	29 (24%)	0 5
40	BU	93/93 (100%)	78 (84%)	15 (16%)	2 16
40	DU	93/93 (100%)	76 (82%)	17 (18%)	1 11
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0 3
41	DV	82/82 (100%)	68 (83%)	14 (17%)	2 14
42	BW	92/92 (100%)	79 (86%)	13 (14%)	3 21
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1 7
43	BX	75/75 (100%)	58 (77%)	17 (23%)	1 6
43	DX	75/75 (100%)	59 (79%)	16 (21%)	1 7
44	BY	88/88 (100%)	65 (74%)	23 (26%)	0 4
44	DY	88/88 (100%)	74 (84%)	14 (16%)	2 16
45	BZ	162/162 (100%)	127 (78%)	35 (22%)	1 7
45	DZ	162/162 (100%)	135 (83%)	27 (17%)	2 15
46	B0	66/66 (100%)	59 (89%)	7 (11%)	6 30
46	D0	66/66 (100%)	53 (80%)	13 (20%)	1 9
47	B1	78/78 (100%)	56 (72%)	22 (28%)	0 2
47	D1	78/78 (100%)	57 (73%)	21 (27%)	0 3
48	B2	66/66 (100%)	56 (85%)	10 (15%)	3 18
48	D2	66/66 (100%)	57 (86%)	9 (14%)	3 22
49	B3	52/52 (100%)	44 (85%)	8 (15%)	2 17
49	D3	52/52 (100%)	45 (86%)	7 (14%)	4 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	B4	31/31 (100%)	23 (74%)	8 (26%)	0 4
50	D4	31/31 (100%)	22 (71%)	9 (29%)	0 2
51	B5	51/51 (100%)	38 (74%)	13 (26%)	0 4
51	D5	51/51 (100%)	45 (88%)	6 (12%)	5 26
52	B6	49/49 (100%)	35 (71%)	14 (29%)	0 2
52	D6	49/49 (100%)	31 (63%)	18 (37%)	0 0
53	B7	42/42 (100%)	35 (83%)	7 (17%)	2 15
53	D7	42/42 (100%)	36 (86%)	6 (14%)	3 20
54	B8	54/54 (100%)	45 (83%)	9 (17%)	2 15
54	D8	54/54 (100%)	42 (78%)	12 (22%)	1 6
55	B9	34/34 (100%)	26 (76%)	8 (24%)	1 5
55	D9	34/34 (100%)	31 (91%)	3 (9%)	10 38
56	Be	54/54 (100%)	48 (89%)	6 (11%)	6 29
56	De	54/54 (100%)	47 (87%)	7 (13%)	4 23
All	All	11130/11172 (100%)	8951 (80%)	2179 (20%)	1 9

All (2179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	8	LYS
1	AB	9	GLU
1	AB	15	VAL
1	AB	17	PHE
1	AB	28	PHE
1	AB	33	TYR
1	AB	36	ARG
1	AB	63	MET
1	AB	64	ARG
1	AB	69	LEU
1	AB	87	ARG
1	AB	96	ARG
1	AB	101	MET
1	AB	103	THR
1	AB	111	ARG
1	AB	113	HIS
1	AB	137	ARG
1	AB	140	HIS

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Mol	Chain	Res	Type
1	AB	144	ARG
1	AB	146	GLN
1	AB	154	LEU
1	AB	155	LEU
1	AB	158	LEU
1	AB	162	ILE
1	AB	165	VAL
1	AB	166	ASP
1	AB	172	ILE
1	AB	176	GLU
1	AB	185	ILE
1	AB	191	ASP
1	AB	195	ASP
1	AB	196	LEU
1	AB	200	ILE
1	AB	205	ASP
1	AB	215	LEU
1	AB	216	SER
1	AB	221	LEU
1	AB	222	ILE
1	AB	230	VAL
1	AB	239	VAL
2	AC	6	HIS
2	AC	8	ILE
2	AC	15	THR
2	AC	20	SER
2	AC	22	TRP
2	AC	26	LYS
2	AC	29	TYR
2	AC	31	HIS
2	AC	34	LEU
2	AC	46	GLU
2	AC	55	VAL
2	AC	69	HIS
2	AC	70	VAL
2	AC	76	VAL
2	AC	79	ARG
2	AC	90	GLU
2	AC	105	GLU
2	AC	107	GLN
2	AC	115	LEU
2	AC	124	ILE

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Mol	Chain	Res	Type
2	AC	125	GLU
2	AC	128	PHE
2	AC	134	ILE
2	AC	139	GLN
2	AC	156	ARG
2	AC	167	TRP
2	AC	173	VAL
2	AC	176	HIS
2	AC	177	THR
2	AC	179	ARG
2	AC	188	LEU
2	AC	204	LEU
3	AD	8	VAL
3	AD	10	ARG
3	AD	12	CYS
3	AD	24	GLU
3	AD	28	SER
3	AD	33	MET
3	AD	35	ARG
3	AD	36	ARG
3	AD	42	GLN
3	AD	43	HIS
3	AD	45	GLN
3	AD	49	ARG
3	AD	50	ARG
3	AD	53	ASP
3	AD	54	TYR
3	AD	56	VAL
3	AD	60	GLU
3	AD	61	LYS
3	AD	65	ARG
3	AD	67	ILE
3	AD	72	GLU
3	AD	79	PHE
3	AD	86	LYS
3	AD	97	LEU
3	AD	101	LEU
3	AD	107	ARG
3	AD	114	ARG
3	AD	127	THR
3	AD	129	ASN
3	AD	138	TYR

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Mol	Chain	Res	Type
3	AD	156	GLU
3	AD	157	LEU
3	AD	173	TRP
3	AD	187	ARG
3	AD	196	LEU
3	AD	200	GLU
3	AD	206	PHE
3	AD	207	TYR
4	AE	12	LEU
4	AE	19	MET
4	AE	24	ARG
4	AE	31	LEU
4	AE	37	ARG
4	AE	41	VAL
4	AE	47	LYS
4	AE	60	TYR
4	AE	61	TYR
4	AE	64	ARG
4	AE	68	GLU
4	AE	69	VAL
4	AE	72	GLN
4	AE	78	HIS
4	AE	80	ILE
4	AE	81	GLU
4	AE	87	SER
4	AE	89	ILE
4	AE	91	LEU
4	AE	119	LEU
4	AE	120	THR
4	AE	125	SER
4	AE	137	GLU
4	AE	150	ARG
5	AF	1	MET
5	AF	10	LEU
5	AF	15	ASP
5	AF	22	GLU
5	AF	31	GLU
5	AF	40	VAL
5	AF	45	LEU
5	AF	46	ARG
5	AF	50	TYR
5	AF	52	ILE

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Mol	Chain	Res	Type
5	AF	55	ASP
5	AF	61	LEU
5	AF	74	ASP
5	AF	82	ARG
5	AF	89	MET
5	AF	91	VAL
5	AF	100	ASN
6	AG	5	ARG
6	AG	13	GLN
6	AG	20	ASP
6	AG	31	MET
6	AG	35	LYS
6	AG	36	LYS
6	AG	75	VAL
6	AG	79	ARG
6	AG	91	VAL
6	AG	97	GLN
6	AG	104	LEU
6	AG	122	HIS
6	AG	136	LYS
6	AG	149	ARG
6	AG	153	HIS
7	AH	10	LEU
7	AH	18	ARG
7	AH	26	VAL
7	AH	30	ARG
7	AH	31	PHE
7	AH	38	ILE
7	AH	39	LEU
7	AH	63	LEU
7	AH	77	GLU
7	AH	82	HIS
7	AH	83	ILE
7	AH	85	ARG
7	AH	95	VAL
7	AH	98	LYS
7	AH	102	ARG
7	AH	104	ARG
7	AH	107	LEU
7	AH	111	ILE
7	AH	120	THR
7	AH	137	VAL

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Mol	Chain	Res	Type
7	AH	138	TRP
8	AI	4	TYR
8	AI	10	ARG
8	AI	25	LYS
8	AI	35	GLU
8	AI	38	GLN
8	AI	79	LEU
8	AI	88	TYR
8	AI	89	ASN
8	AI	91	ASP
8	AI	93	ARG
8	AI	95	LYS
8	AI	104	ARG
8	AI	108	VAL
8	AI	118	LYS
8	AI	126	SER
9	AJ	6	ILE
9	AJ	8	LEU
9	AJ	13	HIS
9	AJ	14	LYS
9	AJ	16	LEU
9	AJ	22	LYS
9	AJ	33	GLN
9	AJ	40	LEU
9	AJ	47	PHE
9	AJ	55	LYS
9	AJ	57	LYS
9	AJ	58	ASP
9	AJ	70	ARG
9	AJ	74	ILE
9	AJ	79	ARG
9	AJ	81	THR
9	AJ	88	LEU
9	AJ	96	ILE
10	AK	14	VAL
10	AK	18	ARG
10	AK	38	ASN
10	AK	40	ILE
10	AK	42	TRP
10	AK	44	SER
10	AK	50	TYR
10	AK	57	THR

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Mol	Chain	Res	Type
10	AK	70	LYS
10	AK	104	GLN
11	AL	17	LYS
11	AL	18	VAL
11	AL	20	LYS
11	AL	33	ARG
11	AL	37	CYS
11	AL	42	THR
11	AL	43	VAL
11	AL	52	LEU
11	AL	53	ARG
11	AL	54	LYS
11	AL	55	VAL
11	AL	59	ARG
11	AL	66	VAL
11	AL	76	ASN
11	AL	77	LEU
11	AL	79	GLU
11	AL	80	HIS
11	AL	85	ILE
11	AL	93	LEU
11	AL	102	ARG
11	AL	104	VAL
11	AL	110	VAL
12	AM	12	ASN
12	AM	15	VAL
12	AM	16	ASP
12	AM	19	LEU
12	AM	21	TYR
12	AM	34	LEU
12	AM	48	LEU
12	AM	56	LEU
12	AM	57	ARG
12	AM	62	ASN
12	AM	81	LEU
12	AM	99	ARG
12	AM	108	ARG
12	AM	120	LYS
12	AM	125	ARG
12	AM	126	LYS
13	AN	16	PHE
13	AN	22	THR

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Mol	Chain	Res	Type
13	AN	25	VAL
13	AN	27	CYS
13	AN	29	ARG
13	AN	35	ARG
13	AN	40	CYS
13	AN	43	CYS
13	AN	61	TRP
14	AO	6	GLU
14	AO	13	GLN
14	AO	17	ARG
14	AO	25	THR
14	AO	26	GLU
14	AO	27	VAL
14	AO	35	ARG
14	AO	37	ASN
14	AO	39	LEU
14	AO	46	HIS
14	AO	47	LYS
14	AO	51	HIS
14	AO	58	MET
14	AO	64	ARG
14	AO	66	LEU
14	AO	71	GLN
14	AO	87	ILE
14	AO	88	ARG
15	AP	27	LYS
15	AP	44	THR
15	AP	72	ARG
15	AP	75	ARG
16	AQ	11	VAL
16	AQ	13	ASP
16	AQ	16	GLN
16	AQ	22	LEU
16	AQ	32	TYR
16	AQ	37	LYS
16	AQ	52	LYS
16	AQ	55	ASP
16	AQ	63	ARG
16	AQ	74	LEU
16	AQ	76	LEU
16	AQ	78	GLU
16	AQ	81	ARG

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Mol	Chain	Res	Type
16	AQ	89	LEU
16	AQ	101	ARG
17	AR	19	LYS
17	AR	23	LYS
17	AR	26	LEU
17	AR	34	TYR
17	AR	37	VAL
17	AR	38	GLU
17	AR	40	LEU
17	AR	44	LEU
17	AR	75	ILE
17	AR	81	PHE
17	AR	82	THR
17	AR	85	LEU
18	AS	5	LEU
18	AS	6	LYS
18	AS	16	LEU
18	AS	22	LEU
18	AS	23	ASN
18	AS	33	THR
18	AS	38	SER
18	AS	41	VAL
18	AS	43	GLU
18	AS	51	VAL
18	AS	57	HIS
18	AS	62	ILE
18	AS	63	THR
18	AS	66	MET
18	AS	71	LEU
18	AS	77	THR
18	AS	81	ARG
19	AT	13	LEU
19	AT	23	ARG
19	AT	26	ASN
19	AT	38	LYS
19	AT	42	GLN
19	AT	57	ARG
19	AT	62	LEU
19	AT	71	THR
19	AT	73	HIS
19	AT	74	LYS
19	AT	84	LEU

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Mol	Chain	Res	Type
19	AT	85	MET
20	AY	9	LEU
20	AY	15	ILE
20	AY	20	HIS
20	AY	26	THR
20	AY	31	ARG
20	AY	33	LEU
20	AY	34	TYR
20	AY	39	ILE
20	AY	72	CYS
20	AY	84	THR
20	AY	89	ASP
20	AY	90	PHE
20	AY	92	ILE
20	AY	98	MET
20	AY	117	GLN
20	AY	119	GLU
20	AY	123	ARG
20	AY	126	GLU
20	AY	132	ARG
20	AY	133	ILE
20	AY	140	ASP
20	AY	146	LEU
20	AY	152	THR
20	AY	153	MET
20	AY	156	ARG
20	AY	170	ARG
20	AY	174	PHE
20	AY	177	ILE
20	AY	178	ILE
20	AY	187	THR
20	AY	197	ARG
20	AY	199	ILE
20	AY	201	ILE
20	AY	203	GLU
20	AY	223	PHE
20	AY	225	GLU
20	AY	238	THR
20	AY	240	GLU
20	AY	241	GLU
20	AY	247	ARG
20	AY	255	ILE

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Mol	Chain	Res	Type
20	AY	260	LEU
20	AY	273	LEU
20	AY	277	VAL
20	AY	278	ASP
20	AY	286	ILE
20	AY	295	GLU
20	AY	300	GLU
20	AY	301	ILE
20	AY	317	MET
20	AY	328	ILE
20	AY	341	VAL
20	AY	344	THR
20	AY	348	ARG
20	AY	355	LEU
20	AY	356	LEU
20	AY	358	MET
20	AY	361	ASN
20	AY	381	LYS
20	AY	398	ILE
20	AY	406	GLU
20	AY	410	ASP
20	AY	420	ASP
20	AY	421	GLN
20	AY	425	SER
20	AY	428	LEU
20	AY	430	ARG
20	AY	431	LEU
20	AY	454	MET
20	AY	457	LEU
20	AY	461	ILE
20	AY	465	ARG
20	AY	481	VAL
20	AY	483	TYR
20	AY	487	ILE
20	AY	504	ARG
20	AY	510	VAL
20	AY	512	ILE
20	AY	523	PHE
20	AY	527	ASN
20	AY	534	ILE
20	AY	542	VAL
20	AY	543	GLN

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Mol	Chain	Res	Type
20	AY	550	MET
20	AY	556	ILE
20	AY	565	VAL
20	AY	567	LEU
20	AY	568	TYR
20	AY	569	ASP
20	AY	572	TYR
20	AY	576	ASP
20	AY	583	LYS
20	AY	588	MET
20	AY	616	TYR
20	AY	617	MET
20	AY	632	LEU
20	AY	635	GLU
20	AY	646	PHE
20	AY	647	VAL
20	AY	652	MET
20	AY	653	PHE
20	AY	657	THR
20	AY	671	MET
20	AY	676	TYR
20	AY	677	GLN
20	AY	679	VAL
20	AY	682	GLN
20	AY	685	GLU
25	BC	3	LYS
25	BC	4	HIS
25	BC	9	ARG
25	BC	12	LEU
25	BC	15	VAL
25	BC	31	LYS
25	BC	38	PHE
25	BC	39	ASP
25	BC	41	THR
25	BC	48	LEU
25	BC	50	ILE
25	BC	53	ARG
25	BC	54	ARG
25	BC	57	GLN
25	BC	59	VAL
25	BC	62	THR
25	BC	63	VAL

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Mol	Chain	Res	Type
25	BC	67	HIS
25	BC	86	GLU
25	BC	110	ASP
25	BC	114	VAL
25	BC	117	THR
25	BC	120	VAL
25	BC	128	LEU
25	BC	138	LEU
25	BC	146	VAL
25	BC	148	PHE
25	BC	150	ILE
25	BC	152	GLU
25	BC	154	ILE
25	BC	158	LYS
25	BC	161	ARG
25	BC	164	PHE
25	BC	165	ARG
25	BC	166	ASN
25	BC	167	ASP
25	BC	169	THR
25	BC	172	ILE
25	BC	173	HIS
25	BC	176	VAL
25	BC	178	LYS
25	BC	182	PRO
25	BC	193	PHE
25	BC	198	GLU
25	BC	201	LYS
25	BC	203	GLU
25	BC	206	LYS
25	BC	216	THR
25	BC	218	THR
25	BC	219	MET
26	BD	5	LYS
26	BD	10	THR
26	BD	14	ARG
26	BD	24	ILE
26	BD	25	THR
26	BD	26	LYS
26	BD	35	LYS
26	BD	37	LEU
26	BD	38	LYS

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Mol	Chain	Res	Type
26	BD	60	ARG
26	BD	63	ARG
26	BD	64	ILE
26	BD	65	ILE
26	BD	78	LYS
26	BD	82	ILE
26	BD	87	ASN
26	BD	96	HIS
26	BD	97	TYR
26	BD	105	ILE
26	BD	115	GLN
26	BD	131	LEU
26	BD	140	THR
26	BD	143	HIS
26	BD	161	THR
26	BD	165	ILE
26	BD	175	LEU
26	BD	177	LEU
26	BD	179	SER
26	BD	186	HIS
26	BD	190	TYR
26	BD	192	THR
26	BD	211	ARG
26	BD	221	VAL
26	BD	252	TRP
26	BD	260	ARG
27	BE	1	MET
27	BE	4	ILE
27	BE	9	VAL
27	BE	11	MET
27	BE	13	ARG
27	BE	26	ILE
27	BE	52	LEU
27	BE	54	GLN
27	BE	58	ARG
27	BE	61	ARG
27	BE	63	LEU
27	BE	67	PHE
27	BE	77	ILE
27	BE	78	LEU
27	BE	79	ARG
27	BE	89	ASP

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Mol	Chain	Res	Type
27	BE	93	VAL
27	BE	95	ILE
27	BE	107	THR
27	BE	113	PHE
27	BE	116	VAL
27	BE	121	ASN
27	BE	132	HIS
27	BE	137	HIS
27	BE	156	MET
27	BE	159	HIS
27	BE	160	TYR
27	BE	174	ASP
27	BE	197	ILE
27	BE	201	THR
27	BE	202	LYS
28	BF	2	LYS
28	BF	6	VAL
28	BF	7	TYR
28	BF	12	LEU
28	BF	17	ARG
28	BF	20	LEU
28	BF	23	ASP
28	BF	24	LEU
28	BF	45	ARG
28	BF	70	THR
28	BF	74	ARG
28	BF	89	VAL
28	BF	100	THR
28	BF	114	VAL
28	BF	120	GLU
28	BF	123	LEU
28	BF	125	LEU
28	BF	126	VAL
28	BF	132	VAL
28	BF	133	ASN
28	BF	139	PHE
28	BF	149	ASP
28	BF	154	VAL
28	BF	155	LEU
28	BF	156	LEU
28	BF	157	VAL
28	BF	158	THR

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Mol	Chain	Res	Type
28	BF	162	LEU
28	BF	168	ARG
28	BF	174	VAL
28	BF	175	THR
28	BF	190	GLU
28	BF	191	ARG
28	BF	192	LEU
28	BF	194	MET
28	BF	202	PHE
29	BG	9	ARG
29	BG	21	ARG
29	BG	26	GLN
29	BG	72	ARG
29	BG	79	ASN
29	BG	86	MET
29	BG	113	ARG
29	BG	125	PHE
29	BG	126	ASP
29	BG	133	LEU
29	BG	135	LEU
29	BG	137	GLU
29	BG	152	LEU
29	BG	155	MET
29	BG	161	THR
30	BH	17	VAL
30	BH	33	LEU
30	BH	34	GLU
30	BH	44	VAL
30	BH	49	VAL
30	BH	58	GLU
30	BH	70	THR
30	BH	83	TYR
30	BH	86	GLU
30	BH	88	LEU
30	BH	95	ARG
30	BH	104	GLU
30	BH	105	LEU
30	BH	107	VAL
30	BH	119	GLU
30	BH	121	ILE
30	BH	123	PHE
30	BH	127	GLU

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Mol	Chain	Res	Type
30	BH	129	THR
30	BH	132	ARG
30	BH	133	VAL
30	BH	136	ILE
30	BH	147	ASN
30	BH	163	TYR
30	BH	164	TYR
32	BK	4	VAL
32	BK	7	VAL
32	BK	9	LYS
32	BK	10	LEU
32	BK	16	LYS
32	BK	29	GLN
32	BK	33	ASN
32	BK	57	ILE
32	BK	59	ILE
32	BK	60	TYR
32	BK	65	PHE
32	BK	67	PHE
32	BK	71	THR
32	BK	78	ILE
32	BK	95	LYS
32	BK	103	GLN
32	BK	105	LEU
32	BK	106	GLU
32	BK	110	GLN
32	BK	115	LEU
32	BK	118	THR
32	BK	119	ASP
32	BK	120	LEU
32	BK	121	GLU
32	BK	126	MET
32	BK	130	SER
32	BK	132	ARG
32	BK	136	VAL
33	BN	4	TYR
33	BN	15	LEU
33	BN	30	ILE
33	BN	37	LYS
33	BN	38	HIS
33	BN	42	TRP
33	BN	45	ASN

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Mol	Chain	Res	Type
33	BN	48	MET
33	BN	51	PHE
33	BN	53	VAL
33	BN	55	VAL
33	BN	56	ASN
33	BN	59	LYS
33	BN	61	ARG
33	BN	71	ILE
33	BN	72	TYR
33	BN	78	TYR
33	BN	82	LEU
33	BN	84	LYS
33	BN	90	MET
33	BN	97	ARG
33	BN	99	LEU
33	BN	101	HIS
33	BN	103	VAL
33	BN	104	LYS
33	BN	107	LEU
33	BN	108	PRO
33	BN	115	ARG
33	BN	127	ASP
33	BN	133	GLN
34	BO	1	MET
34	BO	8	LEU
34	BO	21	CYS
34	BO	23	ARG
34	BO	29	ASN
34	BO	37	ASP
34	BO	56	ASP
34	BO	61	VAL
34	BO	70	LYS
34	BO	71	ARG
34	BO	78	ARG
34	BO	80	ASP
34	BO	82	ASN
34	BO	85	VAL
34	BO	88	ASN
34	BO	91	LEU
34	BO	104	ARG
34	BO	105	GLU
34	BO	114	ILE

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Mol	Chain	Res	Type
34	BO	117	LEU
34	BO	121	VAL
35	BP	7	ARG
35	BP	15	ARG
35	BP	16	ARG
35	BP	18	ARG
35	BP	19	VAL
35	BP	21	ARG
35	BP	39	LYS
35	BP	40	SER
35	BP	49	ARG
35	BP	50	ARG
35	BP	51	PHE
35	BP	55	ARG
35	BP	58	THR
35	BP	61	ARG
35	BP	74	GLU
35	BP	75	ILE
35	BP	85	LEU
35	BP	91	PHE
35	BP	101	VAL
35	BP	106	LEU
35	BP	112	LEU
35	BP	115	LEU
35	BP	123	LEU
35	BP	125	VAL
35	BP	130	PHE
35	BP	135	LEU
35	BP	144	GLU
35	BP	147	LEU
36	BQ	1	MET
36	BQ	3	MET
36	BQ	6	ARG
36	BQ	7	MET
36	BQ	9	TYR
36	BQ	14	ARG
36	BQ	16	ARG
36	BQ	42	ILE
36	BQ	43	THR
36	BQ	45	GLN
36	BQ	46	GLN
36	BQ	48	GLU

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Mol	Chain	Res	Type
36	BQ	57	HIS
36	BQ	58	PHE
36	BQ	59	ARG
36	BQ	66	ILE
36	BQ	68	ILE
36	BQ	74	TYR
36	BQ	91	GLU
36	BQ	93	TYR
36	BQ	96	VAL
36	BQ	103	MET
36	BQ	104	PHE
36	BQ	110	THR
36	BQ	112	GLU
36	BQ	116	GLU
36	BQ	127	ILE
36	BQ	128	LYS
36	BQ	129	THR
36	BQ	131	ILE
36	BQ	132	VAL
36	BQ	135	ASP
36	BQ	137	TYR
37	BR	4	LEU
37	BR	21	TYR
37	BR	23	ASN
37	BR	27	SER
37	BR	29	LEU
37	BR	44	LEU
37	BR	45	ARG
37	BR	47	PHE
37	BR	71	GLN
37	BR	72	ASP
37	BR	75	LEU
37	BR	76	VAL
37	BR	94	TYR
37	BR	95	THR
37	BR	99	LYS
37	BR	100	LEU
37	BR	104	ARG
37	BR	113	LEU
38	BS	12	PHE
38	BS	13	ARG
38	BS	15	ARG

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Mol	Chain	Res	Type
38	BS	18	ILE
38	BS	24	LEU
38	BS	47	THR
38	BS	61	ASN
38	BS	62	LYS
38	BS	64	GLU
38	BS	73	LEU
38	BS	82	ILE
38	BS	95	HIS
38	BS	97	ARG
39	BT	1	MET
39	BT	11	GLU
39	BT	16	ARG
39	BT	18	ASP
39	BT	21	GLU
39	BT	22	PHE
39	BT	27	THR
39	BT	31	SER
39	BT	32	TYR
39	BT	45	PHE
39	BT	48	ILE
39	BT	59	THR
39	BT	62	THR
39	BT	64	ARG
39	BT	70	VAL
39	BT	74	ARG
39	BT	82	LEU
39	BT	90	GLN
39	BT	96	ARG
39	BT	99	LEU
39	BT	104	ASN
39	BT	107	ASP
39	BT	111	ARG
39	BT	115	ARG
39	BT	118	ARG
39	BT	124	ASP
39	BT	134	GLU
40	BU	8	VAL
40	BU	10	ARG
40	BU	14	HIS
40	BU	20	LEU
40	BU	28	ARG

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Mol	Chain	Res	Type
40	BU	51	LYS
40	BU	62	ILE
40	BU	72	HIS
40	BU	74	LEU
40	BU	79	PHE
40	BU	98	LEU
40	BU	102	GLU
40	BU	104	GLN
40	BU	108	GLU
40	BU	117	GLN
41	BV	7	THR
41	BV	15	GLU
41	BV	18	LEU
41	BV	19	LYS
41	BV	21	ARG
41	BV	35	LEU
41	BV	38	LEU
41	BV	40	LEU
41	BV	43	GLU
41	BV	45	THR
41	BV	47	VAL
41	BV	52	VAL
41	BV	57	VAL
41	BV	60	GLU
41	BV	68	LYS
41	BV	72	VAL
41	BV	75	PHE
41	BV	80	GLN
41	BV	81	TYR
41	BV	94	LEU
41	BV	95	LEU
41	BV	98	GLU
41	BV	99	ILE
42	BW	1	MET
42	BW	11	ARG
42	BW	17	VAL
42	BW	22	ASP
42	BW	27	LYS
42	BW	46	PHE
42	BW	61	ASN
42	BW	88	ARG
42	BW	95	ILE

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Mol	Chain	Res	Type
42	BW	96	ILE
42	BW	97	LYS
42	BW	107	LEU
42	BW	113	LYS
43	BX	3	THR
43	BX	12	VAL
43	BX	13	LEU
43	BX	23	GLU
43	BX	27	THR
43	BX	30	VAL
43	BX	35	THR
43	BX	38	GLU
43	BX	44	GLU
43	BX	54	VAL
43	BX	55	ASN
43	BX	57	LEU
43	BX	58	HIS
43	BX	63	LYS
43	BX	68	ARG
43	BX	72	LYS
43	BX	76	ARG
44	BY	2	ARG
44	BY	4	LYS
44	BY	6	HIS
44	BY	7	VAL
44	BY	9	LYS
44	BY	11	ASP
44	BY	13	VAL
44	BY	24	VAL
44	BY	33	LYS
44	BY	35	TYR
44	BY	42	VAL
44	BY	43	ASN
44	BY	44	ILE
44	BY	47	LYS
44	BY	50	ARG
44	BY	51	VAL
44	BY	60	PHE
44	BY	64	GLU
44	BY	76	CYS
44	BY	83	THR
44	BY	90	LEU

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Mol	Chain	Res	Type
44	BY	94	LYS
44	BY	97	ARG
45	BZ	3	TYR
45	BZ	9	TYR
45	BZ	13	GLU
45	BZ	14	LYS
45	BZ	28	MET
45	BZ	29	TYR
45	BZ	32	HIS
45	BZ	36	LYS
45	BZ	42	VAL
45	BZ	44	PHE
45	BZ	50	GLN
45	BZ	60	GLU
45	BZ	63	ASP
45	BZ	65	GLN
45	BZ	77	ASP
45	BZ	82	ARG
45	BZ	87	ASP
45	BZ	89	PHE
45	BZ	98	MET
45	BZ	121	HIS
45	BZ	124	ILE
45	BZ	132	ASN
45	BZ	133	ILE
45	BZ	136	PHE
45	BZ	139	VAL
45	BZ	140	ASP
45	BZ	141	VAL
45	BZ	144	LEU
45	BZ	154	ASP
45	BZ	156	LYS
45	BZ	163	LEU
45	BZ	165	VAL
45	BZ	179	ASP
45	BZ	181	GLU
45	BZ	186	GLU
46	B0	11	ARG
46	B0	20	ARG
46	B0	23	VAL
46	B0	27	GLU
46	B0	36	ILE

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Mol	Chain	Res	Type
46	B0	43	THR
46	B0	80	HIS
47	B1	5	CYS
47	B1	11	ARG
47	B1	17	SER
47	B1	18	ILE
47	B1	20	ARG
47	B1	23	LYS
47	B1	25	LYS
47	B1	35	THR
47	B1	37	ILE
47	B1	39	LYS
47	B1	42	GLN
47	B1	43	TYR
47	B1	46	LEU
47	B1	47	GLN
47	B1	57	GLU
47	B1	60	PHE
47	B1	67	ILE
47	B1	73	LEU
47	B1	80	LEU
47	B1	82	LEU
47	B1	85	LEU
47	B1	86	SER
48	B2	3	LEU
48	B2	11	GLU
48	B2	21	LEU
48	B2	22	GLU
48	B2	24	LEU
48	B2	27	GLU
48	B2	44	LEU
48	B2	50	ILE
48	B2	55	ARG
48	B2	65	ASN
49	B3	5	LYS
49	B3	31	LEU
49	B3	32	GLN
49	B3	36	VAL
49	B3	40	THR
49	B3	52	HIS
49	B3	56	VAL
49	B3	59	VAL

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Mol	Chain	Res	Type
50	B4	1	MET
50	B4	6	HIS
50	B4	9	LEU
50	B4	20	ASN
50	B4	27	THR
50	B4	28	LYS
50	B4	30	GLU
50	B4	33	VAL
51	B5	3	LYS
51	B5	13	LYS
51	B5	20	ARG
51	B5	22	HIS
51	B5	26	THR
51	B5	31	VAL
51	B5	35	GLU
51	B5	40	LYS
51	B5	43	HIS
51	B5	49	CYS
51	B5	51	TYR
51	B5	55	ARG
51	B5	58	LEU
52	B6	6	ARG
52	B6	9	LEU
52	B6	11	LEU
52	B6	18	ARG
52	B6	23	THR
52	B6	27	LYS
52	B6	28	ARG
52	B6	33	LYS
52	B6	36	LEU
52	B6	39	TYR
52	B6	46	HIS
52	B6	48	VAL
52	B6	52	VAL
52	B6	54	ILE
53	B7	5	TRP
53	B7	6	GLN
53	B7	22	MET
53	B7	24	THR
53	B7	40	TRP
53	B7	47	ARG
53	B7	48	LYS

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Mol	Chain	Res	Type
54	B8	14	VAL
54	B8	22	VAL
54	B8	34	TRP
54	B8	48	PHE
54	B8	52	LYS
54	B8	57	ARG
54	B8	59	LYS
54	B8	60	LEU
54	B8	64	TYR
55	B9	4	ARG
55	B9	7	VAL
55	B9	13	LYS
55	B9	17	ILE
55	B9	22	ARG
55	B9	26	ILE
55	B9	28	GLU
55	B9	36	GLN
56	Be	60	PHE
56	Be	64	LEU
56	Be	70	LYS
56	Be	81	ILE
56	Be	84	LEU
56	Be	94	GLU
1	CB	11	LEU
1	CB	15	VAL
1	CB	16	HIS
1	CB	17	PHE
1	CB	28	PHE
1	CB	32	ILE
1	CB	33	TYR
1	CB	36	ARG
1	CB	67	THR
1	CB	69	LEU
1	CB	86	GLU
1	CB	94	ASN
1	CB	96	ARG
1	CB	102	LEU
1	CB	105	PHE
1	CB	121	LEU
1	CB	124	SER
1	CB	129	GLU
1	CB	133	LYS

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Mol	Chain	Res	Type
1	CB	141	GLU
1	CB	143	GLU
1	CB	149	LEU
1	CB	150	SER
1	CB	152	PHE
1	CB	154	LEU
1	CB	155	LEU
1	CB	156	LYS
1	CB	157	ARG
1	CB	158	LEU
1	CB	162	ILE
1	CB	168	THR
1	CB	170	GLU
1	CB	172	ILE
1	CB	175	ARG
1	CB	184	VAL
1	CB	196	LEU
1	CB	200	ILE
1	CB	205	ASP
1	CB	209	ARG
1	CB	212	GLN
1	CB	215	LEU
1	CB	222	ILE
1	CB	230	VAL
1	CB	238	LEU
1	CB	241	GLU
2	CC	3	ASN
2	CC	19	GLU
2	CC	26	LYS
2	CC	29	TYR
2	CC	31	HIS
2	CC	32	LEU
2	CC	36	ASP
2	CC	48	TYR
2	CC	56	ASP
2	CC	67	THR
2	CC	87	LEU
2	CC	90	GLU
2	CC	94	LEU
2	CC	101	LEU
2	CC	103	VAL
2	CC	104	GLN

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Mol	Chain	Res	Type
2	CC	115	LEU
2	CC	119	ARG
2	CC	124	ILE
2	CC	128	PHE
2	CC	136	GLN
2	CC	140	ARG
2	CC	144	SER
2	CC	152	ILE
2	CC	162	GLN
2	CC	166	GLU
2	CC	167	TRP
2	CC	173	VAL
2	CC	175	LEU
2	CC	176	HIS
2	CC	188	LEU
2	CC	193	TYR
2	CC	195	VAL
3	CD	8	VAL
3	CD	10	ARG
3	CD	12	CYS
3	CD	13	ARG
3	CD	19	LEU
3	CD	27	TYR
3	CD	31	CYS
3	CD	33	MET
3	CD	35	ARG
3	CD	43	HIS
3	CD	54	TYR
3	CD	61	LYS
3	CD	67	ILE
3	CD	72	GLU
3	CD	74	GLN
3	CD	76	ARG
3	CD	78	LEU
3	CD	86	LYS
3	CD	105	VAL
3	CD	106	TYR
3	CD	107	ARG
3	CD	127	THR
3	CD	134	ASP
3	CD	140	VAL
3	CD	150	GLU

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Mol	Chain	Res	Type
3	CD	163	GLU
3	CD	165	MET
3	CD	178	VAL
3	CD	190	ASP
3	CD	196	LEU
3	CD	203	VAL
3	CD	207	TYR
4	CE	10	MET
4	CE	12	LEU
4	CE	13	ILE
4	CE	20	GLN
4	CE	36	ASP
4	CE	37	ARG
4	CE	41	VAL
4	CE	47	LYS
4	CE	60	TYR
4	CE	61	TYR
4	CE	64	ARG
4	CE	67	VAL
4	CE	68	GLU
4	CE	76	ILE
4	CE	78	HIS
4	CE	80	ILE
4	CE	84	PHE
4	CE	91	LEU
4	CE	112	LEU
4	CE	119	LEU
4	CE	120	THR
4	CE	125	SER
4	CE	130	ASN
4	CE	135	THR
4	CE	137	GLU
4	CE	150	ARG
4	CE	151	LEU
5	CF	4	TYR
5	CF	11	ASN
5	CF	15	ASP
5	CF	16	GLN
5	CF	38	GLU
5	CF	40	VAL
5	CF	45	LEU
5	CF	46	ARG

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Mol	Chain	Res	Type
5	CF	52	ILE
5	CF	61	LEU
5	CF	70	ASP
5	CF	82	ARG
5	CF	91	VAL
6	CG	4	ARG
6	CG	13	GLN
6	CG	31	MET
6	CG	36	LYS
6	CG	50	ILE
6	CG	52	GLU
6	CG	56	GLN
6	CG	69	VAL
6	CG	79	ARG
6	CG	91	VAL
6	CG	119	ARG
6	CG	122	HIS
6	CG	126	ASP
6	CG	139	GLU
6	CG	140	ASP
6	CG	149	ARG
7	CH	11	THR
7	CH	18	ARG
7	CH	26	VAL
7	CH	30	ARG
7	CH	31	PHE
7	CH	37	ARG
7	CH	41	ARG
7	CH	44	PHE
7	CH	51	VAL
7	CH	52	ASP
7	CH	63	LEU
7	CH	75	ARG
7	CH	82	HIS
7	CH	83	ILE
7	CH	85	ARG
7	CH	98	LYS
7	CH	102	ARG
7	CH	104	ARG
7	CH	107	LEU
7	CH	111	ILE
7	CH	112	LEU

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Mol	Chain	Res	Type
7	CH	114	THR
7	CH	116	LYS
7	CH	129	VAL
7	CH	138	TRP
8	CI	3	GLN
8	CI	4	TYR
8	CI	10	ARG
8	CI	25	LYS
8	CI	35	GLU
8	CI	36	TYR
8	CI	38	GLN
8	CI	41	VAL
8	CI	42	ARG
8	CI	56	LEU
8	CI	66	ARG
8	CI	79	LEU
8	CI	88	TYR
8	CI	93	ARG
8	CI	95	LYS
8	CI	97	LYS
8	CI	107	ARG
8	CI	114	TYR
8	CI	118	LYS
8	CI	121	ARG
9	CJ	6	ILE
9	CJ	8	LEU
9	CJ	11	PHE
9	CJ	17	ASP
9	CJ	21	GLN
9	CJ	22	LYS
9	CJ	25	GLU
9	CJ	33	GLN
9	CJ	35	SER
9	CJ	40	LEU
9	CJ	49	VAL
9	CJ	50	ILE
9	CJ	57	LYS
9	CJ	70	ARG
9	CJ	73	ASP
9	CJ	75	ILE
9	CJ	78	ASN
9	CJ	79	ARG

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Mol	Chain	Res	Type
9	CJ	81	THR
9	CJ	96	ILE
9	CJ	99	LYS
10	CK	29	ILE
10	CK	40	ILE
10	CK	41	THR
10	CK	50	TYR
10	CK	57	THR
10	CK	71	LYS
10	CK	81	ASP
10	CK	84	VAL
10	CK	87	THR
10	CK	112	THR
10	CK	127	LYS
11	CL	15	ARG
11	CL	16	GLU
11	CL	18	VAL
11	CL	20	LYS
11	CL	37	CYS
11	CL	42	THR
11	CL	52	LEU
11	CL	53	ARG
11	CL	54	LYS
11	CL	55	VAL
11	CL	59	ARG
11	CL	60	LEU
11	CL	61	THR
11	CL	75	HIS
11	CL	80	HIS
11	CL	97	ARG
11	CL	101	VAL
11	CL	102	ARG
11	CL	105	TYR
11	CL	106	ASP
11	CL	112	ASP
11	CL	117	ARG
12	CM	3	ARG
12	CM	9	ILE
12	CM	12	ASN
12	CM	19	LEU
12	CM	21	TYR
12	CM	37	THR

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Mol	Chain	Res	Type
12	CM	43	THR
12	CM	46	LYS
12	CM	47	ASP
12	CM	48	LEU
12	CM	49	THR
12	CM	50	GLU
12	CM	56	LEU
12	CM	69	GLU
12	CM	70	LEU
12	CM	81	LEU
12	CM	84	ILE
12	CM	103	THR
12	CM	105	THR
12	CM	108	ARG
12	CM	111	LYS
13	CN	21	TYR
13	CN	22	THR
13	CN	26	ARG
13	CN	32	SER
13	CN	35	ARG
13	CN	40	CYS
13	CN	47	LEU
13	CN	49	HIS
13	CN	53	LEU
13	CN	56	VAL
13	CN	57	ARG
14	CO	17	ARG
14	CO	25	THR
14	CO	26	GLU
14	CO	27	VAL
14	CO	31	LEU
14	CO	38	ARG
14	CO	47	LYS
14	CO	63	ARG
14	CO	72	ARG
14	CO	78	TYR
14	CO	87	ILE
15	CP	2	VAL
15	CP	16	HIS
15	CP	21	VAL
15	CP	29	ASP
15	CP	32	TYR

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Mol	Chain	Res	Type
15	CP	38	TYR
15	CP	42	ARG
15	CP	45	THR
15	CP	49	LEU
15	CP	61	SER
15	CP	67	THR
15	CP	73	LEU
16	CQ	12	SER
16	CQ	31	LEU
16	CQ	37	LYS
16	CQ	40	LYS
16	CQ	46	ASP
16	CQ	52	LYS
16	CQ	63	ARG
16	CQ	74	LEU
16	CQ	78	GLU
16	CQ	81	ARG
16	CQ	84	LEU
16	CQ	86	GLU
16	CQ	89	LEU
16	CQ	98	LEU
17	CR	35	ARG
17	CR	38	GLU
17	CR	40	LEU
17	CR	62	GLU
17	CR	81	PHE
17	CR	83	GLU
17	CR	86	VAL
18	CS	5	LEU
18	CS	6	LYS
18	CS	14	HIS
18	CS	22	LEU
18	CS	31	ILE
18	CS	33	THR
18	CS	37	ARG
18	CS	41	VAL
18	CS	47	HIS
18	CS	51	VAL
18	CS	61	TYR
18	CS	62	ILE
18	CS	63	THR
18	CS	66	MET

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Mol	Chain	Res	Type
18	CS	73	GLU
18	CS	77	THR
19	CT	10	LEU
19	CT	13	LEU
19	CT	33	ILE
19	CT	36	LEU
19	CT	41	ILE
19	CT	50	GLU
19	CT	53	LEU
19	CT	56	MET
19	CT	57	ARG
19	CT	63	ILE
19	CT	64	ASP
19	CT	71	THR
19	CT	73	HIS
19	CT	74	LYS
19	CT	75	ASN
19	CT	84	LEU
19	CT	86	ARG
19	CT	93	GLU
20	CY	6	GLU
20	CY	7	TYR
20	CY	9	LEU
20	CY	20	HIS
20	CY	21	ILE
20	CY	26	THR
20	CY	28	THR
20	CY	33	LEU
20	CY	34	TYR
20	CY	36	THR
20	CY	39	ILE
20	CY	69	VAL
20	CY	73	PHE
20	CY	77	HIS
20	CY	81	ILE
20	CY	83	ASP
20	CY	92	ILE
20	CY	96	ARG
20	CY	98	MET
20	CY	99	ARG
20	CY	105	ILE
20	CY	120	THR

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Mol	Chain	Res	Type
20	CY	121	VAL
20	CY	123	ARG
20	CY	126	GLU
20	CY	132	ARG
20	CY	133	ILE
20	CY	145	ASP
20	CY	170	ARG
20	CY	172	ASP
20	CY	173	THR
20	CY	174	PHE
20	CY	178	ILE
20	CY	194	THR
20	CY	195	ASP
20	CY	199	ILE
20	CY	207	ASP
20	CY	217	VAL
20	CY	223	PHE
20	CY	225	GLU
20	CY	229	LEU
20	CY	232	LEU
20	CY	239	GLU
20	CY	241	GLU
20	CY	253	LEU
20	CY	254	LYS
20	CY	260	LEU
20	CY	266	ASN
20	CY	269	VAL
20	CY	292	THR
20	CY	299	VAL
20	CY	300	GLU
20	CY	304	ASP
20	CY	326	THR
20	CY	327	PHE
20	CY	330	VAL
20	CY	356	LEU
20	CY	358	MET
20	CY	362	HIS
20	CY	370	LYS
20	CY	380	LEU
20	CY	381	LYS
20	CY	383	THR
20	CY	389	LEU

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Mol	Chain	Res	Type
20	CY	406	GLU
20	CY	410	ASP
20	CY	413	ILE
20	CY	414	GLU
20	CY	417	THR
20	CY	428	LEU
20	CY	437	THR
20	CY	442	THR
20	CY	443	HIS
20	CY	449	THR
20	CY	457	LEU
20	CY	465	ARG
20	CY	472	VAL
20	CY	475	ASN
20	CY	487	ILE
20	CY	488	THR
20	CY	491	VAL
20	CY	498	ILE
20	CY	504	ARG
20	CY	510	VAL
20	CY	512	ILE
20	CY	525	PHE
20	CY	537	GLU
20	CY	542	VAL
20	CY	550	MET
20	CY	556	ILE
20	CY	565	VAL
20	CY	568	TYR
20	CY	580	MET
20	CY	588	MET
20	CY	598	ASP
20	CY	605	ILE
20	CY	615	GLU
20	CY	617	MET
20	CY	624	LEU
20	CY	625	ASN
20	CY	634	MET
20	CY	635	GLU
20	CY	651	GLU
20	CY	655	TYR
20	CY	659	LEU
20	CY	660	ARG

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Mol	Chain	Res	Type
20	CY	668	SER
20	CY	671	MET
20	CY	676	TYR
20	CY	677	GLN
20	CY	684	GLN
20	CY	685	GLU
25	DC	4	HIS
25	DC	13	GLU
25	DC	15	VAL
25	DC	19	LYS
25	DC	31	LYS
25	DC	37	LYS
25	DC	48	LEU
25	DC	51	ASP
25	DC	53	ARG
25	DC	54	ARG
25	DC	62	THR
25	DC	106	ASP
25	DC	114	VAL
25	DC	120	VAL
25	DC	130	ARG
25	DC	131	ILE
25	DC	135	ARG
25	DC	137	LEU
25	DC	145	THR
25	DC	148	PHE
25	DC	152	GLU
25	DC	153	ILE
25	DC	158	LYS
25	DC	166	ASN
25	DC	167	ASP
25	DC	169	THR
25	DC	172	ILE
25	DC	173	HIS
25	DC	198	GLU
25	DC	213	VAL
25	DC	215	VAL
25	DC	216	THR
25	DC	219	MET
25	DC	228	HIS
26	DD	5	LYS
26	DD	15	PHE

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Mol	Chain	Res	Type
26	DD	24	ILE
26	DD	25	THR
26	DD	26	LYS
26	DD	28	GLU
26	DD	31	LYS
26	DD	33	LEU
26	DD	35	LYS
26	DD	36	PRO
26	DD	37	LEU
26	DD	38	LYS
26	DD	43	ARG
26	DD	45	ASN
26	DD	49	ILE
26	DD	64	ILE
26	DD	65	ILE
26	DD	78	LYS
26	DD	82	ILE
26	DD	94	LEU
26	DD	105	ILE
26	DD	131	LEU
26	DD	140	THR
26	DD	146	GLU
26	DD	147	LEU
26	DD	150	LYS
26	DD	161	THR
26	DD	172	TYR
26	DD	175	LEU
26	DD	185	VAL
26	DD	186	HIS
26	DD	190	TYR
26	DD	206	LEU
26	DD	226	MET
26	DD	227	ASN
26	DD	230	ASP
26	DD	231	HIS
26	DD	242	ARG
26	DD	244	ARG
26	DD	248	SER
26	DD	252	TRP
26	DD	257	LEU
26	DD	259	THR
26	DD	260	ARG

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Mol	Chain	Res	Type
27	DE	4	ILE
27	DE	13	ARG
27	DE	19	ARG
27	DE	21	VAL
27	DE	23	VAL
27	DE	24	THR
27	DE	35	GLN
27	DE	36	ARG
27	DE	52	LEU
27	DE	58	ARG
27	DE	63	LEU
27	DE	66	HIS
27	DE	72	VAL
27	DE	77	ILE
27	DE	78	LEU
27	DE	79	ARG
27	DE	87	GLU
27	DE	89	ASP
27	DE	95	ILE
27	DE	96	PHE
27	DE	103	ASP
27	DE	104	VAL
27	DE	107	THR
27	DE	111	ARG
27	DE	113	PHE
27	DE	127	ASP
27	DE	132	HIS
27	DE	134	ILE
27	DE	136	ARG
27	DE	146	THR
27	DE	156	MET
27	DE	160	TYR
27	DE	169	ASN
27	DE	172	VAL
27	DE	178	GLU
27	DE	181	LEU
27	DE	196	VAL
27	DE	202	LYS
28	DF	2	LYS
28	DF	7	TYR
28	DF	9	ILE
28	DF	12	LEU

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Mol	Chain	Res	Type
28	DF	17	ARG
28	DF	28	ILE
28	DF	29	ASN
28	DF	31	HIS
28	DF	33	LEU
28	DF	38	ARG
28	DF	45	ARG
28	DF	53	THR
28	DF	65	TRP
28	DF	74	ARG
28	DF	88	VAL
28	DF	89	VAL
28	DF	96	ASP
28	DF	104	LYS
28	DF	114	VAL
28	DF	123	LEU
28	DF	126	VAL
28	DF	132	VAL
28	DF	136	THR
28	DF	149	ASP
28	DF	156	LEU
28	DF	174	VAL
28	DF	186	ILE
28	DF	191	ARG
28	DF	192	LEU
28	DF	194	MET
28	DF	199	TRP
28	DF	205	ARG
28	DF	206	ILE
29	DG	21	ARG
29	DG	26	GLN
29	DG	30	GLU
29	DG	45	GLU
29	DG	48	GLU
29	DG	58	GLN
29	DG	84	LYS
29	DG	86	MET
29	DG	88	ILE
29	DG	113	ARG
29	DG	115	ARG
29	DG	126	ASP
29	DG	133	LEU

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Mol	Chain	Res	Type
29	DG	137	GLU
29	DG	138	GLN
29	DG	139	LEU
29	DG	145	THR
29	DG	146	TYR
29	DG	148	MET
29	DG	150	ASP
29	DG	157	ILE
29	DG	161	THR
29	DG	165	THR
29	DG	170	ARG
30	DH	23	ARG
30	DH	41	MET
30	DH	43	VAL
30	DH	44	VAL
30	DH	49	VAL
30	DH	52	VAL
30	DH	58	GLU
30	DH	65	HIS
30	DH	79	VAL
30	DH	83	TYR
30	DH	104	GLU
30	DH	105	LEU
30	DH	106	THR
30	DH	114	VAL
30	DH	121	ILE
30	DH	127	GLU
30	DH	132	ARG
30	DH	158	HIS
30	DH	171	LEU
32	DK	5	VAL
32	DK	9	LYS
32	DK	10	LEU
32	DK	11	GLN
32	DK	27	LEU
32	DK	29	GLN
32	DK	34	ILE
32	DK	41	PHE
32	DK	48	MET
32	DK	65	PHE
32	DK	78	ILE
32	DK	84	LEU

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Mol	Chain	Res	Type
32	DK	89	HIS
32	DK	95	LYS
32	DK	98	ARG
32	DK	101	TRP
32	DK	105	LEU
32	DK	109	LYS
32	DK	119	ASP
32	DK	125	ARG
32	DK	126	MET
32	DK	127	ILE
32	DK	132	ARG
32	DK	136	VAL
33	DN	13	TRP
33	DN	15	LEU
33	DN	26	LEU
33	DN	39	ARG
33	DN	42	TRP
33	DN	45	ASN
33	DN	48	MET
33	DN	51	PHE
33	DN	55	VAL
33	DN	56	ASN
33	DN	59	LYS
33	DN	62	VAL
33	DN	67	LEU
33	DN	69	GLN
33	DN	71	ILE
33	DN	72	TYR
33	DN	73	THR
33	DN	78	TYR
33	DN	82	LEU
33	DN	84	LYS
33	DN	85	ILE
33	DN	87	LEU
33	DN	91	LEU
33	DN	97	ARG
33	DN	99	LEU
33	DN	101	HIS
33	DN	104	LYS
33	DN	106	MET
33	DN	107	LEU
33	DN	112	LEU

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Mol	Chain	Res	Type
33	DN	114	ARG
33	DN	117	PHE
33	DN	130	HIS
33	DN	139	GLU
34	DO	1	MET
34	DO	2	ILE
34	DO	3	GLN
34	DO	8	LEU
34	DO	17	ARG
34	DO	23	ARG
34	DO	32	TYR
34	DO	45	GLU
34	DO	68	GLU
34	DO	70	LYS
34	DO	71	ARG
34	DO	73	ASP
34	DO	75	SER
34	DO	86	ILE
34	DO	91	LEU
34	DO	102	VAL
34	DO	107	ARG
34	DO	114	ILE
35	DP	7	ARG
35	DP	16	ARG
35	DP	18	ARG
35	DP	19	VAL
35	DP	39	LYS
35	DP	46	LYS
35	DP	50	ARG
35	DP	59	LEU
35	DP	61	ARG
35	DP	68	GLN
35	DP	85	LEU
35	DP	96	THR
35	DP	99	LEU
35	DP	100	LEU
35	DP	107	LYS
35	DP	108	LYS
35	DP	110	TYR
35	DP	115	LEU
35	DP	117	GLU
35	DP	123	LEU

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Mol	Chain	Res	Type
35	DP	128	HIS
35	DP	135	LEU
35	DP	144	GLU
35	DP	146	VAL
36	DQ	7	MET
36	DQ	25	ASP
36	DQ	26	TYR
36	DQ	29	PHE
36	DQ	38	GLU
36	DQ	43	THR
36	DQ	51	ARG
36	DQ	58	PHE
36	DQ	60	ARG
36	DQ	68	ILE
36	DQ	93	TYR
36	DQ	97	VAL
36	DQ	104	PHE
36	DQ	105	GLU
36	DQ	106	VAL
36	DQ	112	GLU
36	DQ	128	LYS
36	DQ	129	THR
36	DQ	132	VAL
36	DQ	137	TYR
37	DR	3	HIS
37	DR	4	LEU
37	DR	17	ARG
37	DR	21	TYR
37	DR	37	THR
37	DR	44	LEU
37	DR	45	ARG
37	DR	47	PHE
37	DR	61	HIS
37	DR	72	ASP
37	DR	74	LYS
37	DR	75	LEU
37	DR	76	VAL
37	DR	80	PHE
37	DR	81	ASP
37	DR	87	TYR
37	DR	88	ARG
37	DR	89	ASP

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Mol	Chain	Res	Type
37	DR	95	THR
37	DR	99	LYS
37	DR	102	GLU
37	DR	107	ASP
38	DS	12	PHE
38	DS	13	ARG
38	DS	15	ARG
38	DS	18	ILE
38	DS	23	ARG
38	DS	24	LEU
38	DS	29	PHE
38	DS	31	SER
38	DS	36	TYR
38	DS	41	ASP
38	DS	42	ASP
38	DS	47	THR
38	DS	69	VAL
38	DS	87	PHE
38	DS	92	TYR
38	DS	97	ARG
38	DS	98	VAL
38	DS	106	ARG
38	DS	107	GLU
39	DT	8	LYS
39	DT	13	ARG
39	DT	16	ARG
39	DT	22	PHE
39	DT	27	THR
39	DT	30	VAL
39	DT	31	SER
39	DT	43	GLN
39	DT	46	GLU
39	DT	55	ASN
39	DT	62	THR
39	DT	64	ARG
39	DT	73	GLU
39	DT	74	ARG
39	DT	75	ILE
39	DT	82	LEU
39	DT	87	ASP
39	DT	90	GLN
39	DT	96	ARG

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Mol	Chain	Res	Type
39	DT	99	LEU
39	DT	101	PHE
39	DT	103	ARG
39	DT	104	ASN
39	DT	107	ASP
39	DT	108	ARG
39	DT	111	ARG
39	DT	118	ARG
39	DT	122	ASP
39	DT	125	ARG
40	DU	14	HIS
40	DU	27	LEU
40	DU	28	ARG
40	DU	30	LYS
40	DU	36	ARG
40	DU	51	LYS
40	DU	57	PHE
40	DU	72	HIS
40	DU	74	LEU
40	DU	83	LEU
40	DU	89	GLU
40	DU	97	ASP
40	DU	102	GLU
40	DU	104	GLN
40	DU	105	VAL
40	DU	108	GLU
40	DU	112	ARG
41	DV	13	ARG
41	DV	19	LYS
41	DV	21	ARG
41	DV	22	VAL
41	DV	34	GLU
41	DV	37	VAL
41	DV	38	LEU
41	DV	40	LEU
41	DV	71	LEU
41	DV	75	PHE
41	DV	80	GLN
41	DV	85	LYS
41	DV	95	LEU
41	DV	99	ILE
42	DW	2	GLU

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Mol	Chain	Res	Type
42	DW	11	ARG
42	DW	16	LYS
42	DW	19	LEU
42	DW	23	LEU
42	DW	25	ARG
42	DW	27	LYS
42	DW	31	GLU
42	DW	45	TYR
42	DW	51	LEU
42	DW	64	MET
42	DW	77	ASP
42	DW	82	LEU
42	DW	88	ARG
42	DW	95	ILE
42	DW	96	ILE
42	DW	99	ARG
42	DW	105	VAL
42	DW	107	LEU
42	DW	110	LYS
43	DX	8	ILE
43	DX	12	VAL
43	DX	23	GLU
43	DX	27	THR
43	DX	30	VAL
43	DX	38	GLU
43	DX	45	THR
43	DX	53	LYS
43	DX	54	VAL
43	DX	57	LEU
43	DX	58	HIS
43	DX	63	LYS
43	DX	66	LEU
43	DX	72	LYS
43	DX	75	ASP
43	DX	80	ILE
44	DY	4	LYS
44	DY	7	VAL
44	DY	9	LYS
44	DY	27	VAL
44	DY	28	LYS
44	DY	31	LEU
44	DY	33	LYS

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Mol	Chain	Res	Type
44	DY	35	TYR
44	DY	44	ILE
44	DY	50	ARG
44	DY	64	GLU
44	DY	83	THR
44	DY	97	ARG
44	DY	106	LEU
45	DZ	3	TYR
45	DZ	9	TYR
45	DZ	28	MET
45	DZ	29	TYR
45	DZ	36	LYS
45	DZ	39	VAL
45	DZ	57	ILE
45	DZ	61	LEU
45	DZ	63	ASP
45	DZ	70	LEU
45	DZ	71	VAL
45	DZ	74	VAL
45	DZ	81	ARG
45	DZ	90	VAL
45	DZ	98	MET
45	DZ	104	PHE
45	DZ	117	LEU
45	DZ	124	ILE
45	DZ	144	LEU
45	DZ	145	GLU
45	DZ	151	HIS
45	DZ	155	LEU
45	DZ	162	GLU
45	DZ	163	LEU
45	DZ	181	GLU
45	DZ	183	LEU
45	DZ	185	GLU
46	D0	11	ARG
46	D0	20	ARG
46	D0	27	GLU
46	D0	32	ARG
46	D0	36	ILE
46	D0	41	ARG
46	D0	44	ARG
46	D0	60	PHE

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Mol	Chain	Res	Type
46	D0	63	VAL
46	D0	64	ASP
46	D0	67	VAL
46	D0	70	GLN
46	D0	82	ARG
47	D1	5	CYS
47	D1	18	ILE
47	D1	20	ARG
47	D1	32	LYS
47	D1	33	LYS
47	D1	34	THR
47	D1	39	LYS
47	D1	40	ARG
47	D1	41	ARG
47	D1	42	GLN
47	D1	46	LEU
47	D1	50	ARG
47	D1	56	GLN
47	D1	57	GLU
47	D1	58	ILE
47	D1	59	THR
47	D1	60	PHE
47	D1	67	ILE
47	D1	73	LEU
47	D1	80	LEU
47	D1	85	LEU
48	D2	22	GLU
48	D2	24	LEU
48	D2	34	GLU
48	D2	44	LEU
48	D2	50	ILE
48	D2	55	ARG
48	D2	64	LEU
48	D2	66	GLU
48	D2	68	ARG
49	D3	15	TYR
49	D3	26	LEU
49	D3	29	ARG
49	D3	31	LEU
49	D3	35	ARG
49	D3	37	LEU
49	D3	44	ARG

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Mol	Chain	Res	Type
50	D4	1	MET
50	D4	8	LYS
50	D4	9	LEU
50	D4	10	VAL
50	D4	22	ILE
50	D4	28	LYS
50	D4	30	GLU
50	D4	32	TYR
50	D4	33	VAL
51	D5	3	LYS
51	D5	29	THR
51	D5	36	CYS
51	D5	43	HIS
51	D5	45	VAL
51	D5	55	ARG
52	D6	6	ARG
52	D6	9	LEU
52	D6	10	LEU
52	D6	11	LEU
52	D6	18	ARG
52	D6	19	ARG
52	D6	20	ASN
52	D6	23	THR
52	D6	25	LYS
52	D6	28	ARG
52	D6	37	ARG
52	D6	39	TYR
52	D6	46	HIS
52	D6	48	VAL
52	D6	49	HIS
52	D6	50	ARG
52	D6	51	GLU
52	D6	53	LYS
53	D7	18	PHE
53	D7	24	THR
53	D7	34	ARG
53	D7	35	ARG
53	D7	36	GLN
53	D7	40	TRP
54	D8	5	LYS
54	D8	16	ILE
54	D8	22	VAL

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Mol	Chain	Res	Type
54	D8	34	TRP
54	D8	36	LYS
54	D8	40	GLU
54	D8	48	PHE
54	D8	49	VAL
54	D8	53	PRO
54	D8	57	ARG
54	D8	59	LYS
54	D8	61	LEU
55	D9	12	ASP
55	D9	16	VAL
55	D9	20	HIS
56	De	72	LEU
56	De	73	GLU
56	De	74	VAL
56	De	92	LEU
56	De	95	LYS
56	De	99	VAL
56	De	107	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	40	HIS
1	AB	78	GLN
2	AC	123	GLN
3	AD	45	GLN
3	AD	123	HIS
3	AD	125	HIS
3	AD	161	ASN
10	AK	38	ASN
20	AY	165	GLN
20	AY	448	GLN
20	AY	500	GLN
28	BF	67	GLN
28	BF	169	ASN
30	BH	111	HIS
32	BK	30	HIS
32	BK	42	ASN
33	BN	38	HIS
33	BN	101	HIS
34	BO	29	ASN

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Mol	Chain	Res	Type
35	BP	27	HIS
35	BP	38	GLN
36	BQ	46	GLN
37	BR	24	GLN
38	BS	61	ASN
40	BU	81	HIS
40	BU	104	GLN
40	BU	117	GLN
42	BW	57	ASN
42	BW	61	ASN
45	BZ	73	GLN
48	B2	48	HIS
52	B6	20	ASN
55	B9	34	GLN
1	CB	94	ASN
1	CB	95	GLN
3	CD	125	HIS
5	CF	7	ASN
6	CG	153	HIS
8	CI	3	GLN
10	CK	27	ASN
10	CK	116	HIS
11	CL	8	ASN
11	CL	49	ASN
12	CM	92	HIS
12	CM	101	GLN
18	CS	53	ASN
20	CY	77	HIS
20	CY	117	GLN
20	CY	625	ASN
20	CY	630	GLN
25	DC	45	HIS
25	DC	67	HIS
26	DD	45	ASN
26	DD	164	GLN
27	DE	35	GLN
27	DE	129	HIS
28	DF	40	GLN
28	DF	75	HIS
28	DF	169	ASN
29	DG	138	GLN
30	DH	61	HIS

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Mol	Chain	Res	Type
32	DK	116	ASN
33	DN	38	HIS
33	DN	56	ASN
33	DN	101	HIS
34	DO	29	ASN
35	DP	68	GLN
37	DR	71	GLN
39	DT	43	GLN
39	DT	84	GLN
42	DW	57	ASN
42	DW	102	HIS
44	DY	43	ASN
44	DY	68	HIS
45	DZ	73	GLN
45	DZ	75	ASN
47	D1	42	GLN
47	D1	47	GLN
55	D9	34	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1510/1511 (99%)	358 (23%)	16 (1%)
21	CA	1511/1511 (100%)	377 (24%)	16 (1%)
22	AW	76/77 (98%)	37 (48%)	1 (1%)
22	CW	76/77 (98%)	42 (55%)	2 (2%)
23	AV	35/36 (97%)	24 (68%)	9 (25%)
23	CV	35/36 (97%)	27 (77%)	7 (20%)
24	AX	75/78 (96%)	29 (38%)	1 (1%)
24	CX	75/78 (96%)	30 (40%)	0
59	BA	2878/2879 (99%)	748 (25%)	28 (0%)
59	DA	2878/2879 (99%)	715 (24%)	29 (1%)
60	BB	118/119 (99%)	27 (22%)	0
60	DB	118/119 (99%)	32 (27%)	0
All	All	9385/9400 (99%)	2446 (26%)	109 (1%)

All (2446) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G

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Mol	Chain	Res	Type
21	AA	9	G
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	60	A
21	AA	65	U
21	AA	68	G
21	AA	68(A)	G
21	AA	68(H)	G
21	AA	68(L)	U
21	AA	68(M)	U
21	AA	68(P)	C
21	AA	68(Q)	U
21	AA	68(S)	C
21	AA	101	A
21	AA	115	G
21	AA	121	C
21	AA	122	G
21	AA	126	G
21	AA	129(A)	G
21	AA	131	C
21	AA	134	A
21	AA	135	C
21	AA	147	G
21	AA	151	A
21	AA	163	C
21	AA	170	U
21	AA	174	C
21	AA	176	C
21	AA	182	U
21	AA	186(J)	G
21	AA	192	U
21	AA	195	A
21	AA	196	A
21	AA	197	A
21	AA	198	G
21	AA	201(C)	U
21	AA	216	G
21	AA	222	U

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Mol	Chain	Res	Type
21	AA	231	G
21	AA	236	G
21	AA	244	U
21	AA	247	G
21	AA	251	G
21	AA	253	U
21	AA	258	G
21	AA	267	C
21	AA	275	G
21	AA	279	A
21	AA	280	C
21	AA	281	G
21	AA	289	G
21	AA	298	A
21	AA	300	A
21	AA	301	G
21	AA	324	G
21	AA	325	A
21	AA	328	C
21	AA	329	A
21	AA	331	G
21	AA	332	G
21	AA	335	C
21	AA	345	C
21	AA	346	G
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	367	U
21	AA	372	C
21	AA	373	A
21	AA	388	G
21	AA	396	G
21	AA	397	A
21	AA	398	C
21	AA	408	A
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	422	C

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Mol	Chain	Res	Type
21	AA	423	G
21	AA	424	G
21	AA	429	U
21	AA	440	A
21	AA	443	C
21	AA	452	A
21	AA	453	A
21	AA	458(B)	A
21	AA	481	G
21	AA	484	G
21	AA	485	G
21	AA	491	G
21	AA	497	A
21	AA	498	U
21	AA	505	G
21	AA	509	A
21	AA	510	A
21	AA	511	C
21	AA	514	C
21	AA	517	G
21	AA	518	C
21	AA	520	A
21	AA	523	A
21	AA	524	G
21	AA	527	G
21	AA	531	U
21	AA	532	A
21	AA	533	A
21	AA	536	C
21	AA	547	A
21	AA	559	A
21	AA	560	U
21	AA	562	C
21	AA	564	C
21	AA	565	U
21	AA	567	G
21	AA	568	G
21	AA	572	A
21	AA	574	A
21	AA	576	G
21	AA	603	U
21	AA	616	G

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Mol	Chain	Res	Type
21	AA	618	C
21	AA	623	C
21	AA	628	G
21	AA	629	G
21	AA	642	A
21	AA	653	A
21	AA	654	G
21	AA	659	U
21	AA	665	A
21	AA	671	G
21	AA	685	G
21	AA	688	G
21	AA	698	G
21	AA	702	A
21	AA	704	A
21	AA	717	C
21	AA	721	G
21	AA	723	U
21	AA	732	C
21	AA	733	A
21	AA	734	G
21	AA	735	C
21	AA	737	A
21	AA	742	G
21	AA	743	U
21	AA	749	C
21	AA	750	G
21	AA	754	C
21	AA	755	G
21	AA	756	C
21	AA	776	G
21	AA	777	A
21	AA	793	U
21	AA	794	A
21	AA	803	G
21	AA	811	C
21	AA	812	C
21	AA	815	A
21	AA	816	A
21	AA	817	C
21	AA	818	G
21	AA	819	A

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Mol	Chain	Res	Type
21	AA	828	A
21	AA	829	G
21	AA	836	G
21	AA	837	G
21	AA	838(A)	U
21	AA	838(B)	C
21	AA	838(C)	U
21	AA	848	C
21	AA	853	G
21	AA	855	G
21	AA	858	G
21	AA	859	A
21	AA	867	G
21	AA	873	A
21	AA	875	C
21	AA	876	G
21	AA	877	C
21	AA	879	C
21	AA	882	C
21	AA	889	A
21	AA	902	G
21	AA	914	A
21	AA	922	G
21	AA	923	A
21	AA	925	G
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	935	A
21	AA	961	U
21	AA	966	G
21	AA	967	C
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	974	A
21	AA	975	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	980	C

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Mol	Chain	Res	Type
21	AA	981	U
21	AA	992	U
21	AA	993	G
21	AA	1004	A
21	AA	1015	A
21	AA	1022	G
21	AA	1023	G
21	AA	1024	G
21	AA	1025	U
21	AA	1026	G
21	AA	1028(B)	C
21	AA	1050	G
21	AA	1054	C
21	AA	1060	C
21	AA	1064	G
21	AA	1065	U
21	AA	1066	C
21	AA	1072	G
21	AA	1078	U
21	AA	1089	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1104	G
21	AA	1108	G
21	AA	1109	C
21	AA	1117	G
21	AA	1123	A
21	AA	1126	U
21	AA	1127	G
21	AA	1129	C
21	AA	1130	A
21	AA	1131	G
21	AA	1137	C
21	AA	1138	G
21	AA	1139	G
21	AA	1140	C
21	AA	1146	A
21	AA	1156	G
21	AA	1157	A
21	AA	1158	C
21	AA	1159	U

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Mol	Chain	Res	Type
21	AA	1160	G
21	AA	1171	G
21	AA	1178	G
21	AA	1181	G
21	AA	1182	G
21	AA	1183	A
21	AA	1188	A
21	AA	1196	U
21	AA	1197	G
21	AA	1200	C
21	AA	1201	A
21	AA	1202	G
21	AA	1206	G
21	AA	1211	U
21	AA	1212	U
21	AA	1213	A
21	AA	1214	C
21	AA	1225	A
21	AA	1227	A
21	AA	1229	A
21	AA	1238	A
21	AA	1241	G
21	AA	1253	G
21	AA	1256	A
21	AA	1257	U
21	AA	1261	A
21	AA	1262	C
21	AA	1268	A
21	AA	1274	G
21	AA	1275	A
21	AA	1278	U
21	AA	1280	A
21	AA	1281	U
21	AA	1282	C
21	AA	1286	A
21	AA	1287	A
21	AA	1291	G
21	AA	1297	C
21	AA	1298	C
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U

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Mol	Chain	Res	Type
21	AA	1303	C
21	AA	1305	G
21	AA	1306	A
21	AA	1312	G
21	AA	1317	C
21	AA	1320	C
21	AA	1321	C
21	AA	1322	C
21	AA	1330	U
21	AA	1331	G
21	AA	1335	C
21	AA	1336	C
21	AA	1347	G
21	AA	1348	U
21	AA	1359	C
21	AA	1363	A
21	AA	1365	G
21	AA	1370	G
21	AA	1376	U
21	AA	1377	A
21	AA	1379	G
21	AA	1381	U
21	AA	1382	C
21	AA	1394	A
21	AA	1397	C
21	AA	1413	A
21	AA	1419	G
21	AA	1435	G
21	AA	1436	U
21	AA	1440(B)	G
21	AA	1440(C)	G
21	AA	1440(D)	A
21	AA	1440(I)	A
21	AA	1440(J)	C
21	AA	1440(K)	G
21	AA	1440(L)	G
21	AA	1475	G
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1495	U
21	AA	1497	G

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Mol	Chain	Res	Type
21	AA	1499	A
21	AA	1503	A
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
21	AA	1507	A
21	AA	1510	U
21	AA	1517	G
21	AA	1519	A
21	AA	1520	G
21	AA	1525	G
21	AA	1529	G
21	AA	1530	G
21	AA	1531	A
21	AA	1532	U
21	AA	1533	C
21	AA	1534	A
21	AA	1535	C
21	AA	1537	U
21	AA	1538	C
22	AW	2	G
22	AW	4	U
22	AW	8	U
22	AW	10	G
22	AW	14	A
22	AW	15	G
22	AW	16	U
22	AW	18	G
22	AW	19	G
22	AW	20	U
22	AW	20(A)	U
22	AW	21	A
22	AW	22	G
22	AW	24	G
22	AW	26	A
22	AW	27	C
22	AW	28	A
22	AW	37	A
22	AW	38	A
22	AW	42	U
22	AW	43	G
22	AW	44	G

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Mol	Chain	Res	Type
22	AW	45	G
22	AW	46	G
22	AW	48	C
22	AW	55	U
22	AW	56	C
22	AW	57	G
22	AW	58	A
22	AW	59	A
22	AW	61	C
22	AW	62	C
22	AW	63	C
22	AW	64	G
22	AW	69	A
22	AW	72	C
22	AW	74	C
23	AV	4	A
23	AV	5	A
23	AV	7	G
23	AV	8	A
23	AV	10	G
23	AV	11	U
23	AV	12	A
23	AV	13	A
23	AV	14	A
23	AV	15	A
23	AV	16	A
23	AV	17	U
23	AV	19	G
23	AV	20	U
23	AV	22	U
23	AV	26	A
23	AV	27	A
23	AV	28	A
23	AV	30	A
23	AV	31	A
23	AV	32	U
23	AV	33	C
23	AV	35	A
23	AV	36	A
24	AX	6	A
24	AX	8	U
24	AX	9	A

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Mol	Chain	Res	Type
24	AX	16	C
24	AX	17	U
24	AX	18	G
24	AX	20	G
24	AX	21	A
24	AX	34	U
24	AX	39	G
24	AX	42	G
24	AX	45	G
24	AX	46	G
24	AX	47	U
24	AX	48	C
24	AX	50	G
24	AX	51	C
24	AX	52	G
24	AX	55	U
24	AX	60	C
24	AX	63	G
24	AX	64	U
24	AX	66	A
24	AX	68	C
24	AX	72	C
24	AX	73	A
24	AX	74	C
24	AX	75	C
24	AX	76	A
59	BA	7	G
59	BA	8	A
59	BA	10	G
59	BA	11	G
59	BA	13	A
59	BA	15	G
59	BA	18	C
59	BA	33	U
59	BA	35	G
59	BA	40	C
59	BA	46	C
59	BA	50	U
59	BA	51	G
59	BA	58	G
59	BA	61	G
59	BA	64	A

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Mol	Chain	Res	Type
59	BA	67	U
59	BA	70	G
59	BA	72	U
59	BA	73	A
59	BA	75	G
59	BA	83	G
59	BA	84	A
59	BA	88	G
59	BA	91	A
59	BA	99	U
59	BA	101	G
59	BA	102	G
59	BA	105	C
59	BA	113	G
59	BA	117	G
59	BA	118	A
59	BA	120	U
59	BA	122	G
59	BA	128	C
59	BA	134	C
59	BA	137(B)	G
59	BA	137(C)	G
59	BA	137(E)	A
59	BA	137(F)	C
59	BA	149	A
59	BA	171	G
59	BA	177	G
59	BA	186	G
59	BA	196	A
59	BA	197	A
59	BA	200	U
59	BA	201	C
59	BA	204	A
59	BA	205	G
59	BA	215	G
59	BA	216	A
59	BA	220	G
59	BA	221	A
59	BA	222	A
59	BA	225	A
59	BA	226	G
59	BA	228	A

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Mol	Chain	Res	Type
59	BA	229	A
59	BA	230	U
59	BA	233	A
59	BA	248	G
59	BA	252	G
59	BA	253	C
59	BA	268	C
59	BA	270(D)	C
59	BA	270(K)	C
59	BA	270(L)	U
59	BA	270(M)	U
59	BA	270(Q)	C
59	BA	271(B)	G
59	BA	271(C)	U
59	BA	271(D)	G
59	BA	271(J)	C
59	BA	271(M)	G
59	BA	271(N)	G
59	BA	271(R)	C
59	BA	271(T)	G
59	BA	283	U
59	BA	299	A
59	BA	302	C
59	BA	310	A
59	BA	322	A
59	BA	325	G
59	BA	329	G
59	BA	330	A
59	BA	349	G
59	BA	352	G
59	BA	357(C)	G
59	BA	357(K)	U
59	BA	357(M)	C
59	BA	373	U
59	BA	377	C
59	BA	380	U
59	BA	386	G
59	BA	387	U
59	BA	391	G
59	BA	396	G
59	BA	405	U
59	BA	406	G

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Mol	Chain	Res	Type
59	BA	411	G
59	BA	412	A
59	BA	418	G
59	BA	436	C
59	BA	444	C
59	BA	451	C
59	BA	456	C
59	BA	457	A
59	BA	467	G
59	BA	470	A
59	BA	473	G
59	BA	475	U
59	BA	480	A
59	BA	481	G
59	BA	484	C
59	BA	487	C
59	BA	491	G
59	BA	492	A
59	BA	504	U
59	BA	505	A
59	BA	508	G
59	BA	509	C
59	BA	512	G
59	BA	518	G
59	BA	527	C
59	BA	530	G
59	BA	531	C
59	BA	532	A
59	BA	533	G
59	BA	541	C
59	BA	550	G
59	BA	556	G
59	BA	563	G
59	BA	572	A
59	BA	573	G
59	BA	584	C
59	BA	588	U
59	BA	589	C
59	BA	591	C
59	BA	593	G
59	BA	602	G
59	BA	603	A

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Mol	Chain	Res	Type
59	BA	611(D)	U
59	BA	611(E)	G
59	BA	611(F)	A
59	BA	611(G)	G
59	BA	620	G
59	BA	621	A
59	BA	627	A
59	BA	628	G
59	BA	634	C
59	BA	637	A
59	BA	645	C
59	BA	646	A
59	BA	653	C
59	BA	654	U
59	BA	655	A
59	BA	656	G
59	BA	661	C
59	BA	666	G
59	BA	668	G
59	BA	684	G
59	BA	686	G
59	BA	689	A
59	BA	692	C
59	BA	699	A
59	BA	719	C
59	BA	730	C
59	BA	738	G
59	BA	746	A
59	BA	747	U
59	BA	748	G
59	BA	750	A
59	BA	752	A
59	BA	757	U
59	BA	761	A
59	BA	764	A
59	BA	765	G
59	BA	772	C
59	BA	776	G
59	BA	777	A
59	BA	782	A
59	BA	784	A
59	BA	785	G

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Mol	Chain	Res	Type
59	BA	791	C
59	BA	792	G
59	BA	793	A
59	BA	798	G
59	BA	799	G
59	BA	805	G
59	BA	807	U
59	BA	812	C
59	BA	819	A
59	BA	827	U
59	BA	828	U
59	BA	831	G
59	BA	833	U
59	BA	843	G
59	BA	845	G
59	BA	846	C
59	BA	847	U
59	BA	857	C
59	BA	861	A
59	BA	865	C
59	BA	866	A
59	BA	868	U
59	BA	872	A
59	BA	881	G
59	BA	883	G
59	BA	885	C
59	BA	886	C
59	BA	887	A
59	BA	889	C
59	BA	890	A
59	BA	895	U
59	BA	896	A
59	BA	897	C
59	BA	906	G
59	BA	910	A
59	BA	914	C
59	BA	917	A
59	BA	919	G
59	BA	930	U
59	BA	932	G
59	BA	933	A
59	BA	938	G

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Mol	Chain	Res	Type
59	BA	939	G
59	BA	941	A
59	BA	943	U
59	BA	945	A
59	BA	946	G
59	BA	957	A
59	BA	959	A
59	BA	961	C
59	BA	962	G
59	BA	963	U
59	BA	964	C
59	BA	974	G
59	BA	974(A)	C
59	BA	980	A
59	BA	983	A
59	BA	988	A
59	BA	990	A
59	BA	996	A
59	BA	1003	G
59	BA	1004	C
59	BA	1005	C
59	BA	1008	C
59	BA	1009	A
59	BA	1011	G
59	BA	1012	U
59	BA	1013	C
59	BA	1022	G
59	BA	1023	U
59	BA	1025	G
59	BA	1026	U
59	BA	1027	A
59	BA	1033	U
59	BA	1035	U
59	BA	1042	G
59	BA	1046	A
59	BA	1047	G
59	BA	1048	A
59	BA	1052	C
59	BA	1061	U
59	BA	1062	G
59	BA	1064	C
59	BA	1070	A

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Mol	Chain	Res	Type
59	BA	1071	G
59	BA	1072	C
59	BA	1073	A
59	BA	1077	A
59	BA	1078	U
59	BA	1079	C
59	BA	1082	U
59	BA	1088	A
59	BA	1090	U
59	BA	1095	A
59	BA	1097	U
59	BA	1098	A
59	BA	1101	U
59	BA	1112	G
59	BA	1129	A
59	BA	1130	U
59	BA	1131	G
59	BA	1132	A
59	BA	1133	U
59	BA	1135	C
59	BA	1136	G
59	BA	1139	G
59	BA	1142	A
59	BA	1144	G
59	BA	1155	A
59	BA	1157	G
59	BA	1173	A
59	BA	1174	U
59	BA	1186	G
59	BA	1188	U
59	BA	1199	U
59	BA	1204	A
59	BA	1205	U
59	BA	1210	A
59	BA	1211	U
59	BA	1212	G
59	BA	1213	A
59	BA	1215	G
59	BA	1219(A)	A
59	BA	1220	C
59	BA	1225	G
59	BA	1236	G

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Mol	Chain	Res	Type
59	BA	1239	G
59	BA	1241	A
59	BA	1248	G
59	BA	1250	G
59	BA	1252	G
59	BA	1253	A
59	BA	1256	G
59	BA	1257	C
59	BA	1265	A
59	BA	1266	G
59	BA	1272	A
59	BA	1273	U
59	BA	1274	A
59	BA	1275	A
59	BA	1284	A
59	BA	1287	A
59	BA	1288	U
59	BA	1299	G
59	BA	1300	U
59	BA	1301	A
59	BA	1302	A
59	BA	1303	G
59	BA	1313	U
59	BA	1314	C
59	BA	1321	A
59	BA	1329	U
59	BA	1330	C
59	BA	1331	A
59	BA	1332	G
59	BA	1341	U
59	BA	1345	C
59	BA	1349	A
59	BA	1352	U
59	BA	1359	A
59	BA	1360	A
59	BA	1371	G
59	BA	1378	A
59	BA	1380	G
59	BA	1384	A
59	BA	1385	G
59	BA	1386	C
59	BA	1395	A

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Mol	Chain	Res	Type
59	BA	1396	U
59	BA	1416	G
59	BA	1417	C
59	BA	1420	U
59	BA	1421	G
59	BA	1422	G
59	BA	1427	A
59	BA	1428	C
59	BA	1438	U
59	BA	1444(A)	A
59	BA	1453	A
59	BA	1454	U
59	BA	1455	G
59	BA	1458	C
59	BA	1459	G
59	BA	1461	G
59	BA	1465	G
59	BA	1467	C
59	BA	1468(C)	A
59	BA	1483	G
59	BA	1486	A
59	BA	1490	A
59	BA	1491	G
59	BA	1493	C
59	BA	1494	A
59	BA	1495	A
59	BA	1497	U
59	BA	1498	C
59	BA	1506(C)	A
59	BA	1506(K)	C
59	BA	1506(O)	G
59	BA	1536	A
59	BA	1538	G
59	BA	1541	U
59	BA	1542	G
59	BA	1543	A
59	BA	1543(A)	C
59	BA	1544	A
59	BA	1545	A
59	BA	1546	C
59	BA	1547	C
59	BA	1553	A

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Mol	Chain	Res	Type
59	BA	1554	A
59	BA	1555	G
59	BA	1558	A
59	BA	1559	G
59	BA	1560	G
59	BA	1565	C
59	BA	1566	A
59	BA	1569	A
59	BA	1579	A
59	BA	1581	G
59	BA	1584	C
59	BA	1586	A
59	BA	1598	C
59	BA	1603	A
59	BA	1607	C
59	BA	1610	A
59	BA	1615	C
59	BA	1617	C
59	BA	1618	A
59	BA	1619	G
59	BA	1631	A
59	BA	1635	G
59	BA	1640	C
59	BA	1646	C
59	BA	1648	C
59	BA	1651	G
59	BA	1653	G
59	BA	1654	A
59	BA	1664	A
59	BA	1671	U
59	BA	1673	U
59	BA	1674	G
59	BA	1690	A
59	BA	1695	G
59	BA	1696	G
59	BA	1698	A
59	BA	1702	G
59	BA	1705	G
59	BA	1712(H)	A
59	BA	1712(J)	G
59	BA	1712(K)	A
59	BA	1712(O)	C

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Mol	Chain	Res	Type
59	BA	1750	G
59	BA	1756	G
59	BA	1759	A
59	BA	1763	G
59	BA	1764	G
59	BA	1773	A
59	BA	1781	C
59	BA	1782	C
59	BA	1783	A
59	BA	1784	A
59	BA	1787	A
59	BA	1788	C
59	BA	1793	C
59	BA	1794	U
59	BA	1800	C
59	BA	1801	G
59	BA	1806	C
59	BA	1815	A
59	BA	1816	G
59	BA	1821	A
59	BA	1829	A
59	BA	1831	G
59	BA	1835	G
59	BA	1839	G
59	BA	1840	G
59	BA	1841	U
59	BA	1847	A
59	BA	1848	A
59	BA	1860	G
59	BA	1878	G
59	BA	1888	G
59	BA	1895	C
59	BA	1899	G
59	BA	1900	A
59	BA	1901	A
59	BA	1902	C
59	BA	1906	G
59	BA	1913	A
59	BA	1914	C
59	BA	1915	U
59	BA	1917	U
59	BA	1923	U

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Mol	Chain	Res	Type
59	BA	1927	A
59	BA	1929	G
59	BA	1930	G
59	BA	1933	G
59	BA	1935	G
59	BA	1936	A
59	BA	1938	A
59	BA	1939	U
59	BA	1940	U
59	BA	1944	U
59	BA	1951	U
59	BA	1955	U
59	BA	1961	C
59	BA	1962	C
59	BA	1963	U
59	BA	1965	C
59	BA	1967	C
59	BA	1968	G
59	BA	1970	A
59	BA	1971	A
59	BA	1972	A
59	BA	1981	A
59	BA	1982	C
59	BA	1991	U
59	BA	1992	G
59	BA	1993	U
59	BA	1997	G
59	BA	1998	G
59	BA	2009	G
59	BA	2015	A
59	BA	2019	A
59	BA	2020	A
59	BA	2023	G
59	BA	2025	C
59	BA	2031	A
59	BA	2032	G
59	BA	2033	A
59	BA	2036	C
59	BA	2041	U
59	BA	2042	A
59	BA	2043	C
59	BA	2045	C

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Mol	Chain	Res	Type
59	BA	2047	U
59	BA	2050	C
59	BA	2051	A
59	BA	2055	C
59	BA	2056	G
59	BA	2059	A
59	BA	2060	A
59	BA	2061	G
59	BA	2068	U
59	BA	2069	G
59	BA	2075	U
59	BA	2104	G
59	BA	2105	C
59	BA	2107	C
59	BA	2111	C
59	BA	2112	G
59	BA	2113	U
59	BA	2114	A
59	BA	2116	G
59	BA	2120	G
59	BA	2131	G
59	BA	2132	U
59	BA	2133	G
59	BA	2136	C
59	BA	2144	U
59	BA	2145	C
59	BA	2148	G
59	BA	2154	G
59	BA	2156	G
59	BA	2158	A
59	BA	2159	G
59	BA	2161	C
59	BA	2169	A
59	BA	2170	A
59	BA	2171	A
59	BA	2172	U
59	BA	2185	C
59	BA	2186	G
59	BA	2198	A
59	BA	2202(D)	G
59	BA	2202(E)	A
59	BA	2202(F)	U

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Mol	Chain	Res	Type
59	BA	2223	G
59	BA	2225	A
59	BA	2226	C
59	BA	2232	U
59	BA	2235	G
59	BA	2238	G
59	BA	2243	U
59	BA	2245	U
59	BA	2246	G
59	BA	2247	A
59	BA	2249	U
59	BA	2250	G
59	BA	2251	G
59	BA	2252	G
59	BA	2253	G
59	BA	2254	C
59	BA	2255	G
59	BA	2256	G
59	BA	2259	G
59	BA	2266	A
59	BA	2268	A
59	BA	2270	G
59	BA	2275	C
59	BA	2277	G
59	BA	2278	A
59	BA	2283	C
59	BA	2285	C
59	BA	2286	A
59	BA	2287	A
59	BA	2304	G
59	BA	2305	A
59	BA	2306	C
59	BA	2307	G
59	BA	2308	G
59	BA	2309	A
59	BA	2310	A
59	BA	2319	G
59	BA	2320	A
59	BA	2325	G
59	BA	2334	G
59	BA	2336	A
59	BA	2343	C

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Mol	Chain	Res	Type
59	BA	2345	G
59	BA	2346	A
59	BA	2347	C
59	BA	2367	G
59	BA	2377	A
59	BA	2379	G
59	BA	2382	G
59	BA	2383	G
59	BA	2385	C
59	BA	2402	C
59	BA	2403	C
59	BA	2413	G
59	BA	2423	U
59	BA	2424	C
59	BA	2425	A
59	BA	2427	C
59	BA	2428	G
59	BA	2429	G
59	BA	2430	A
59	BA	2435	A
59	BA	2436	G
59	BA	2439	A
59	BA	2441	C
59	BA	2445	G
59	BA	2446	G
59	BA	2447	G
59	BA	2448	A
59	BA	2449	U
59	BA	2451	A
59	BA	2452	C
59	BA	2456	C
59	BA	2468	G
59	BA	2469	A
59	BA	2470	G
59	BA	2476	A
59	BA	2477	C
59	BA	2478	A
59	BA	2479	G
59	BA	2480	C
59	BA	2484	G
59	BA	2498	C
59	BA	2502	G

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Mol	Chain	Res	Type
59	BA	2503	A
59	BA	2505	G
59	BA	2506	U
59	BA	2516	G
59	BA	2520	C
59	BA	2529	G
59	BA	2533	A
59	BA	2540	C
59	BA	2542	A
59	BA	2543	G
59	BA	2544	G
59	BA	2551	C
59	BA	2552	U
59	BA	2553	G
59	BA	2554	U
59	BA	2555	U
59	BA	2556	C
59	BA	2557	G
59	BA	2558	C
59	BA	2560	C
59	BA	2566	A
59	BA	2567	G
59	BA	2572	A
59	BA	2573	C
59	BA	2574	G
59	BA	2576	G
59	BA	2578	G
59	BA	2582	G
59	BA	2586	C
59	BA	2587	A
59	BA	2602	A
59	BA	2609	U
59	BA	2610	C
59	BA	2611	U
59	BA	2612	C
59	BA	2614	A
59	BA	2620	C
59	BA	2621	A
59	BA	2629	A
59	BA	2630	G
59	BA	2635	C
59	BA	2636	U

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Mol	Chain	Res	Type
59	BA	2639	A
59	BA	2645	G
59	BA	2646	C
59	BA	2653	U
59	BA	2654	A
59	BA	2660	A
59	BA	2665	A
59	BA	2671	A
59	BA	2682	U
59	BA	2686	G
59	BA	2689	U
59	BA	2690	C
59	BA	2691	C
59	BA	2692	C
59	BA	2701	C
59	BA	2702	U
59	BA	2703	C
59	BA	2707	G
59	BA	2712(A)	A
59	BA	2713	A
59	BA	2714	G
59	BA	2725	A
59	BA	2726	U
59	BA	2727	G
59	BA	2732	G
59	BA	2733	A
59	BA	2748	A
59	BA	2751	G
59	BA	2757	A
59	BA	2758	A
59	BA	2764	A
59	BA	2765	A
59	BA	2766	G
59	BA	2772	C
59	BA	2778	A
59	BA	2779	U
59	BA	2780	G
59	BA	2781	A
59	BA	2782	G
59	BA	2790	A
59	BA	2792	G
59	BA	2793	G

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Mol	Chain	Res	Type
59	BA	2794(B)	U
59	BA	2794(E)	A
59	BA	2804	C
59	BA	2805	G
59	BA	2808	U
59	BA	2811	G
59	BA	2820	A
59	BA	2821	A
59	BA	2833	G
59	BA	2835	A
59	BA	2849	U
59	BA	2872	G
59	BA	2876	G
59	BA	2880	C
59	BA	2884	U
59	BA	2892	A
59	BA	2894	G
59	BA	2895	U
60	BB	4	C
60	BB	7	G
60	BB	13	A
60	BB	14	U
60	BB	15	A
60	BB	16	G
60	BB	21	G
60	BB	25	A
60	BB	30	C
60	BB	41	U
60	BB	44	G
60	BB	46	A
60	BB	52	A
60	BB	56	G
60	BB	66	A
60	BB	73	A
60	BB	74	U
60	BB	79	C
60	BB	80	U
60	BB	82	G
60	BB	86	G
60	BB	87	G
60	BB	89(A)	G
60	BB	91	C

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Mol	Chain	Res	Type
60	BB	97	G
60	BB	100	G
60	BB	117	G
21	CA	6	G
21	CA	9	G
21	CA	16	A
21	CA	31	G
21	CA	32	A
21	CA	39	G
21	CA	47	C
21	CA	48	C
21	CA	49	U
21	CA	51	A
21	CA	59	A
21	CA	65	U
21	CA	66	G
21	CA	68	G
21	CA	68(H)	G
21	CA	68(L)	U
21	CA	68(M)	U
21	CA	68(P)	C
21	CA	68(S)	C
21	CA	68(T)	G
21	CA	68(V)	G
21	CA	68(W)	G
21	CA	68(X)	U
21	CA	101	A
21	CA	108	G
21	CA	109	A
21	CA	116	A
21	CA	120	A
21	CA	121	C
21	CA	123	C
21	CA	129	U
21	CA	129(A)	G
21	CA	131	C
21	CA	136	C
21	CA	144	G
21	CA	151	A
21	CA	161	A
21	CA	163	C
21	CA	174	C

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Mol	Chain	Res	Type
21	CA	176	C
21	CA	185	A
21	CA	186(C)	G
21	CA	186(H)	U
21	CA	186(J)	G
21	CA	186(K)	G
21	CA	186(M)	G
21	CA	195	A
21	CA	197	A
21	CA	201	C
21	CA	201(C)	U
21	CA	216	G
21	CA	219	C
21	CA	230	G
21	CA	231	G
21	CA	247	G
21	CA	250	A
21	CA	251	G
21	CA	258	G
21	CA	262	A
21	CA	264	U
21	CA	267	C
21	CA	268	C
21	CA	279	A
21	CA	280	C
21	CA	281	G
21	CA	283	C
21	CA	289	G
21	CA	291	C
21	CA	306	G
21	CA	308	C
21	CA	315	A
21	CA	316	G
21	CA	328	C
21	CA	329	A
21	CA	332	G
21	CA	340	U
21	CA	345	C
21	CA	346	G
21	CA	347	G
21	CA	352	C
21	CA	353	A

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Mol	Chain	Res	Type
21	CA	354	G
21	CA	367	U
21	CA	372	C
21	CA	373	A
21	CA	378	G
21	CA	384	G
21	CA	389	A
21	CA	397	A
21	CA	398	C
21	CA	404	U
21	CA	412	A
21	CA	413	G
21	CA	414	A
21	CA	422	C
21	CA	423	G
21	CA	424	G
21	CA	427	U
21	CA	429	U
21	CA	430	A
21	CA	434	U
21	CA	440	A
21	CA	441	A
21	CA	452	A
21	CA	453	A
21	CA	455	C
21	CA	478	A
21	CA	481	G
21	CA	485	G
21	CA	497	A
21	CA	498	U
21	CA	499	A
21	CA	501	C
21	CA	505	G
21	CA	511	C
21	CA	514	C
21	CA	516	U
21	CA	518	C
21	CA	519	C
21	CA	521	G
21	CA	524	G
21	CA	527	G
21	CA	532	A

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Mol	Chain	Res	Type
21	CA	533	A
21	CA	535	A
21	CA	536	C
21	CA	547	A
21	CA	555	C
21	CA	559	A
21	CA	562	C
21	CA	567	G
21	CA	568	G
21	CA	572	A
21	CA	573	A
21	CA	574	A
21	CA	576	G
21	CA	585	G
21	CA	590	C
21	CA	596	C
21	CA	598	U
21	CA	603	U
21	CA	607	A
21	CA	616	G
21	CA	618	C
21	CA	620	C
21	CA	629	G
21	CA	638	G
21	CA	641	U
21	CA	652	U
21	CA	653	A
21	CA	661	G
21	CA	665	A
21	CA	671	G
21	CA	676	A
21	CA	687	A
21	CA	688	G
21	CA	702	A
21	CA	704	A
21	CA	717	C
21	CA	721	G
21	CA	723	U
21	CA	734	G
21	CA	735	C
21	CA	741	G
21	CA	749	C

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Mol	Chain	Res	Type
21	CA	754	C
21	CA	755	G
21	CA	762	C
21	CA	766	A
21	CA	777	A
21	CA	781	A
21	CA	782	A
21	CA	789	U
21	CA	793	U
21	CA	794	A
21	CA	796	C
21	CA	815	A
21	CA	816	A
21	CA	817	C
21	CA	818	G
21	CA	819	A
21	CA	828	A
21	CA	838(A)	U
21	CA	838(B)	C
21	CA	838(C)	U
21	CA	848	C
21	CA	853	G
21	CA	855	G
21	CA	859	A
21	CA	867	G
21	CA	870	U
21	CA	873	A
21	CA	876	G
21	CA	885	G
21	CA	887	G
21	CA	889	A
21	CA	890	G
21	CA	892	A
21	CA	900	A
21	CA	907	A
21	CA	908	A
21	CA	909	A
21	CA	914	A
21	CA	916	G
21	CA	926	G
21	CA	927	G
21	CA	930	C

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Mol	Chain	Res	Type
21	CA	936	C
21	CA	939	G
21	CA	941	G
21	CA	945	G
21	CA	950	U
21	CA	958	A
21	CA	960	U
21	CA	961	U
21	CA	965	A
21	CA	966	G
21	CA	967	C
21	CA	968	A
21	CA	969	A
21	CA	971	G
21	CA	974	A
21	CA	976	G
21	CA	977	A
21	CA	978	A
21	CA	979	C
21	CA	980	C
21	CA	992	U
21	CA	993	G
21	CA	1004	A
21	CA	1005	A
21	CA	1006	C
21	CA	1008	C
21	CA	1017	G
21	CA	1020	U
21	CA	1024	G
21	CA	1025	U
21	CA	1028(B)	C
21	CA	1028(C)	G
21	CA	1036	G
21	CA	1037	C
21	CA	1041	A
21	CA	1046	A
21	CA	1049	U
21	CA	1054	C
21	CA	1062	U
21	CA	1065	U
21	CA	1066	C
21	CA	1068	G

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Mol	Chain	Res	Type
21	CA	1092	A
21	CA	1094	G
21	CA	1095	U
21	CA	1100	C
21	CA	1101	A
21	CA	1108	G
21	CA	1117	G
21	CA	1123	A
21	CA	1125	U
21	CA	1126	U
21	CA	1130	A
21	CA	1131	G
21	CA	1136	U
21	CA	1137	C
21	CA	1138	G
21	CA	1139	G
21	CA	1140	C
21	CA	1145	C
21	CA	1146	A
21	CA	1152	A
21	CA	1157	A
21	CA	1158	C
21	CA	1159	U
21	CA	1178	G
21	CA	1181	G
21	CA	1184	G
21	CA	1191	A
21	CA	1193	G
21	CA	1196	U
21	CA	1197	G
21	CA	1201	A
21	CA	1202	G
21	CA	1211	U
21	CA	1212	U
21	CA	1213	A
21	CA	1219	U
21	CA	1225	A
21	CA	1226	C
21	CA	1227	A
21	CA	1229	A
21	CA	1237	C
21	CA	1238	A

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Mol	Chain	Res	Type
21	CA	1239	A
21	CA	1240	U
21	CA	1241	G
21	CA	1251	A
21	CA	1252	A
21	CA	1256	A
21	CA	1257	U
21	CA	1262	C
21	CA	1272	G
21	CA	1273	G
21	CA	1278	U
21	CA	1279	A
21	CA	1280	A
21	CA	1281	U
21	CA	1282	C
21	CA	1285	A
21	CA	1286	A
21	CA	1287	A
21	CA	1290	G
21	CA	1298	C
21	CA	1299	A
21	CA	1300	G
21	CA	1301	U
21	CA	1303	C
21	CA	1305	G
21	CA	1306	A
21	CA	1307	U
21	CA	1317	C
21	CA	1321	C
21	CA	1322	C
21	CA	1323	G
21	CA	1330	U
21	CA	1331	G
21	CA	1335	C
21	CA	1336	C
21	CA	1345	U
21	CA	1347	G
21	CA	1359	C
21	CA	1361	G
21	CA	1362(A)	C
21	CA	1363	A
21	CA	1364	U

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Mol	Chain	Res	Type
21	CA	1370	G
21	CA	1374	A
21	CA	1379	G
21	CA	1381	U
21	CA	1386	G
21	CA	1394	A
21	CA	1397	C
21	CA	1401	G
21	CA	1402	C
21	CA	1419	G
21	CA	1422	G
21	CA	1436	U
21	CA	1439	C
21	CA	1440(C)	G
21	CA	1440(D)	A
21	CA	1440(E)	G
21	CA	1440(I)	A
21	CA	1440(J)	C
21	CA	1440(K)	G
21	CA	1440(O)	A
21	CA	1484	C
21	CA	1487	G
21	CA	1492	A
21	CA	1494	G
21	CA	1497	G
21	CA	1502	A
21	CA	1503	A
21	CA	1504	G
21	CA	1505	G
21	CA	1506	U
21	CA	1507	A
21	CA	1517	G
21	CA	1519	A
21	CA	1520	G
21	CA	1525	G
21	CA	1528	U
21	CA	1530	G
21	CA	1531	A
21	CA	1532	U
21	CA	1533	C
21	CA	1534	A
21	CA	1535	C

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Mol	Chain	Res	Type
21	CA	1536	C
21	CA	1538	C
23	CV	3	C
23	CV	4	A
23	CV	5	A
23	CV	8	A
23	CV	9	G
23	CV	10	G
23	CV	11	U
23	CV	12	A
23	CV	13	A
23	CV	14	A
23	CV	15	A
23	CV	16	A
23	CV	17	U
23	CV	18	G
23	CV	19	G
23	CV	20	U
23	CV	21	A
23	CV	22	U
23	CV	24	C
23	CV	26	A
23	CV	27	A
23	CV	28	A
23	CV	30	A
23	CV	31	A
23	CV	32	U
23	CV	35	A
23	CV	36	A
22	CW	2	G
22	CW	3	C
22	CW	8	U
22	CW	10	G
22	CW	12	U
22	CW	13	C
22	CW	14	A
22	CW	15	G
22	CW	16	U
22	CW	18	G
22	CW	19	G
22	CW	20	U
22	CW	20(A)	U

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Mol	Chain	Res	Type
22	CW	21	A
22	CW	22	G
22	CW	24	G
22	CW	25	C
22	CW	26	A
22	CW	27	C
22	CW	29	U
22	CW	32	C
22	CW	34	C
22	CW	37	A
22	CW	38	A
22	CW	42	U
22	CW	43	G
22	CW	44	G
22	CW	45	G
22	CW	46	G
22	CW	47	U
22	CW	48	C
22	CW	50	C
22	CW	52	G
22	CW	56	C
22	CW	57	G
22	CW	58	A
22	CW	59	A
22	CW	60	U
22	CW	61	C
22	CW	63	C
22	CW	64	G
22	CW	74	C
24	CX	5	G
24	CX	8	U
24	CX	16	C
24	CX	17	U
24	CX	18	G
24	CX	20	G
24	CX	21	A
24	CX	24	G
24	CX	25	C
24	CX	28	C
24	CX	42	G
24	CX	44	G
24	CX	45	G

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Mol	Chain	Res	Type
24	CX	47	U
24	CX	48	C
24	CX	49	G
24	CX	50	G
24	CX	52	G
24	CX	53	G
24	CX	57	G
24	CX	58	A
24	CX	60	C
24	CX	61	C
24	CX	64	U
24	CX	65	C
24	CX	68	C
24	CX	72	C
24	CX	73	A
24	CX	74	C
24	CX	76	A
59	DA	8	A
59	DA	10	G
59	DA	11	G
59	DA	12	U
59	DA	17	G
59	DA	25	U
59	DA	34	C
59	DA	35	G
59	DA	46	C
59	DA	49	A
59	DA	51	G
59	DA	57	C
59	DA	63	U
59	DA	64	A
59	DA	73	A
59	DA	74	A
59	DA	75	G
59	DA	84	A
59	DA	88	G
59	DA	91	A
59	DA	95	G
59	DA	98	G
59	DA	101	G
59	DA	102	G
59	DA	115	C

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Mol	Chain	Res	Type
59	DA	116	C
59	DA	117	G
59	DA	118	A
59	DA	120	U
59	DA	137(B)	G
59	DA	137(D)	A
59	DA	150	C
59	DA	155(B)	U
59	DA	155(C)	U
59	DA	155(D)	U
59	DA	175	G
59	DA	181	A
59	DA	186	G
59	DA	193	U
59	DA	195	A
59	DA	196	A
59	DA	197	A
59	DA	204	A
59	DA	205	G
59	DA	210	C
59	DA	216	A
59	DA	221	A
59	DA	222	A
59	DA	225	A
59	DA	228	A
59	DA	229	A
59	DA	230	U
59	DA	233	A
59	DA	235	U
59	DA	241	A
59	DA	248	G
59	DA	252	G
59	DA	256	A
59	DA	264	C
59	DA	269	U
59	DA	270	A
59	DA	270(B)	A
59	DA	270(G)	C
59	DA	270(K)	C
59	DA	270(L)	U
59	DA	270(M)	U
59	DA	270(P)	C

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Mol	Chain	Res	Type
59	DA	270(Q)	C
59	DA	270(S)	G
59	DA	270(U)	C
59	DA	271(C)	U
59	DA	271(D)	G
59	DA	271(F)	G
59	DA	271(M)	G
59	DA	271(N)	G
59	DA	271(P)	C
59	DA	271(Q)	A
59	DA	271(R)	C
59	DA	271(T)	G
59	DA	293	U
59	DA	294	A
59	DA	299	A
59	DA	302	C
59	DA	317	G
59	DA	321	G
59	DA	322	A
59	DA	323	G
59	DA	324	A
59	DA	329	G
59	DA	330	A
59	DA	345	A
59	DA	346	A
59	DA	352	G
59	DA	353	G
59	DA	357(F)	G
59	DA	357(K)	U
59	DA	357(L)	A
59	DA	357(M)	C
59	DA	372	G
59	DA	375	C
59	DA	380	U
59	DA	386	G
59	DA	389	G
59	DA	390	A
59	DA	394	A
59	DA	405	U
59	DA	409	C
59	DA	411	G
59	DA	412	A

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Mol	Chain	Res	Type
59	DA	421	U
59	DA	431	U
59	DA	439	G
59	DA	444	C
59	DA	449	A
59	DA	451	C
59	DA	456	C
59	DA	457	A
59	DA	467	G
59	DA	470	A
59	DA	473	G
59	DA	475	U
59	DA	476	G
59	DA	480	A
59	DA	481	G
59	DA	482	A
59	DA	505	A
59	DA	508	G
59	DA	509	C
59	DA	510	C
59	DA	517	C
59	DA	527	C
59	DA	528	A
59	DA	530	G
59	DA	531	C
59	DA	532	A
59	DA	540	C
59	DA	543(B)	C
59	DA	543(C)	A
59	DA	550	G
59	DA	559	G
59	DA	563	G
59	DA	573	G
59	DA	575	A
59	DA	577	G
59	DA	582	G
59	DA	586	A
59	DA	588	U
59	DA	603	A
59	DA	604	G
59	DA	611	C
59	DA	611(A)	C

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Mol	Chain	Res	Type
59	DA	611(E)	G
59	DA	611(F)	A
59	DA	611(G)	G
59	DA	621	A
59	DA	627	A
59	DA	629	G
59	DA	634	C
59	DA	636	G
59	DA	637	A
59	DA	645	C
59	DA	646	A
59	DA	654	U
59	DA	655	A
59	DA	662	G
59	DA	668	G
59	DA	670	A
59	DA	671	C
59	DA	686	G
59	DA	699	A
59	DA	701	G
59	DA	723	G
59	DA	730	C
59	DA	734	A
59	DA	747	U
59	DA	748	G
59	DA	755	C
59	DA	760	G
59	DA	764	A
59	DA	765	G
59	DA	771	G
59	DA	775	G
59	DA	776	G
59	DA	782	A
59	DA	784	A
59	DA	785	G
59	DA	788	A
59	DA	790	C
59	DA	791	C
59	DA	792	G
59	DA	796	C
59	DA	800	A
59	DA	805	G

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Mol	Chain	Res	Type
59	DA	806	C
59	DA	808	G
59	DA	812	C
59	DA	819	A
59	DA	827	U
59	DA	828	U
59	DA	843	G
59	DA	844	C
59	DA	846	C
59	DA	847	U
59	DA	859	G
59	DA	861	A
59	DA	874	G
59	DA	882	G
59	DA	885	C
59	DA	886	C
59	DA	887	A
59	DA	890	A
59	DA	896	A
59	DA	897	C
59	DA	898	C
59	DA	903	C
59	DA	907	U
59	DA	910	A
59	DA	917	A
59	DA	918	A
59	DA	919	G
59	DA	921	G
59	DA	929	G
59	DA	932	G
59	DA	933	A
59	DA	938	G
59	DA	941	A
59	DA	945	A
59	DA	946	G
59	DA	948	G
59	DA	959	A
59	DA	961	C
59	DA	962	G
59	DA	963	U
59	DA	964	C
59	DA	967	C

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Mol	Chain	Res	Type
59	DA	972	G
59	DA	974	G
59	DA	974(A)	C
59	DA	980	A
59	DA	983	A
59	DA	985	C
59	DA	988	A
59	DA	990	A
59	DA	996	A
59	DA	1003	G
59	DA	1004	C
59	DA	1005	C
59	DA	1006	C
59	DA	1009	A
59	DA	1011	G
59	DA	1012	U
59	DA	1013	C
59	DA	1022	G
59	DA	1023	U
59	DA	1025	G
59	DA	1026	U
59	DA	1033	U
59	DA	1047	G
59	DA	1048	A
59	DA	1051	G
59	DA	1053	C
59	DA	1060	U
59	DA	1065	U
59	DA	1070	A
59	DA	1072	C
59	DA	1073	A
59	DA	1074	G
59	DA	1077	A
59	DA	1083	U
59	DA	1086	A
59	DA	1088	A
59	DA	1090	U
59	DA	1098	A
59	DA	1100	C
59	DA	1105	U
59	DA	1111	A
59	DA	1112	G

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Mol	Chain	Res	Type
59	DA	1115	G
59	DA	1129	A
59	DA	1130	U
59	DA	1135	C
59	DA	1136	G
59	DA	1137	G
59	DA	1142	A
59	DA	1143	A
59	DA	1146	C
59	DA	1154	G
59	DA	1155	A
59	DA	1157	G
59	DA	1173	A
59	DA	1174	U
59	DA	1175	G
59	DA	1178	C
59	DA	1186	G
59	DA	1198	U
59	DA	1199	U
59	DA	1204	A
59	DA	1205	U
59	DA	1210	A
59	DA	1211	U
59	DA	1212	G
59	DA	1219(A)	A
59	DA	1220	C
59	DA	1221	C
59	DA	1229	G
59	DA	1235	G
59	DA	1241	A
59	DA	1244	G
59	DA	1248	G
59	DA	1250	G
59	DA	1253	A
59	DA	1255	U
59	DA	1256	G
59	DA	1271	G
59	DA	1272	A
59	DA	1273	U
59	DA	1285	G
59	DA	1287	A
59	DA	1289	C

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Mol	Chain	Res	Type
59	DA	1295	C
59	DA	1296	G
59	DA	1300	U
59	DA	1301	A
59	DA	1302	A
59	DA	1303	G
59	DA	1309	G
59	DA	1313	U
59	DA	1314	C
59	DA	1324	G
59	DA	1325	G
59	DA	1329	U
59	DA	1332	G
59	DA	1341	U
59	DA	1343	G
59	DA	1345	C
59	DA	1349	A
59	DA	1352	U
59	DA	1359	A
59	DA	1360	A
59	DA	1366	A
59	DA	1372	U
59	DA	1378	A
59	DA	1380	G
59	DA	1382	G
59	DA	1384	A
59	DA	1385	G
59	DA	1392	A
59	DA	1395	A
59	DA	1396	U
59	DA	1398	C
59	DA	1416	G
59	DA	1420	U
59	DA	1421	G
59	DA	1428	C
59	DA	1438	U
59	DA	1441	G
59	DA	1443	G
59	DA	1444(A)	A
59	DA	1453	A
59	DA	1454	U
59	DA	1455	G

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Mol	Chain	Res	Type
59	DA	1461	G
59	DA	1465	G
59	DA	1467	C
59	DA	1468(C)	A
59	DA	1468(H)	C
59	DA	1468(I)	A
59	DA	1483	G
59	DA	1484	G
59	DA	1490	A
59	DA	1491	G
59	DA	1493	C
59	DA	1494	A
59	DA	1495	A
59	DA	1497	U
59	DA	1498	C
59	DA	1506(B)	A
59	DA	1506(C)	A
59	DA	1538	G
59	DA	1540	G
59	DA	1541	U
59	DA	1542	G
59	DA	1543(A)	C
59	DA	1545	A
59	DA	1547	C
59	DA	1551	C
59	DA	1554	A
59	DA	1558	A
59	DA	1565	C
59	DA	1566	A
59	DA	1569	A
59	DA	1572	A
59	DA	1575	C
59	DA	1576	U
59	DA	1579	A
59	DA	1581	G
59	DA	1584	C
59	DA	1586	A
59	DA	1589	C
59	DA	1598	C
59	DA	1607	C
59	DA	1608	A
59	DA	1610	A

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Mol	Chain	Res	Type
59	DA	1613	G
59	DA	1615	C
59	DA	1617	C
59	DA	1618	A
59	DA	1627	G
59	DA	1645	G
59	DA	1646	C
59	DA	1648	C
59	DA	1651	G
59	DA	1653	G
59	DA	1654	A
59	DA	1664	A
59	DA	1665	A
59	DA	1667	G
59	DA	1670	C
59	DA	1671	U
59	DA	1674	G
59	DA	1678	G
59	DA	1696	G
59	DA	1698	A
59	DA	1708	C
59	DA	1712(F)	U
59	DA	1712(J)	G
59	DA	1712(K)	A
59	DA	1712(L)	G
59	DA	1712(Q)	G
59	DA	1756	G
59	DA	1763	G
59	DA	1764	G
59	DA	1769	G
59	DA	1773	A
59	DA	1775	U
59	DA	1793	C
59	DA	1800	C
59	DA	1801	G
59	DA	1803	A
59	DA	1816	G
59	DA	1819	A
59	DA	1821	A
59	DA	1829	A
59	DA	1830	C
59	DA	1832	C

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Mol	Chain	Res	Type
59	DA	1835	G
59	DA	1840	G
59	DA	1847	A
59	DA	1878	G
59	DA	1888	G
59	DA	1889	A
59	DA	1895	C
59	DA	1900	A
59	DA	1902	C
59	DA	1904	G
59	DA	1905	C
59	DA	1906	G
59	DA	1913	A
59	DA	1914	C
59	DA	1919	A
59	DA	1927	A
59	DA	1929	G
59	DA	1930	G
59	DA	1934	C
59	DA	1936	A
59	DA	1937	A
59	DA	1938	A
59	DA	1939	U
59	DA	1955	U
59	DA	1964	G
59	DA	1965	C
59	DA	1966	A
59	DA	1967	C
59	DA	1968	G
59	DA	1970	A
59	DA	1971	A
59	DA	1972	A
59	DA	1974	C
59	DA	1981	A
59	DA	1982	C
59	DA	1984	G
59	DA	1987	G
59	DA	1992	G
59	DA	1993	U
59	DA	1997	G
59	DA	2011	U
59	DA	2014	A

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Mol	Chain	Res	Type
59	DA	2020	A
59	DA	2027	G
59	DA	2031	A
59	DA	2032	G
59	DA	2033	A
59	DA	2034	U
59	DA	2036	C
59	DA	2041	U
59	DA	2043	C
59	DA	2045	C
59	DA	2047	U
59	DA	2052	G
59	DA	2055	C
59	DA	2056	G
59	DA	2060	A
59	DA	2061	G
59	DA	2069	G
59	DA	2077	A
59	DA	2080	G
59	DA	2093	G
59	DA	2108	C
59	DA	2111	C
59	DA	2112	G
59	DA	2118	U
59	DA	2120	G
59	DA	2126	A
59	DA	2132	U
59	DA	2133	G
59	DA	2136	C
59	DA	2147	G
59	DA	2153	G
59	DA	2156	G
59	DA	2158	A
59	DA	2159	G
59	DA	2160	G
59	DA	2172	U
59	DA	2185	C
59	DA	2190	G
59	DA	2193	G
59	DA	2195	C
59	DA	2202(D)	G
59	DA	2202(E)	A

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Mol	Chain	Res	Type
59	DA	2202(F)	U
59	DA	2202(G)	G
59	DA	2225	A
59	DA	2238	G
59	DA	2239	G
59	DA	2245	U
59	DA	2247	A
59	DA	2250	G
59	DA	2251	G
59	DA	2252	G
59	DA	2253	G
59	DA	2254	C
59	DA	2257	U
59	DA	2259	G
59	DA	2266	A
59	DA	2267	A
59	DA	2268	A
59	DA	2269	A
59	DA	2272	U
59	DA	2273	A
59	DA	2275	C
59	DA	2282	G
59	DA	2283	C
59	DA	2285	C
59	DA	2287	A
59	DA	2288	A
59	DA	2304	G
59	DA	2305	A
59	DA	2306	C
59	DA	2309	A
59	DA	2310	A
59	DA	2311	A
59	DA	2319	G
59	DA	2320	A
59	DA	2322	A
59	DA	2323	G
59	DA	2325	G
59	DA	2327	A
59	DA	2334	G
59	DA	2336	A
59	DA	2343	C
59	DA	2345	G

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Mol	Chain	Res	Type
59	DA	2347	C
59	DA	2348	U
59	DA	2350	C
59	DA	2353	G
59	DA	2354	G
59	DA	2379	G
59	DA	2381	C
59	DA	2383	G
59	DA	2385	C
59	DA	2387	U
59	DA	2391	G
59	DA	2392	A
59	DA	2400	G
59	DA	2402	C
59	DA	2403	C
59	DA	2418	A
59	DA	2423	U
59	DA	2425	A
59	DA	2427	C
59	DA	2428	G
59	DA	2429	G
59	DA	2430	A
59	DA	2431	U
59	DA	2435	A
59	DA	2436	G
59	DA	2439	A
59	DA	2441	C
59	DA	2447	G
59	DA	2448	A
59	DA	2451	A
59	DA	2452	C
59	DA	2464	C
59	DA	2468	G
59	DA	2469	A
59	DA	2470	G
59	DA	2476	A
59	DA	2484	G
59	DA	2495	G
59	DA	2498	C
59	DA	2501	C
59	DA	2502	G
59	DA	2504	U

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Mol	Chain	Res	Type
59	DA	2505	G
59	DA	2506	U
59	DA	2507	C
59	DA	2508	G
59	DA	2513	G
59	DA	2518	A
59	DA	2520	C
59	DA	2529	G
59	DA	2531	A
59	DA	2534	A
59	DA	2542	A
59	DA	2543	G
59	DA	2549	G
59	DA	2552	U
59	DA	2553	G
59	DA	2554	U
59	DA	2555	U
59	DA	2558	C
59	DA	2561	A
59	DA	2562	U
59	DA	2564	A
59	DA	2566	A
59	DA	2567	G
59	DA	2572	A
59	DA	2573	C
59	DA	2576	G
59	DA	2579	C
59	DA	2586	C
59	DA	2587	A
59	DA	2599	G
59	DA	2602	A
59	DA	2604	U
59	DA	2610	C
59	DA	2611	U
59	DA	2612	C
59	DA	2613	U
59	DA	2620	C
59	DA	2621	A
59	DA	2629	A
59	DA	2630	G
59	DA	2632	A
59	DA	2634	G

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Mol	Chain	Res	Type
59	DA	2637	U
59	DA	2638	G
59	DA	2645	G
59	DA	2646	C
59	DA	2651	C
59	DA	2654	A
59	DA	2662	A
59	DA	2664	G
59	DA	2665	A
59	DA	2682	U
59	DA	2687	U
59	DA	2689	U
59	DA	2690	C
59	DA	2691	C
59	DA	2693	A
59	DA	2702	U
59	DA	2703	C
59	DA	2712(A)	A
59	DA	2713	A
59	DA	2714	G
59	DA	2726	U
59	DA	2733	A
59	DA	2751	G
59	DA	2757	A
59	DA	2764	A
59	DA	2765	A
59	DA	2768	C
59	DA	2769	C
59	DA	2778	A
59	DA	2779	U
59	DA	2780	G
59	DA	2781	A
59	DA	2782	G
59	DA	2790	A
59	DA	2791	C
59	DA	2792	G
59	DA	2793	G
59	DA	2794	C
59	DA	2794(B)	U
59	DA	2794(D)	A
59	DA	2802	G
59	DA	2808	U

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Mol	Chain	Res	Type
59	DA	2819	G
59	DA	2820	A
59	DA	2821	A
59	DA	2833	G
59	DA	2835	A
59	DA	2842	G
59	DA	2849	U
59	DA	2850	A
59	DA	2854	G
59	DA	2861	G
59	DA	2872	G
59	DA	2876	G
59	DA	2877	G
59	DA	2880	C
59	DA	2881	C
59	DA	2884	U
59	DA	2886	G
59	DA	2892	A
60	DB	2	C
60	DB	12	C
60	DB	13	A
60	DB	14	U
60	DB	15	A
60	DB	16	G
60	DB	20	C
60	DB	21	G
60	DB	23	G
60	DB	25	A
60	DB	30	C
60	DB	40	U
60	DB	41	U
60	DB	44	G
60	DB	50	G
60	DB	52	A
60	DB	56	G
60	DB	60	C
60	DB	64	C
60	DB	66	A
60	DB	67	G
60	DB	73	A
60	DB	74	U
60	DB	79	C

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Mol	Chain	Res	Type
60	DB	80	U
60	DB	82	G
60	DB	86	G
60	DB	90	C
60	DB	97	G
60	DB	99	A
60	DB	108	C
60	DB	109	G

All (109) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	266	G
21	AA	328	C
21	AA	687	A
21	AA	748	C
21	AA	815	A
21	AA	992	U
21	AA	1139	G
21	AA	1182	G
21	AA	1200	C
21	AA	1280	A
21	AA	1285	A
21	AA	1297	C
21	AA	1300	G
21	AA	1358	U
21	AA	1504	G
21	AA	1537	U
22	AW	7	G
23	AV	6	G
23	AV	14	A
23	AV	16	A
23	AV	26	A
23	AV	27	A
23	AV	29	A
23	AV	30	A
23	AV	34	A
23	AV	35	A
24	AX	71	C
59	BA	214	G
59	BA	221	A
59	BA	271(B)	G

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Mol	Chain	Res	Type
59	BA	357(L)	A
59	BA	474	G
59	BA	479	A
59	BA	611(F)	A
59	BA	775	G
59	BA	846	C
59	BA	880	G
59	BA	895	U
59	BA	961	C
59	BA	963	U
59	BA	1012	U
59	BA	1022	G
59	BA	1187	G
59	BA	1210	A
59	BA	1240	U
59	BA	1300	U
59	BA	1558	A
59	BA	1663	C
59	BA	2111	C
59	BA	2250	G
59	BA	2422	A
59	BA	2447	G
59	BA	2585	U
59	BA	2613	U
59	BA	2780	G
21	CA	5	U
21	CA	68(U)	U
21	CA	115	G
21	CA	266	G
21	CA	328	C
21	CA	429	U
21	CA	748	C
21	CA	992	U
21	CA	1064	G
21	CA	1067	A
21	CA	1200	C
21	CA	1280	A
21	CA	1285	A
21	CA	1300	G
21	CA	1504	G
21	CA	1537	U
23	CV	14	A

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Mol	Chain	Res	Type
23	CV	16	A
23	CV	18	G
23	CV	26	A
23	CV	27	A
23	CV	34	A
23	CV	35	A
22	CW	7	G
22	CW	26	A
59	DA	137(E)	A
59	DA	221	A
59	DA	271(B)	G
59	DA	479	A
59	DA	481	G
59	DA	611(F)	A
59	DA	733	G
59	DA	775	G
59	DA	846	C
59	DA	889	C
59	DA	1022	G
59	DA	1110	G
59	DA	1210	A
59	DA	1240	U
59	DA	1300	U
59	DA	1506(A)	A
59	DA	1964	G
59	DA	1966	A
59	DA	2202(E)	A
59	DA	2422	A
59	DA	2438	U
59	DA	2447	G
59	DA	2497	A
59	DA	2503	A
59	DA	2553	G
59	DA	2585	U
59	DA	2598	A
59	DA	2689	U
59	DA	2756	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
63	NMY	BA	2903	-	45,45,45	0.60	0	63,67,67	0.97	4 (6%)
63	NMY	AA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	BA	2904	-	45,45,45	0.59	0	63,67,67	0.97	4 (6%)
61	GDP	CY	701	-	24,30,30	1.30	3 (12%)	30,47,47	1.69	8 (26%)
63	NMY	CA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	DA	2901	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	BA	2902	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
62	FUA	CY	702	-	39,40,40	1.67	7 (17%)	49,64,64	1.52	6 (12%)
62	FUA	AY	702	-	39,40,40	1.67	7 (17%)	49,64,64	1.52	6 (12%)
61	GDP	AY	701	-	24,30,30	1.37	4 (16%)	30,47,47	1.76	8 (26%)

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
63	NMY	BA	2903	-	-	12/18/94/94	0/4/4/4
63	NMY	AA	1601	-	-	12/18/94/94	0/4/4/4
63	NMY	BA	2904	-	-	12/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	5/12/32/32	0/3/3/3
63	NMY	CA	1601	-	-	12/18/94/94	0/4/4/4
63	NMY	DA	2901	-	-	12/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	NMY	BA	2902	-	-	12/18/94/94	0/4/4/4
62	FUA	CY	702	-	-	6/15/92/92	0/4/4/4
62	FUA	AY	702	-	-	6/15/92/92	0/4/4/4
61	GDP	AY	701	-	-	3/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-4.39	1.39	1.51
62	AY	702	FUA	C23-C22	-4.33	1.40	1.51
62	AY	702	FUA	C23-C24	-4.28	1.39	1.53
62	CY	702	FUA	C23-C24	-4.26	1.39	1.53
61	AY	701	GDP	C5-C6	-4.22	1.38	1.47
62	CY	702	FUA	C29-C22	4.17	1.53	1.47
62	AY	702	FUA	C29-C22	4.17	1.53	1.47
61	CY	701	GDP	C5-C6	-3.97	1.39	1.47
62	AY	702	FUA	C24-C25	-3.27	1.39	1.50
62	CY	702	FUA	C24-C25	-3.26	1.39	1.50
62	CY	702	FUA	C14-C8	-3.15	1.53	1.59
62	AY	702	FUA	C14-C8	-3.14	1.53	1.59
62	CY	702	FUA	C25-C26	2.41	1.39	1.32
62	AY	702	FUA	C25-C26	2.39	1.39	1.32
61	CY	701	GDP	O4'-C1'	2.16	1.44	1.41
61	AY	701	GDP	O4'-C1'	2.16	1.44	1.41
62	AY	702	FUA	C10-C9	-2.13	1.53	1.57
61	AY	701	GDP	C8-N7	-2.10	1.31	1.35
62	CY	702	FUA	C10-C9	-2.08	1.53	1.57
61	CY	701	GDP	PB-O3B	-2.05	1.46	1.54
61	AY	701	GDP	C5-C4	-2.05	1.37	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	CY	702	FUA	C13-C12-C11	-4.32	105.84	111.90
62	AY	702	FUA	C13-C12-C11	-4.31	105.87	111.90
62	AY	702	FUA	C16-O2-C31	-3.90	111.13	117.06
62	CY	702	FUA	C16-O2-C31	-3.88	111.16	117.06
61	CY	701	GDP	C2-N1-C6	-3.85	118.01	125.10
61	AY	701	GDP	PA-O3A-PB	-3.53	120.70	132.83
62	CY	702	FUA	C8-C9-C10	-3.51	112.75	116.34
62	AY	702	FUA	C8-C9-C10	-3.47	112.79	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	CY	701	GDP	C5-C6-N1	3.30	119.78	113.95
61	AY	701	GDP	C5'-C4'-C3'	-3.08	103.62	115.18
61	AY	701	GDP	O5'-C5'-C4'	3.02	119.39	108.99
61	AY	701	GDP	C5-C6-N1	3.00	119.25	113.95
62	AY	702	FUA	O2-C31-C32	2.98	116.56	111.09
62	CY	702	FUA	O2-C31-C32	2.97	116.56	111.09
61	CY	701	GDP	C8-N7-C5	2.93	108.56	102.99
61	AY	701	GDP	C8-N7-C5	2.91	108.53	102.99
63	CA	1601	NMY	C13-O11-C11	-2.86	110.89	117.96
63	AA	1601	NMY	C13-O11-C11	-2.86	110.89	117.96
63	BA	2903	NMY	C13-O11-C11	-2.86	110.89	117.96
63	BA	2904	NMY	C13-O11-C11	-2.86	110.89	117.96
63	BA	2902	NMY	C13-O11-C11	-2.85	110.92	117.96
63	DA	2901	NMY	C13-O11-C11	-2.85	110.92	117.96
61	CY	701	GDP	PA-O3A-PB	-2.83	123.12	132.83
61	CY	701	GDP	C5'-C4'-C3'	-2.82	104.61	115.18
61	AY	701	GDP	C2-N1-C6	-2.79	119.96	125.10
61	AY	701	GDP	O4'-C1'-C2'	-2.70	102.98	106.93
61	CY	701	GDP	O4'-C1'-C2'	-2.64	103.06	106.93
61	CY	701	GDP	O6-C6-C5	-2.36	119.76	124.37
62	AY	702	FUA	C28-C26-C27	2.35	119.79	114.60
62	CY	702	FUA	C28-C26-C27	2.35	119.79	114.60
63	BA	2903	NMY	O22-C22-C23	2.32	110.32	106.01
63	AA	1601	NMY	O22-C22-C23	2.29	110.27	106.01
63	BA	2904	NMY	O22-C22-C23	2.28	110.26	106.01
63	CA	1601	NMY	O22-C22-C23	2.28	110.25	106.01
63	BA	2902	NMY	O22-C22-C23	2.27	110.23	106.01
63	DA	2901	NMY	O22-C22-C23	2.26	110.21	106.01
61	CY	701	GDP	O2B-PB-O1B	2.25	119.50	110.68
63	BA	2902	NMY	C13-C14-C15	2.22	104.78	102.10
63	CA	1601	NMY	C13-C14-C15	2.22	104.78	102.10
63	BA	2904	NMY	C13-C14-C15	2.22	104.77	102.10
63	DA	2901	NMY	C13-C14-C15	2.21	104.76	102.10
63	AA	1601	NMY	C13-C14-C15	2.21	104.76	102.10
63	BA	2903	NMY	C13-C14-C15	2.20	104.75	102.10
61	AY	701	GDP	N1-C2-N3	-2.16	119.28	123.32
63	BA	2904	NMY	C1-O1-C10	-2.10	112.77	117.96
63	BA	2902	NMY	C1-O1-C10	-2.08	112.81	117.96
63	DA	2901	NMY	C1-O1-C10	-2.08	112.81	117.96
63	BA	2903	NMY	C1-O1-C10	-2.08	112.82	117.96
63	CA	1601	NMY	C1-O1-C10	-2.07	112.83	117.96
62	CY	702	FUA	C21-C14-C8	-2.07	110.36	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	AA	1601	NMY	C1-O1-C10	-2.06	112.86	117.96
62	AY	702	FUA	C21-C14-C8	-2.05	110.38	112.27

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	GDP	PA-O3A-PB-O3B
61	CY	701	GDP	C5'-O5'-PA-O3A
61	CY	701	GDP	C5'-O5'-PA-O1A
61	CY	701	GDP	C5'-O5'-PA-O2A
61	CY	701	GDP	O4'-C4'-C5'-O5'
62	AY	702	FUA	C13-C17-C22-C29
62	AY	702	FUA	C17-C22-C23-C24
62	AY	702	FUA	C29-C22-C23-C24
62	CY	702	FUA	C13-C17-C22-C29
62	CY	702	FUA	C17-C22-C23-C24
62	CY	702	FUA	C29-C22-C23-C24
63	AA	1601	NMY	C4-C5-C6-N6
63	AA	1601	NMY	O5-C5-C6-N6
63	AA	1601	NMY	C14-C13-O11-C11
63	AA	1601	NMY	C16-C15-O18-C18
63	AA	1601	NMY	C19-C18-O18-C15
63	BA	2902	NMY	C4-C5-C6-N6
63	BA	2902	NMY	O5-C5-C6-N6
63	BA	2902	NMY	C14-C13-O11-C11
63	BA	2902	NMY	C16-C15-O18-C18
63	BA	2902	NMY	C19-C18-O18-C15
63	BA	2903	NMY	C4-C5-C6-N6
63	BA	2903	NMY	O5-C5-C6-N6
63	BA	2903	NMY	C14-C13-O11-C11
63	BA	2903	NMY	C16-C15-O18-C18
63	BA	2903	NMY	C19-C18-O18-C15
63	BA	2904	NMY	C4-C5-C6-N6
63	BA	2904	NMY	O5-C5-C6-N6
63	BA	2904	NMY	C14-C13-O11-C11
63	BA	2904	NMY	C16-C15-O18-C18
63	BA	2904	NMY	C19-C18-O18-C15
63	CA	1601	NMY	C4-C5-C6-N6
63	CA	1601	NMY	O5-C5-C6-N6
63	CA	1601	NMY	C14-C13-O11-C11
63	CA	1601	NMY	C16-C15-O18-C18

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Mol	Chain	Res	Type	Atoms
63	CA	1601	NMY	C19-C18-O18-C15
63	DA	2901	NMY	C4-C5-C6-N6
63	DA	2901	NMY	O5-C5-C6-N6
63	DA	2901	NMY	C14-C13-O11-C11
63	DA	2901	NMY	C16-C15-O18-C18
63	DA	2901	NMY	C19-C18-O18-C15
63	AA	1601	NMY	C15-C16-C17-O17
63	BA	2902	NMY	C15-C16-C17-O17
63	BA	2903	NMY	C15-C16-C17-O17
63	BA	2904	NMY	C15-C16-C17-O17
63	CA	1601	NMY	C15-C16-C17-O17
63	DA	2901	NMY	C15-C16-C17-O17
62	AY	702	FUA	C32-C31-O2-C16
62	CY	702	FUA	C32-C31-O2-C16
62	AY	702	FUA	O3-C31-O2-C16
62	CY	702	FUA	O3-C31-O2-C16
63	AA	1601	NMY	O16-C16-C17-O17
63	BA	2902	NMY	O16-C16-C17-O17
63	BA	2903	NMY	O16-C16-C17-O17
63	BA	2904	NMY	O16-C16-C17-O17
63	CA	1601	NMY	O16-C16-C17-O17
63	DA	2901	NMY	O16-C16-C17-O17
61	CY	701	GDP	C3'-C4'-C5'-O5'
63	AA	1601	NMY	O16-C13-O11-C11
63	BA	2902	NMY	O16-C13-O11-C11
63	BA	2903	NMY	O16-C13-O11-C11
63	BA	2904	NMY	O16-C13-O11-C11
63	CA	1601	NMY	O16-C13-O11-C11
63	DA	2901	NMY	O16-C13-O11-C11
63	AA	1601	NMY	O22-C18-O18-C15
63	BA	2904	NMY	O22-C18-O18-C15
63	CA	1601	NMY	O22-C18-O18-C15
63	BA	2902	NMY	O22-C18-O18-C15
63	BA	2903	NMY	O22-C18-O18-C15
63	DA	2901	NMY	O22-C18-O18-C15
63	AA	1601	NMY	C11-C10-O1-C1
63	BA	2902	NMY	C11-C10-O1-C1
63	BA	2903	NMY	C11-C10-O1-C1
63	BA	2904	NMY	C11-C10-O1-C1
63	CA	1601	NMY	C11-C10-O1-C1
63	DA	2901	NMY	C11-C10-O1-C1
63	AA	1601	NMY	C12-C11-O11-C13

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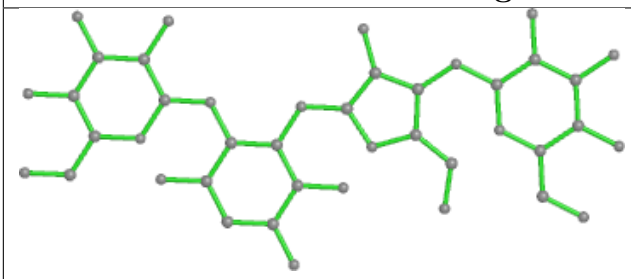
Mol	Chain	Res	Type	Atoms
63	BA	2902	NMY	C12-C11-O11-C13
63	BA	2904	NMY	C12-C11-O11-C13
63	CA	1601	NMY	C12-C11-O11-C13
63	DA	2901	NMY	C12-C11-O11-C13
63	BA	2903	NMY	C12-C11-O11-C13
61	AY	701	GDP	C5'-O5'-PA-O3A
63	CA	1601	NMY	C10-C11-O11-C13
63	AA	1601	NMY	C10-C11-O11-C13
63	BA	2902	NMY	C10-C11-O11-C13
63	BA	2903	NMY	C10-C11-O11-C13
63	BA	2904	NMY	C10-C11-O11-C13
63	DA	2901	NMY	C10-C11-O11-C13
62	AY	702	FUA	C23-C24-C25-C26
62	CY	702	FUA	C23-C24-C25-C26
61	AY	701	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

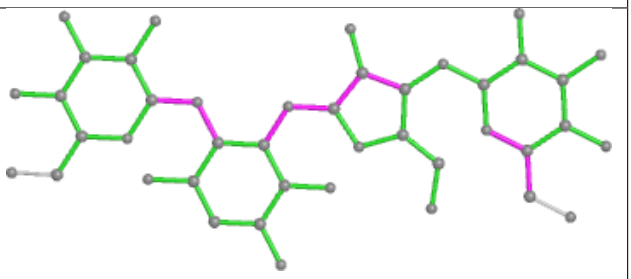
No monomer is involved in short contacts.

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 then 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.

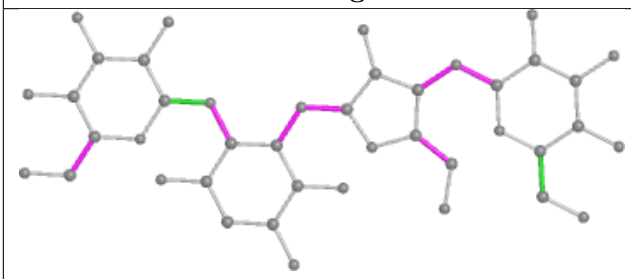
Ligand NMY BA 2903



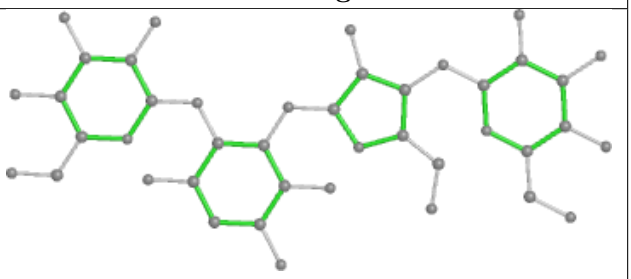
Bond lengths



Bond angles

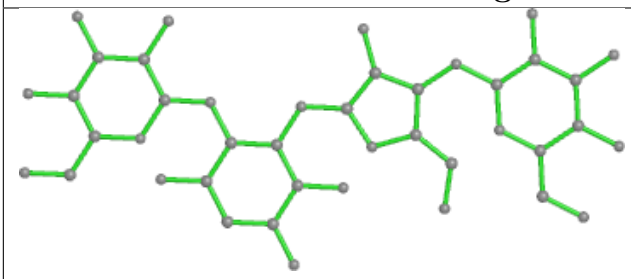


Torsions

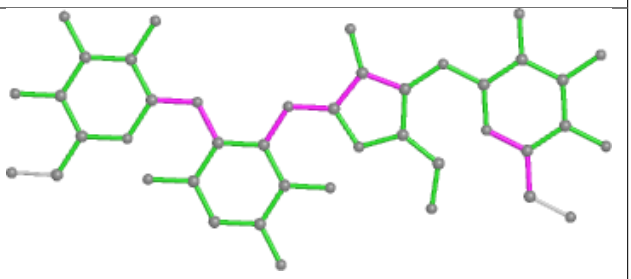


Rings

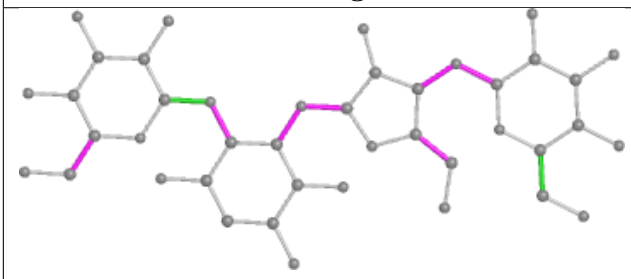
Ligand NMY AA 1601



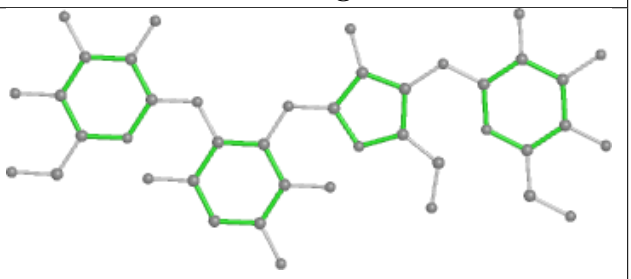
Bond lengths



Bond angles

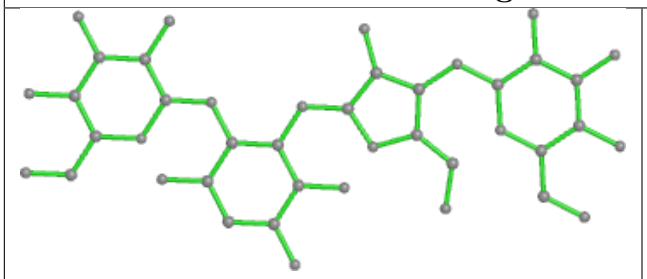


Torsions

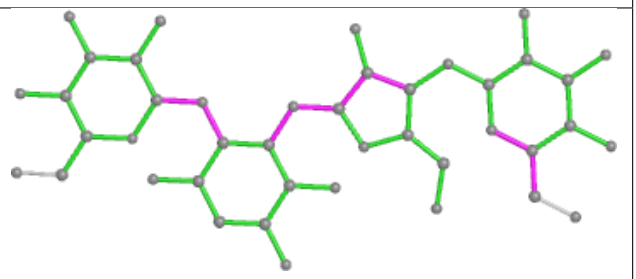


Rings

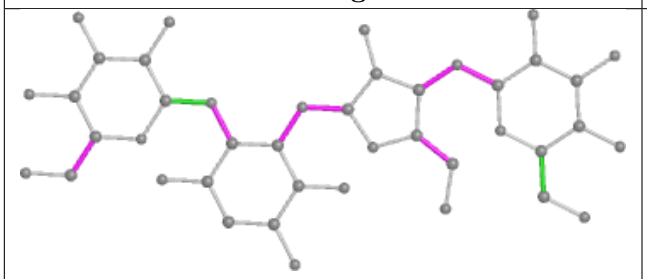
Ligand NMY BA 2904



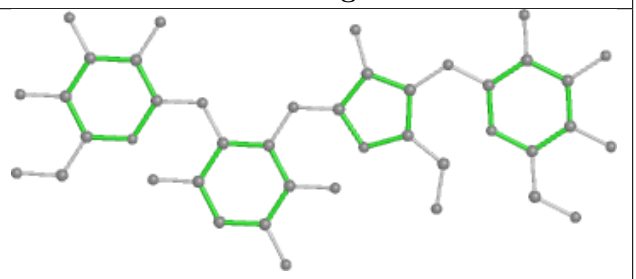
Bond lengths



Bond angles

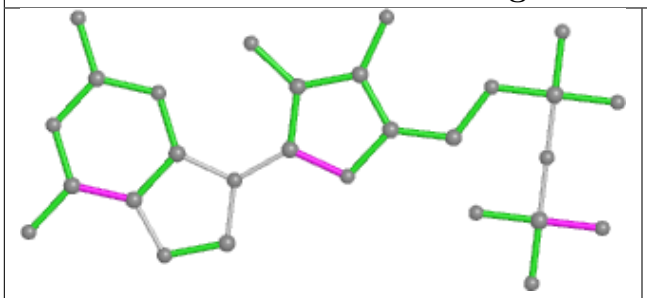


Torsions

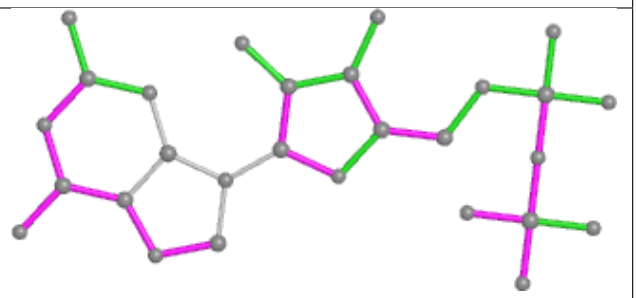


Rings

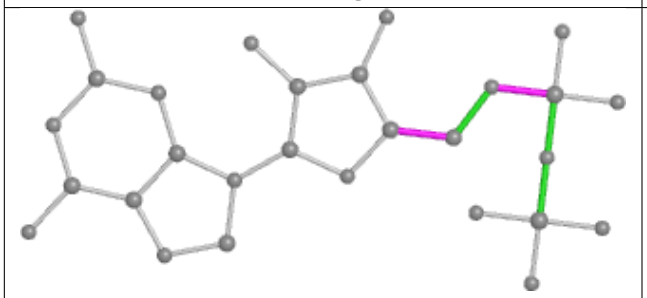
Ligand GDP CY 701



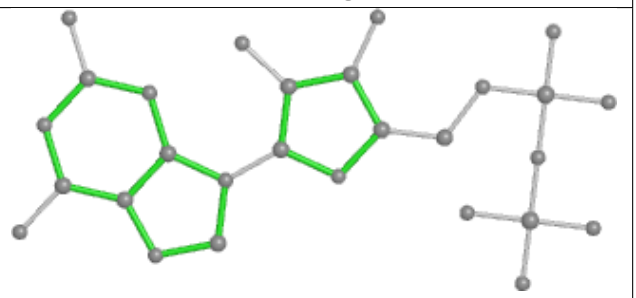
Bond lengths



Bond angles

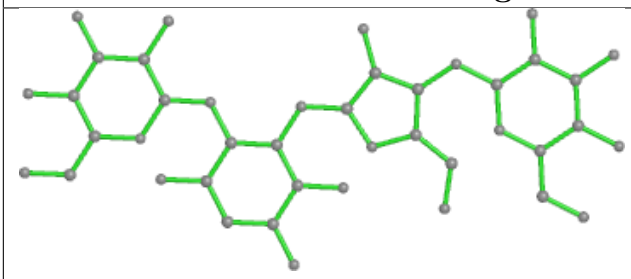


Torsions

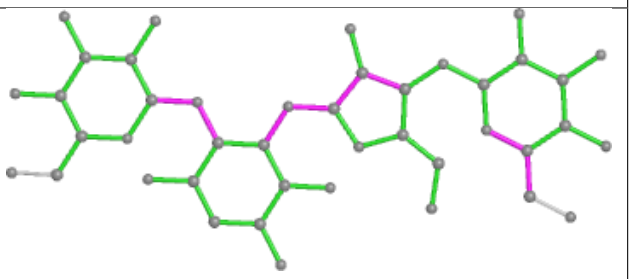


Rings

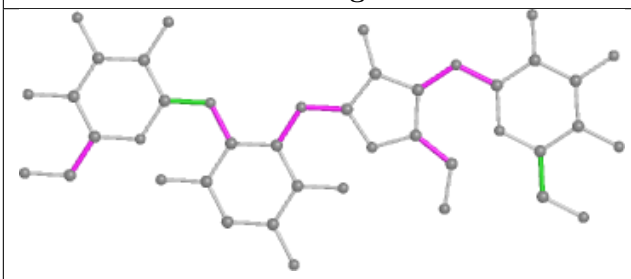
Ligand NMY CA 1601



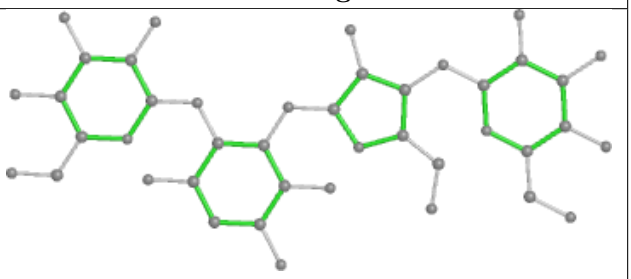
Bond lengths



Bond angles

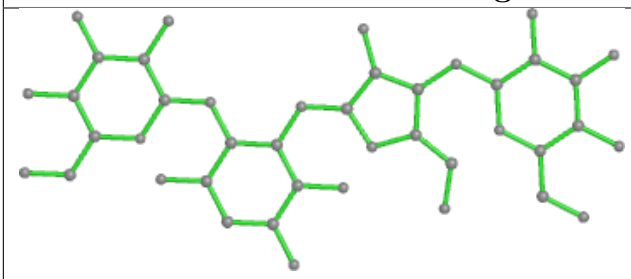


Torsions

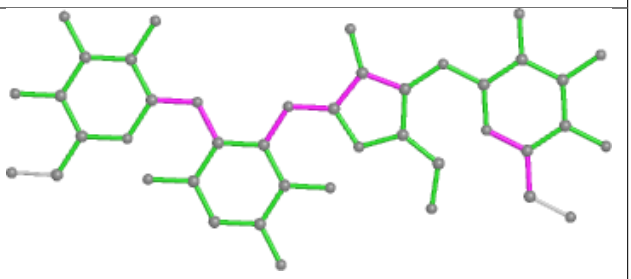


Rings

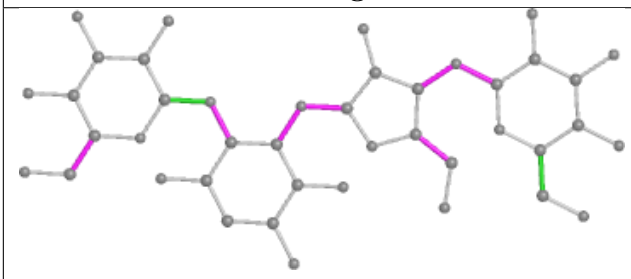
Ligand NMY DA 2901



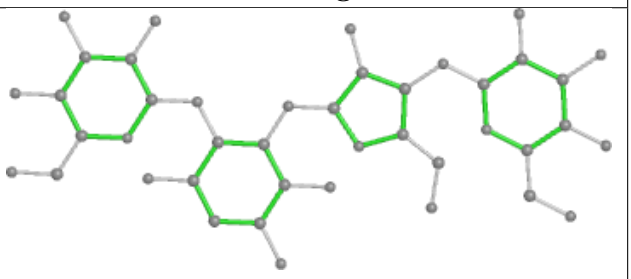
Bond lengths



Bond angles

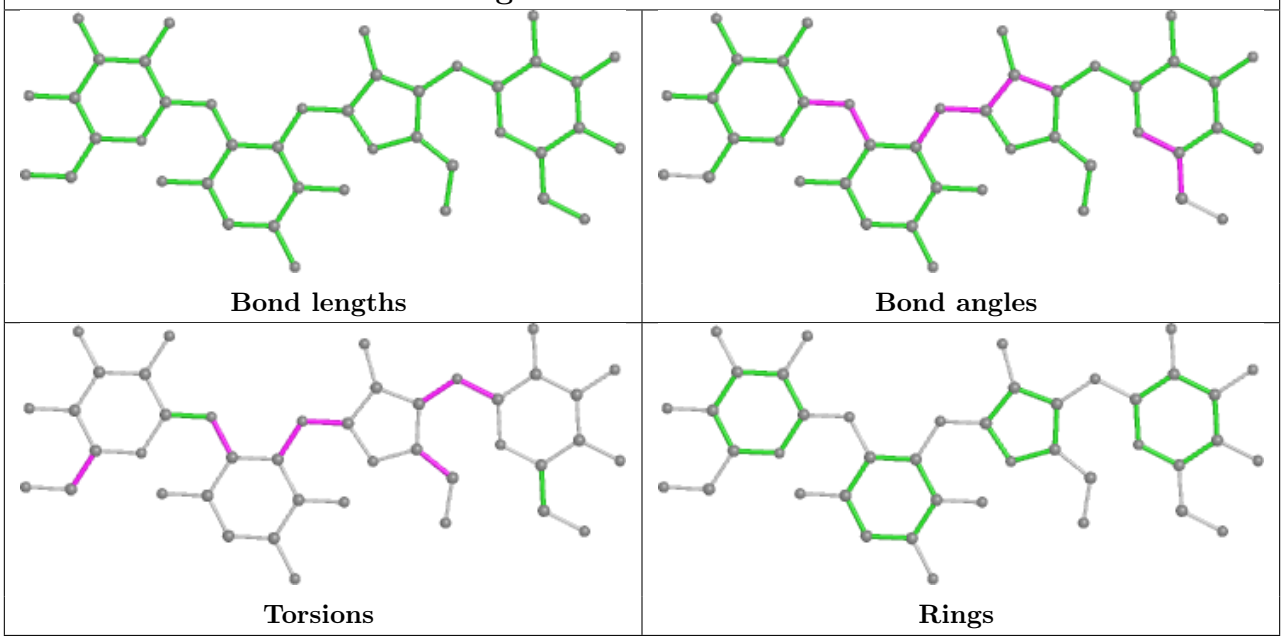


Torsions

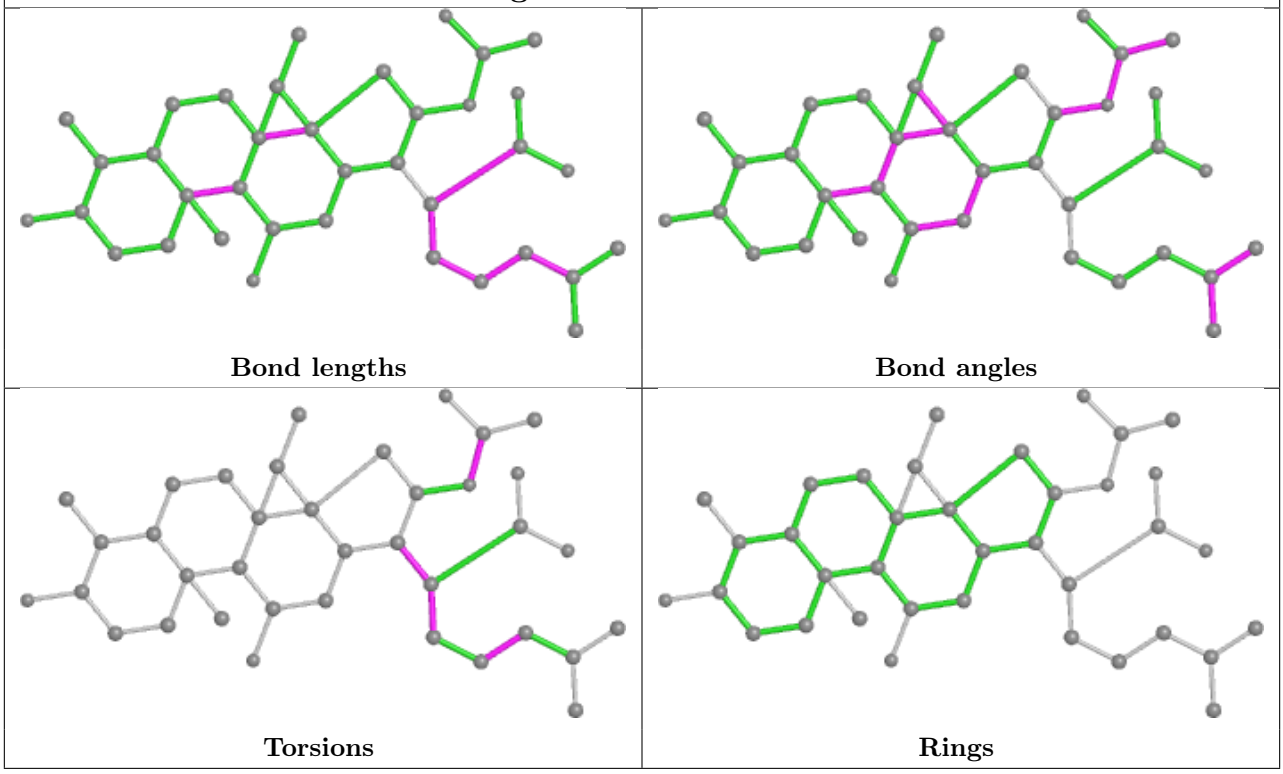


Rings

Ligand NMY BA 2902



Ligand FUA CY 702



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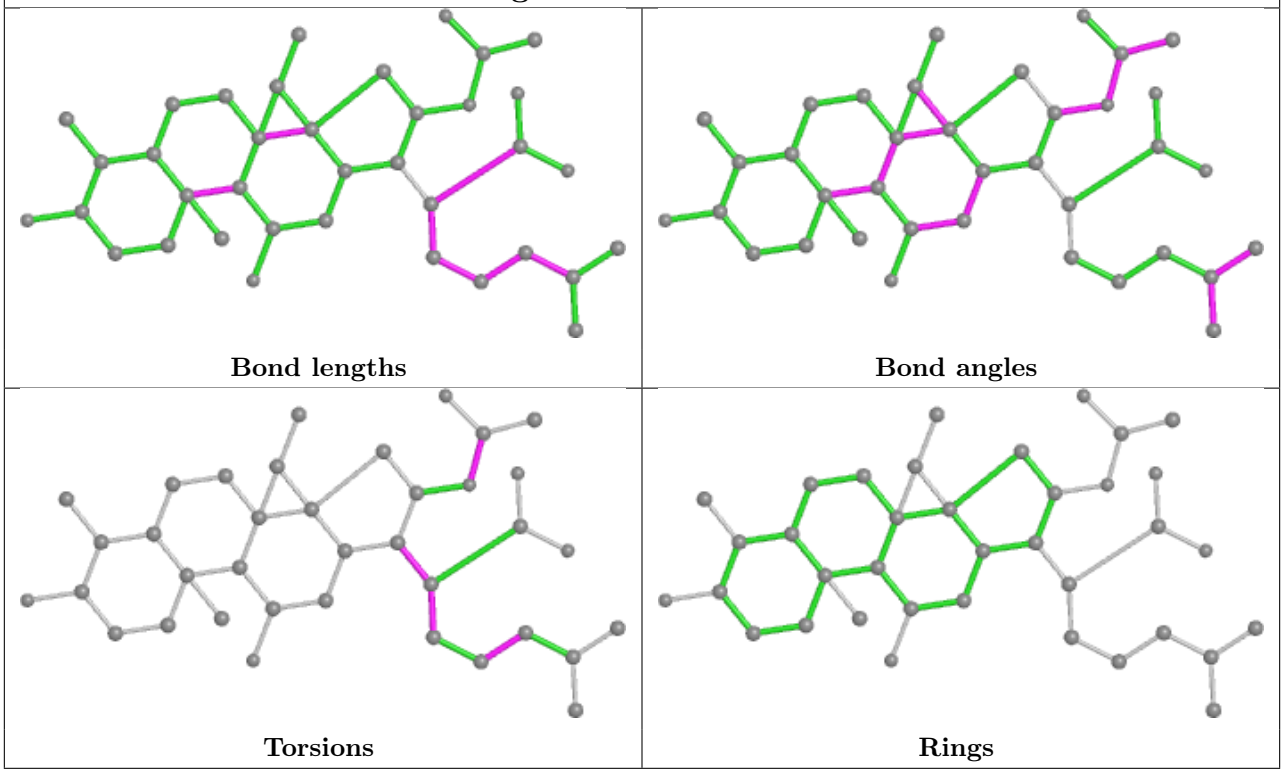
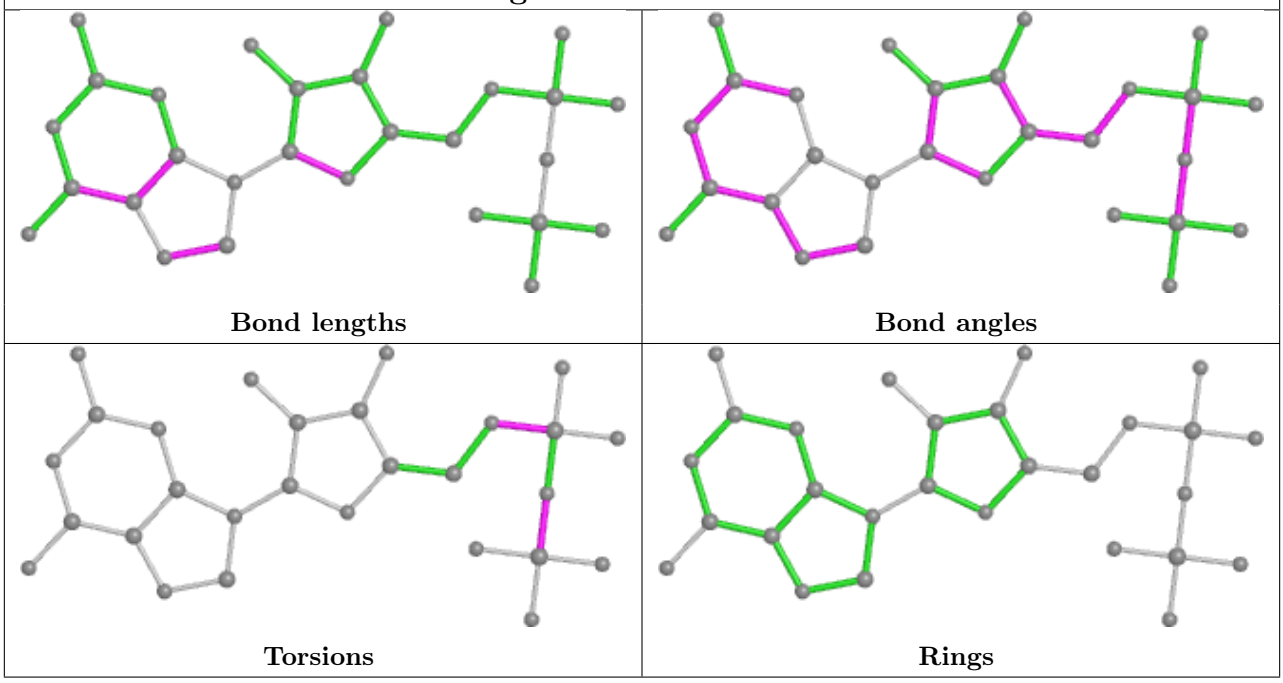


Ligand GDP AY 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	CX	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CX	76:A	O3'	77:VAL	N	3.06

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	AB	235/235 (100%)	-0.33	4 (1%)	70	62	17, 55, 103, 129	0
1	CB	235/235 (100%)	-0.09	3 (1%)	77	70	17, 63, 111, 140	0
2	AC	207/207 (100%)	1.77	89 (42%)	0	0	18, 52, 99, 118	0
2	CC	207/207 (100%)	1.85	81 (39%)	0	0	15, 58, 99, 132	0
3	AD	208/208 (100%)	-0.46	2 (0%)	82	76	14, 59, 107, 137	0
3	CD	208/208 (100%)	-0.32	1 (0%)	91	87	20, 52, 102, 136	0
4	AE	151/151 (100%)	0.08	15 (9%)	7	6	26, 62, 96, 129	0
4	CE	151/151 (100%)	-0.05	9 (5%)	21	17	19, 56, 99, 143	0
5	AF	101/101 (100%)	-0.60	0	100	100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-0.65	0	100	100	19, 56, 106, 128	0
6	AG	155/155 (100%)	-0.28	7 (4%)	33	28	26, 78, 122, 150	0
6	CG	155/155 (100%)	-0.32	6 (3%)	39	32	38, 85, 120, 147	0
7	AH	138/138 (100%)	-0.75	0	100	100	16, 43, 87, 109	0
7	CH	138/138 (100%)	-0.63	0	100	100	10, 49, 86, 102	0
8	AI	127/127 (100%)	-0.59	3 (2%)	59	50	30, 64, 101, 127	0
8	CI	127/127 (100%)	-0.59	1 (0%)	86	81	9, 77, 108, 134	0
9	AJ	99/99 (100%)	1.69	37 (37%)	0	0	34, 64, 104, 146	0
9	CJ	99/99 (100%)	1.63	35 (35%)	0	0	22, 57, 107, 115	0
10	AK	119/119 (100%)	0.03	10 (8%)	11	9	13, 74, 139, 160	0
10	CK	119/119 (100%)	-0.03	3 (2%)	57	49	21, 71, 125, 161	0
11	AL	125/125 (100%)	-0.27	4 (3%)	47	38	15, 73, 145, 164	0
11	CL	125/125 (100%)	0.00	6 (4%)	30	26	27, 85, 148, 170	0
12	AM	125/125 (100%)	0.06	6 (4%)	30	26	43, 86, 129, 159	0
12	CM	125/125 (100%)	-0.10	8 (6%)	19	15	27, 63, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	60/60 (100%)	1.04	13 (21%) 0 1	33, 70, 116, 128	0
13	CN	60/60 (100%)	0.81	10 (16%) 1 2	30, 58, 105, 128	0
14	AO	88/88 (100%)	-0.36	1 (1%) 80 74	26, 53, 99, 110	0
14	CO	88/88 (100%)	-0.42	0 100 100	8, 44, 84, 109	0
15	AP	84/84 (100%)	0.40	7 (8%) 11 9	33, 71, 110, 143	0
15	CP	84/84 (100%)	0.45	10 (11%) 4 5	39, 69, 111, 165	0
16	AQ	100/100 (100%)	-0.52	0 100 100	27, 62, 107, 131	0
16	CQ	100/100 (100%)	-0.34	2 (2%) 65 58	22, 66, 120, 135	0
17	AR	70/70 (100%)	-0.30	4 (5%) 23 19	19, 61, 102, 130	0
17	CR	70/70 (100%)	-0.29	3 (4%) 35 30	24, 56, 100, 125	0
18	AS	79/79 (100%)	-0.49	1 (1%) 77 70	17, 69, 111, 124	0
18	CS	79/79 (100%)	-0.13	5 (6%) 20 15	28, 65, 108, 130	0
19	AT	99/99 (100%)	-0.17	5 (5%) 28 24	17, 51, 85, 128	0
19	CT	99/99 (100%)	0.52	16 (16%) 1 2	26, 69, 110, 139	0
20	AY	661/687 (96%)	-0.44	23 (3%) 44 36	19, 64, 113, 178	0
20	CY	661/687 (96%)	-0.36	22 (3%) 46 38	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	-0.46	14 (0%) 84 79	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	-0.47	28 (1%) 66 59	10, 88, 160, 242	0
22	AW	77/77 (100%)	-0.15	9 (11%) 4 5	15, 71, 130, 150	0
22	CW	77/77 (100%)	0.09	7 (9%) 9 7	30, 88, 145, 178	0
23	AV	36/36 (100%)	1.73	8 (22%) 0 0	32, 89, 137, 186	0
23	CV	36/36 (100%)	3.53	16 (44%) 0 0	23, 139, 232, 237	0
24	AX	77/78 (98%)	-0.49	3 (3%) 39 32	3, 65, 233, 320	0
24	CX	77/78 (98%)	-0.36	2 (2%) 56 47	37, 123, 185, 285	0
25	BC	228/228 (100%)	1.24	65 (28%) 0 0	54, 104, 139, 159	0
25	DC	228/228 (100%)	0.75	48 (21%) 1 1	37, 90, 130, 169	0
26	BD	275/275 (100%)	-0.08	21 (7%) 13 11	10, 61, 103, 125	0
26	DD	275/275 (100%)	-0.03	14 (5%) 28 24	16, 57, 100, 127	0
27	BE	205/205 (100%)	0.16	10 (4%) 29 25	21, 60, 107, 131	0
27	DE	205/205 (100%)	0.15	8 (3%) 39 32	22, 57, 97, 142	0
28	BF	208/208 (100%)	0.37	22 (10%) 6 5	20, 67, 108, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DF	208/208 (100%)	0.58	31 (14%)	2	2	23, 75, 120, 140	0
29	BG	181/181 (100%)	0.77	22 (12%)	4	4	28, 69, 113, 148	0
29	DG	181/181 (100%)	0.67	25 (13%)	2	3	25, 71, 113, 148	0
30	BH	167/167 (100%)	0.00	7 (4%)	36	30	29, 65, 108, 121	0
30	DH	167/167 (100%)	-0.01	8 (4%)	30	26	24, 59, 100, 132	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	-0.28	7 (5%)	28	25	32, 71, 114, 126	0
32	DK	140/140 (100%)	-0.08	7 (5%)	28	25	34, 77, 113, 138	0
33	BN	139/139 (100%)	2.00	56 (40%)	0	0	23, 105, 298, 334	0
33	DN	139/139 (100%)	2.07	57 (41%)	0	0	16, 116, 252, 312	0
34	BO	122/122 (100%)	1.65	45 (36%)	0	0	12, 50, 93, 111	0
34	DO	122/122 (100%)	2.17	56 (45%)	0	0	28, 59, 103, 132	0
35	BP	146/146 (100%)	-0.51	4 (2%)	54	45	25, 63, 106, 123	0
35	DP	146/146 (100%)	-0.45	3 (2%)	63	55	25, 67, 104, 131	0
36	BQ	141/141 (100%)	-0.35	4 (2%)	53	43	5, 54, 93, 109	0
36	DQ	141/141 (100%)	0.02	8 (5%)	23	19	27, 70, 113, 141	0
37	BR	117/117 (100%)	-0.62	0	100	100	29, 65, 116, 145	0
37	DR	117/117 (100%)	-0.71	1 (0%)	84	79	27, 62, 97, 126	0
38	BS	99/99 (100%)	1.00	20 (20%)	1	1	14, 70, 108, 117	0
38	DS	99/99 (100%)	0.78	11 (11%)	5	5	19, 52, 96, 120	0
39	BT	138/138 (100%)	1.23	43 (31%)	0	0	16, 59, 101, 123	0
39	DT	138/138 (100%)	1.14	34 (24%)	0	0	15, 51, 109, 140	0
40	BU	117/117 (100%)	-0.48	1 (0%)	84	79	20, 56, 96, 121	0
40	DU	117/117 (100%)	-0.45	1 (0%)	84	79	13, 53, 94, 142	0
41	BV	101/101 (100%)	0.22	5 (4%)	28	25	21, 66, 108, 127	0
41	DV	101/101 (100%)	0.13	5 (4%)	28	25	15, 65, 101, 126	0
42	BW	113/113 (100%)	-0.42	3 (2%)	54	45	13, 54, 99, 111	0
42	DW	113/113 (100%)	-0.35	5 (4%)	34	29	15, 64, 116, 148	0
43	BX	93/93 (100%)	-0.25	4 (4%)	35	30	20, 54, 96, 115	0
43	DX	93/93 (100%)	-0.34	2 (2%)	62	54	13, 45, 87, 126	0
44	BY	107/107 (100%)	0.31	10 (9%)	8	7	29, 58, 109, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	DY	107/107 (100%)	0.10	6 (5%) 24 20	25, 62, 97, 138	0
45	BZ	185/185 (100%)	-0.34	0 100 100	17, 58, 97, 113	0
45	DZ	185/185 (100%)	-0.22	4 (2%) 62 54	33, 64, 101, 138	0
46	B0	84/84 (100%)	0.60	15 (17%) 1 1	26, 75, 117, 131	0
46	D0	84/84 (100%)	0.06	4 (4%) 30 26	19, 65, 108, 116	0
47	B1	93/93 (100%)	1.11	20 (21%) 0 1	21, 84, 140, 156	0
47	D1	93/93 (100%)	1.41	27 (29%) 0 0	31, 103, 148, 181	0
48	B2	71/71 (100%)	-0.72	0 100 100	23, 55, 95, 116	0
48	D2	71/71 (100%)	-0.44	2 (2%) 53 43	35, 61, 103, 118	0
49	B3	60/60 (100%)	-0.50	1 (1%) 70 62	29, 60, 99, 112	0
49	D3	60/60 (100%)	-0.39	0 100 100	36, 68, 94, 110	0
50	B4	35/35 (100%)	1.49	11 (31%) 0 0	26, 71, 110, 122	0
50	D4	35/35 (100%)	1.26	8 (22%) 0 0	64, 109, 144, 185	0
51	B5	59/59 (100%)	-0.69	0 100 100	24, 63, 106, 123	0
51	D5	59/59 (100%)	-0.64	2 (3%) 45 37	31, 68, 113, 138	0
52	B6	50/50 (100%)	1.20	14 (28%) 0 0	13, 57, 107, 154	0
52	D6	50/50 (100%)	0.96	13 (26%) 0 0	26, 65, 120, 154	0
53	B7	49/49 (100%)	1.24	16 (32%) 0 0	46, 91, 136, 164	0
53	D7	49/49 (100%)	0.91	10 (20%) 1 1	51, 73, 109, 134	0
54	B8	64/64 (100%)	1.05	10 (15%) 2 2	26, 58, 109, 132	0
54	D8	64/64 (100%)	0.61	7 (10%) 5 5	30, 64, 104, 118	0
55	B9	37/37 (100%)	-0.34	1 (2%) 54 45	39, 64, 109, 116	0
55	D9	37/37 (100%)	-0.62	0 100 100	34, 65, 116, 134	0
56	Be	72/103 (69%)	0.63	12 (16%) 1 2	15, 49, 122, 163	0
56	De	72/103 (69%)	0.69	9 (12%) 3 4	14, 57, 118, 157	0
57	Bf	0/31	-	-	-	-
57	Bg	0/31	-	-	-	-
57	Df	0/31	-	-	-	-
57	Dg	0/31	-	-	-	-
58	Bh	0/30	-	-	-	-
58	Dh	0/30	-	-	-	-
59	BA	2879/2879 (100%)	-0.49	31 (1%) 80 74	11, 89, 164, 284	0
59	DA	2879/2879 (100%)	-0.49	31 (1%) 80 74	9, 88, 171, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	BB	119/119 (100%)	-0.37	6 (5%) 28 25	18, 80, 158, 172	0
60	DB	119/119 (100%)	-0.36	0 100 100	30, 88, 150, 175	0
All	All	22852/23492 (97%)	-0.09	1472 (6%) 19 15	3, 73, 146, 334	0

All (1472) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	CV	36	A	21.2
23	CV	34	A	20.9
23	CV	35	A	18.6
23	AV	35	A	18.0
23	AV	34	A	13.7
33	BN	99	LEU	11.7
59	BA	2897	U	10.7
23	AV	36	A	10.2
34	DO	96	THR	10.0
33	BN	80	GLY	9.5
19	CT	8	ARG	9.1
33	BN	86	PRO	9.1
56	Be	51	ALA	8.9
33	BN	103	VAL	8.8
56	De	54	ALA	8.5
33	DN	80	GLY	8.5
33	BN	123	TYR	8.4
2	CC	150	LYS	8.4
6	CG	81	GLY	8.3
56	De	53	PRO	8.2
23	CV	2	G	8.2
33	DN	103	VAL	8.2
34	DO	95	GLY	8.0
33	DN	99	LEU	8.0
33	BN	120	LEU	8.0
25	BC	57	GLN	8.0
28	DF	97	TYR	7.9
36	DQ	141	GLN	7.8
33	BN	119	ARG	7.8
33	DN	107	LEU	7.7
59	BA	180	G	7.7
25	BC	58	ASN	7.7
47	D1	60	PHE	7.6
2	CC	201	TYR	7.5

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Mol	Chain	Res	Type	RSRZ
23	CV	33	C	7.5
59	DA	2897	U	7.4
33	DN	51	PHE	7.4
2	CC	206	GLU	7.3
19	CT	9	ASN	7.3
47	D1	19	GLN	7.2
19	CT	11	SER	7.2
34	DO	9	GLU	7.2
25	BC	50	ILE	7.1
33	DN	86	PRO	7.0
25	BC	163	GLU	7.0
34	DO	99	PHE	7.0
9	CJ	48	THR	6.9
39	DT	105	LEU	6.8
33	BN	121	LYS	6.7
25	BC	56	ASP	6.7
28	DF	96	ASP	6.6
23	CV	5	A	6.6
34	DO	84	ALA	6.6
25	DC	203	GLU	6.6
2	AC	201	TYR	6.6
23	CV	28	A	6.6
25	BC	49	GLY	6.6
33	BN	102	ALA	6.6
34	BO	50	GLY	6.5
33	DN	98	VAL	6.5
33	DN	89	LYS	6.5
47	D1	59	THR	6.5
34	BO	96	THR	6.4
4	CE	25	ARG	6.4
2	CC	208	ILE	6.3
33	DN	108	PRO	6.3
34	DO	17	ARG	6.3
56	Be	54	ALA	6.3
25	BC	48	LEU	6.3
39	BT	104	ASN	6.3
33	DN	52	VAL	6.2
16	CQ	101	ARG	6.2
34	BO	18	LYS	6.2
33	BN	79	PRO	6.1
47	B1	60	PHE	6.1
25	DC	49	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
47	B1	14	VAL	6.1
25	BC	204	GLY	6.1
33	BN	107	LEU	6.0
56	De	52	ALA	6.0
47	D1	16	ASN	6.0
33	BN	100	GLU	6.0
33	DN	95	PRO	6.0
44	BY	8	LYS	6.0
47	B1	59	THR	6.0
25	DC	204	GLY	5.9
33	DN	94	HIS	5.9
47	D1	29	GLY	5.9
19	CT	10	LEU	5.9
25	DC	165	ARG	5.9
56	De	51	ALA	5.9
33	DN	79	PRO	5.9
59	BA	45	G	5.9
34	BO	9	GLU	5.8
34	DO	94	ARG	5.8
34	DO	100	GLY	5.8
33	DN	49	GLY	5.8
34	DO	83	ALA	5.8
25	DC	200	HIS	5.7
59	DA	2502	G	5.7
34	BO	84	ALA	5.7
33	BN	118	LYS	5.7
25	BC	165	ARG	5.6
59	DA	887	A	5.6
2	CC	59	ARG	5.6
59	BA	34	C	5.6
59	BA	508	G	5.6
33	DN	83	LYS	5.5
59	BA	179	G	5.5
34	DO	101	PRO	5.5
23	AV	33	C	5.5
34	DO	102	VAL	5.5
52	B6	35	GLU	5.5
11	CL	20	LYS	5.5
56	Be	52	ALA	5.5
33	BN	122	VAL	5.4
33	DN	11	PRO	5.4
33	DN	102	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
59	BA	47	C	5.4
46	B0	70	GLN	5.3
25	DC	163	GLU	5.3
34	DO	80	ASP	5.3
33	DN	12	ARG	5.3
23	CV	4	A	5.3
2	CC	205	GLY	5.3
47	B1	41	ARG	5.3
2	AC	208	ILE	5.3
33	BN	81	GLY	5.3
9	AJ	11	PHE	5.3
39	DT	106	SER	5.2
44	BY	4	LYS	5.2
59	BA	214	G	5.2
2	CC	202	ILE	5.2
38	DS	11	LYS	5.2
44	BY	3	VAL	5.2
20	AY	361	ASN	5.2
2	CC	196	LEU	5.1
4	AE	31	LEU	5.1
18	CS	82	GLY	5.1
2	AC	168	ALA	5.1
2	CC	104	GLN	5.1
34	BO	17	ARG	5.1
56	De	55	GLU	5.1
6	CG	82	GLY	5.1
25	BC	161	ARG	5.1
23	CV	29	A	5.1
19	CT	71	THR	5.1
9	CJ	10	GLY	5.1
33	DN	81	GLY	5.1
2	CC	129	ALA	5.1
9	CJ	8	LEU	5.1
34	DO	122	LEU	5.1
9	CJ	47	PHE	5.0
33	BN	89	LYS	5.0
47	B1	95	LEU	5.0
2	AC	202	ILE	5.0
33	BN	126	PRO	5.0
56	Be	53	PRO	5.0
38	BS	89	ARG	5.0
33	DN	100	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
39	BT	103	ARG	5.0
39	DT	100	TYR	5.0
2	AC	151	VAL	5.0
2	AC	169	ALA	4.9
26	DD	276	LYS	4.9
6	CG	80	VAL	4.9
34	BO	12	ASP	4.9
25	BC	51	ASP	4.9
33	BN	98	VAL	4.9
23	CV	1	G	4.9
38	DS	91	PRO	4.8
42	DW	85	VAL	4.8
9	CJ	11	PHE	4.8
2	CC	168	ALA	4.8
29	BG	137	GLU	4.8
28	BF	97	TYR	4.8
33	DN	34	LEU	4.8
52	B6	36	LEU	4.8
21	AA	351	G	4.8
9	CJ	95	GLU	4.8
2	CC	147	LYS	4.8
33	DN	14	VAL	4.8
25	BC	47	LYS	4.8
34	DO	10	VAL	4.8
33	BN	11	PRO	4.8
28	BF	90	PHE	4.8
13	AN	52	GLN	4.8
33	DN	16	ILE	4.8
56	Be	55	GLU	4.8
33	DN	15	LEU	4.7
2	CC	149	ALA	4.7
59	DA	889	C	4.7
33	DN	17	ASP	4.7
47	B1	58	ILE	4.7
34	DO	18	LYS	4.7
33	BN	12	ARG	4.7
44	BY	5	MET	4.7
39	DT	104	ASN	4.7
2	CC	183	ASP	4.7
21	CA	1190	G	4.7
25	BC	60	ARG	4.7
36	DQ	140	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
26	DD	40	THR	4.6
15	CP	29	ASP	4.6
34	BO	81	ASP	4.6
50	B4	31	ILE	4.6
2	CC	169	ALA	4.6
34	DO	98	VAL	4.6
23	CV	3	C	4.6
23	CV	11	U	4.6
2	AC	188	LEU	4.6
21	CA	57	G	4.6
34	DO	82	ASN	4.6
2	AC	177	THR	4.6
21	CA	1534	A	4.5
2	CC	179	ARG	4.5
33	BN	87	LEU	4.5
21	AA	388	G	4.5
44	DY	3	VAL	4.5
34	BO	51	ALA	4.5
34	DO	77	ILE	4.5
25	DC	48	LEU	4.5
39	DT	103	ARG	4.5
9	AJ	15	THR	4.5
9	AJ	87	THR	4.5
26	BD	2	ALA	4.5
15	CP	59	TRP	4.5
34	BO	10	VAL	4.5
2	CC	167	TRP	4.5
21	AA	328	C	4.5
50	B4	6	HIS	4.5
2	CC	200	ALA	4.4
2	CC	2	GLY	4.4
25	BC	59	VAL	4.4
2	CC	131	ARG	4.4
11	CL	129	ALA	4.4
25	BC	136	GLY	4.4
33	DN	71	ILE	4.4
59	BA	588	U	4.4
2	AC	181	ASN	4.4
52	B6	34	LEU	4.4
53	B7	39	ARG	4.4
59	BA	2896	C	4.4
59	DA	1712(O)	C	4.4

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Mol	Chain	Res	Type	RSRZ
38	DS	89	ARG	4.4
29	DG	34	LEU	4.4
25	DC	58	ASN	4.4
13	CN	58	LYS	4.4
34	BO	46	ALA	4.4
25	DC	131	ILE	4.3
9	CJ	12	ASP	4.3
13	CN	49	HIS	4.3
10	AK	129	SER	4.3
12	AM	93	ARG	4.3
2	CC	172	ARG	4.3
12	CM	122	LYS	4.3
28	DF	40	GLN	4.3
39	DT	22	PHE	4.3
2	AC	150	LYS	4.3
12	AM	122	LYS	4.3
52	D6	54	ILE	4.3
2	AC	107	GLN	4.3
9	AJ	61	GLU	4.3
52	D6	12	GLU	4.3
23	CV	31	A	4.3
33	DN	109	LYS	4.3
34	BO	80	ASP	4.3
34	BO	11	ALA	4.3
39	BT	105	LEU	4.3
34	DO	85	VAL	4.3
28	DF	98	SER	4.3
47	D1	8	SER	4.3
59	BA	1706	U	4.3
59	DA	2896	C	4.3
29	BG	96	ARG	4.2
33	DN	112	LEU	4.3
39	BT	22	PHE	4.2
25	DC	59	VAL	4.2
13	AN	49	HIS	4.2
33	BN	34	LEU	4.2
36	DQ	97	VAL	4.2
4	CE	24	ARG	4.2
29	BG	136	ARG	4.2
9	AJ	47	PHE	4.2
25	BC	164	PHE	4.2
47	B1	38	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	AC	2	GLY	4.2
34	BO	47	ILE	4.2
39	BT	50	ILE	4.2
59	BA	215	G	4.2
6	CG	6	ARG	4.2
39	DT	43	GLN	4.2
22	CW	53	G	4.2
15	AP	27	LYS	4.2
39	BT	72	VAL	4.1
41	DV	101	GLY	4.1
2	CC	182	ILE	4.1
2	AC	17	ASP	4.1
53	D7	39	ARG	4.1
47	D1	61	ARG	4.1
13	AN	50	LYS	4.1
34	BO	13	ASN	4.1
9	AJ	62	HIS	4.1
34	BO	45	GLU	4.1
28	DF	133	ASN	4.1
34	DO	81	ASP	4.1
59	BA	213	A	4.1
30	BH	167	GLU	4.1
9	AJ	49	VAL	4.1
59	DA	1712(P)	C	4.1
34	DO	97	ARG	4.0
3	AD	50	ARG	4.0
9	AJ	48	THR	4.0
26	BD	40	THR	4.0
38	BS	34	HIS	4.0
17	AR	88	LYS	4.0
53	B7	41	ARG	4.0
2	AC	49	SER	4.0
59	BA	1755	A	4.0
25	BC	140	ASN	4.0
47	B1	92	LYS	4.0
59	DA	508	G	4.0
9	AJ	98	ILE	4.0
52	B6	25	LYS	4.0
53	D7	32	LYS	4.0
9	CJ	49	VAL	4.0
53	B7	49	ARG	4.0
33	BN	10	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
25	BC	62	THR	3.9
10	AK	48	ILE	3.9
21	CA	1440(C)	G	3.9
2	AC	205	GLY	3.9
11	CL	67	THR	3.9
2	AC	108	ASN	3.9
33	BN	61	ARG	3.9
52	D6	35	GLU	3.9
13	AN	48	ALA	3.9
59	DA	214	G	3.9
39	DT	65	LYS	3.9
28	DF	78	ILE	3.9
10	AK	21	ILE	3.9
59	DA	1554	A	3.9
22	AW	54	U	3.9
9	CJ	96	ILE	3.9
33	DN	87	LEU	3.9
13	AN	51	GLY	3.9
18	CS	81	ARG	3.9
33	BN	49	GLY	3.9
9	AJ	12	ASP	3.9
47	B1	16	ASN	3.9
43	BX	31	HIS	3.9
54	B8	65	GLU	3.9
2	AC	51	GLY	3.9
24	AX	20	G	3.9
52	D6	11	LEU	3.9
28	BF	188	ARG	3.9
50	B4	14	ILE	3.9
47	D1	14	VAL	3.9
2	CC	136	GLN	3.9
33	DN	116	LEU	3.9
34	DO	64	ARG	3.9
25	BC	141	PRO	3.9
28	DF	52	LYS	3.9
35	DP	22	GLY	3.9
39	BT	68	TYR	3.9
56	De	56	GLU	3.8
33	DN	119	ARG	3.8
25	BC	193	PHE	3.8
36	DQ	25	ASP	3.8
54	B8	43	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
6	AG	81	GLY	3.8
12	AM	121	LYS	3.8
29	BG	2	PRO	3.8
18	AS	82	GLY	3.8
25	BC	33	LEU	3.8
59	DA	215	G	3.8
25	DC	62	THR	3.8
2	CC	4	LYS	3.8
34	DO	79	PHE	3.8
52	B6	26	ASN	3.8
9	CJ	86	MET	3.8
19	CT	12	ALA	3.8
47	D1	12	PRO	3.8
9	AJ	86	MET	3.8
1	CB	137	ARG	3.8
10	CK	50	TYR	3.8
12	CM	116	THR	3.8
55	B9	9	ARG	3.8
39	BT	69	GLY	3.8
23	CV	7	G	3.8
2	CC	189	ALA	3.8
19	CT	72	LEU	3.8
34	DO	8	LEU	3.8
39	BT	71	GLY	3.8
52	B6	54	ILE	3.7
54	D8	37	SER	3.7
15	AP	60	LEU	3.7
34	BO	102	VAL	3.7
20	CY	324	ARG	3.7
34	BO	111	PHE	3.7
47	D1	15	ALA	3.7
28	BF	89	VAL	3.7
2	AC	200	ALA	3.7
2	CC	185	GLY	3.7
2	CC	130	VAL	3.7
2	CC	165	THR	3.7
34	BO	16	ALA	3.7
1	AB	241	GLU	3.7
38	DS	88	ASP	3.7
25	BC	172	ILE	3.7
39	BT	101	PHE	3.7
2	CC	152	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
60	BB	35	U	3.7
2	CC	190	ARG	3.7
15	CP	27	LYS	3.7
2	CC	145	GLY	3.7
34	BO	14	THR	3.7
2	AC	143	GLU	3.7
2	AC	62	ASP	3.7
39	BT	106	SER	3.7
2	AC	183	ASP	3.7
2	CC	123	GLN	3.7
2	AC	204	LEU	3.7
56	Be	102	GLY	3.6
2	CC	151	VAL	3.6
19	CT	15	ARG	3.6
9	AJ	96	ILE	3.6
59	DA	1712(N)	U	3.6
2	AC	50	ALA	3.6
21	CA	1112	C	3.6
54	B8	14	VAL	3.6
25	BC	162	ILE	3.6
2	CC	177	THR	3.6
44	BY	30	VAL	3.6
33	BN	17	ASP	3.6
39	DT	68	TYR	3.6
21	CA	1066	C	3.6
46	B0	75	LEU	3.6
2	CC	127	ARG	3.6
38	DS	92	TYR	3.6
9	CJ	94	VAL	3.6
34	DO	76	ALA	3.6
28	BF	91	GLY	3.6
29	BG	146	TYR	3.6
34	BO	48	PRO	3.6
11	AL	68	ALA	3.6
33	BN	124	ALA	3.6
47	D1	11	ARG	3.6
28	DF	114	VAL	3.6
2	CC	199	LYS	3.6
32	DK	118	THR	3.6
39	BT	102	ILE	3.6
33	DN	123	TYR	3.6
44	BY	31	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
27	BE	10	GLY	3.6
33	DN	61	ARG	3.6
25	BC	225	ILE	3.6
33	DN	13	TRP	3.6
25	BC	52	PRO	3.6
39	BT	48	ILE	3.5
25	BC	224	ARG	3.5
2	CC	128	PHE	3.5
12	CM	117	VAL	3.5
26	BD	22	SER	3.5
11	AL	67	THR	3.5
32	DK	25	PRO	3.5
2	CC	63	ASN	3.5
20	CY	67	ALA	3.5
39	DT	102	ILE	3.5
56	Be	56	GLU	3.5
13	CN	7	ILE	3.5
29	DG	150	ASP	3.5
52	D6	34	LEU	3.5
2	AC	175	LEU	3.5
39	BT	100	TYR	3.5
33	BN	116	LEU	3.5
9	CJ	87	THR	3.5
33	BN	95	PRO	3.5
9	AJ	72	VAL	3.5
9	AJ	89	ASP	3.5
50	D4	22	ILE	3.5
9	CJ	9	ARG	3.5
20	AY	104	ALA	3.5
39	DT	67	SER	3.5
34	BO	108	GLU	3.5
52	B6	12	GLU	3.5
54	B8	63	PRO	3.5
2	CC	98	ASN	3.5
25	DC	201	LYS	3.5
25	BC	203	GLU	3.5
25	DC	55	SER	3.5
20	AY	378	VAL	3.5
29	BG	26	GLN	3.5
34	DO	103	ALA	3.5
33	DN	134	ARG	3.4
28	DF	27	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	AC	112	SER	3.4
21	AA	1190	G	3.4
33	DN	104	LYS	3.4
2	CC	207	VAL	3.4
32	BK	47	ASN	3.4
33	BN	14	VAL	3.4
42	BW	83	LYS	3.4
32	DK	24	GLY	3.4
59	DA	2060	A	3.4
20	AY	308	PRO	3.4
21	AA	352	C	3.4
2	CC	181	ASN	3.4
34	DO	56	ASP	3.4
52	D6	33	LYS	3.4
2	AC	111	LEU	3.4
28	BF	27	GLU	3.4
39	BT	64	ARG	3.4
4	AE	47	LYS	3.4
28	BF	52	LYS	3.4
25	DC	119	ASP	3.4
25	DC	164	PHE	3.4
34	BO	15	GLY	3.4
34	DO	63	VAL	3.4
4	AE	10	MET	3.4
59	DA	1551	C	3.4
2	CC	184	TYR	3.4
2	AC	203	PHE	3.4
2	CC	140	ARG	3.4
39	BT	73	GLU	3.4
39	DT	101	PHE	3.4
59	BA	589	C	3.4
33	BN	104	LYS	3.4
28	BF	56	GLU	3.4
59	DA	2334	G	3.4
2	AC	162	GLN	3.4
47	D1	23	LYS	3.4
21	AA	1066	C	3.4
41	DV	71	LEU	3.4
52	D6	51	GLU	3.4
33	BN	15	LEU	3.4
2	CC	203	PHE	3.4
28	DF	95	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
9	AJ	84	GLN	3.3
33	BN	135	PRO	3.3
9	CJ	63	PHE	3.3
34	BO	52	VAL	3.3
39	BT	29	ARG	3.3
2	AC	14	ILE	3.3
2	AC	157	ILE	3.3
2	CC	108	ASN	3.3
4	AE	89	ILE	3.3
25	BC	176	VAL	3.3
25	DC	133	GLY	3.3
39	DT	99	LEU	3.3
28	DF	42	ALA	3.3
59	BA	2141	G	3.3
25	BC	142	LYS	3.3
47	B1	15	ALA	3.3
53	D7	49	ARG	3.3
9	CJ	33	GLN	3.3
26	BD	20	ASP	3.3
33	BN	54	VAL	3.3
9	AJ	71	LEU	3.3
59	BA	46	C	3.3
33	DN	85	ILE	3.3
23	CV	6	G	3.3
26	DD	56	GLY	3.3
33	DN	120	LEU	3.3
33	BN	8	GLN	3.3
59	DA	2133	G	3.3
26	BD	3	VAL	3.3
47	B1	37	ILE	3.3
47	B1	39	LYS	3.3
26	DD	236	GLY	3.3
10	AK	128	ALA	3.3
20	CY	377	VAL	3.3
29	DG	136	ARG	3.3
34	DO	62	VAL	3.3
59	BA	2060	A	3.3
47	D1	48	LYS	3.3
2	AC	167	TRP	3.3
2	AC	48	TYR	3.3
8	AI	115	GLY	3.3
36	DQ	21	THR	3.3

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Mol	Chain	Res	Type	RSRZ
20	CY	38	ARG	3.3
38	BS	87	PHE	3.3
25	BC	211	ARG	3.2
29	BG	68	PRO	3.2
43	DX	33	LYS	3.2
21	CA	68(D)	C	3.2
59	DA	34	C	3.2
10	AK	49	GLY	3.2
38	BS	55	ALA	3.2
2	CC	58	GLU	3.2
25	BC	202	PRO	3.2
2	AC	149	ALA	3.2
44	DY	33	LYS	3.2
22	AW	53	G	3.2
35	BP	22	GLY	3.2
15	CP	26	ARG	3.2
34	BO	53	LYS	3.2
47	B1	11	ARG	3.2
2	CC	176	HIS	3.2
39	DT	71	GLY	3.2
46	B0	76	GLY	3.2
17	CR	88	LYS	3.2
25	DC	130	ARG	3.2
9	AJ	69	ASN	3.2
22	CW	57	G	3.2
21	CA	162	A	3.2
25	DC	209	PHE	3.2
59	DA	1379	A	3.2
2	CC	204	LEU	3.2
9	CJ	84	GLN	3.2
9	CJ	85	LEU	3.2
9	CJ	7	LYS	3.2
26	DD	54	ARG	3.2
32	BK	141	ALA	3.2
45	DZ	117	LEU	3.2
33	BN	16	ILE	3.2
21	CA	1440(B)	G	3.2
2	CC	135	LYS	3.2
44	BY	7	VAL	3.2
50	B4	1	MET	3.2
9	CJ	50	ILE	3.2
39	BT	46	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
22	CW	56	C	3.2
34	BO	85	VAL	3.2
2	CC	188	LEU	3.2
51	D5	23	HIS	3.2
28	BF	53	THR	3.1
39	BT	70	VAL	3.1
20	AY	363	ARG	3.1
32	DK	2	LYS	3.1
9	AJ	67	THR	3.1
23	AV	4	A	3.1
21	AA	332	G	3.1
22	AW	64	G	3.1
15	AP	64	ALA	3.1
39	BT	97	ALA	3.1
29	DG	36	LYS	3.1
44	BY	34	LYS	3.1
21	CA	58	C	3.1
47	B1	13	ILE	3.1
53	B7	45	ALA	3.1
59	DA	2153	G	3.1
28	BF	98	SER	3.1
13	CN	59	ALA	3.1
26	BD	31	LYS	3.1
39	DT	19	LEU	3.1
21	CA	1189	C	3.1
29	BG	118	ARG	3.1
30	BH	51	ARG	3.1
41	BV	21	ARG	3.1
53	B7	43	THR	3.1
21	CA	1064	G	3.1
34	BO	19	ILE	3.1
34	DO	69	ILE	3.1
33	BN	136	GLU	3.1
17	AR	19	LYS	3.1
27	BE	24	THR	3.1
2	AC	182	ILE	3.1
34	DO	86	ILE	3.1
23	AV	6	G	3.1
34	DO	72	PRO	3.1
34	BO	95	GLY	3.1
35	BP	15	ARG	3.1
39	DT	44	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	CC	134	ILE	3.1
48	D2	72	ALA	3.1
34	BO	112	MET	3.1
2	AC	47	LEU	3.1
25	DC	47	LYS	3.1
33	DN	127	ASP	3.1
33	BN	52	VAL	3.1
20	CY	4	LYS	3.1
22	AW	47	U	3.1
52	B6	24	GLU	3.1
4	AE	11	ILE	3.1
15	CP	25	ARG	3.1
52	D6	22	ALA	3.1
33	DN	29	LYS	3.1
44	BY	29	GLU	3.1
47	B1	34	THR	3.1
52	B6	11	LEU	3.1
39	BT	94	ALA	3.0
39	DT	72	VAL	3.0
34	BO	65	THR	3.0
59	BA	587	C	3.0
2	AC	164	ARG	3.0
47	D1	39	LYS	3.0
28	DF	38	ARG	3.0
9	AJ	83	GLU	3.0
59	DA	6	A	3.0
25	DC	132	LEU	3.0
46	D0	62	LEU	3.0
1	AB	128	GLU	3.0
2	CC	109	PRO	3.0
9	CJ	98	ILE	3.0
12	CM	126	LYS	3.0
38	BS	90	GLY	3.0
53	B7	38	GLY	3.0
25	DC	134	PRO	3.0
41	DV	70	ILE	3.0
38	DS	109	GLY	3.0
20	CY	376	ALA	3.0
25	BC	46	ALA	3.0
42	DW	93	ALA	3.0
34	DO	105	GLU	3.0
21	AA	421	U	3.0

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Mol	Chain	Res	Type	RSRZ
2	CC	62	ASP	3.0
29	DG	120	LEU	3.0
23	CV	30	A	3.0
25	BC	200	HIS	3.0
25	BC	11	LEU	3.0
59	DA	456	C	3.0
25	DC	60	ARG	3.0
2	AC	46	GLU	3.0
15	CP	21	VAL	3.0
47	D1	13	ILE	3.0
50	D4	35	VAL	3.0
10	CK	42	TRP	3.0
20	CY	393	ASP	3.0
25	BC	205	ALA	3.0
53	B7	44	PRO	3.0
38	BS	39	ILE	3.0
25	BC	222	SER	3.0
27	BE	118	LYS	3.0
59	DA	888	C	3.0
11	CL	13	LYS	3.0
29	DG	98	ARG	3.0
34	BO	64	ARG	3.0
39	BT	65	LYS	3.0
9	CJ	19	SER	3.0
2	CC	191	THR	3.0
50	D4	21	VAL	3.0
4	AE	9	LYS	3.0
56	Be	122	VAL	2.9
2	AC	45	LYS	2.9
53	B7	6	GLN	2.9
4	CE	91	LEU	2.9
1	CB	163	PHE	2.9
33	DN	53	VAL	2.9
9	CJ	60	ARG	2.9
2	CC	51	GLY	2.9
21	AA	1065	U	2.9
28	DF	134	GLY	2.9
9	AJ	88	LEU	2.9
29	BG	28	VAL	2.9
26	BD	33	LEU	2.9
25	DC	202	PRO	2.9
33	BN	85	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
4	AE	27	ARG	2.9
21	CA	110	C	2.9
6	AG	82	GLY	2.9
33	BN	109	LYS	2.9
2	AC	178	LEU	2.9
21	CA	1385	G	2.9
25	BC	166	ASN	2.9
34	DO	19	ILE	2.9
2	CC	141	VAL	2.9
33	DN	54	VAL	2.9
39	DT	66	VAL	2.9
54	B8	36	LYS	2.9
33	DN	97	ARG	2.9
2	AC	152	ILE	2.9
29	DG	2	PRO	2.9
34	BO	97	ARG	2.9
38	DS	90	GLY	2.9
34	DO	45	GLU	2.9
29	DG	55	LYS	2.9
13	AN	59	ALA	2.9
25	DC	207	GLY	2.9
53	B7	16	HIS	2.9
60	BB	33	G	2.9
25	BC	178	LYS	2.9
29	DG	75	LYS	2.9
36	DQ	26	TYR	2.9
39	BT	95	ARG	2.9
2	CC	133	ALA	2.9
33	BN	94	HIS	2.9
54	B8	11	LYS	2.9
34	BO	49	ARG	2.9
47	B1	42	GLN	2.9
2	CC	137	ALA	2.9
25	DC	61	GLY	2.9
29	BG	151	ALA	2.9
21	CA	1191	A	2.9
2	AC	199	LYS	2.9
28	BF	88	VAL	2.9
43	BX	32	PRO	2.9
54	B8	30	ARG	2.9
21	AA	1464	G	2.9
34	DO	50	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	AC	195	VAL	2.8
33	DN	126	PRO	2.8
2	AC	11	ARG	2.8
25	DC	50	ILE	2.8
2	AC	16	ARG	2.8
29	DG	35	GLU	2.8
13	AN	57	ARG	2.8
33	DN	118	LYS	2.8
34	DO	39	ILE	2.8
15	AP	29	ASP	2.8
21	CA	388	G	2.8
42	BW	82	LEU	2.8
2	CC	146	ALA	2.8
19	AT	18	GLN	2.8
25	DC	46	ALA	2.8
20	AY	320	PRO	2.8
25	BC	175	PRO	2.8
46	B0	78	TYR	2.8
2	CC	175	LEU	2.8
13	AN	47	LEU	2.8
34	BO	82	ASN	2.8
29	DG	151	ALA	2.8
39	BT	93	ARG	2.8
20	AY	365	GLU	2.8
26	DD	23	GLU	2.8
34	BO	79	PHE	2.8
30	DH	51	ARG	2.8
26	DD	59	LYS	2.8
2	AC	44	GLU	2.8
36	BQ	141	GLN	2.8
28	DF	39	TRP	2.8
2	AC	159	GLY	2.8
29	BG	39	ILE	2.8
2	AC	207	VAL	2.8
27	BE	25	VAL	2.8
33	DN	44	PRO	2.8
33	DN	84	LYS	2.8
33	DN	82	LEU	2.8
29	DG	54	GLU	2.8
47	D1	38	SER	2.8
2	CC	97	LYS	2.8
34	DO	11	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
38	BS	60	GLY	2.8
19	CT	13	LEU	2.8
20	AY	356	LEU	2.8
41	DV	94	LEU	2.8
9	CJ	6	ILE	2.8
2	AC	54	ARG	2.8
46	B0	41	ARG	2.8
28	DF	65	TRP	2.8
25	BC	134	PRO	2.8
34	DO	93	PRO	2.8
30	DH	13	LYS	2.8
25	DC	208	THR	2.8
19	AT	8	ARG	2.7
24	AX	54	U	2.7
27	DE	14	ILE	2.7
46	B0	79	VAL	2.7
50	B4	5	ILE	2.7
2	AC	170	GLN	2.7
13	AN	44	LEU	2.7
19	CT	20	LEU	2.7
33	DN	50	ASP	2.7
35	DP	5	ASP	2.7
53	D7	40	TRP	2.7
38	DS	65	VAL	2.7
39	BT	38	ASN	2.7
4	AE	15	ARG	2.7
6	AG	5	ARG	2.7
38	BS	37	ALA	2.7
9	AJ	85	LEU	2.7
25	BC	210	LEU	2.7
26	BD	245	PRO	2.7
28	DF	41	LEU	2.7
12	CM	118	ALA	2.7
20	CY	379	GLY	2.7
8	CI	111	ARG	2.7
9	CJ	69	ASN	2.7
21	CA	369	C	2.7
59	DA	2794(A)	G	2.7
4	CE	22	GLY	2.7
4	CE	23	GLY	2.7
20	AY	324	ARG	2.7
41	DV	68	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
50	D4	13	ARG	2.7
13	CN	48	ALA	2.7
21	CA	1183	A	2.7
59	BA	1757	U	2.7
39	DT	45	PHE	2.7
25	DC	166	ASN	2.7
2	CC	143	GLU	2.7
39	BT	21	GLU	2.7
29	DG	131	TYR	2.7
53	B7	31	LEU	2.7
35	BP	20	GLY	2.7
2	CC	166	GLU	2.7
34	BO	44	LYS	2.7
34	DO	47	ILE	2.7
39	DT	50	ILE	2.7
44	DY	107	ASP	2.7
23	AV	28	A	2.7
21	CA	1062	U	2.7
25	DC	146	VAL	2.7
15	CP	30	GLY	2.7
52	B6	7	ILE	2.7
13	AN	46	GLU	2.7
25	BC	138	LEU	2.7
25	BC	208	THR	2.7
46	B0	74	ARG	2.7
34	DO	46	ALA	2.7
47	D1	7	ILE	2.7
59	BA	2315	G	2.7
25	DC	161	ARG	2.7
30	DH	47	GLU	2.7
53	B7	12	ARG	2.7
2	AC	158	GLY	2.7
33	DN	20	GLY	2.7
26	BD	249	PRO	2.7
34	BO	8	LEU	2.7
39	BT	20	PRO	2.7
22	CW	47	U	2.7
47	D1	6	GLU	2.7
59	BA	1750	G	2.7
32	BK	114	ASP	2.6
2	AC	109	PRO	2.6
20	AY	377	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
26	BD	246	PRO	2.6
2	AC	135	LYS	2.6
33	BN	84	LYS	2.6
46	B0	17	GLN	2.6
25	BC	69	LEU	2.6
11	AL	129	ALA	2.6
27	BE	16	ARG	2.6
36	BQ	33	GLY	2.6
18	CS	27	GLU	2.6
2	CC	124	ILE	2.6
20	AY	358	MET	2.6
26	DD	39	LYS	2.6
13	CN	52	GLN	2.6
59	DA	1552	G	2.6
25	DC	137	LEU	2.6
59	DA	588	U	2.6
21	CA	1113	C	2.6
52	B6	33	LYS	2.6
20	CY	384	ILE	2.6
19	AT	9	ASN	2.6
39	BT	99	LEU	2.6
47	D1	28	GLY	2.6
9	AJ	63	PHE	2.6
15	CP	60	LEU	2.6
29	BG	139	LEU	2.6
39	DT	70	VAL	2.6
34	DO	114	ILE	2.6
53	D7	41	ARG	2.6
25	DC	197	LEU	2.6
29	DG	179	PRO	2.6
22	CW	54	U	2.6
20	AY	354	ARG	2.6
20	CY	368	GLU	2.6
28	DF	184	TYR	2.6
33	BN	51	PHE	2.6
10	AK	31	THR	2.6
30	DH	12	PRO	2.6
17	CR	19	LYS	2.6
25	BC	16	ASP	2.6
28	DF	185	ASP	2.6
60	BB	34	U	2.6
2	AC	121	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
44	DY	4	LYS	2.6
54	D8	26	LYS	2.6
9	AJ	50	ILE	2.6
24	AX	42	G	2.6
22	CW	20(A)	U	2.6
9	AJ	97	GLU	2.6
39	BT	61	PHE	2.6
39	DT	138	ALA	2.6
41	BV	19	LYS	2.6
46	B0	18	ALA	2.6
53	B7	48	LYS	2.6
21	CA	111	G	2.6
38	BS	54	LEU	2.6
12	CM	85	GLY	2.6
33	DN	46	VAL	2.6
38	BS	109	GLY	2.6
42	DW	91	GLY	2.6
54	D8	2	PRO	2.6
27	BE	73	GLU	2.6
9	AJ	29	ARG	2.6
20	CY	321	TYR	2.6
43	DX	32	PRO	2.6
34	BO	103	ALA	2.6
14	AO	19	PRO	2.5
15	CP	19	ILE	2.5
47	D1	71	TYR	2.5
47	D1	93	GLU	2.5
39	BT	66	VAL	2.5
2	AC	189	ALA	2.5
6	AG	155	ARG	2.5
21	CA	1065	U	2.5
2	AC	42	LEU	2.5
44	BY	14	LEU	2.5
19	CT	16	HIS	2.5
19	CT	21	LYS	2.5
34	DO	78	ARG	2.5
59	BA	53	A	2.5
9	AJ	64	GLU	2.5
33	DN	122	VAL	2.5
25	BC	14	LYS	2.5
28	BF	26	ALA	2.5
25	BC	212	SER	2.5

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Mol	Chain	Res	Type	RSRZ
33	BN	44	PRO	2.5
36	DQ	104	PHE	2.5
29	DG	108	ASN	2.5
2	AC	130	VAL	2.5
2	AC	131	ARG	2.5
12	AM	94	ARG	2.5
22	AW	16	U	2.5
39	DT	109	GLU	2.5
2	AC	185	GLY	2.5
34	DO	75	SER	2.5
50	B4	13	ARG	2.5
1	CB	140	HIS	2.5
34	DO	117	LEU	2.5
52	D6	26	ASN	2.5
25	DC	8	TYR	2.5
47	D1	10	LYS	2.5
1	AB	183	PRO	2.5
19	CT	18	GLN	2.5
28	DF	187	VAL	2.5
29	DG	26	GLN	2.5
2	CC	144	SER	2.5
38	DS	26	LEU	2.5
38	BS	107	GLU	2.5
53	B7	32	LYS	2.5
36	DQ	20	ALA	2.5
39	DT	69	GLY	2.5
52	D6	10	LEU	2.5
34	BO	101	PRO	2.5
59	DA	1711	C	2.5
29	DG	178	PHE	2.5
34	DO	113	LYS	2.5
2	CC	153	VAL	2.5
50	B4	15	ILE	2.5
54	D8	23	VAL	2.5
9	AJ	65	LEU	2.5
29	DG	56	ALA	2.5
30	DH	49	VAL	2.5
32	BK	2	LYS	2.5
2	CC	178	LEU	2.5
19	CT	17	ARG	2.5
28	BF	96	ASP	2.5
38	BS	41	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
46	B0	77	ARG	2.5
20	CY	155	GLU	2.5
49	B3	12	PRO	2.5
20	CY	157	LEU	2.5
9	CJ	4	ILE	2.5
12	CM	125	ARG	2.5
59	DA	2132	U	2.5
2	AC	23	TYR	2.5
2	AC	110	ASN	2.5
6	AG	11	GLN	2.5
47	B1	93	GLU	2.5
52	B6	51	GLU	2.5
33	DN	90	MET	2.5
2	CC	45	LYS	2.5
59	DA	2321	G	2.4
2	CC	52	LEU	2.4
20	CY	383	THR	2.4
27	DE	105	THR	2.4
30	DH	50	VAL	2.4
12	CM	2	ALA	2.4
20	CY	16	GLY	2.4
42	DW	113	LYS	2.4
27	DE	15	PHE	2.4
2	AC	104	GLN	2.4
2	AC	106	VAL	2.4
16	CQ	99	SER	2.4
25	DC	129	GLY	2.4
27	DE	25	VAL	2.4
52	D6	29	ASN	2.4
53	B7	36	GLN	2.4
34	DO	108	GLU	2.4
39	DT	11	GLU	2.4
54	B8	64	TYR	2.4
20	AY	322	VAL	2.4
26	BD	39	LYS	2.4
39	BT	63	VAL	2.4
25	BC	174	ALA	2.4
2	AC	52	LEU	2.4
2	AC	141	VAL	2.4
2	AC	144	SER	2.4
22	AW	63	C	2.4
28	DF	119	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
39	BT	41	ARG	2.4
15	AP	65	GLN	2.4
56	Be	121	VAL	2.4
25	DC	211	ARG	2.4
20	CY	375	GLY	2.4
28	DF	186	ILE	2.4
34	DO	104	ARG	2.4
56	De	82	THR	2.4
28	BF	69	HIS	2.4
2	AC	43	LEU	2.4
35	BP	21	ARG	2.4
2	AC	186	PHE	2.4
26	BD	4	LYS	2.4
2	AC	139	GLN	2.4
2	AC	196	LEU	2.4
21	CA	1192	C	2.4
27	BE	120	TRP	2.4
39	BT	52	ILE	2.4
2	AC	145	GLY	2.4
10	CK	41	THR	2.4
25	BC	180	SER	2.4
56	Be	58	THR	2.4
2	AC	69	HIS	2.4
1	AB	68	ILE	2.4
2	CC	112	SER	2.4
26	BD	32	SER	2.4
30	BH	16	SER	2.4
30	DH	48	GLY	2.4
38	BS	88	ASP	2.4
4	AE	91	LEU	2.4
39	BT	62	THR	2.4
47	B1	35	THR	2.4
25	BC	227	PRO	2.4
28	BF	182	ASN	2.4
21	AA	317	G	2.4
38	BS	33	LYS	2.4
10	AK	41	THR	2.4
25	BC	12	LEU	2.4
25	BC	22	THR	2.4
27	BE	98	PRO	2.4
28	DF	66	PRO	2.4
38	BS	38	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
50	D4	14	ILE	2.4
52	D6	27	LYS	2.4
6	AG	79	ARG	2.4
29	DG	96	ARG	2.4
25	BC	55	SER	2.4
39	BT	78	LEU	2.4
2	AC	15	THR	2.4
9	AJ	100	THR	2.4
4	AE	88	LYS	2.4
13	CN	50	LYS	2.4
47	D1	20	ARG	2.4
39	DT	114	LEU	2.4
29	BG	97	ASP	2.4
26	DD	57	GLY	2.3
34	DO	16	ALA	2.3
50	B4	22	ILE	2.3
38	DS	58	LEU	2.3
50	B4	33	VAL	2.3
2	AC	147	LYS	2.3
45	DZ	79	ARG	2.3
30	BH	168	PRO	2.3
32	BK	120	LEU	2.3
42	DW	86	LEU	2.3
2	CC	60	ALA	2.3
4	AE	30	ALA	2.3
9	CJ	3	LYS	2.3
24	CX	18	G	2.3
29	BG	143	GLU	2.3
39	DT	111	ARG	2.3
56	De	101	GLU	2.3
22	CW	61	C	2.3
34	BO	122	LEU	2.3
9	CJ	61	GLU	2.3
2	AC	71	ALA	2.3
2	CC	170	GLN	2.3
39	BT	87	ASP	2.3
22	AW	17	U	2.3
2	AC	187	ALA	2.3
34	DO	53	LYS	2.3
2	CC	15	THR	2.3
54	B8	57	ARG	2.3
28	BF	176	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
20	AY	105	ILE	2.3
21	AA	1185	G	2.3
26	BD	29	PRO	2.3
59	DA	2794(C)	C	2.3
26	BD	30	GLU	2.3
46	D0	75	LEU	2.3
2	AC	142	MET	2.3
28	DF	79	GLY	2.3
29	BG	99	MET	2.3
50	B4	20	ASN	2.3
46	B0	55	ARG	2.3
4	AE	135	THR	2.3
30	BH	24	VAL	2.3
33	BN	137	LYS	2.3
33	DN	55	VAL	2.3
43	BX	33	LYS	2.3
46	B0	71	ASP	2.3
46	D0	46	LYS	2.3
47	D1	30	VAL	2.3
46	B0	52	GLY	2.3
59	BA	2286	A	2.3
60	BB	25	A	2.3
39	DT	95	ARG	2.3
53	D7	45	ALA	2.3
59	BA	351	G	2.3
25	DC	57	GLN	2.3
29	BG	66	GLN	2.3
56	De	63	ILE	2.3
38	BS	26	LEU	2.3
20	AY	383	THR	2.3
9	AJ	14	LYS	2.3
20	CY	339	SER	2.3
25	BC	189	ASN	2.3
28	DF	37	VAL	2.3
27	DE	26	ILE	2.3
50	D4	8	LYS	2.3
56	Be	73	GLU	2.3
20	AY	228	MET	2.3
29	BG	127	GLY	2.3
10	AK	11	LYS	2.3
39	BT	85	LYS	2.3
33	BN	53	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
41	BV	14	VAL	2.3
19	CT	70	SER	2.3
34	DO	48	PRO	2.3
20	AY	396	ARG	2.3
25	DC	205	ALA	2.3
29	BG	88	ILE	2.3
6	CG	79	ARG	2.2
15	AP	30	GLY	2.2
32	DK	111	LYS	2.2
34	DO	112	MET	2.2
39	BT	67	SER	2.2
25	BC	137	LEU	2.2
25	BC	221	PRO	2.2
27	DE	126	PRO	2.2
33	BN	83	LYS	2.2
36	BQ	97	VAL	2.2
21	CA	1086	U	2.2
26	DD	217	ARG	2.2
25	BC	61	GLY	2.2
40	DU	19	LYS	2.2
59	BA	611(E)	G	2.2
25	DC	118	PRO	2.2
34	DO	106	LEU	2.2
6	CG	154	TYR	2.2
9	CJ	22	LYS	2.2
24	CX	54	U	2.2
53	D7	38	GLY	2.2
4	AE	32	VAL	2.2
25	BC	143	ALA	2.2
34	DO	61	VAL	2.2
47	B1	12	PRO	2.2
33	BN	134	ARG	2.2
21	CA	1386	G	2.2
22	AW	52	G	2.2
32	DK	115	LEU	2.2
52	D6	9	LEU	2.2
34	BO	94	ARG	2.2
9	AJ	8	LEU	2.2
18	CS	68	GLY	2.2
46	B0	21	LEU	2.2
2	CC	121	ALA	2.2
27	BE	72	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
25	BC	35	THR	2.2
51	D5	24	ALA	2.2
29	BG	170	ARG	2.2
2	AC	105	GLU	2.2
23	AV	29	A	2.2
28	DF	89	VAL	2.2
29	DG	152	LEU	2.2
47	D1	95	LEU	2.2
59	BA	472	A	2.2
25	DC	113	ALA	2.2
28	BF	40	GLN	2.2
26	BD	27	THR	2.2
38	BS	62	LYS	2.2
39	DT	41	ARG	2.2
47	B1	61	ARG	2.2
27	DE	9	VAL	2.2
54	D8	40	GLU	2.2
39	BT	88	ILE	2.2
15	CP	28	ARG	2.2
50	D4	1	MET	2.2
33	BN	127	ASP	2.2
2	AC	172	ARG	2.2
9	CJ	5	ARG	2.2
9	CJ	93	GLY	2.2
20	AY	39	ILE	2.2
26	BD	5	LYS	2.2
3	AD	183	GLY	2.2
2	CC	10	PHE	2.2
10	AK	12	ARG	2.2
25	DC	199	ALA	2.2
33	DN	72	TYR	2.2
38	DS	32	LEU	2.2
13	AN	26	ARG	2.2
26	DD	52	ARG	2.2
33	BN	70	LYS	2.2
39	DT	96	ARG	2.2
53	B7	2	LYS	2.2
20	CY	378	VAL	2.2
26	BD	23	GLU	2.2
33	BN	1	MET	2.2
52	B6	13	CYS	2.2
33	BN	9	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
20	AY	379	GLY	2.2
54	D8	28	GLY	2.2
9	CJ	62	HIS	2.2
20	CY	311	ALA	2.2
25	DC	136	GLY	2.2
34	DO	2	ILE	2.2
59	BA	889	C	2.2
2	CC	17	ASP	2.2
2	AC	136	GLN	2.2
20	AY	357	ARG	2.2
39	BT	115	ARG	2.2
2	CC	46	GLU	2.2
6	AG	8	GLU	2.2
30	BH	21	PRO	2.1
4	AE	12	LEU	2.1
9	AJ	70	ARG	2.1
17	CR	42	ARG	2.1
26	DD	95	LEU	2.1
36	BQ	132	VAL	2.1
29	DG	52	ILE	2.1
59	DA	2294	C	2.1
2	AC	72	LYS	2.1
9	CJ	71	LEU	2.1
13	AN	12	ARG	2.1
29	BG	150	ASP	2.1
9	AJ	95	GLU	2.1
11	AL	127	GLU	2.1
30	DH	18	GLU	2.1
26	DD	2	ALA	2.1
2	AC	138	VAL	2.1
17	AR	42	ARG	2.1
29	DG	3	LEU	2.1
2	AC	161	GLU	2.1
9	AJ	21	GLN	2.1
2	CC	7	PRO	2.1
26	BD	91	ARG	2.1
27	DE	5	LEU	2.1
33	BN	108	PRO	2.1
42	BW	85	VAL	2.1
9	CJ	64	GLU	2.1
39	DT	85	LYS	2.1
28	DF	191	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
60	BB	42	C	2.1
2	AC	53	ALA	2.1
34	DO	43	VAL	2.1
13	AN	21	TYR	2.1
25	BC	139	PRO	2.1
50	D4	29	PRO	2.1
54	D8	41	ILE	2.1
18	CS	28	LYS	2.1
3	CD	48	ALA	2.1
9	AJ	92	THR	2.1
39	BT	19	LEU	2.1
47	D1	94	LEU	2.1
8	AI	114	TYR	2.1
33	BN	56	ASN	2.1
33	DN	135	PRO	2.1
37	DR	21	TYR	2.1
59	BA	125	G	2.1
9	AJ	60	ARG	2.1
2	CC	139	GLN	2.1
9	AJ	68	HIS	2.1
9	CJ	21	GLN	2.1
28	BF	192	LEU	2.1
29	DG	82	LEU	2.1
25	DC	169	THR	2.1
11	CL	19	ARG	2.1
39	BT	47	GLY	2.1
4	CE	48	ALA	2.1
20	AY	355	LEU	2.1
25	BC	223	VAL	2.1
34	BO	106	LEU	2.1
21	CA	333	G	2.1
25	BC	157	ILE	2.1
2	CC	195	VAL	2.1
28	DF	35	GLU	2.1
13	CN	6	LEU	2.1
25	BC	199	ALA	2.1
53	D7	31	LEU	2.1
20	CY	328	ILE	2.1
53	D7	43	THR	2.1
29	BG	149	VAL	2.1
38	BS	106	ARG	2.1
4	CE	13	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
25	DC	172	ILE	2.1
32	DK	110	GLN	2.1
33	BN	133	GLN	2.1
10	AK	110	ASP	2.1
20	CY	326	THR	2.1
25	BC	160	GLY	2.1
26	BD	56	GLY	2.1
28	BF	41	LEU	2.1
28	DF	192	LEU	2.1
39	BT	92	GLY	2.1
47	D1	24	ALA	2.1
59	BA	291	C	2.1
8	AI	113	LYS	2.1
33	BN	7	LYS	2.1
44	DY	8	LYS	2.1
13	CN	47	LEU	2.1
29	BG	152	LEU	2.1
25	DC	167	ASP	2.1
43	BX	34	ALA	2.1
2	AC	124	ILE	2.1
45	DZ	78	LYS	2.1
12	AM	104	ARG	2.1
26	DD	13	ARG	2.1
21	CA	1195	C	2.1
46	B0	80	HIS	2.1
12	AM	88	ARG	2.1
39	DT	38	ASN	2.1
9	AJ	90	LEU	2.1
28	DF	36	VAL	2.1
19	AT	19	SER	2.0
22	AW	51	A	2.0
59	DA	7	G	2.0
25	DC	210	LEU	2.0
34	BO	89	ASN	2.0
48	D2	71	ASN	2.0
59	BA	1543(A)	C	2.0
25	BC	70	GLY	2.0
50	B4	8	LYS	2.0
20	AY	360	ALA	2.0
28	DF	26	ALA	2.0
2	AC	38	ARG	2.0
4	CE	27	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
28	DF	64	ILE	2.0
46	D0	53	MET	2.0
52	B6	6	ARG	2.0
2	AC	103	VAL	2.0
9	CJ	88	LEU	2.0
28	BF	193	VAL	2.0
41	BV	5	VAL	2.0
13	CN	37	PHE	2.0
20	CY	381	LYS	2.0
38	BS	59	LYS	2.0
41	BV	6	LYS	2.0
56	Be	96	GLY	2.0
2	AC	134	ILE	2.0
21	AA	1189	C	2.0
28	BF	78	ILE	2.0
30	BH	162	ILE	2.0
54	B8	2	PRO	2.0
29	DG	146	TYR	2.0
26	BD	34	VAL	2.0
25	DC	168	LYS	2.0
39	DT	21	GLU	2.0
39	DT	73	GLU	2.0
44	DY	32	PRO	2.0
19	CT	73	HIS	2.0
27	BE	23	VAL	2.0
34	BO	115	VAL	2.0
4	AE	46	GLY	2.0
29	DG	145	THR	2.0
4	CE	15	ARG	2.0
21	AA	110	C	2.0
60	BB	28	C	2.0
38	BS	48	LEU	2.0
11	CL	78	GLN	2.0
34	BO	114	ILE	2.0
53	B7	35	ARG	2.0
2	AC	97	LYS	2.0
2	CC	106	VAL	2.0
32	BK	3	LYS	2.0
40	BU	72	HIS	2.0
20	AY	386	GLY	2.0
21	CA	163	C	2.0
15	AP	56	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
32	BK	118	THR	2.0
35	DP	21	ARG	2.0
45	DZ	81	ARG	2.0
17	AR	22	VAL	2.0
25	DC	196	ALA	2.0
28	BF	185	ASP	2.0
53	D7	14	LYS	2.0
2	AC	206	GLU	2.0
19	AT	15	ARG	2.0
33	DN	96	GLU	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)

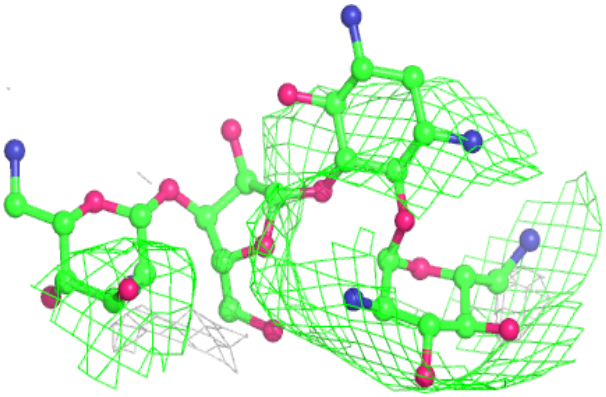
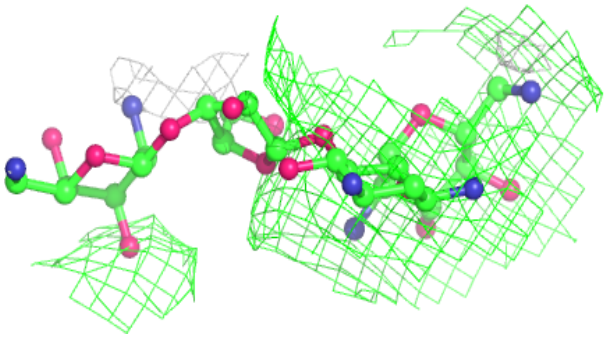
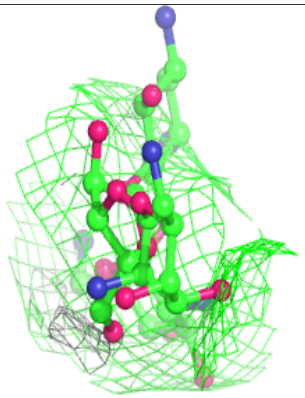
There are no monosaccharides in this entry.

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.

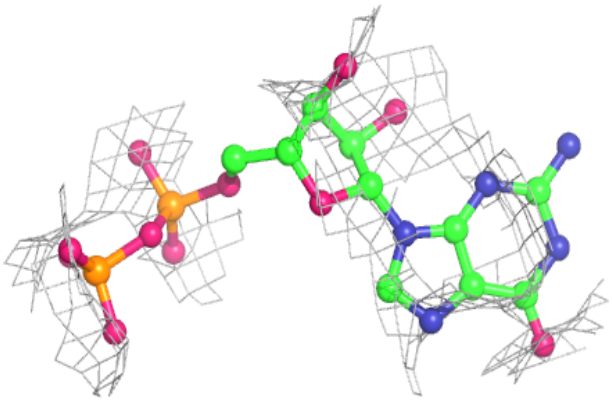
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
64	MG	CY	703	1/1	0.74	0.18	6,6,6,6	0
64	MG	BA	2901	1/1	0.75	0.12	2,2,2,2	0
63	NMY	BA	2904	42/42	0.79	0.26	42,50,59,62	42
61	GDP	AY	701	28/28	0.80	0.24	179,183,185,185	0
62	FUA	AY	702	37/37	0.81	0.69	198,199,200,201	0
63	NMY	DA	2901	42/42	0.81	0.24	31,42,51,53	42
62	FUA	CY	702	37/37	0.82	0.89	194,196,197,197	0
63	NMY	BA	2902	42/42	0.82	0.22	14,24,43,44	42
63	NMY	AA	1601	42/42	0.87	0.31	16,27,36,38	42
63	NMY	BA	2903	42/42	0.87	0.28	18,29,38,41	42
61	GDP	CY	701	28/28	0.88	0.14	104,108,109,110	0
63	NMY	CA	1601	42/42	0.90	0.23	14,25,34,37	42

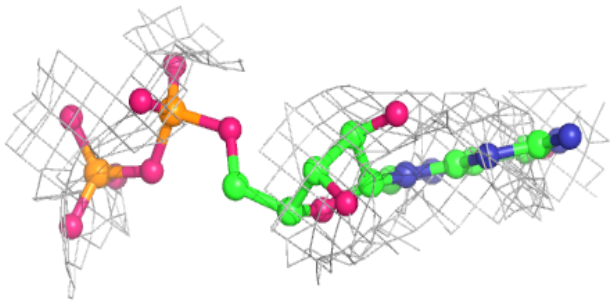
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

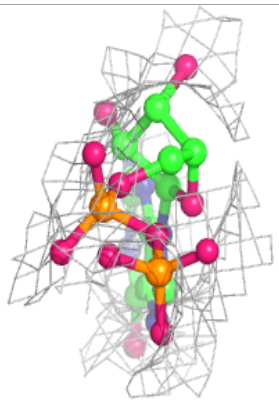
Electron density around NMY BA 2904: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around GDP AY 701:

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

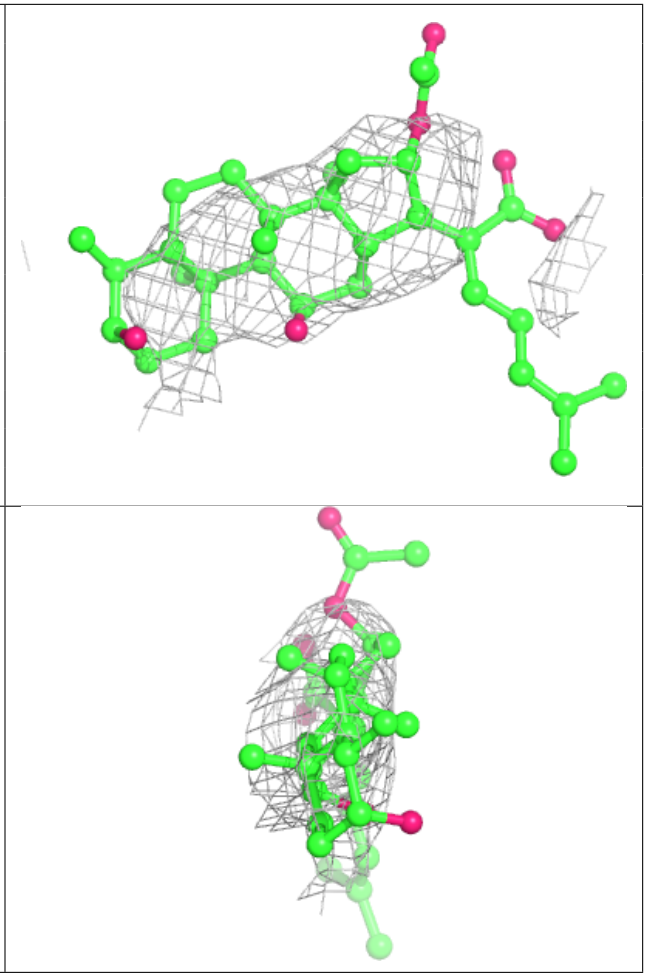






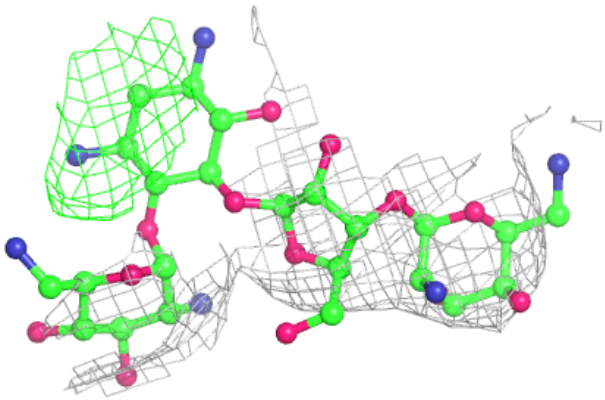
Electron density around FUA AY 702:

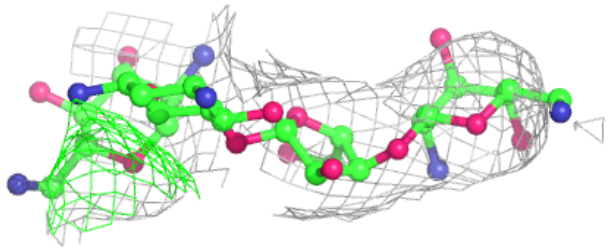
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

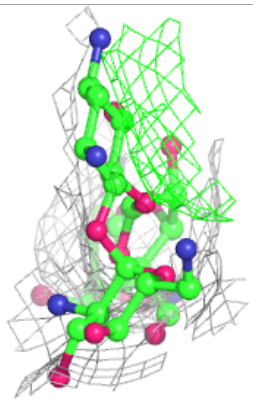


Electron density around NMY DA 2901:

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

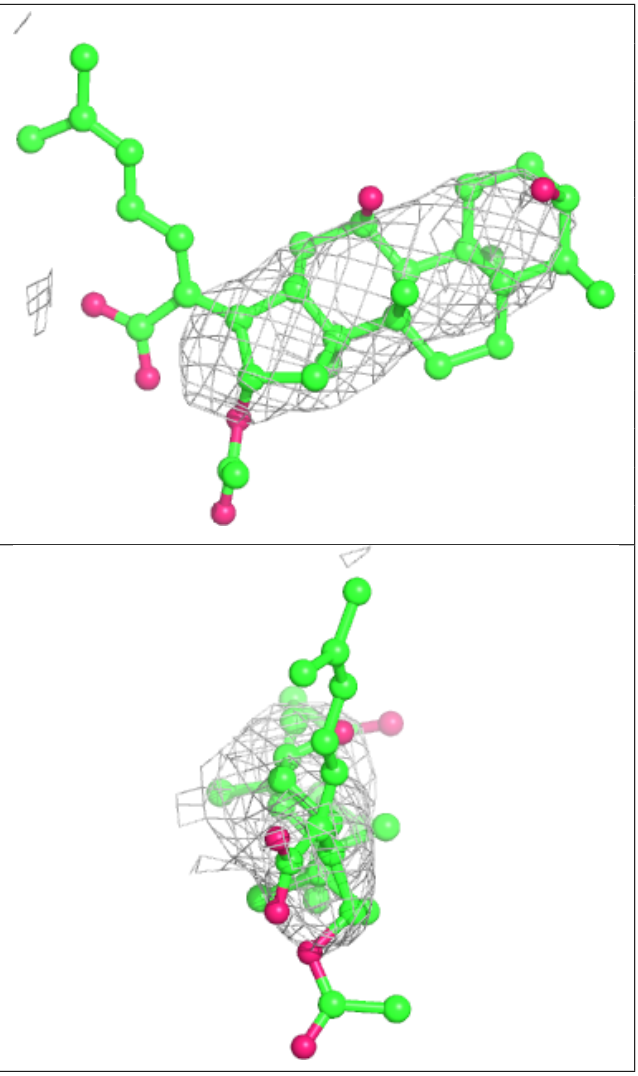






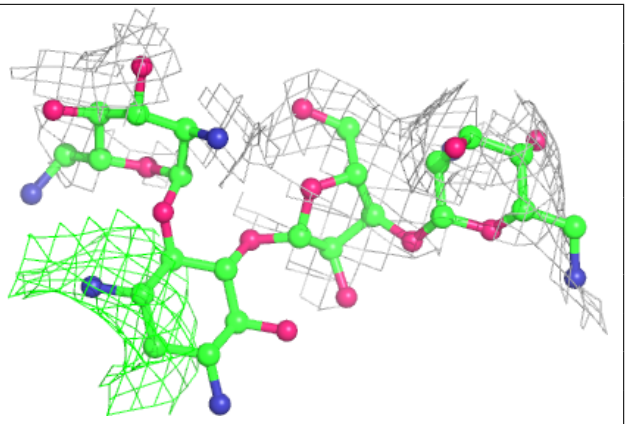
Electron density around FUA CY 702:

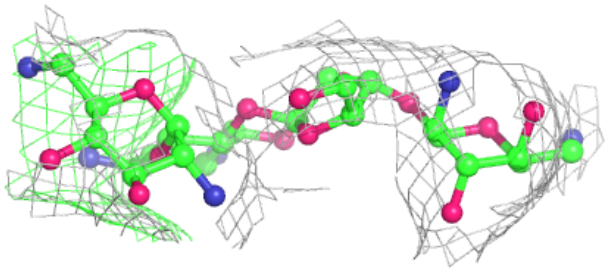
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

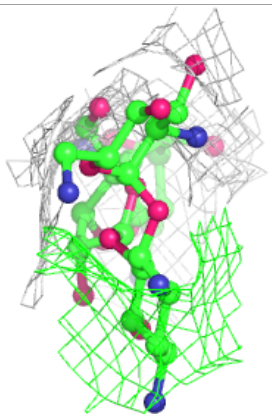


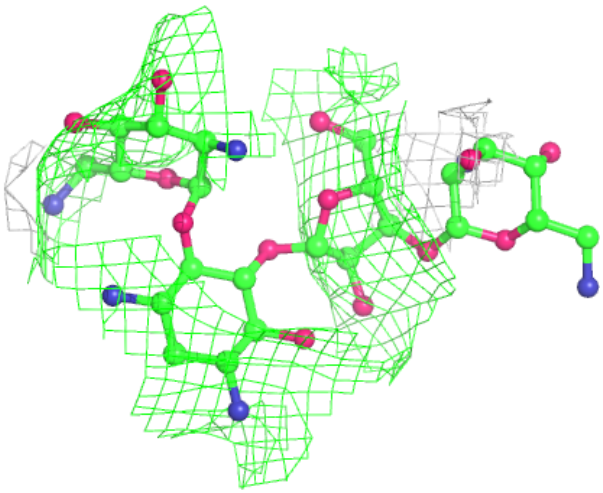
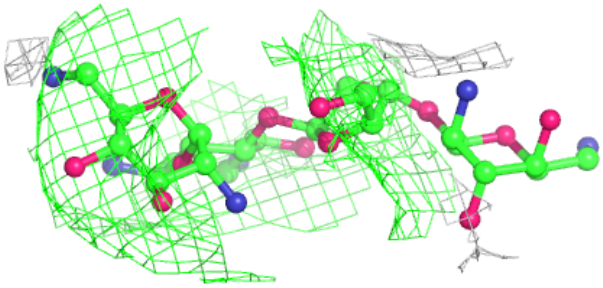
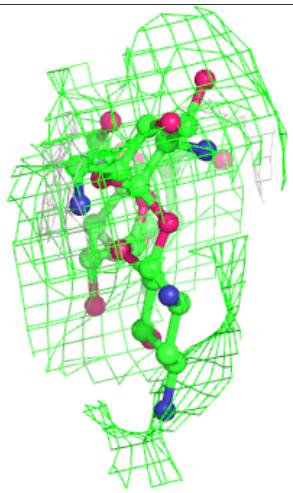
Electron density around NMY BA 2902:

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



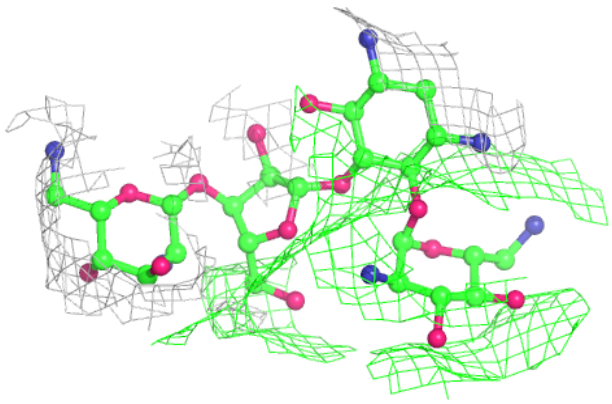


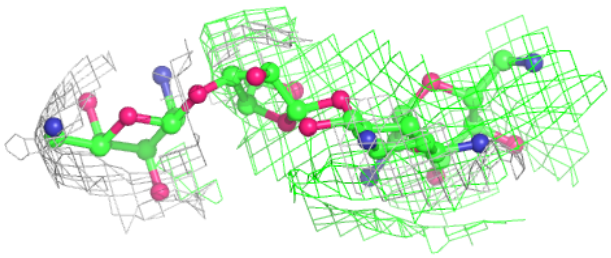


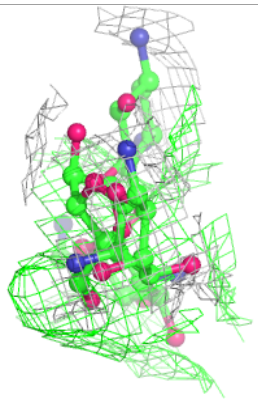
Electron density around NMY AA 1601: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around NMY BA 2903:

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

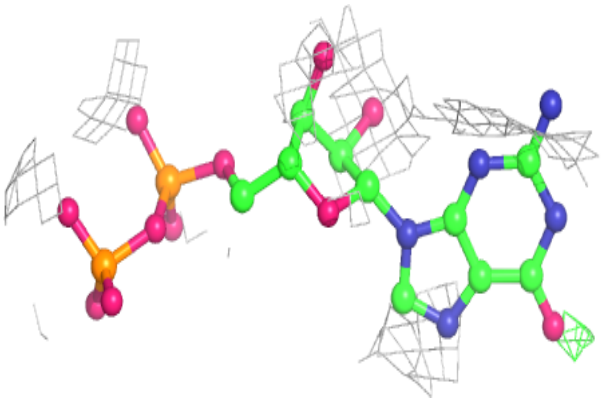


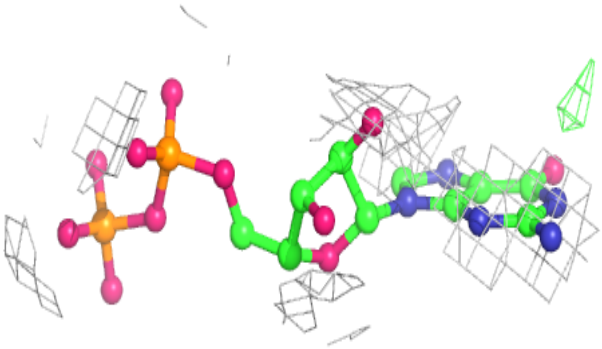


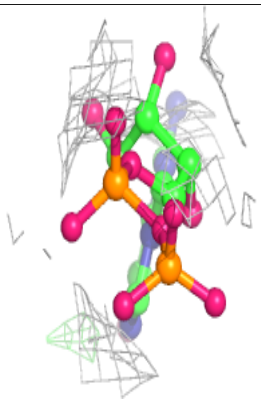


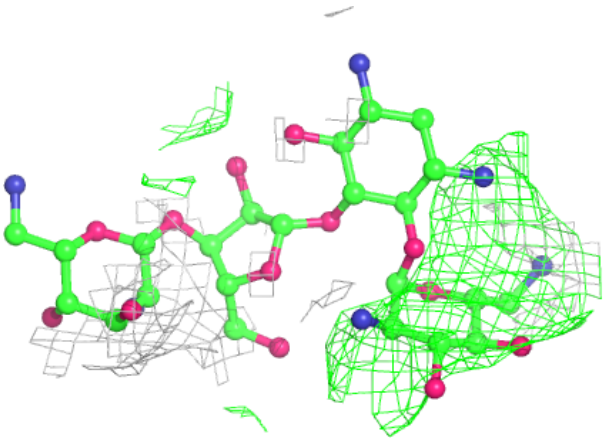
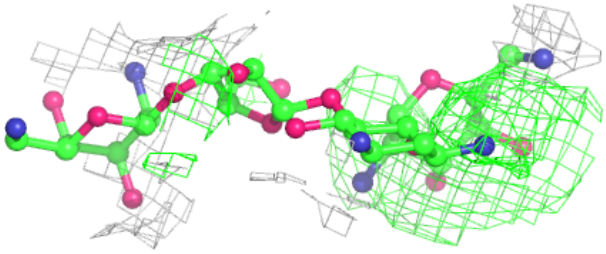
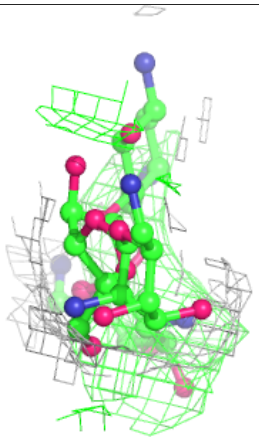
Electron density around GDP CY 701:

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







Electron density around NMY CA 1601: 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.