



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 12:48 PM EDT

PDB ID : 4V9L
Title : 70S Ribosome translocation intermediate FA-3.6A containing elongation factor EFG/FUSIDIC ACID/GDP, mRNA, and tRNA bound in the pe*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

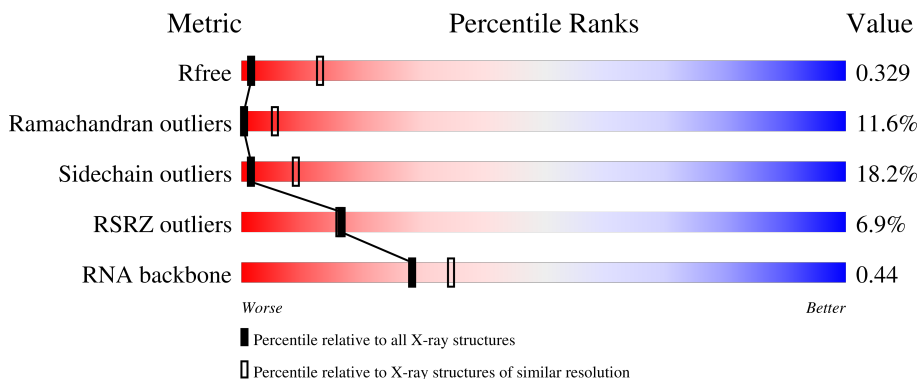
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



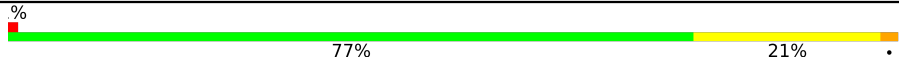

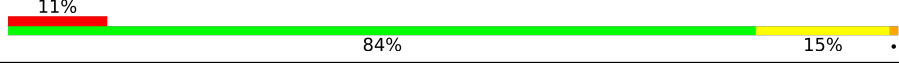

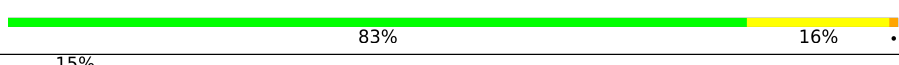
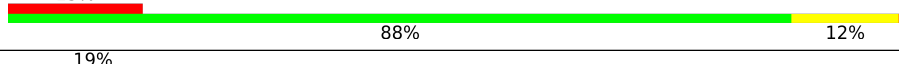
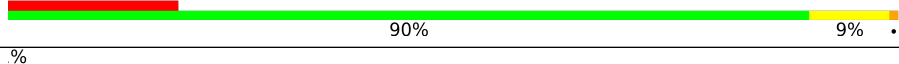

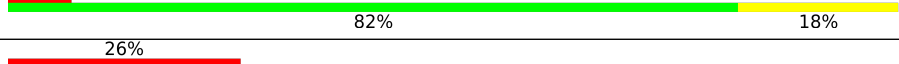


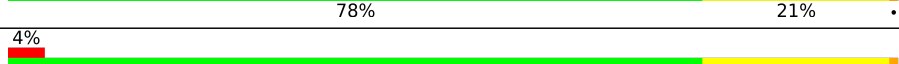
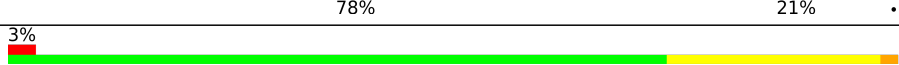
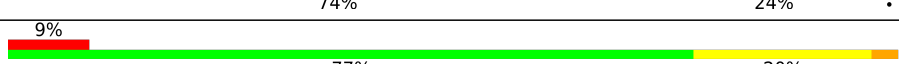


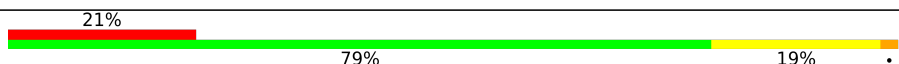
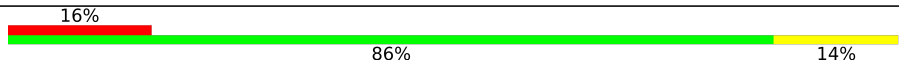
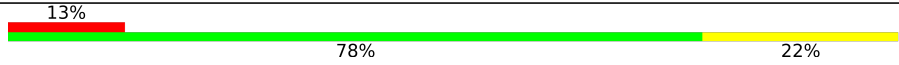


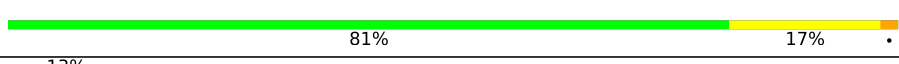
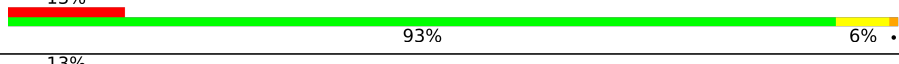


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AB	235	
1	CB	235	
2	AC	207	
2	CC	207	
3	AD	208	

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Mol	Chain	Length	Quality of chain
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	

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Mol	Chain	Length	Quality of chain
16	AQ	100	6% 77% 22%
16	CQ	100	11% 75% 24%
17	AR	70	% 77% 21%
17	CR	70	6% 81% 16%
18	AS	79	15% 66% 34%
18	CS	79	10% 66% 32%
19	AT	99	4% 86% 12%
19	CT	99	8% 86% 13%
20	AA	1511	2% 78% 21%
20	CA	1511	2% 80% 19%
21	AW	77	% 69% 31%
21	CW	77	8% 69% 29%
22	AV	23	22% 65% 35%
22	CV	23	39% 61% 39%
23	AY	687	7% 74% 22%
23	CY	687	9% 74% 20%
24	AU	6	50% 50%
24	CU	6	33% 67%
25	BC	228	22% 64% 32%
25	DC	228	34% 66% 29%
26	BD	275	2% 66% 31%
26	DD	275	3% 66% 31%
27	BE	205	% 71% 25%
27	DE	205	3% 66% 31%
28	BF	208	13% 72% 25%

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Mol	Chain	Length	Quality of chain
28	DF	208	16% 71% 25% .
29	BG	181	31% 81% 18% .
29	DG	181	32% 79% 20% .
30	BH	167	% 78% 19% .
30	DH	167	3% 82% 17% .
31	BJ	170	99% .
31	DJ	170	99% .
32	BK	140	28% 81% 18% .
32	DK	140	31% 84% 16% .
33	BN	138	17% 70% 29% .
33	DN	138	14% 75% 25% .
34	BO	122	2% 78% 20% .
34	DO	122	3% 80% 19% .
35	BP	146	9% 71% 27% .
35	DP	146	8% 71% 29% .
36	BQ	141	% 70% 29% .
36	DQ	141	4% 74% 24% .
37	BR	117	4% 83% 16% .
37	DR	117	5% 78% 19% .
38	BS	99	23% 69% 25% 5% .
38	DS	99	40% 65% 29% 5% .
39	BT	138	5% 67% 28% .
39	DT	138	8% 68% 28% .
40	BU	117	4% 78% 21% .
40	DU	117	3% 75% 24% .

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Mol	Chain	Length	Quality of chain
41	BV	101	5% 65% 30% 5%
41	DV	101	3% 65% 33% .
42	BW	113	5% 69% 27% ..
42	DW	113	4% 74% 22% .
43	BX	93	3% 84% 16%
43	DX	93	5% 78% 20% .
44	BY	107	7% 62% 36% .
44	DY	107	6% 62% 31% 7%
45	BZ	185	4% 76% 22% .
45	DZ	185	4% 77% 21% .
46	B0	84	2% 77% 23%
46	D0	84	2% 73% 25% .
47	B2	71	90% 8% .
47	D2	71	87% 13%
48	B3	60	85% 12% .
48	D3	60	78% 22%
49	B5	59	2% 85% 14% .
49	D5	59	76% 24%
50	B6	50	8% 72% 20% 6% .
50	D6	50	20% 58% 38% .
51	B7	49	22% 78% 22%
51	D7	49	27% 82% 16% .
52	B8	64	5% 64% 33% .
52	D8	64	5% 66% 30% 5%
53	B9	37	73% 24% .

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Mol	Chain	Length	Quality of chain
53	D9	37	86% 14%
54	Be	102	40% 86% 13%
54	De	102	28% 88% 10%
55	Bf	31	100%
55	Bg	31	100%
55	Df	31	100%
55	Dg	31	100%
56	Bh	30	100%
56	Dh	30	100%
57	B1	93	24% 66% 33%
57	D1	93	28% 62% 33%
58	B4	35	49% 66% 31%
58	D4	35	66% 69% 29%
59	BA	2879	75% 24%
59	DA	2879	75% 24%
60	BB	119	3% 78% 22%
60	DB	119	8% 82% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	FUA	CY	701	-	-	-	X

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 308166 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	Total 1910	C 1218	N 342	O 345	S 5	0	0	0
1	CB	235	Total 1910	C 1218	N 342	O 345	S 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	Total 1621	C 1022	N 315	O 283	S 1	0	0	0
2	CC	207	Total 1621	C 1022	N 315	O 283	S 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	Total 1703	C 1066	N 339	O 291	S 7	0	0	0
3	CD	208	Total 1703	C 1066	N 339	O 291	S 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	Total 1156	C 729	N 218	O 205	S 4	0	0	0
4	CE	151	Total 1156	C 729	N 218	O 205	S 4	0	0	0

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	HIS	ARG	conflict	UNP P62669
CI	58	HIS	ARG	conflict	UNP P62669

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	96	GLU	GLN	conflict	UNP P62658
CQ	96	GLU	GLN	conflict	UNP P62658

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	41	ILE	VAL	conflict	UNP P62661
CT	41	ILE	VAL	conflict	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

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

- Molecule 21 is a RNA chain called transfer RNA.

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

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			
22	CV	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			
23	CY	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

There are 4 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total	C	N	O	0	0	0
			48	25	13	10			
24	CU	6	Total	C	N	O	0	0	0
			48	25	13	10			

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	conflict	UNP Q72GV9
BC	28	ARG	HIS	conflict	UNP Q72GV9
DC	20	VAL	ILE	conflict	UNP Q72GV9
DC	28	ARG	HIS	conflict	UNP Q72GV9

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

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

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

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

- 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	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			
28	DF	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	insertion	UNP Q72I05
BF	3	GLU	-	insertion	UNP Q72I05
BF	4	VAL	-	insertion	UNP Q72I05
BF	5	ALA	-	insertion	UNP Q72I05
BF	6	VAL	-	insertion	UNP Q72I05
DF	2	LYS	-	insertion	UNP Q72I05
DF	3	GLU	-	insertion	UNP Q72I05
DF	4	VAL	-	insertion	UNP Q72I05
DF	5	ALA	-	insertion	UNP Q72I05
DF	6	VAL	-	insertion	UNP Q72I05

- 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	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
29	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	conflict	UNP Q72I16
DG	5	VAL	LEU	conflict	UNP Q72I16

- 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	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			
30	DH	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- 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	138	1104	712	206	182	4	0	0	0
33	DN	138	1104	712	206	182	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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	conflict	UNP Q72I14
DO	69	ILE	VAL	conflict	UNP Q72I14

- 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

Continued on next page...

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	conflict	UNP Q72JU9
BT	135	ALA	VAL	conflict	UNP Q72JU9
DT	123	GLN	LYS	conflict	UNP Q72JU9
DT	135	ALA	VAL	conflict	UNP Q72JU9

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	conflict	UNP Q72HR3
D0	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	conflict	UNP P62652
D5	29	THR	ILE	conflict	UNP P62652

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
53	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 54 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

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

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

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

- Molecule 57 is a protein called 50S ribosomal protein L28.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	conflict	UNP Q72G84
D1	81	LYS	ARG	conflict	UNP Q72G84

- Molecule 58 is a protein called 50S ribosomal protein L31.

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

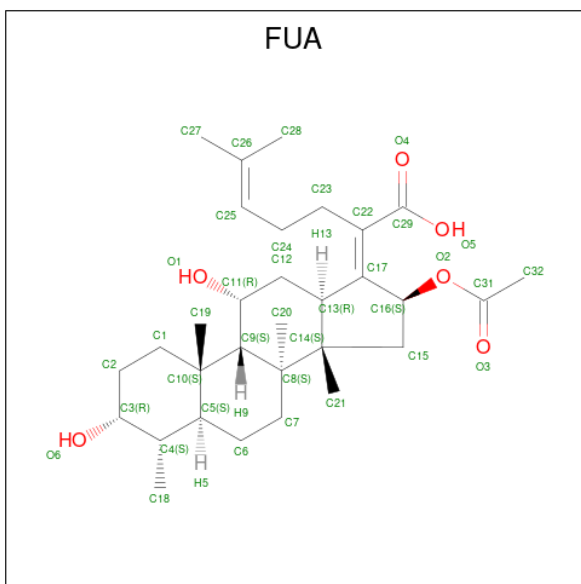
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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

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

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

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).

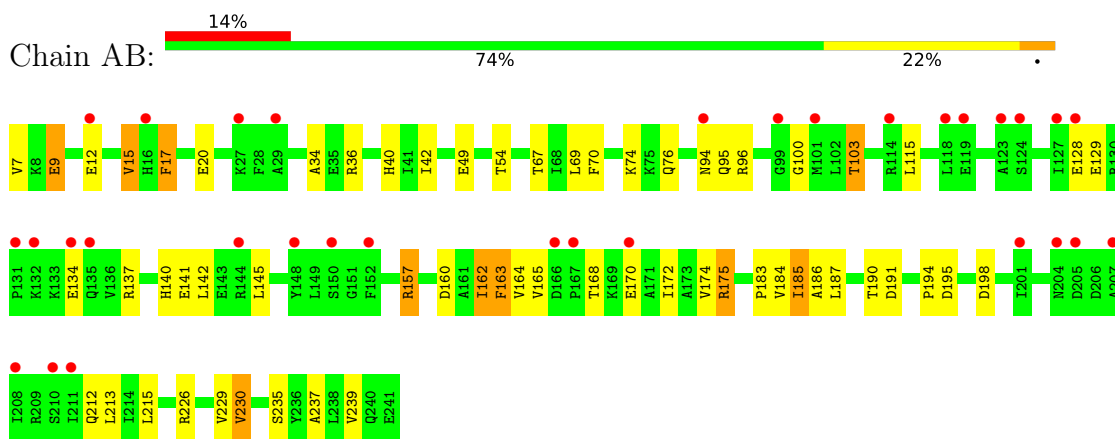


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	1	Total	C O	0	0
			37	31 6		
61	CY	1	Total	C O	0	0
			37	31 6		

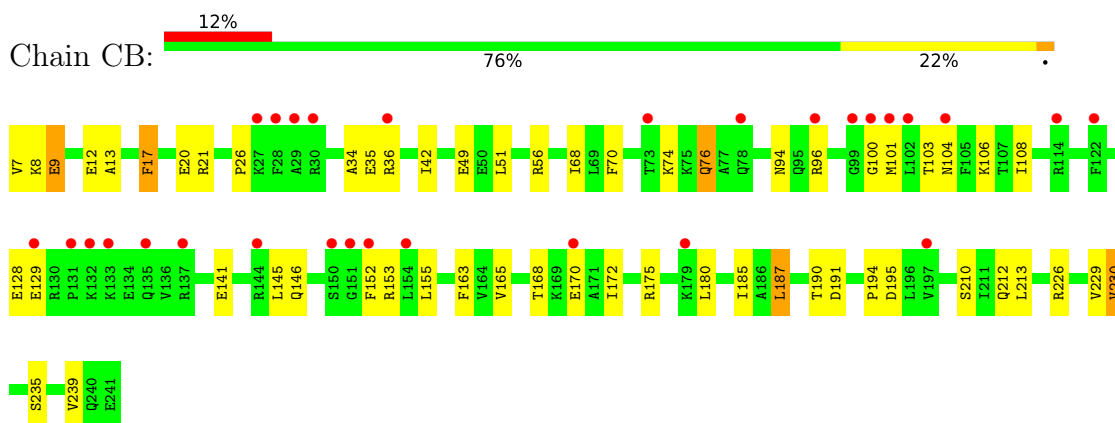
3 Residue-property plots [i](#)

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.

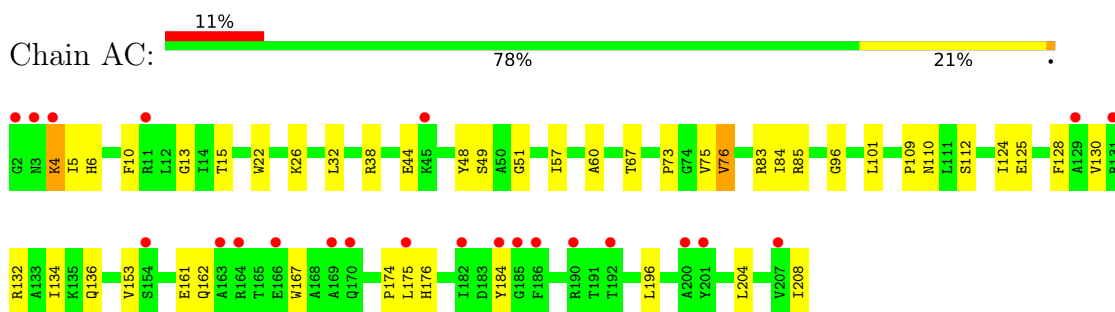
- Molecule 1: 30S ribosomal protein S2



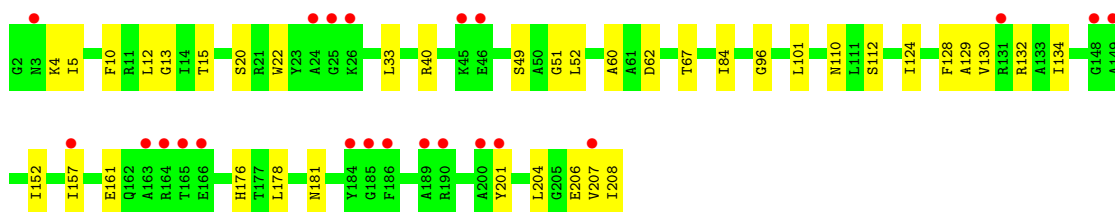
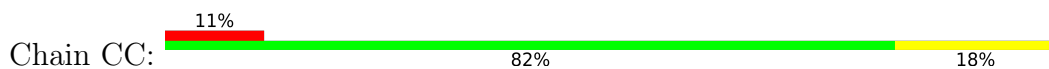
- Molecule 1: 30S ribosomal protein S2



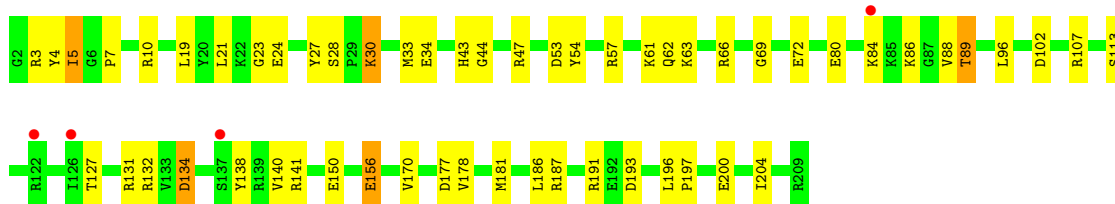
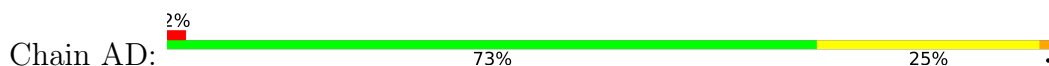
- Molecule 2: 30S ribosomal protein S3



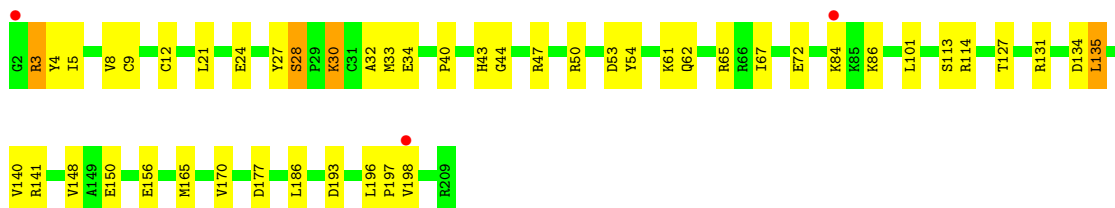
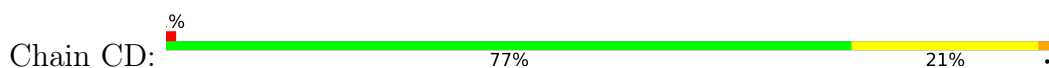
- Molecule 2: 30S ribosomal protein S3



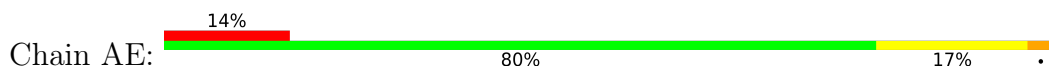
- Molecule 3: 30S ribosomal protein S4



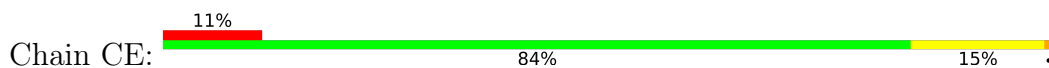
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5

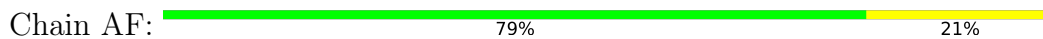


- Molecule 4: 30S ribosomal protein S5

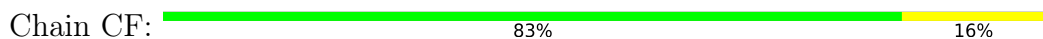




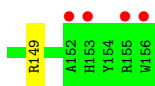
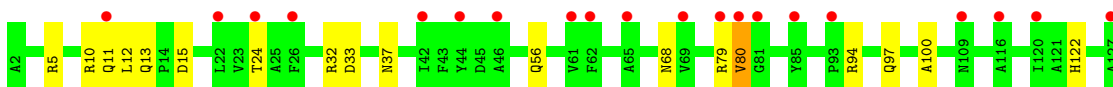
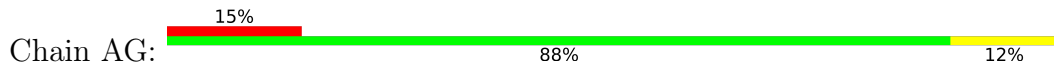
- Molecule 5: 30S ribosomal protein S6



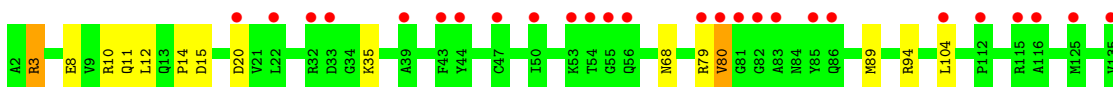
- Molecule 5: 30S ribosomal protein S6



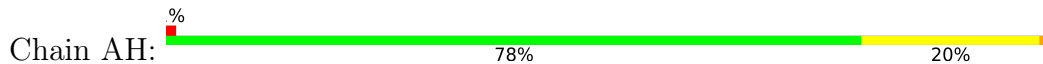
- Molecule 6: 30S ribosomal protein S7



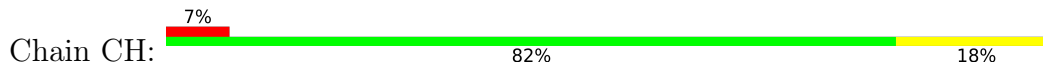
- Molecule 6: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S8

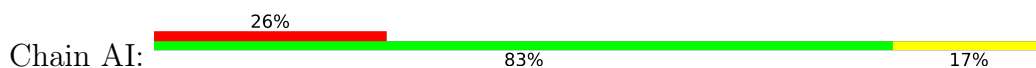


- Molecule 7: 30S ribosomal protein S8

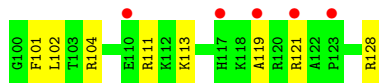




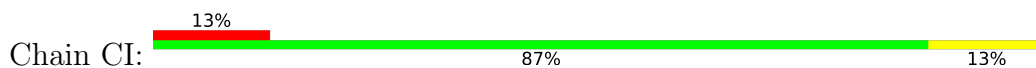
- Molecule 8: 30S ribosomal protein S9



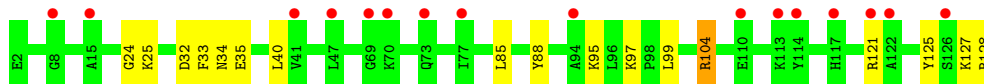
Chain AI:



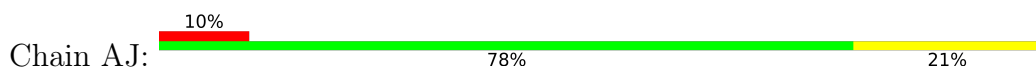
- Molecule 8: 30S ribosomal protein S9



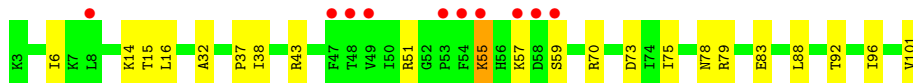
Chain CI:



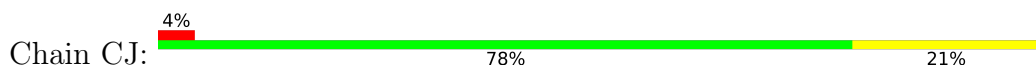
- Molecule 9: 30S ribosomal protein S10



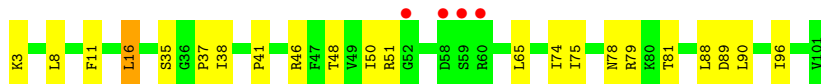
Chain AJ:



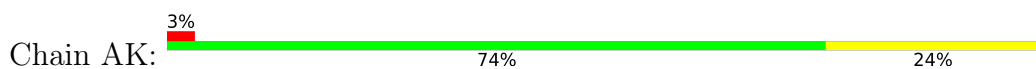
- Molecule 9: 30S ribosomal protein S10



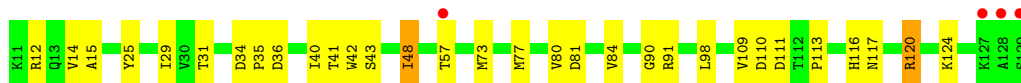
Chain CJ:



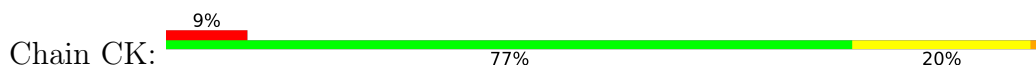
- Molecule 10: 30S ribosomal protein S11



Chain AK:



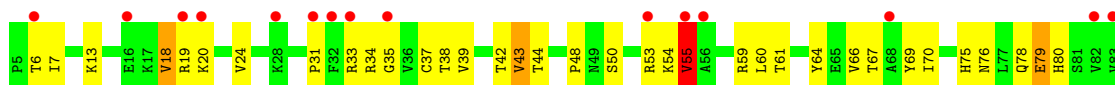
- Molecule 10: 30S ribosomal protein S11



Chain CK:



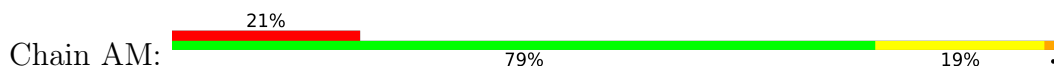
- Molecule 11: 30S ribosomal protein S12



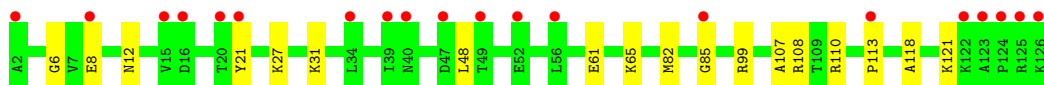
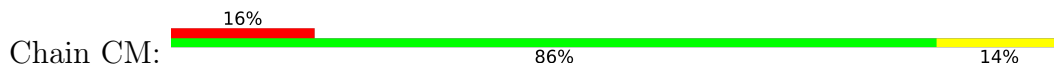
- Molecule 11: 30S ribosomal protein S12



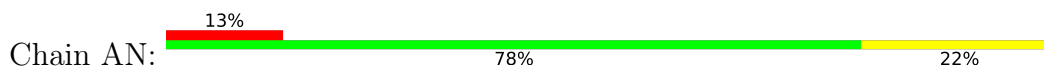
- Molecule 12: 30S ribosomal protein S13




- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14 type Z




- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:  85% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  2% 84% 15%



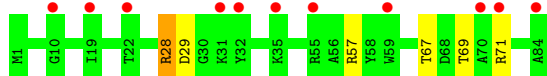
- Molecule 14: 30S ribosomal protein S15

Chain CO:  81% 17%




- Molecule 15: 30S ribosomal protein S16

Chain AP:  13% 93% 6%




- Molecule 15: 30S ribosomal protein S16

Chain CP:  13% 83% 17%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  6% 77% 22%

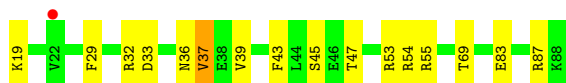
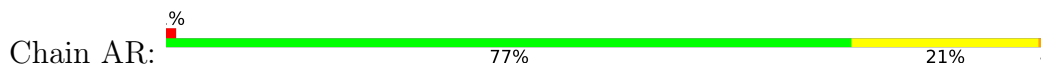


- Molecule 16: 30S ribosomal protein S17

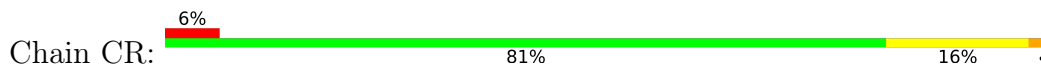
Chain CQ:  11% 75% 24%



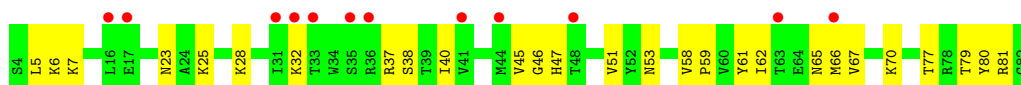
- Molecule 17: 30S ribosomal protein S18



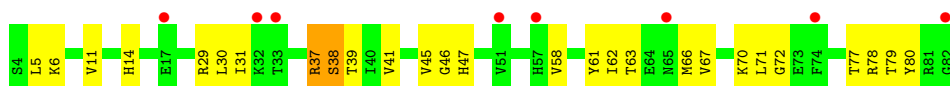
- Molecule 17: 30S ribosomal protein S18



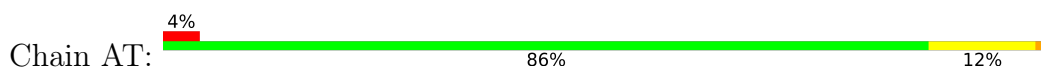
- Molecule 18: 30S ribosomal protein S19



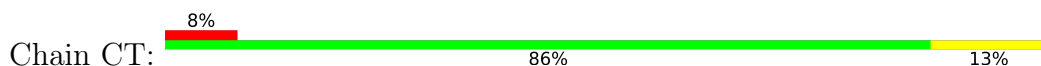
- Molecule 18: 30S ribosomal protein S19



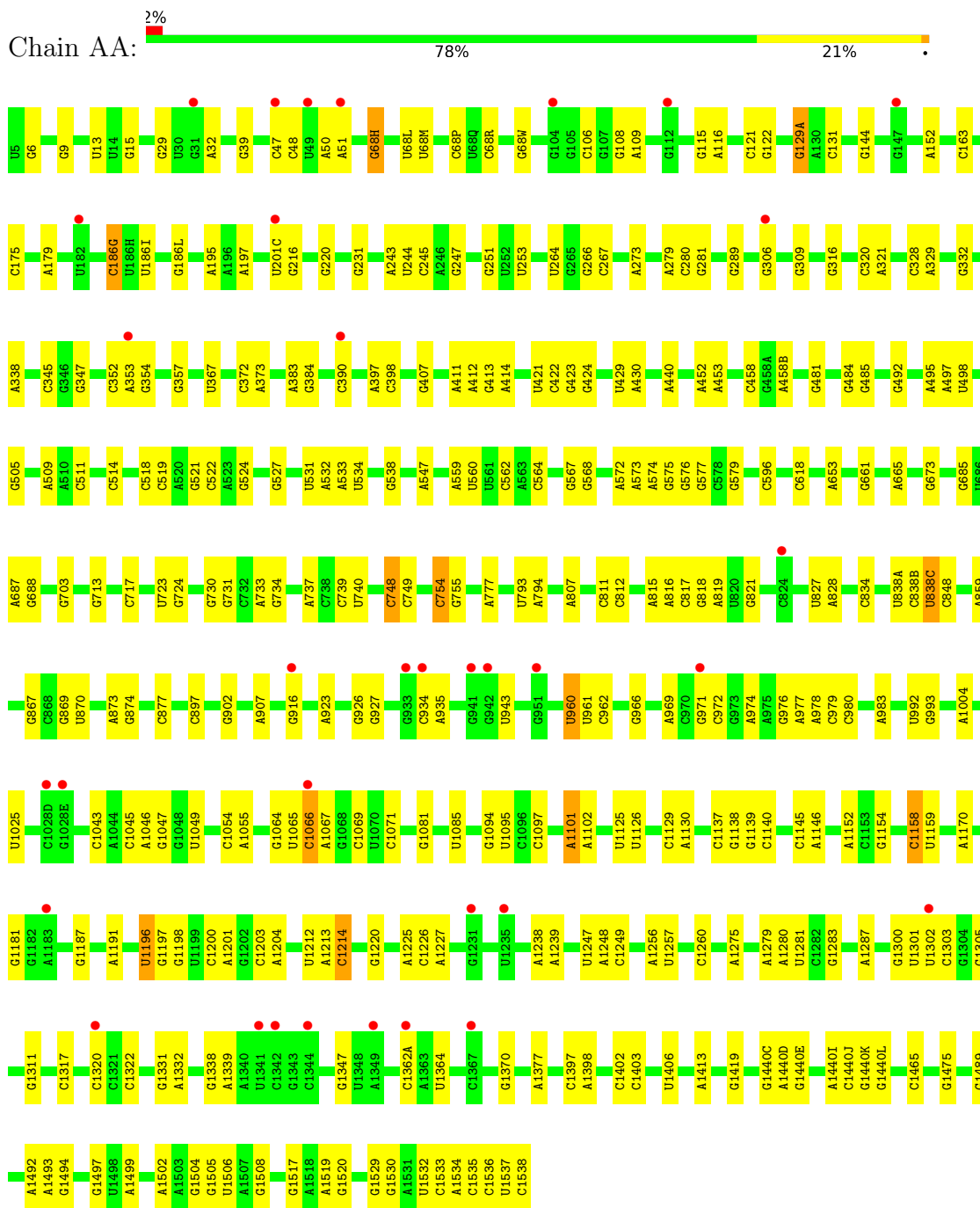
- Molecule 19: 30S ribosomal protein S20



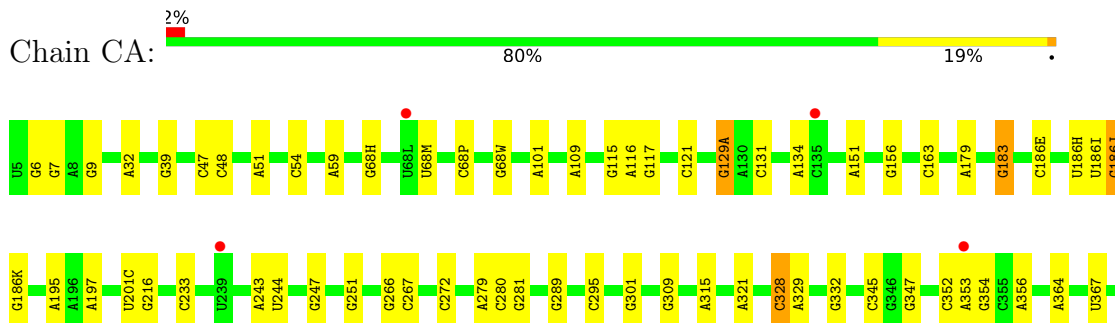
- Molecule 19: 30S ribosomal protein S20

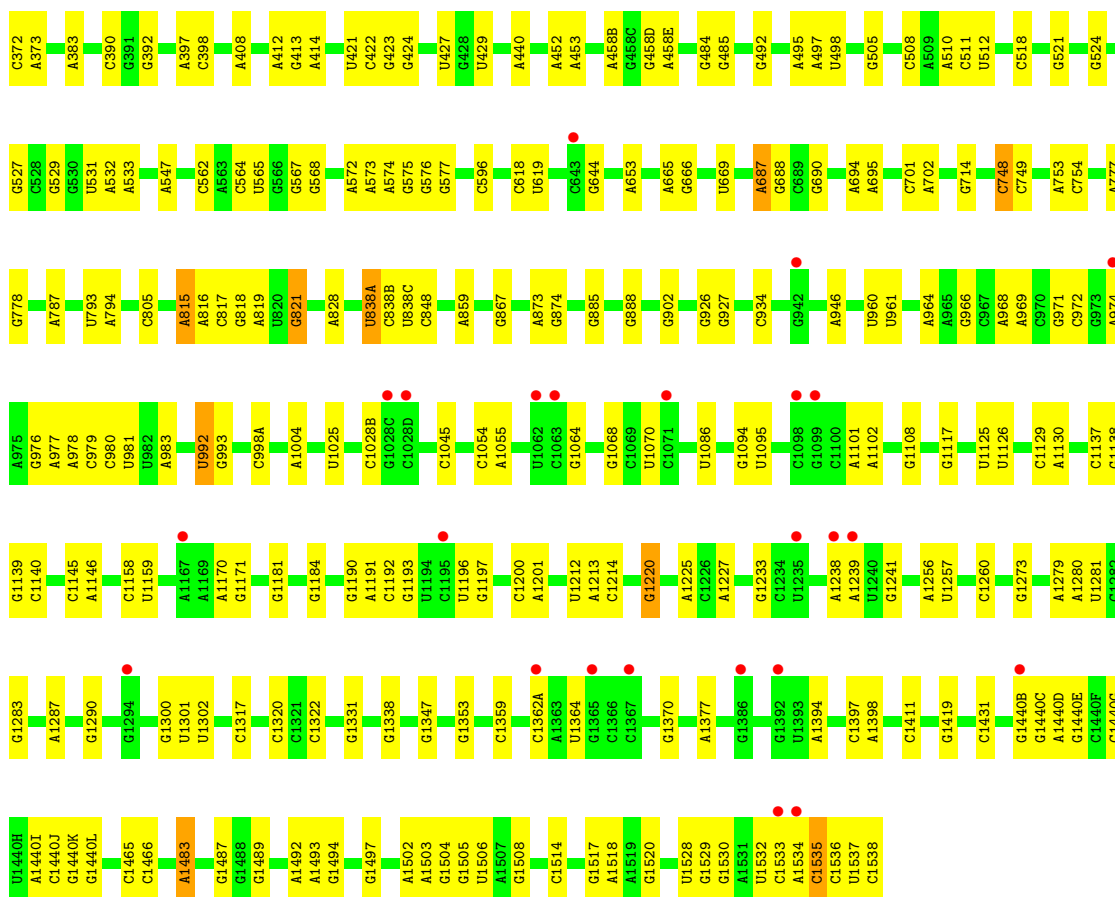


- Molecule 20: ribosomal RNA 16S

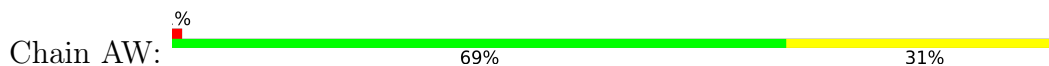


- Molecule 20: ribosomal RNA 16S

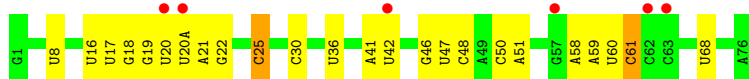
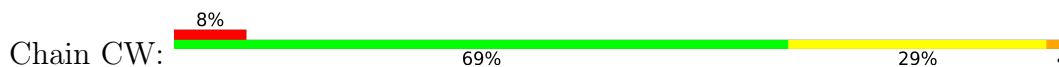




- Molecule 21: transfer RNA



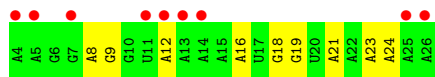
- Molecule 21: transfer RNA



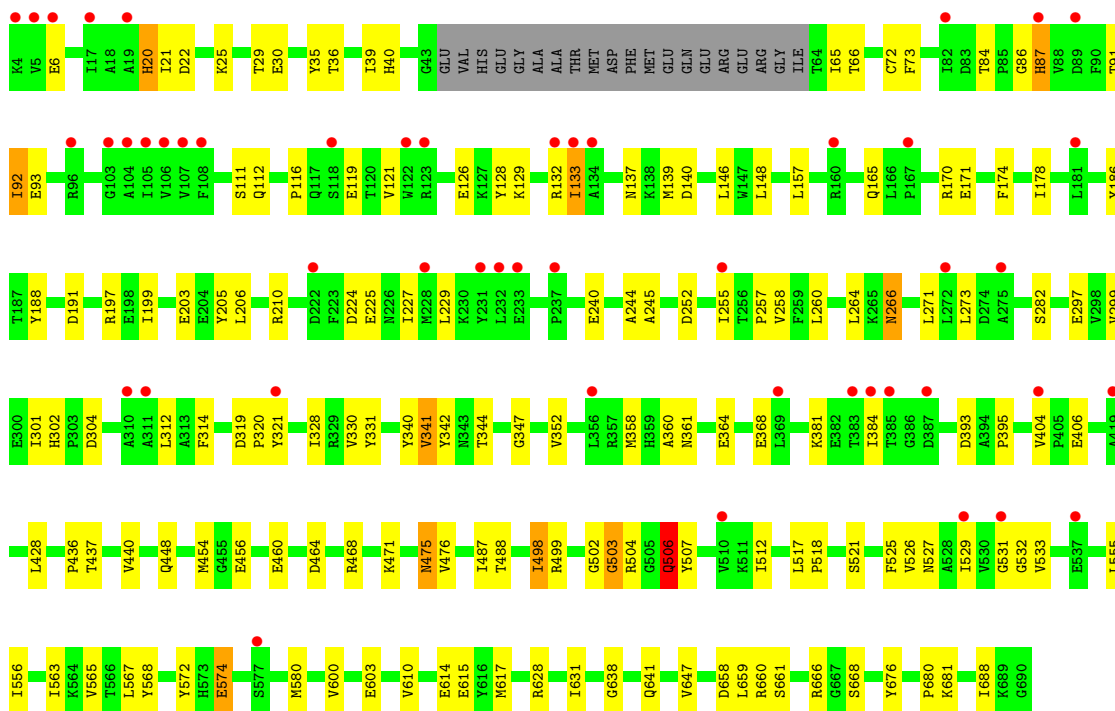
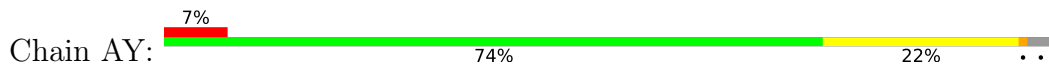
- Molecule 22: messenger RNA



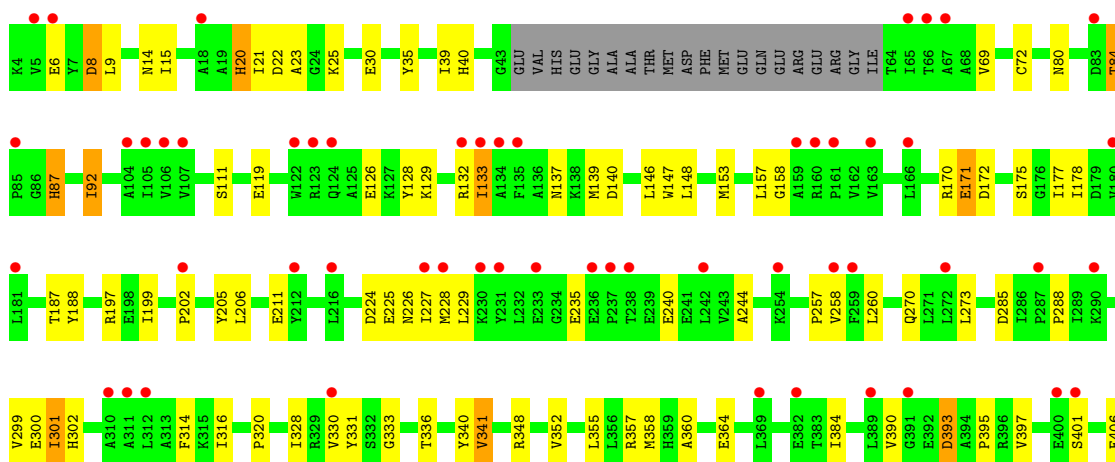
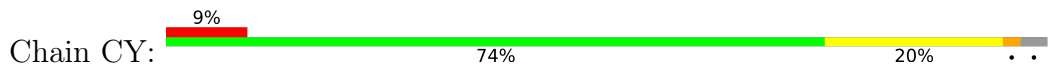
- Molecule 22: messenger RNA

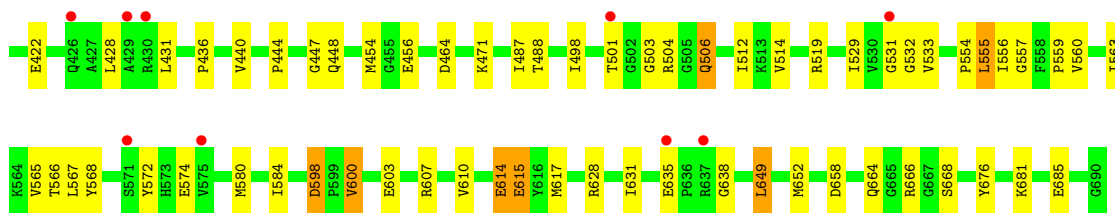


• Molecule 23: Elongation factor G



• Molecule 23: Elongation factor G

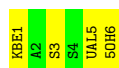




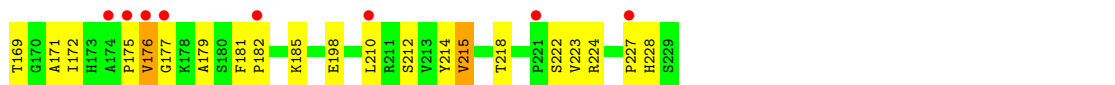
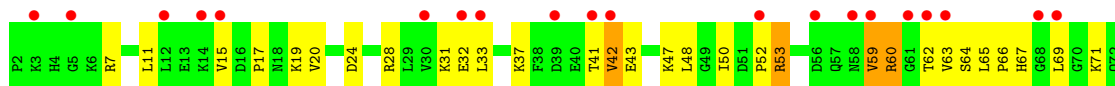
- Molecule 24: VIOMYCIN



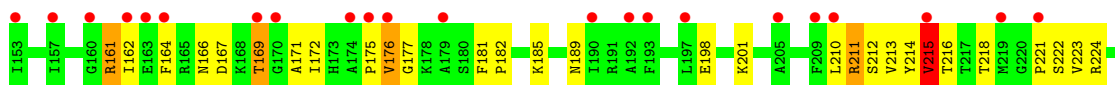
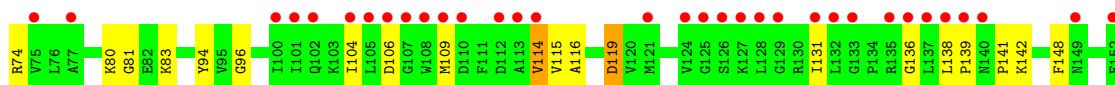
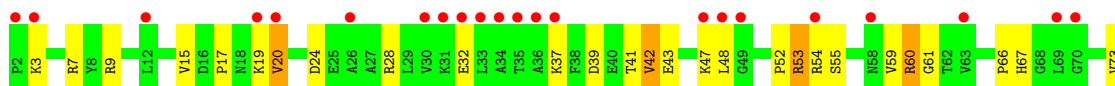
- Molecule 24: VIOMYCIN



- Molecule 25: 50S ribosomal protein L1



- Molecule 25: 50S ribosomal protein L1



P227
R228
S229

• Molecule 26: 50S ribosomal protein L2

Chain BD: 2% 66% 31%

A2 V3 K4 K5 Y9 T10 P11 S12 D20 V113 E23 T24 T25 T26 K26 E28 P29 E30 L33 V34 K35 P36 L37 K38 K39 G41 G42 R43 R44 M45 R48 R49 F53 I64 I65 I66 D66 F67 F68 R69 P76 A77 K78 V79 I82 I87 N87 P88 S89 L94 L95

H96 Y97 V98 D99 G100 I105 I106 Q112 V113 G114 Q115 T117 V118 A119 G120 E28 P29 D121 D122 A123 V127 L131 P137 T140 T141 V142 L147 E148 A158 Q164 I165 Q166 E169 G170 D171 L177 P178 R183 Y190 G197 D200 N203 G207

P219 H220 V221 R222 G223 A224 A225 M226 P232 H233 G238 R239 R242 G243 R244 P245 P246 A247 W250 T254 L257 K258 T259 R260 R268 A272 R273 K276

• Molecule 26: 50S ribosomal protein L2

Chain DD: 3% 66% 31%

A2 V3 K4 K5 Y9 R13 E23 T24 T25 T27 E28 E30 L33 V34 K35 P36 L37 K38 K39 G41 G42 R43 R44 M45 R48 R49 T50 V51 R52 F53 R59 R60 R63 I64 I65 D171 R69 V70 D71 K78 V79 I82 I87 N87 R88 S89 L95

H96 Y97 V98 D99 G100 I105 I106 D109 G110 V113 G114 Q115 V117 V118 A123 V127 P137 T140 V141 V142 L147 E148 P149 K150 A158 T161 S162 A163 Q164 I165 Q166 D171 Y172 V173 L174 L175 P178 S179 G180 Y190 G197 S212

M226 V229 D230 H231 H233 G235 G236 E237 G238 R239 R240 P241 R242 P245 P246 W250 T254 L257 K258 T259 R260 K261 R262 S267 R272 R273 K276

• Molecule 27: 50S ribosomal protein L3

Chain BE: 71% 25%

M1 I4 K8 M11 M12 T12 R13 I14 D17 I26 L27 V33 V34 T38 P39 Y44 T45 L49 G50 F51 G54 N55 P56 M60 R61 P62 L63 H66 F67 A68 V72 E73 P74 P75 R76 I77 L78 R79 N85 P86 E87 T90 E94 V104

F113 R119 W120 M121 F122 A123 P126 H129 G130 I134 S140 R144 K145 T146 P147 K154 K155 A162 E163 R164 V175 V184 K185 G186 I197 E200 A205

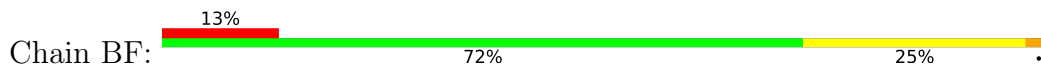
• Molecule 27: 50S ribosomal protein L3

Chain DE: 3% 66% 31%

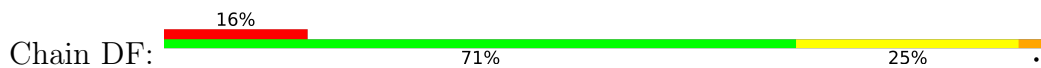
M1 I4 M11 T12 R13 I14 F15 R16 D17 D18 V21 T24 V25 I26 L27 P30 V33 R36 R37 T38 T45 Q48 L49 G50 F51 L52 P53 Q54 N55 P56 N60 R61 P62 L63 H66 F67 A68 V72 E73 P74 P75 R76 I77 L78 R79 F84 N85



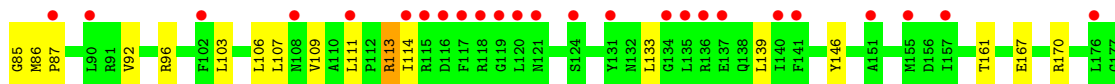
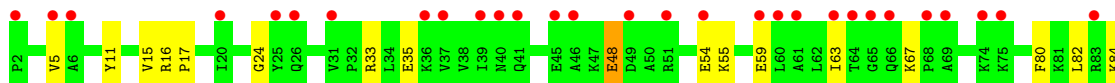
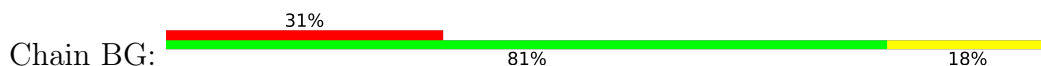
- Molecule 28: 50S ribosomal protein L4



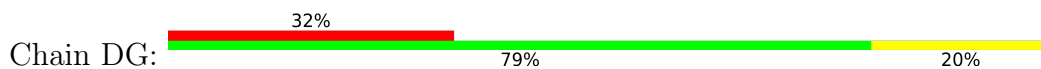
- Molecule 28: 50S ribosomal protein L4

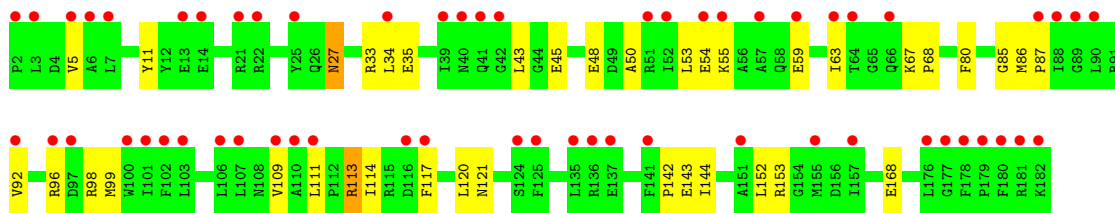


- Molecule 29: 50S ribosomal protein L5

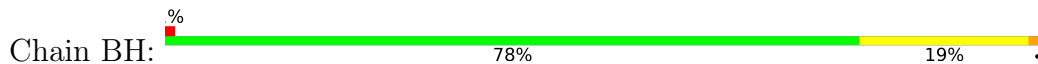


- Molecule 29: 50S ribosomal protein L5

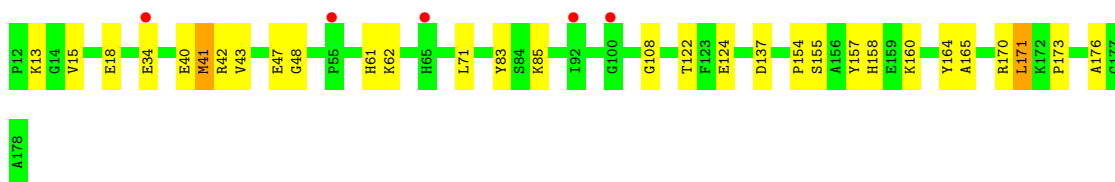
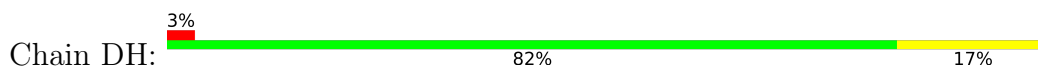




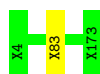
• Molecule 30: 50S ribosomal protein L6



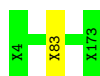
• Molecule 30: 50S ribosomal protein L6



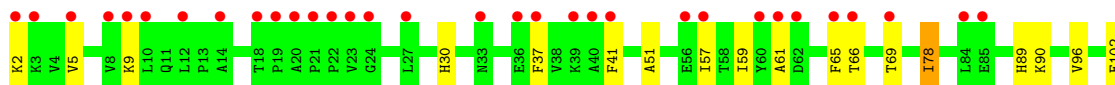
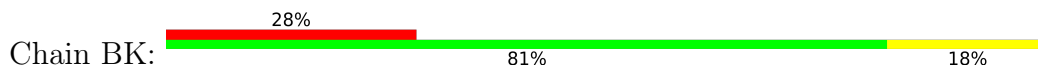
• Molecule 31: 50S RIBOSOMAL PROTEIN L10



• Molecule 31: 50S RIBOSOMAL PROTEIN L10

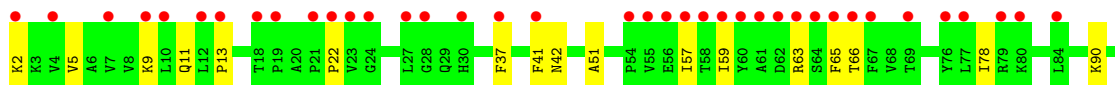
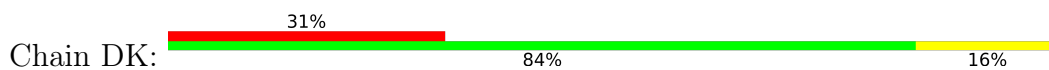


• Molecule 32: 50S ribosomal protein L11

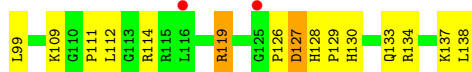
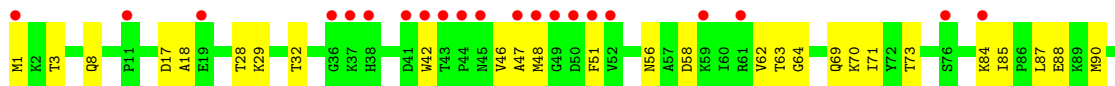
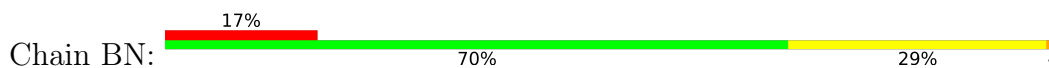




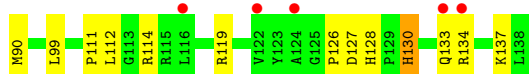
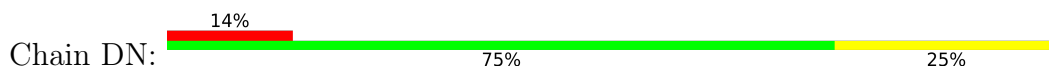
- Molecule 32: 50S ribosomal protein L11



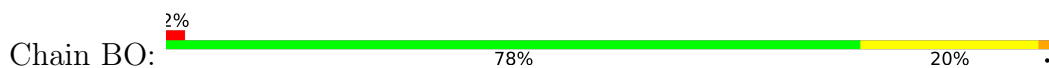
- Molecule 33: 50S ribosomal protein L13



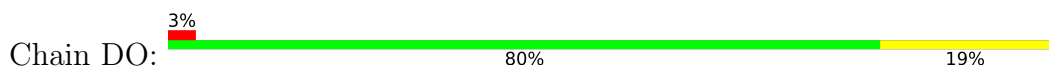
- Molecule 33: 50S ribosomal protein L13



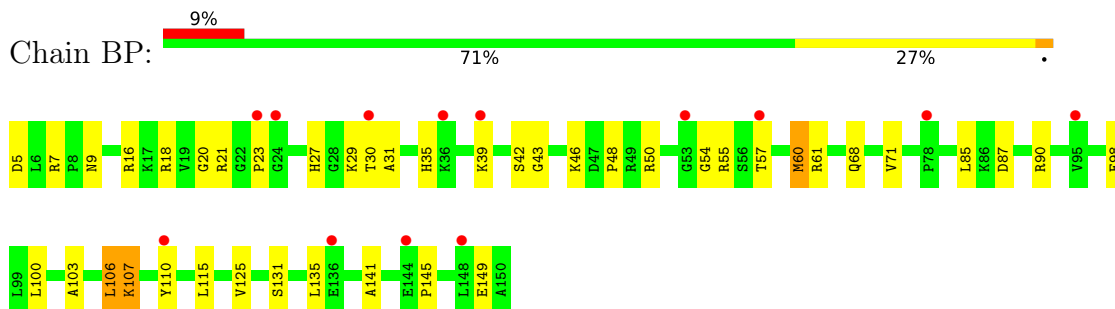
- Molecule 34: 50S ribosomal protein L14



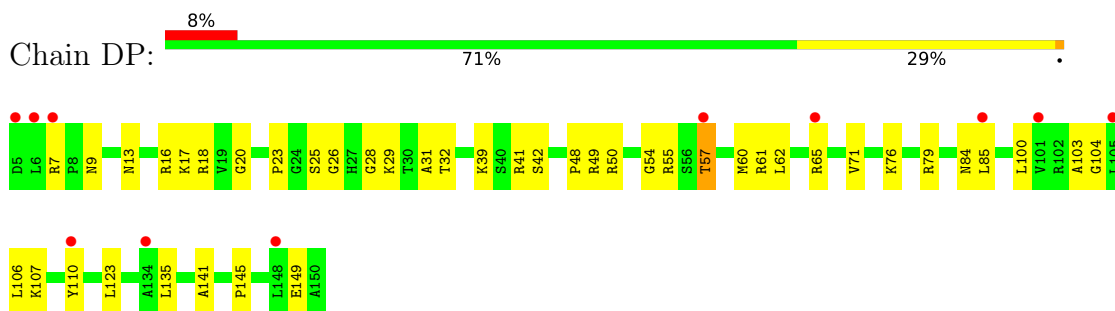
- Molecule 34: 50S ribosomal protein L14



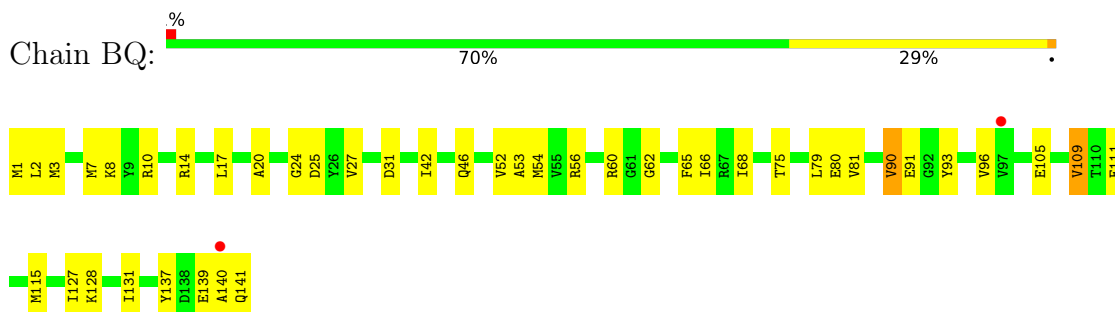
- Molecule 35: 50S ribosomal protein L15



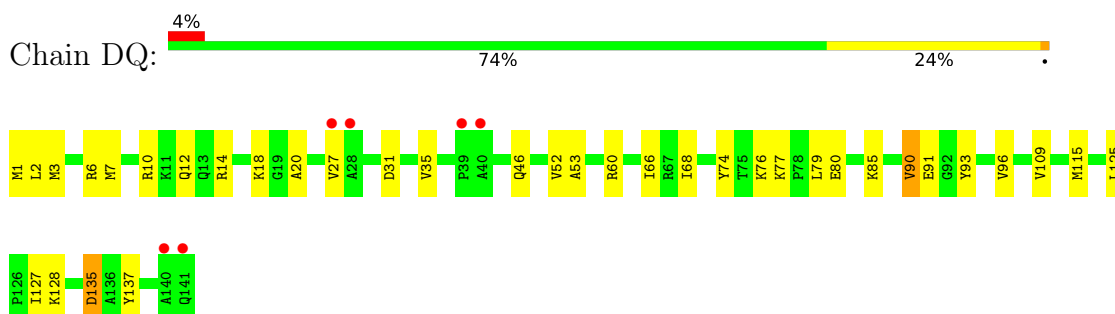
- Molecule 35: 50S ribosomal protein L15



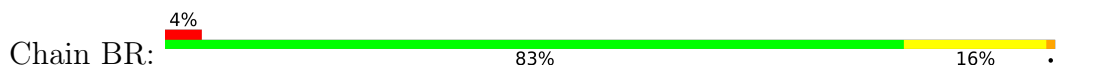
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

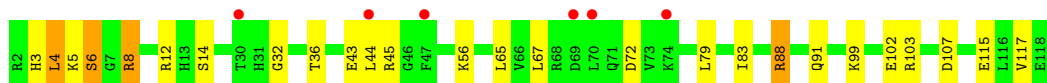
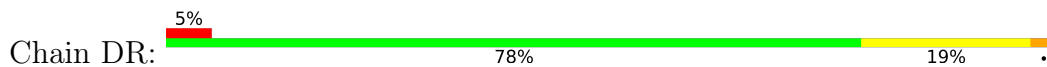


- Molecule 37: 50S ribosomal protein L17

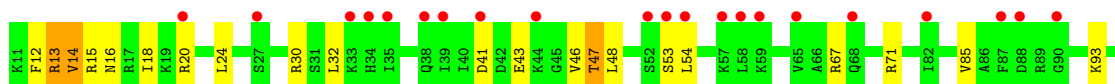




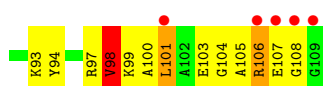
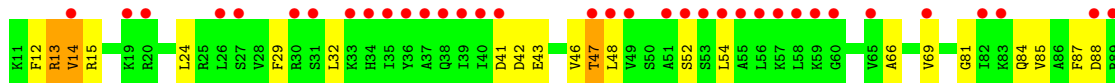
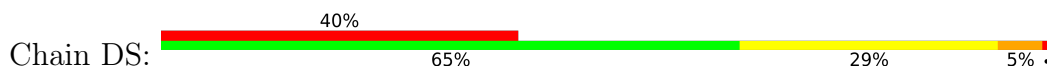
- Molecule 37: 50S ribosomal protein L17



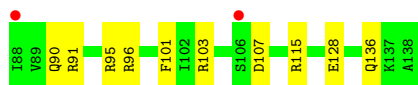
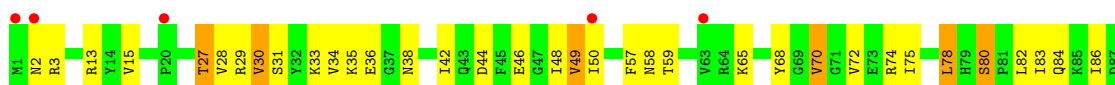
- Molecule 38: 50S ribosomal protein L18



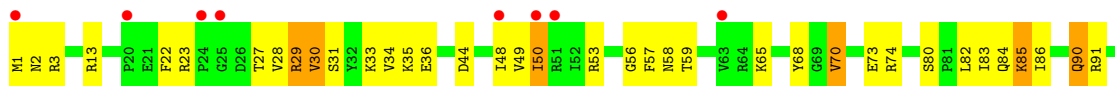
- Molecule 38: 50S ribosomal protein L18

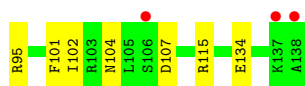


- Molecule 39: 50S ribosomal protein L19

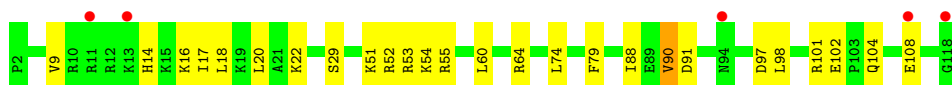
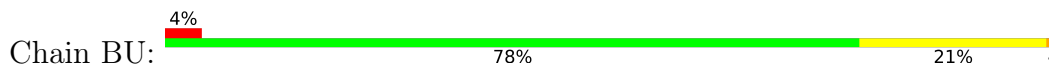


- Molecule 39: 50S ribosomal protein L19

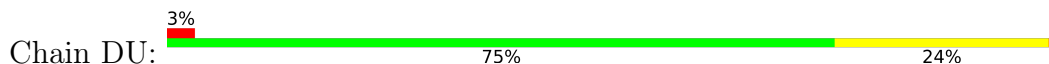




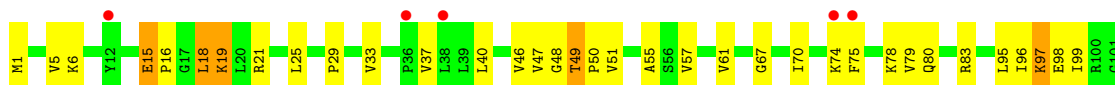
- Molecule 40: 50S ribosomal protein L20



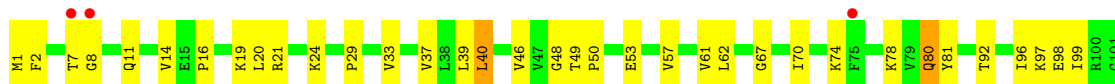
- Molecule 40: 50S ribosomal protein L20



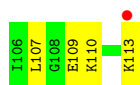
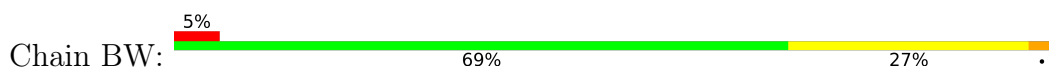
- Molecule 41: 50S ribosomal protein L21



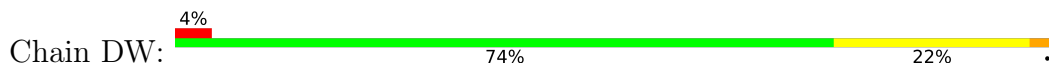
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22

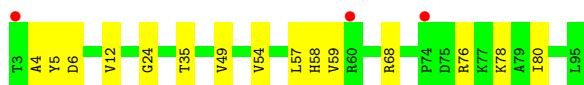
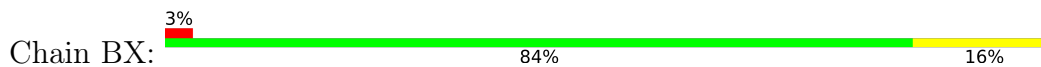


- Molecule 42: 50S ribosomal protein L22

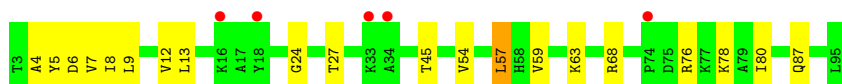
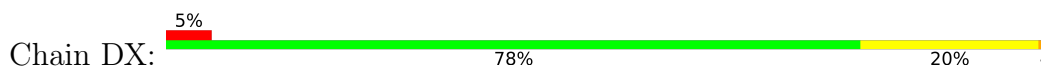




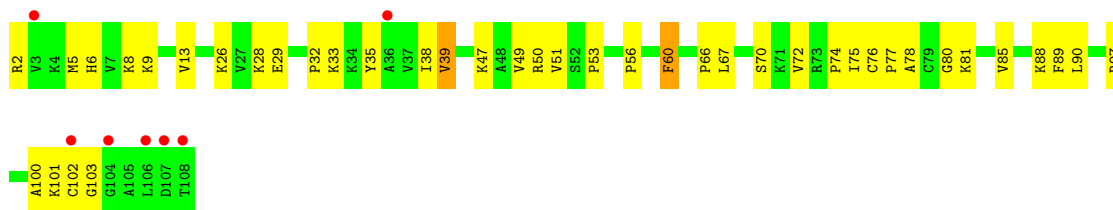
- Molecule 43: 50S ribosomal protein L23



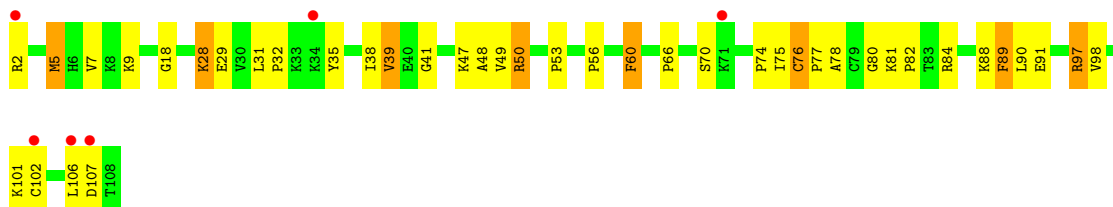
- Molecule 43: 50S ribosomal protein L23



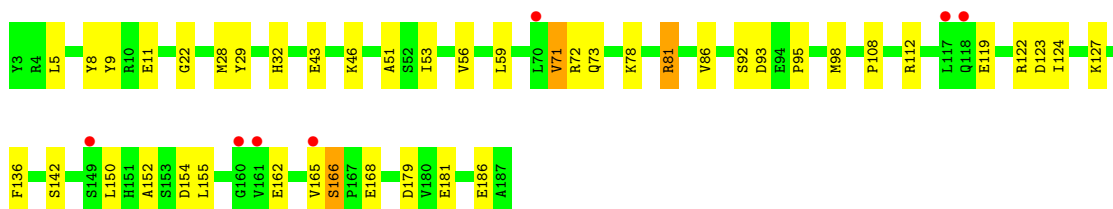
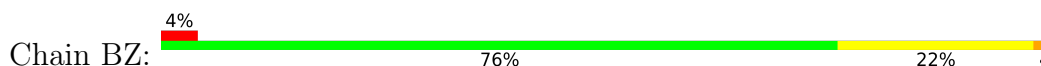
- Molecule 44: 50S ribosomal protein L24



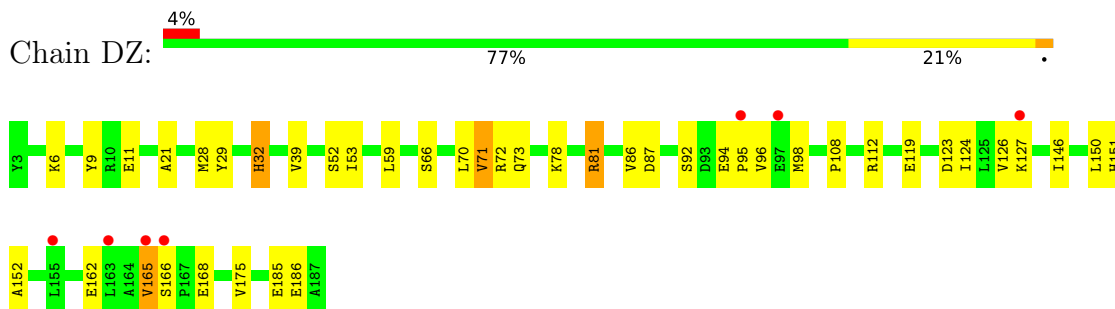
- Molecule 44: 50S ribosomal protein L24



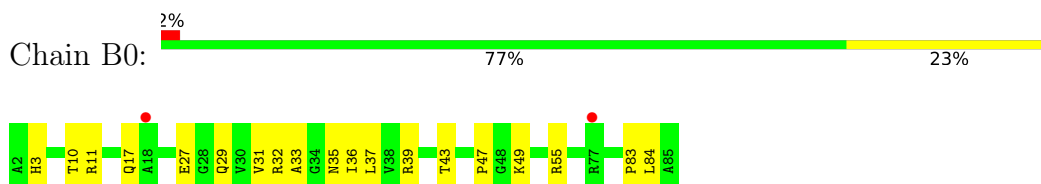
- Molecule 45: 50S ribosomal protein L25



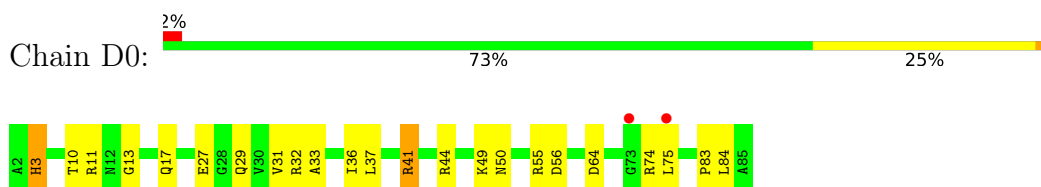
- Molecule 45: 50S ribosomal protein L25



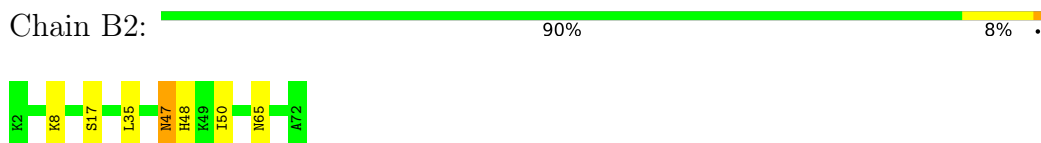
- Molecule 46: 50S ribosomal protein L27



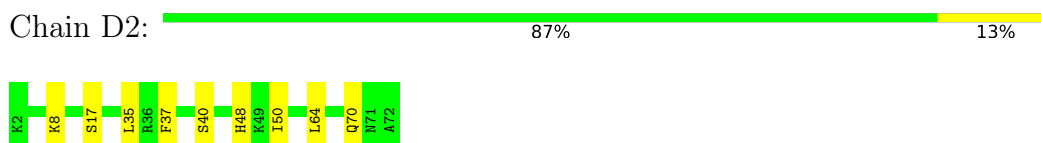
- Molecule 46: 50S ribosomal protein L27



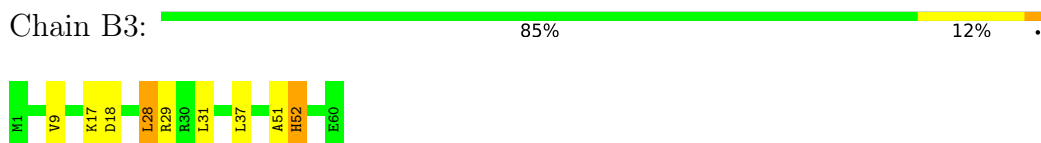
- Molecule 47: 50S ribosomal protein L29



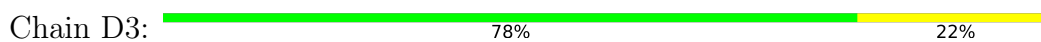
- Molecule 47: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L30

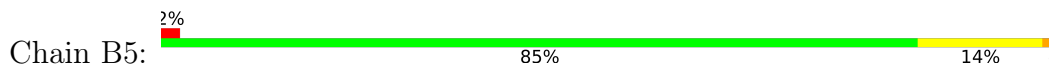


- Molecule 48: 50S ribosomal protein L30

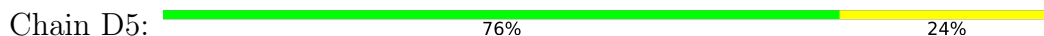




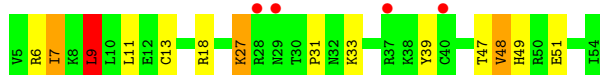
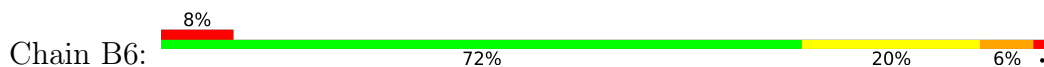
- Molecule 49: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L32



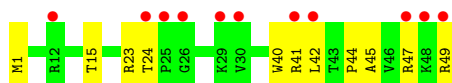
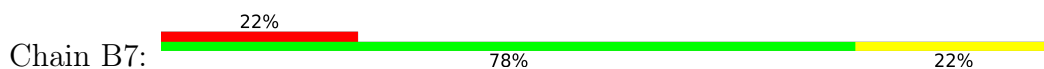
- Molecule 50: 50S ribosomal protein L33



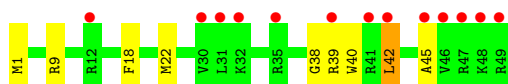
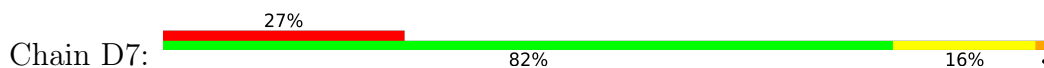
- Molecule 50: 50S ribosomal protein L33



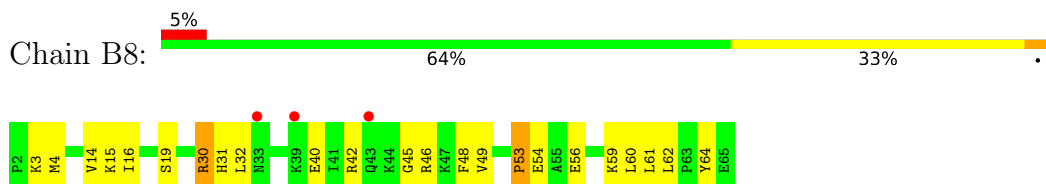
- Molecule 51: 50S ribosomal protein L34



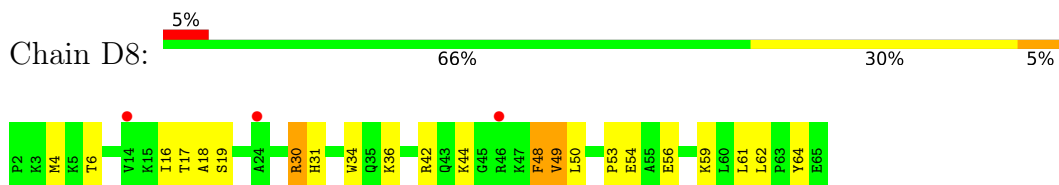
- Molecule 51: 50S ribosomal protein L34



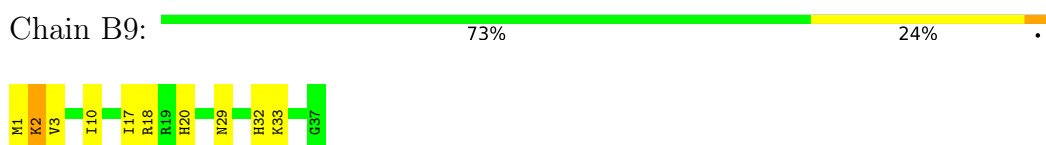
- Molecule 52: 50S ribosomal protein L35



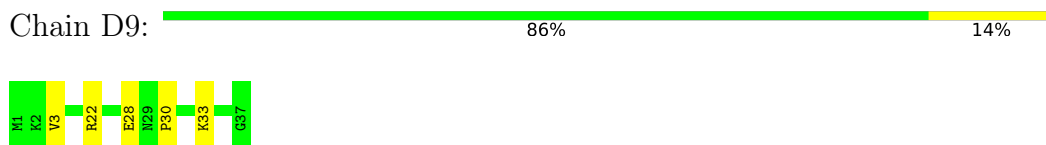
- Molecule 52: 50S ribosomal protein L35



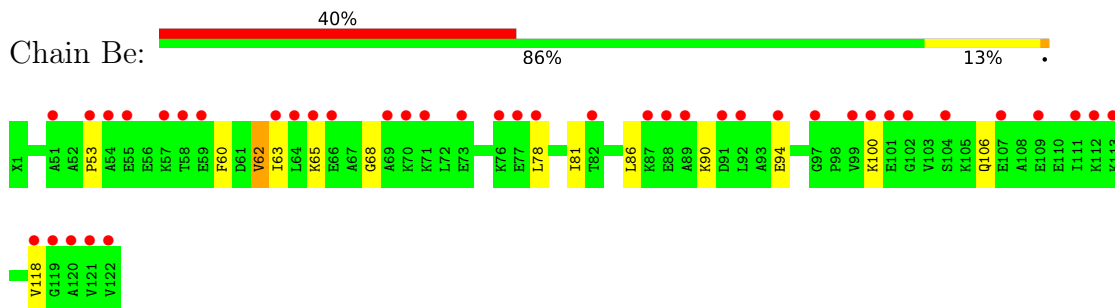
- Molecule 53: 50S ribosomal protein L36



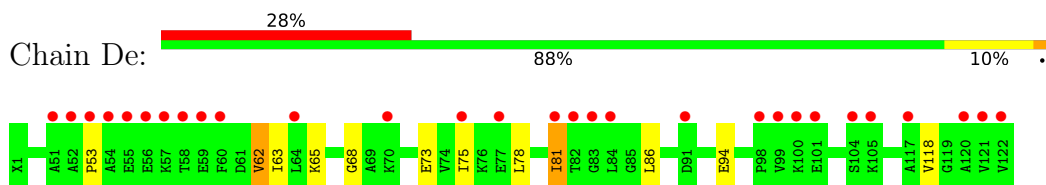
- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 54: 50S ribosomal protein L7/L12



- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12



There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh:  100%

There are no outlier residues recorded for this chain.

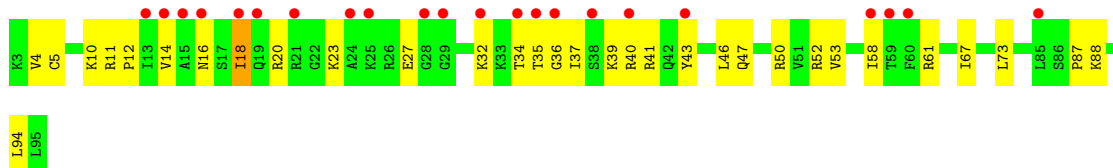
- Molecule 56: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

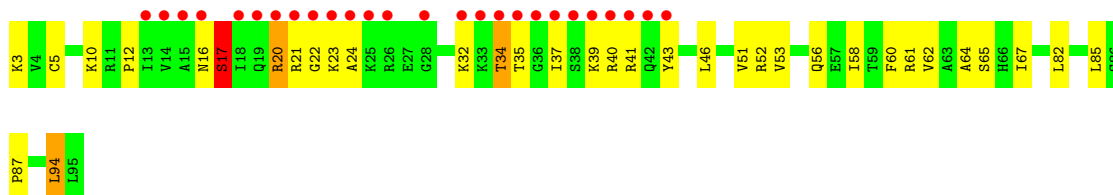
- Molecule 57: 50S ribosomal protein L28

Chain B1:  24% 66% 33%

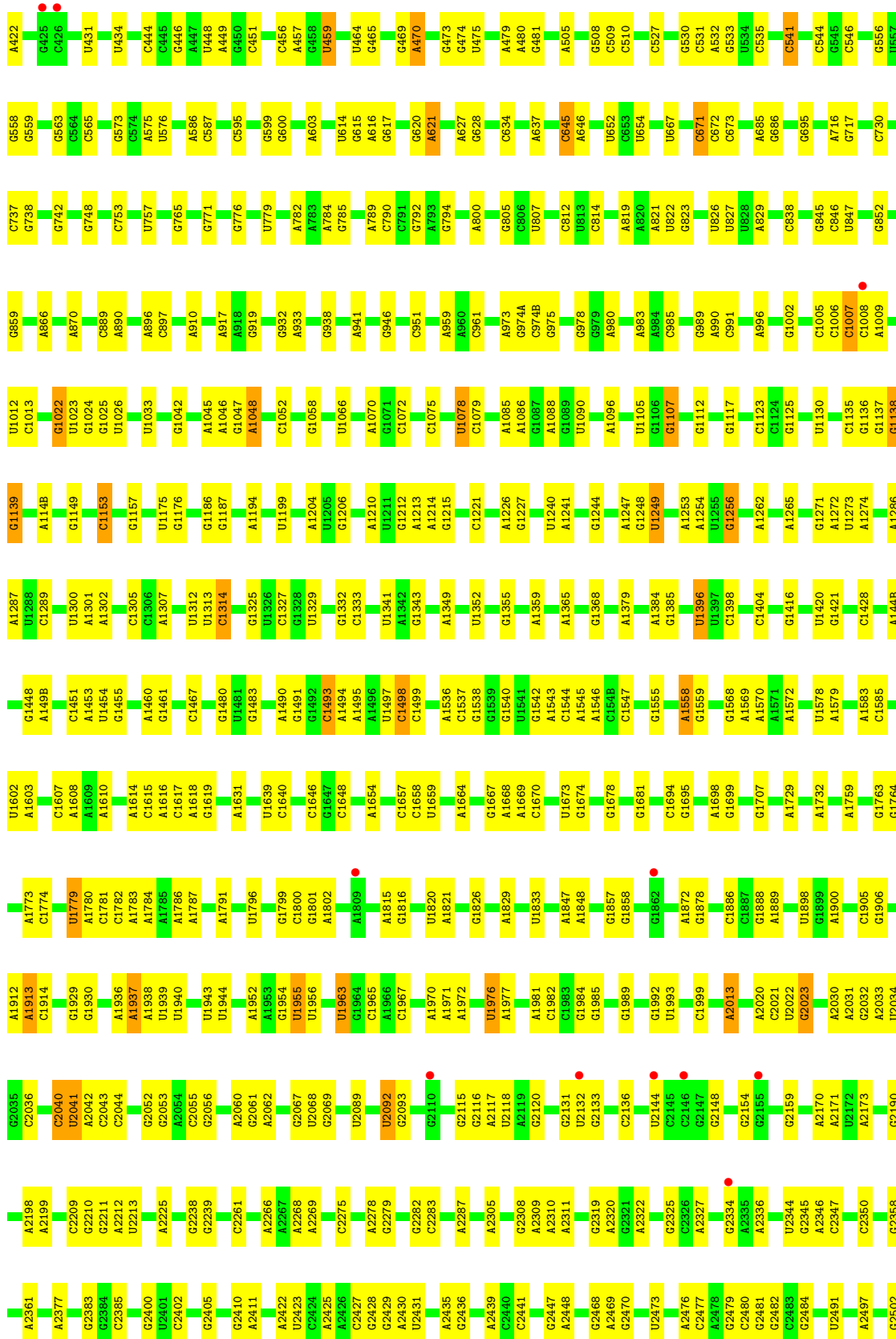


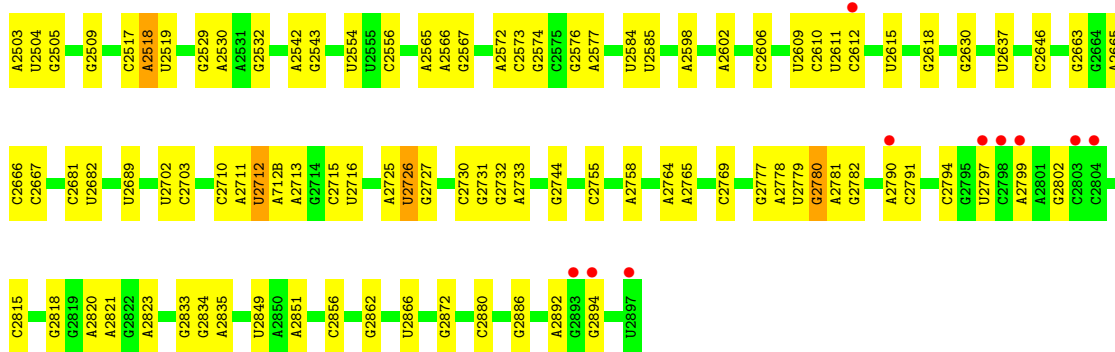
- Molecule 57: 50S ribosomal protein L28

Chain D1:  28% 62% 33%

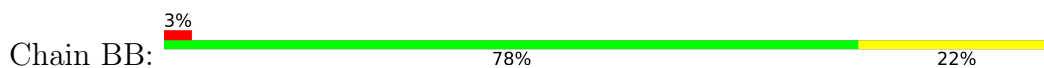


- Molecule 58: 50S ribosomal protein L31

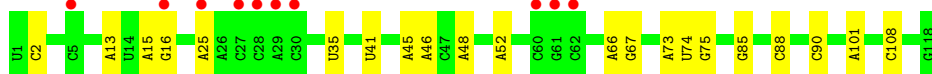
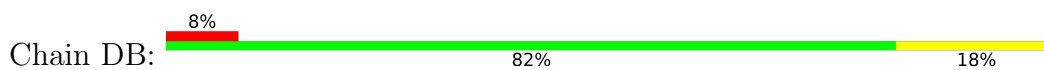




- Molecule 60: 5S ribosomal RNA



- Molecule 60: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 140.20 – 3.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.7 (140.20-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.58Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.328 0.289 , 0.329	Depositor DCC
R_{free} test set	33495 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtrriage
Anisotropy	0.660	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtrriage
Estimated twinning fraction	0.258 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5OH, KBE, UAL, MG, DPP, FUA, 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	0.38	0/1945	0.72	1/2621 (0.0%)
1	CB	0.37	0/1945	0.67	1/2621 (0.0%)
2	AC	0.28	0/1645	0.53	0/2216
2	CC	0.28	0/1645	0.52	0/2216
3	AD	0.30	0/1733	0.58	0/2318
3	CD	0.30	0/1733	0.58	1/2318 (0.0%)
4	AE	0.32	0/1172	0.58	1/1576 (0.1%)
4	CE	0.31	0/1172	0.58	1/1576 (0.1%)
5	AF	0.31	0/856	0.59	0/1154
5	CF	0.31	0/856	0.56	1/1154 (0.1%)
6	AG	0.29	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.52	0/1709
7	AH	0.30	0/1136	0.57	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.29	0/1029	0.53	0/1379
8	CI	0.27	0/1029	0.49	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.57	1/1095 (0.1%)
10	AK	0.33	0/900	0.61	0/1213
10	CK	0.36	0/900	0.65	0/1213
11	AL	0.40	0/992	0.83	2/1327 (0.2%)
11	CL	0.40	0/992	0.82	1/1327 (0.1%)
12	AM	0.29	0/1008	0.59	1/1347 (0.1%)
12	CM	0.28	0/1008	0.54	0/1347
13	AN	0.30	0/501	0.52	0/664
13	CN	0.26	0/501	0.46	0/664
14	AO	0.31	0/745	0.52	0/992
14	CO	0.31	0/745	0.53	0/992
15	AP	0.28	0/722	0.50	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.36	0/848	0.65	0/1131
16	CQ	0.37	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.31	0/579	0.59	0/768
17	CR	0.30	0/579	0.55	0/768
18	AS	0.31	0/647	0.60	0/870
18	CS	0.31	0/647	0.61	0/870
19	AT	0.33	0/765	0.56	0/1007
19	CT	0.32	0/765	0.55	0/1007
20	AA	0.37	0/36351	1.02	61/56736 (0.1%)
20	CA	0.36	0/36351	0.99	53/56736 (0.1%)
21	AW	0.33	0/1827	1.03	0/2845
21	CW	0.33	0/1827	1.01	5/2845 (0.2%)
22	AV	0.27	0/568	0.81	0/886
22	CV	0.29	0/568	0.92	0/886
23	AY	0.34	1/5317 (0.0%)	0.66	7/7198 (0.1%)
23	CY	0.37	2/5317 (0.0%)	0.61	1/7198 (0.0%)
24	AU	0.95	0/11	1.28	0/13
24	CU	0.92	0/11	1.04	0/13
25	BC	0.41	0/1774	0.74	1/2391 (0.0%)
25	DC	0.43	0/1774	0.72	1/2391 (0.0%)
26	BD	0.33	0/2195	0.65	1/2955 (0.0%)
26	DD	0.35	0/2195	0.65	0/2955
27	BE	0.32	0/1602	0.66	0/2160
27	DE	0.31	0/1602	0.66	0/2160
28	BF	0.35	0/1663	0.73	2/2249 (0.1%)
28	DF	0.37	0/1663	0.76	3/2249 (0.1%)
29	BG	0.40	1/1499 (0.1%)	0.59	0/2016
29	DG	0.38	1/1499 (0.1%)	0.61	0/2016
30	BH	0.30	0/1298	0.60	0/1751
30	DH	0.29	0/1298	0.57	0/1751
32	BK	0.27	0/1054	0.51	0/1427
32	DK	0.27	0/1054	0.50	0/1427
33	BN	0.45	0/1131	0.77	0/1525
33	DN	0.48	0/1131	0.74	0/1525
34	BO	0.30	0/943	0.57	0/1269
34	DO	0.29	0/943	0.55	0/1269
35	BP	0.30	0/1131	0.62	0/1504
35	DP	0.29	0/1131	0.62	0/1504
36	BQ	0.35	0/1143	0.63	0/1527
36	DQ	0.34	0/1143	0.60	0/1527
37	BR	0.30	0/974	0.60	0/1302
37	DR	0.31	0/974	0.61	0/1302
38	BS	0.34	0/783	0.69	0/1041
38	DS	0.33	0/783	0.70	0/1041
39	BT	0.34	0/1161	0.67	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.36	0/1161	0.66	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.40	0/982	0.60	0/1306
41	BV	0.38	0/790	0.70	1/1057 (0.1%)
41	DV	0.38	0/790	0.67	0/1057
42	BW	0.31	0/911	0.59	0/1220
42	DW	0.31	0/911	0.61	1/1220 (0.1%)
43	BX	0.30	0/748	0.55	0/1004
43	DX	0.29	0/748	0.54	1/1004 (0.1%)
44	BY	0.32	0/831	0.62	0/1108
44	DY	0.33	0/831	0.66	0/1108
45	BZ	0.29	0/1505	0.58	0/2042
45	DZ	0.28	0/1505	0.58	0/2042
46	B0	0.28	0/671	0.49	0/892
46	D0	0.28	0/671	0.54	0/892
47	B2	0.31	0/600	0.55	0/793
47	D2	0.32	0/600	0.55	0/793
48	B3	0.27	0/482	0.53	0/646
48	D3	0.27	0/482	0.55	0/646
49	B5	0.33	0/473	0.59	0/639
49	D5	0.31	0/473	0.57	0/639
50	B6	0.29	0/440	0.70	1/586 (0.2%)
50	D6	0.30	0/440	0.66	0/586
51	B7	0.33	0/438	0.64	0/575
51	D7	0.31	0/438	0.59	0/575
52	B8	0.34	0/525	0.68	0/691
52	D8	0.30	0/525	0.64	0/691
53	B9	0.30	0/310	0.55	0/407
53	D9	0.32	0/310	0.52	0/407
54	Be	0.28	0/538	0.50	0/715
54	De	0.26	0/538	0.49	0/715
57	B1	0.46	0/739	0.82	0/981
57	D1	0.47	0/739	0.84	1/981 (0.1%)
58	B4	0.32	0/276	0.58	0/372
58	D4	0.35	0/276	0.62	0/372
59	BA	0.40	0/69437	1.04	158/108401 (0.1%)
59	DA	0.40	3/69437 (0.0%)	1.03	149/108401 (0.1%)
60	BB	0.37	0/2853	1.08	11/4451 (0.2%)
60	DB	0.35	0/2853	1.03	5/4451 (0.1%)
All	All	0.37	8/330576 (0.0%)	0.92	474/492228 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	3
1	CB	0	1
11	CL	0	2
23	AY	0	3
23	CY	0	2
25	BC	0	1
25	DC	0	3
26	BD	0	1
26	DD	0	2
28	BF	0	2
28	DF	0	2
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
35	DP	0	1
38	BS	0	3
38	DS	0	3
42	BW	0	1
42	DW	0	1
57	B1	0	2
57	D1	0	2
All	All	0	41

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	506	GLN	C-N	8.35	1.53	1.34
29	BG	114	ILE	N-CA	-7.50	1.31	1.46
29	DG	114	ILE	N-CA	-7.47	1.31	1.46
23	CY	25	LYS	C-N	6.18	1.48	1.34
23	AY	506	GLN	C-N	-5.48	1.21	1.34
59	DA	459	U	C2-O2	-5.47	1.17	1.22
59	DA	459	U	N1-C2	-5.46	1.33	1.38
59	DA	459	U	N3-C4	-5.16	1.33	1.38

All (474) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1006	C	C6-N1-C2	-13.61	114.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	459	U	N1-C2-N3	12.63	122.48	114.90
59	BA	1006	C	C6-N1-C2	-12.54	115.28	120.30
23	AY	506	GLN	O-C-N	-12.49	102.72	122.70
20	AA	815	A	C5-C6-N6	11.75	133.10	123.70
20	CA	815	A	C5-C6-N6	11.67	133.04	123.70
59	DA	459	U	C6-N1-C2	-11.47	114.12	121.00
59	BA	1139	G	O5'-P-OP1	-11.12	95.69	105.70
20	AA	815	A	N1-C6-N6	-11.03	111.98	118.60
20	CA	815	A	N1-C6-N6	-10.84	112.10	118.60
59	BA	1007	C	C6-N1-C1'	-9.64	109.23	120.80
59	DA	2040	C	C5-C6-N1	9.42	125.71	121.00
59	DA	459	U	N1-C2-O2	-9.28	116.30	122.80
59	DA	1006	C	N3-C2-O2	-9.28	115.41	121.90
59	BA	2040	C	C5-C6-N1	9.26	125.63	121.00
59	DA	459	U	N3-C4-C5	-9.23	109.06	114.60
28	DF	193	VAL	N-CA-C	-9.19	86.18	111.00
59	BA	1249	U	C2-N1-C1'	8.87	128.35	117.70
59	BA	2023	G	N1-C6-O6	8.87	125.22	119.90
59	BA	1007	C	C6-N1-C2	8.75	123.80	120.30
59	BA	1132	A	N1-C2-N3	8.71	133.66	129.30
20	AA	1508	G	N1-C2-N3	8.68	129.11	123.90
60	BB	101	A	C6-N1-C2	-8.49	113.51	118.60
59	DA	459	U	C5-C4-O4	8.44	130.96	125.90
59	BA	1008	C	C6-N1-C2	-8.20	117.02	120.30
20	AA	1158	C	C2-N1-C1'	8.16	127.78	118.80
20	CA	838(C)	U	C2-N1-C1'	8.15	127.48	117.70
59	BA	1048	A	N1-C6-N6	8.11	123.47	118.60
59	DA	1006	C	O4'-C1'-N1	8.11	114.69	108.20
20	AA	838(C)	U	C2-N1-C1'	8.04	127.35	117.70
59	DA	1287	A	N1-C2-N3	8.01	133.31	129.30
23	AY	502	GLY	CA-C-N	-7.95	100.30	116.20
23	AY	503	GLY	O-C-N	-7.83	110.17	122.70
59	DA	2041	U	C5-C6-N1	7.83	126.62	122.70
23	AY	506	GLN	CA-C-N	7.81	134.39	117.20
59	BA	2023	G	C4-C5-N7	7.80	113.92	110.80
59	DA	459	U	C6-N1-C1'	7.75	132.04	121.20
59	BA	621	A	N1-C6-N6	-7.72	113.97	118.60
20	AA	815	A	N3-C4-N9	-7.71	121.23	127.40
59	DA	1493	C	N1-C2-O2	7.70	123.52	118.90
20	AA	1508	G	C2-N3-C4	-7.64	108.08	111.90
60	DB	101	A	C6-N1-C2	-7.59	114.04	118.60
59	BA	673	C	C2-N3-C4	-7.58	116.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	1136	G	C5-C6-O6	-7.57	124.06	128.60
59	DA	1138	G	N3-C4-N9	-7.55	121.47	126.00
20	AA	815	A	C6-N1-C2	7.53	123.12	118.60
20	CA	129(A)	G	N3-C2-N2	7.52	125.16	119.90
59	DA	470	A	N1-C6-N6	7.51	123.11	118.60
59	DA	2041	U	O5'-P-OP2	-7.51	98.94	105.70
59	DA	459	U	C4-C5-C6	7.47	124.18	119.70
20	AA	1158	C	N1-C2-O2	7.46	123.38	118.90
59	DA	1153	C	C2-N1-C1'	7.45	127.00	118.80
60	BB	75	G	C6-N1-C2	-7.41	120.65	125.10
59	DA	1249	U	C2-N1-C1'	7.41	126.59	117.70
59	BA	1313	U	C2-N1-C1'	7.38	126.56	117.70
20	CA	815	A	N9-C4-C5	7.38	108.75	105.80
20	CA	1158	C	C2-N1-C1'	7.35	126.88	118.80
59	DA	1493	C	C2-N1-C1'	7.33	126.86	118.80
59	BA	1007	C	N1-C2-N3	-7.31	114.08	119.20
59	DA	1022	G	P-O3'-C3'	7.30	128.46	119.70
20	AA	815	A	N9-C4-C5	7.30	108.72	105.80
59	BA	2585	U	C2-N1-C1'	7.29	126.45	117.70
23	AY	506	GLN	C-N-CA	7.28	139.91	121.70
59	BA	1963	U	C2-N1-C1'	7.24	126.38	117.70
59	BA	2023	G	N9-C4-C5	-7.22	102.51	105.40
59	BA	1136	G	N1-C6-O6	7.21	124.22	119.90
1	AB	163	PHE	N-CA-C	-7.20	91.55	111.00
59	DA	1078	U	C2-N1-C1'	7.20	126.34	117.70
23	AY	502	GLY	O-C-N	7.18	135.41	123.20
59	DA	103	A	N1-C6-N6	7.18	122.91	118.60
59	BA	2712	U	N1-C2-O2	7.18	127.83	122.80
59	DA	2585	U	C2-N1-C1'	7.13	126.25	117.70
20	CA	1170	A	N1-C6-N6	7.08	122.85	118.60
20	AA	1170	A	N1-C6-N6	7.07	122.84	118.60
59	BA	2712	U	C2-N1-C1'	7.07	126.18	117.70
20	AA	838(C)	U	N1-C2-O2	7.07	127.75	122.80
59	BA	2023	G	C5-C6-O6	-7.07	124.36	128.60
59	DA	1006	C	C2-N1-C1'	7.06	126.57	118.80
59	BA	1774	C	C2-N1-C1'	7.04	126.55	118.80
59	DA	673	C	C2-N3-C4	-7.04	116.38	119.90
59	BA	2040	C	P-O3'-C3'	7.02	128.13	119.70
59	DA	470	A	N7-C8-N9	7.00	117.30	113.80
20	CA	1535	C	C2-N1-C1'	6.96	126.45	118.80
20	AA	421	U	C2-N1-C1'	6.95	126.03	117.70
20	AA	815	A	C6-C5-N7	6.89	137.12	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	2344	U	N1-C2-O2	-6.87	117.99	122.80
59	DA	1048	A	N1-C6-N6	6.87	122.72	118.60
59	DA	2585	U	N1-C2-O2	6.87	127.61	122.80
59	BA	2710	C	C6-N1-C2	-6.87	117.55	120.30
20	AA	754	C	C2-N1-C1'	6.85	126.33	118.80
59	BA	95	G	N3-C4-N9	-6.79	121.92	126.00
59	BA	963	U	N3-C2-O2	-6.77	117.46	122.20
59	BA	1914	C	C2-N1-C1'	6.76	126.24	118.80
59	BA	103	A	N1-C6-N6	6.75	122.65	118.60
20	CA	1508	G	N1-C2-N3	6.75	127.95	123.90
60	BB	101	A	C5-C6-N1	6.73	121.06	117.70
59	DA	1963	U	N1-C2-O2	6.70	127.49	122.80
20	CA	815	A	N3-C4-N9	-6.69	122.05	127.40
59	BA	1774	C	N1-C2-O2	6.68	122.91	118.90
59	DA	1139	G	N7-C8-N9	6.66	116.43	113.10
20	CA	838(C)	U	N1-C2-O2	6.66	127.46	122.80
60	DB	75	G	C6-N1-C2	-6.64	121.11	125.10
59	DA	1138	G	N3-C4-C5	6.64	131.92	128.60
20	AA	838(C)	U	N3-C2-O2	-6.63	117.56	122.20
59	BA	673	C	C5-C4-N4	-6.63	115.56	120.20
59	DA	1314	C	C2-N1-C1'	6.63	126.09	118.80
20	AA	618	C	C6-N1-C1'	6.62	128.75	120.80
60	BB	101	A	C5-C6-N6	-6.61	118.41	123.70
59	DA	1963	U	C2-N1-C1'	6.60	125.62	117.70
20	CA	815	A	C6-C5-N7	6.59	136.91	132.30
59	DA	83	G	C2-N3-C4	-6.58	108.61	111.90
60	DB	88	C	C2-N1-C1'	6.57	126.02	118.80
59	BA	1007	C	C2-N1-C1'	6.55	126.00	118.80
20	CA	1508	G	N3-C2-N2	-6.54	115.32	119.90
59	BA	1137	G	N3-C4-C5	-6.54	125.33	128.60
59	DA	1007	C	N1-C1'-C2'	6.51	122.47	114.00
60	BB	9	G	C5-C6-O6	6.51	132.51	128.60
59	DA	470	A	C6-C5-N7	-6.51	127.75	132.30
59	DA	2681	C	C2-N1-C1'	6.50	125.95	118.80
20	CA	618	C	N3-C4-C5	-6.48	119.31	121.90
21	CW	61	C	C2-N1-C1'	6.46	125.91	118.80
20	CA	1158	C	N1-C2-O2	6.46	122.77	118.90
60	BB	75	G	C5-C6-O6	-6.45	124.73	128.60
25	BC	138	LEU	CA-CB-CG	6.45	130.13	115.30
59	BA	1137	G	N3-C4-N9	6.43	129.86	126.00
59	BA	963	U	N1-C2-O2	6.42	127.30	122.80
59	BA	1136	G	C4-C5-N7	6.41	113.36	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CD	28	SER	C-N-CD	6.41	141.86	128.40
20	CA	618	C	C5-C4-N4	6.41	124.69	120.20
20	AA	618	C	C5-C4-N4	6.40	124.68	120.20
59	DA	2585	U	N3-C2-O2	-6.40	117.72	122.20
59	BA	1132	A	C2-N3-C4	-6.38	107.41	110.60
20	CA	129(A)	G	N3-C4-N9	6.38	129.83	126.00
59	BA	2040	C	C6-N1-C2	-6.36	117.75	120.30
4	CE	12	LEU	CA-CB-CG	6.35	129.91	115.30
20	CA	815	A	C6-N1-C2	6.35	122.41	118.60
59	DA	1313	U	C2-N1-C1'	6.33	125.30	117.70
59	DA	2794	C	C2-N1-C1'	6.33	125.77	118.80
59	BA	1494	A	C2-N3-C4	6.31	113.76	110.60
20	AA	717	C	C2-N1-C1'	6.30	125.74	118.80
59	BA	459	U	C5-C6-N1	6.30	125.85	122.70
60	BB	75	G	C5-C6-N1	6.29	114.65	111.50
59	DA	673	C	C5-C4-N4	-6.29	115.79	120.20
59	DA	2344	U	N1-C2-O2	-6.29	118.40	122.80
59	BA	1136	G	N9-C4-C5	-6.27	102.89	105.40
59	BA	2802	G	N3-C4-N9	6.26	129.76	126.00
59	DA	576	U	C5-C4-O4	-6.26	122.14	125.90
28	BF	155	LEU	N-CA-C	-6.24	94.16	111.00
59	BA	1007	C	N1-C1'-C2'	6.23	122.09	114.00
59	BA	1420	U	C2-N1-C1'	6.22	125.17	117.70
20	AA	1158	C	C6-N1-C1'	-6.22	113.33	120.80
59	BA	226	G	C2-N3-C4	6.21	115.01	111.90
59	BA	463	G	C2-N3-C4	-6.21	108.79	111.90
59	BA	1313	U	N1-C2-O2	6.21	127.15	122.80
20	CA	1514	C	C5-C6-N1	6.21	124.10	121.00
59	DA	621	A	N1-C6-N6	-6.18	114.89	118.60
4	AE	12	LEU	CA-CB-CG	6.18	129.51	115.30
59	DA	1937	A	P-O3'-C3'	6.17	127.10	119.70
41	BV	49	THR	C-N-CD	6.17	141.35	128.40
59	DA	294	A	N1-C6-N6	6.17	122.30	118.60
59	BA	1542	G	P-O3'-C3'	6.17	127.10	119.70
59	DA	1139	G	C6-C5-N7	-6.16	126.71	130.40
20	AA	421	U	N1-C2-O2	6.15	127.11	122.80
59	BA	527	C	C6-N1-C2	-6.14	117.84	120.30
59	DA	985	C	C2-N1-C1'	6.14	125.55	118.80
59	DA	121	G	N3-C4-N9	6.13	129.68	126.00
59	BA	2688	U	N3-C2-O2	-6.12	117.91	122.20
20	AA	68(R)	C	N1-C2-O2	-6.12	115.23	118.90
59	BA	2585	U	N1-C2-O2	6.11	127.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	754	C	C2-N1-C1'	6.10	125.51	118.80
59	BA	1494	A	N1-C6-N6	-6.09	114.94	118.60
20	CA	1508	G	C2-N3-C4	-6.08	108.86	111.90
59	DA	114	U	C2-N1-C1'	6.06	124.97	117.70
59	BA	95	G	C4-N9-C1'	-6.06	118.62	126.50
59	BA	2712	U	N3-C2-O2	-6.06	117.96	122.20
20	CA	421	U	N1-C2-O2	6.06	127.04	122.80
59	BA	2598	A	N1-C6-N6	6.06	122.23	118.60
59	BA	1048	A	C6-C5-N7	-6.05	128.06	132.30
59	DA	671	C	C2-N1-C1'	6.05	125.45	118.80
59	BA	1314	C	N1-C2-O2	6.04	122.53	118.90
59	BA	1920	C	C6-N1-C2	-6.04	117.89	120.30
20	AA	618	C	O4'-C1'-N1	6.03	113.02	108.20
20	AA	383	A	N1-C6-N6	6.02	122.21	118.60
59	BA	1006	C	N3-C2-O2	-6.02	117.69	121.90
59	BA	1673	U	O4'-C1'-N1	6.01	113.01	108.20
59	BA	30	G	N3-C4-N9	6.01	129.61	126.00
59	DA	30	G	N3-C4-N9	6.00	129.60	126.00
20	AA	1066	C	C2-N1-C1'	6.00	125.40	118.80
59	BA	278	A	P-O3'-C3'	6.00	126.89	119.70
20	AA	1158	C	N3-C2-O2	-5.99	117.71	121.90
59	BA	1963	U	N1-C2-O2	5.99	126.99	122.80
59	BA	2407	G	C4-N9-C1'	5.99	134.29	126.50
20	CA	421	U	C2-N1-C1'	5.99	124.89	117.70
59	BA	1249	U	C6-N1-C1'	-5.99	112.82	121.20
12	AM	56	LEU	CA-CB-CG	5.99	129.06	115.30
28	DF	155	LEU	N-CA-C	-5.98	94.86	111.00
59	BA	1249	U	N1-C2-O2	5.96	126.97	122.80
59	BA	1048	A	C4-C5-C6	5.95	119.98	117.00
59	DA	1448	G	N9-C4-C5	5.94	107.78	105.40
9	CJ	16	LEU	CA-CB-CG	5.93	128.95	115.30
20	CA	1535	C	C5-C6-N1	5.93	123.97	121.00
20	CA	838(A)	U	C2-N1-C1'	5.92	124.81	117.70
59	DA	737	C	C2-N1-C1'	5.92	125.31	118.80
59	DA	30	G	N3-C4-C5	-5.92	125.64	128.60
59	BA	2119	A	C5-C6-N6	5.92	128.43	123.70
59	BA	1006	C	C5-C6-N1	5.90	123.95	121.00
20	CA	992	U	P-O3'-C3'	5.88	126.76	119.70
20	AA	1332	A	N1-C6-N6	5.87	122.12	118.60
59	BA	329	G	N3-C4-N9	5.87	129.52	126.00
20	AA	618	C	N3-C4-C5	-5.87	119.55	121.90
59	DA	2041	U	O4'-C1'-N1	5.87	112.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	618	C	C2-N1-C1'	-5.86	112.35	118.80
59	DA	1006	C	C5-C6-N1	5.86	123.93	121.00
59	BA	1287	A	N1-C2-N3	5.85	132.23	129.30
60	BB	81	G	C5-C6-O6	-5.85	125.09	128.60
21	CW	25	C	C2-N1-C1'	5.85	125.23	118.80
50	B6	9	LEU	CA-CB-CG	5.84	128.73	115.30
59	BA	1107	G	N3-C4-N9	-5.84	122.50	126.00
20	AA	129(A)	G	N3-C2-N2	5.84	123.99	119.90
59	DA	1570	A	N1-C6-N6	5.83	122.10	118.60
20	AA	1043	C	O4'-C1'-N1	5.81	112.85	108.20
59	DA	2710	C	C6-N1-C2	-5.81	117.98	120.30
20	AA	1214	C	C2-N1-C1'	5.80	125.18	118.80
59	BA	103	A	C4-C5-C6	5.79	119.89	117.00
59	BA	95	G	C8-N9-C1'	5.76	134.49	127.00
21	CW	61	C	N1-C2-O2	5.76	122.35	118.90
59	DA	1327	C	C6-N1-C2	-5.76	118.00	120.30
60	BB	101	A	N3-C4-N9	5.75	132.00	127.40
60	DB	88	C	N1-C2-O2	5.74	122.35	118.90
59	BA	1774	C	N3-C2-O2	-5.74	117.88	121.90
59	DA	103	A	C4-C5-C6	5.74	119.87	117.00
59	BA	1872	A	N1-C6-N6	5.72	122.03	118.60
59	DA	807	U	C2-N3-C4	-5.72	123.57	127.00
59	DA	2681	C	C6-N1-C1'	-5.72	113.94	120.80
20	CA	1483	A	N9-C4-C5	-5.72	103.51	105.80
59	BA	2040	C	O4'-C1'-N1	-5.71	103.63	108.20
20	AA	1214	C	N1-C2-O2	5.71	122.32	118.90
59	BA	1022	G	P-O3'-C3'	5.70	126.53	119.70
59	DA	510	C	N1-C2-O2	5.70	122.32	118.90
59	DA	1107	G	N9-C4-C5	5.69	107.68	105.40
59	BA	527	C	C2-N1-C1'	5.68	125.05	118.80
59	DA	1153	C	C6-N1-C1'	-5.68	113.98	120.80
28	DF	174	VAL	N-CA-C	-5.67	95.69	111.00
59	BA	1493	C	N1-C2-O2	5.67	122.30	118.90
20	CA	815	A	C5-C6-N1	-5.67	114.87	117.70
59	DA	1774	C	C6-N1-C2	-5.67	118.03	120.30
59	BA	1007	C	C4-C5-C6	-5.66	114.57	117.40
59	BA	45	G	N3-C4-N9	-5.66	122.60	126.00
20	CA	838(C)	U	N3-C2-O2	-5.66	118.24	122.20
59	DA	270(L)	C	C6-N1-C2	-5.64	118.04	120.30
20	AA	960	U	N1-C2-O2	5.63	126.74	122.80
20	AA	1170	A	C4-C5-C6	5.62	119.81	117.00
59	BA	1497	U	C2-N1-C1'	5.62	124.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1493	C	N3-C2-O2	-5.62	117.97	121.90
59	DA	1955	U	C2-N1-C1'	5.62	124.44	117.70
59	DA	1913	A	P-O3'-C3'	5.62	126.44	119.70
20	AA	186(G)	C	C6-N1-C2	-5.61	118.06	120.30
59	DA	645	C	C2-N1-C1'	5.61	124.97	118.80
20	AA	717	C	C6-N1-C1'	-5.60	114.08	120.80
59	BA	1327	C	C6-N1-C2	-5.60	118.06	120.30
59	BA	1332	G	C4-N9-C1'	5.59	133.77	126.50
59	DA	1658	C	C2-N1-C1'	5.59	124.95	118.80
20	AA	68(H)	G	C8-N9-C4	-5.59	104.17	106.40
59	BA	1143	A	C2-N3-C4	-5.58	107.81	110.60
59	DA	401	A	N1-C2-N3	5.58	132.09	129.30
20	AA	815	A	C5-C6-N1	-5.58	114.91	117.70
20	CA	1465	C	C2-N3-C4	-5.57	117.11	119.90
20	AA	68(R)	C	C2-N1-C1'	-5.57	112.67	118.80
59	DA	2023	G	N1-C2-N2	5.57	121.21	116.20
59	DA	1976	U	O4'-C1'-N1	5.57	112.65	108.20
59	BA	24	G	N3-C4-N9	-5.56	122.66	126.00
20	AA	1465	C	C2-N3-C4	-5.55	117.12	119.90
59	DA	1107	G	N3-C4-N9	-5.55	122.67	126.00
59	BA	114	U	C2-N1-C1'	5.55	124.36	117.70
59	DA	1779	U	C2-N1-C1'	5.55	124.36	117.70
59	DA	1673	U	O4'-C1'-N1	5.54	112.64	108.20
59	BA	1558	A	P-O3'-C3'	5.54	126.35	119.70
59	DA	1937	A	OP1-P-O3'	5.54	117.39	105.20
60	DB	75	G	N3-C4-C5	-5.54	125.83	128.60
20	CA	129(A)	G	N9-C4-C5	-5.53	103.19	105.40
59	DA	2518	A	P-O3'-C3'	5.53	126.34	119.70
20	AA	68(H)	G	N9-C4-C5	5.53	107.61	105.40
20	CA	821	G	N9-C4-C5	-5.53	103.19	105.40
59	BA	2447	G	P-O3'-C3'	5.53	126.33	119.70
59	BA	1007	C	C5'-C4'-C3'	5.52	124.83	116.00
59	BA	2119	A	N1-C6-N6	-5.52	115.29	118.60
20	AA	748	C	P-O3'-C3'	5.51	126.31	119.70
20	AA	68(R)	C	C6-N1-C1'	5.51	127.41	120.80
59	BA	2407	G	C8-N9-C1'	-5.51	119.84	127.00
59	DA	1052	C	C2-N1-C1'	-5.50	112.75	118.80
59	BA	1153	C	C2-N1-C1'	5.50	124.85	118.80
20	CA	838(C)	U	C6-N1-C1'	-5.50	113.50	121.20
20	AA	1508	G	C6-C5-N7	-5.49	127.10	130.40
59	DA	1052	C	C6-N1-C1'	5.49	127.39	120.80
20	CA	748	C	P-O3'-C3'	5.49	126.28	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1963	U	N3-C2-O2	-5.49	118.36	122.20
59	DA	1774	C	C2-N1-C1'	5.48	124.83	118.80
42	DW	51	LEU	CA-CB-CG	5.48	127.90	115.30
59	BA	329	G	C8-N9-C1'	-5.48	119.88	127.00
59	BA	1313	U	C6-N1-C1'	-5.47	113.54	121.20
20	CA	821	G	N3-C4-N9	5.47	129.28	126.00
59	BA	1136	G	C6-C5-N7	-5.47	127.12	130.40
59	DA	470	A	C5-N7-C8	-5.46	101.17	103.90
59	BA	2794	C	N1-C2-O2	5.45	122.17	118.90
59	BA	1090	U	O4'-C1'-N1	5.45	112.56	108.20
20	CA	815	A	C4-C5-N7	-5.45	107.98	110.70
20	CA	1170	A	C4-C5-C6	5.45	119.72	117.00
59	DA	2040	C	O5'-P-OP1	5.44	117.23	110.70
59	BA	1249	U	C5-C6-N1	5.44	125.42	122.70
59	BA	1985	G	N3-C4-N9	-5.43	122.74	126.00
11	AL	55	VAL	CB-CA-C	-5.43	101.08	111.40
21	CW	30	C	C2-N1-C1'	5.43	124.77	118.80
59	BA	1774	C	C6-N1-C2	-5.42	118.13	120.30
20	AA	943	U	C5-C4-O4	5.42	129.15	125.90
60	BB	101	A	N3-C4-C5	-5.42	123.01	126.80
59	DA	1048	A	C4-C5-C6	5.42	119.71	117.00
59	DA	1558	A	P-O3'-C3'	5.41	126.20	119.70
20	AA	1196	U	C2-N1-C1'	5.41	124.19	117.70
59	BA	1019	U	N3-C2-O2	-5.41	118.41	122.20
59	BA	576	U	C5-C4-O4	-5.41	122.66	125.90
20	CA	1158	C	N3-C2-O2	-5.40	118.12	121.90
59	BA	737	C	C2-N1-C1'	5.40	124.74	118.80
59	DA	422	A	C8-N9-C4	-5.38	103.65	105.80
59	DA	2473	U	C2-N1-C1'	5.37	124.15	117.70
59	BA	2780	G	C4-C5-N7	-5.37	108.65	110.80
59	DA	1137	G	N3-C4-C5	-5.37	125.91	128.60
59	DA	544	C	C6-N1-C1'	-5.37	114.36	120.80
59	BA	2119	A	N9-C4-C5	5.36	107.94	105.80
59	BA	294	A	N1-C6-N6	5.36	121.82	118.60
20	AA	383	A	C4-C5-C6	5.36	119.68	117.00
59	DA	2726	U	C2-N1-C1'	5.36	124.13	117.70
20	CA	186(J)	G	OP2-P-O3'	5.35	116.97	105.20
59	DA	1249	U	C6-N1-C1'	-5.34	113.72	121.20
20	AA	1071	C	C5-C6-N1	5.34	123.67	121.00
59	DA	130	C	N1-C2-O2	5.34	122.10	118.90
59	DA	541	C	O4'-C1'-N1	5.34	112.47	108.20
59	BA	2429	G	O4'-C1'-N9	5.33	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	186(G)	C	N3-C2-O2	-5.33	118.17	121.90
59	DA	2598	A	N1-C6-N6	5.33	121.80	118.60
59	DA	985	C	C6-N1-C1'	-5.32	114.41	120.80
59	DA	1213	A	N1-C6-N6	5.32	121.79	118.60
59	BA	2681	C	C2-N1-C1'	5.32	124.65	118.80
59	BA	2801	A	N1-C6-N6	5.32	121.79	118.60
59	DA	2023	G	N3-C4-C5	5.32	131.26	128.60
59	BA	2578	G	C8-N9-C1'	5.31	133.91	127.00
59	DA	1256	G	N3-C4-N9	5.31	129.19	126.00
20	CA	687	A	P-O3'-C3'	5.31	126.07	119.70
59	BA	2802	G	N9-C4-C5	-5.29	103.28	105.40
59	BA	1963	U	N3-C2-O2	-5.29	118.50	122.20
59	DA	2344	U	C2-N3-C4	-5.28	123.83	127.00
23	CY	567	LEU	CA-CB-CG	5.28	127.44	115.30
59	BA	673	C	N3-C4-C5	5.27	124.01	121.90
59	DA	544	C	C2-N1-C1'	5.27	124.60	118.80
59	DA	1157	G	C8-N9-C1'	-5.27	120.15	127.00
59	BA	2041	U	C5-C4-O4	-5.27	122.74	125.90
20	CA	1158	C	C6-N1-C1'	-5.27	114.48	120.80
59	DA	757	U	N1-C2-O2	5.27	126.49	122.80
59	DA	270(L)	C	C2-N1-C1'	5.26	124.59	118.80
59	DA	1493	C	C6-N1-C2	-5.26	118.19	120.30
59	DA	270(L)	C	N1-C2-O2	5.26	122.06	118.90
59	BA	1007	C	C5-C4-N4	-5.26	116.52	120.20
20	CA	383	A	N1-C6-N6	5.26	121.76	118.60
20	CA	618	C	C6-N1-C1'	5.26	127.11	120.80
59	BA	2041	U	N3-C2-O2	5.26	125.88	122.20
59	BA	2598	A	C4-C5-C6	5.25	119.63	117.00
59	BA	2786	U	C2-N1-C1'	5.25	124.01	117.70
59	BA	1048	A	C4-N9-C1'	5.25	135.76	126.30
59	DA	2040	C	OP1-P-O3'	5.25	116.75	105.20
20	CA	129(A)	G	C8-N9-C1'	-5.25	120.18	127.00
59	DA	2802	G	N3-C4-N9	5.24	129.14	126.00
59	DA	671	C	C6-N1-C1'	-5.23	114.52	120.80
59	BA	95	G	C6-C5-N7	5.23	133.54	130.40
59	BA	121	G	N3-C4-N9	5.23	129.14	126.00
20	CA	838(A)	U	N1-C2-O2	5.23	126.46	122.80
59	DA	2712	U	N1-C2-O2	5.22	126.46	122.80
20	CA	183	G	N3-C4-N9	5.22	129.13	126.00
20	AA	421	U	N3-C2-O2	-5.22	118.55	122.20
59	BA	2710	C	N3-C2-O2	-5.22	118.25	121.90
59	DA	1022	G	C8-N9-C4	-5.22	104.31	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1498	C	N3-C2-O2	-5.22	118.25	121.90
20	AA	320	C	O4'-C1'-N1	5.22	112.37	108.20
59	BA	1287	A	C2-N3-C4	-5.22	107.99	110.60
59	BA	1048	A	N3-C4-N9	5.21	131.57	127.40
59	DA	130	C	C2-N1-C1'	5.21	124.53	118.80
59	DA	2053	G	N3-C4-N9	5.21	129.13	126.00
20	AA	838(C)	U	C6-N1-C1'	-5.21	113.90	121.20
59	BA	1914	C	N1-C2-O2	5.21	122.03	118.90
59	DA	1448	G	N3-C4-N9	-5.21	122.88	126.00
59	BA	510	C	N1-C2-O2	5.20	122.02	118.90
59	BA	226	G	N9-C4-C5	5.19	107.48	105.40
59	DA	1249	U	C5-C6-N1	5.19	125.30	122.70
59	BA	83	G	C2-N3-C4	-5.19	109.31	111.90
20	CA	129(A)	G	C4-N9-C1'	5.18	133.24	126.50
59	DA	565	C	C5-C4-N4	-5.18	116.58	120.20
59	DA	1287	A	C2-N3-C4	-5.18	108.01	110.60
59	DA	1078	U	N3-C2-O2	-5.17	118.58	122.20
59	DA	1138	G	N3-C2-N2	-5.17	116.28	119.90
20	AA	1465	C	C5-C4-N4	-5.17	116.58	120.20
59	BA	1138	G	N3-C4-N9	-5.17	122.90	126.00
59	DA	1006	C	N1-C2-O2	5.17	122.00	118.90
20	AA	717	C	N1-C2-O2	5.16	121.99	118.90
59	BA	1048	A	N9-C4-C5	-5.16	103.74	105.80
59	DA	130	C	C6-N1-C1'	-5.16	114.61	120.80
59	BA	2532	G	C2-N3-C4	5.15	114.48	111.90
59	DA	1985	G	N3-C2-N2	-5.15	116.30	119.90
59	BA	2595	G	C2-N3-C4	-5.15	109.33	111.90
59	BA	2769	C	C6-N1-C1'	5.15	126.98	120.80
20	CA	129(A)	G	C6-C5-N7	-5.15	127.31	130.40
59	BA	1314	C	N3-C2-O2	-5.13	118.31	121.90
59	DA	329	G	C4-N9-C1'	5.13	133.17	126.50
59	DA	1139	G	C4-C5-N7	5.13	112.85	110.80
20	AA	1066	C	C6-N1-C1'	-5.13	114.65	120.80
59	DA	1007	C	C5-C6-N1	5.13	123.56	121.00
20	AA	1101	A	P-O3'-C3'	5.12	125.85	119.70
20	AA	1170	A	C6-C5-N7	-5.12	128.71	132.30
59	DA	1149	G	N3-C4-N9	5.12	129.07	126.00
59	DA	2598	A	C4-C5-C6	5.12	119.56	117.00
26	BD	177	LEU	CA-CB-CG	5.12	127.08	115.30
59	DA	671	C	N1-C2-O2	5.12	121.97	118.90
59	DA	1493	C	C5-C6-N1	5.11	123.56	121.00
59	DA	344	G	C2-N3-C4	-5.11	109.34	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DC	215	VAL	CB-CA-C	-5.11	101.70	111.40
59	BA	1931	U	N3-C2-O2	-5.11	118.63	122.20
59	DA	2041	U	C6-N1-C2	-5.10	117.94	121.00
20	CA	1290	G	C5-C6-O6	-5.09	125.55	128.60
20	AA	754	C	C6-N1-C2	-5.09	118.27	120.30
59	DA	1157	G	N3-C4-N9	5.09	129.05	126.00
11	AL	60	LEU	CA-CB-CG	5.08	126.99	115.30
59	BA	1048	A	C8-N9-C1'	-5.08	118.55	127.70
20	AA	129(A)	G	N9-C4-C5	-5.08	103.37	105.40
59	BA	95	G	C4-C5-N7	-5.08	108.77	110.80
57	D1	17	SER	N-CA-C	-5.08	97.30	111.00
59	DA	1872	A	N1-C6-N6	5.08	121.65	118.60
59	DA	470	A	C4-C5-C6	5.07	119.53	117.00
59	BA	1009	A	C5-N7-C8	5.07	106.43	103.90
59	BA	1851	U	C5-C6-N1	5.07	125.23	122.70
60	BB	88	C	C2-N1-C1'	5.07	124.37	118.80
59	DA	1139	G	C5-N7-C8	-5.06	101.77	104.30
59	BA	1420	U	C5-C6-N1	5.06	125.23	122.70
59	DA	2092	U	P-O3'-C3'	5.06	125.78	119.70
59	DA	2780	G	P-O3'-C3'	5.06	125.78	119.70
1	CB	187	LEU	CA-CB-CG	5.06	126.93	115.30
59	DA	1007	C	C2-N1-C1'	5.06	124.36	118.80
59	BA	9	U	N1-C2-O2	5.05	126.34	122.80
59	BA	474	G	P-O3'-C3'	5.05	125.77	119.70
23	AY	502	GLY	C-N-CA	-5.05	111.69	122.30
59	BA	2578	G	N3-C4-N9	-5.05	122.97	126.00
21	CW	25	C	N1-C2-O2	5.05	121.93	118.90
28	BF	191	ARG	N-CA-C	5.05	124.62	111.00
5	CF	19	LEU	CA-CB-CG	5.05	126.91	115.30
59	BA	1802	A	N1-C6-N6	5.04	121.63	118.60
59	DA	737	C	N1-C2-O2	5.04	121.93	118.90
20	CA	328	C	P-O3'-C3'	5.04	125.75	119.70
59	BA	1743	G	O4'-C1'-N9	5.03	112.23	108.20
20	CA	1483	A	C8-N9-C4	5.03	107.81	105.80
59	DA	673	C	N3-C4-C5	5.03	123.91	121.90
59	DA	1396	U	C2-N1-C1'	5.03	123.73	117.70
59	DA	2013	A	N1-C6-N6	-5.03	115.58	118.60
59	BA	671	C	C2-N1-C1'	5.03	124.33	118.80
20	CA	838(C)	U	C5-C6-N1	5.03	125.21	122.70
59	BA	2576	G	C4-N9-C1'	5.02	133.03	126.50
59	BA	1090	U	C2-N1-C1'	-5.02	111.68	117.70
11	CL	33	ARG	N-CA-C	5.02	124.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	1220	G	N3-C4-N9	5.02	129.01	126.00
59	DA	2040	C	C4-C5-C6	-5.02	114.89	117.40
59	BA	329	G	C4-N9-C1'	5.01	133.01	126.50
59	BA	1090	U	C6-N1-C1'	5.01	128.21	121.20
59	BA	2712	U	C6-N1-C1'	-5.01	114.19	121.20
43	DX	57	LEU	CA-CB-CG	5.01	126.82	115.30
59	BA	2407	G	N3-C4-N9	5.01	129.00	126.00
59	BA	1090	U	C5-C4-O4	5.00	128.90	125.90
59	BA	2040	C	C4-C5-C6	-5.00	114.90	117.40
20	AA	1248	A	N1-C6-N6	-5.00	115.60	118.60
59	DA	130	C	C5-C4-N4	-5.00	116.70	120.20

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
23	AY	133	ILE	Peptide
23	AY	503	GLY	Mainchain
23	AY	506	GLN	Mainchain
57	B1	16	ASN	Peptide
57	B1	18	ILE	Peptide
25	BC	171	ALA	Peptide
26	BD	164	GLN	Peptide
28	BF	154	VAL	Peptide
28	BF	173	VAL	Peptide
29	BG	111	LEU	Mainchain
29	BG	113	ARG	Peptide
31	BJ	83	UNK	Peptide
38	BS	14	VAL	Peptide
38	BS	46	VAL	Peptide
38	BS	98	VAL	Peptide
42	BW	75	TYR	Peptide
1	CB	170	GLU	Peptide
11	CL	32	PHE	Peptide
11	CL	57	LYS	Peptide
23	CY	133	ILE	Peptide
23	CY	503	GLY	Mainchain
57	D1	16	ASN	Peptide
57	D1	17	SER	Peptide

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Mol	Chain	Res	Type	Group
25	DC	161	ARG	Peptide
25	DC	171	ALA	Peptide
25	DC	211	ARG	Peptide
26	DD	164	GLN	Peptide
26	DD	78	LYS	Peptide
28	DF	154	VAL	Peptide
28	DF	173	VAL	Peptide
29	DG	111	LEU	Mainchain
29	DG	113	ARG	Peptide
31	DJ	83	UNK	Peptide
35	DP	57	THR	Peptide
38	DS	14	VAL	Peptide
38	DS	46	VAL	Peptide
38	DS	98	VAL	Peptide
42	DW	75	TYR	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%)	154 (66%)	51 (22%)	28 (12%)	0	5
1	CB	233/235 (99%)	159 (68%)	50 (22%)	24 (10%)	0	7
2	AC	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	0	8
2	CC	205/207 (99%)	156 (76%)	36 (18%)	13 (6%)	1	14
3	AD	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	5
3	CD	206/208 (99%)	153 (74%)	32 (16%)	21 (10%)	0	7
4	AE	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CE	149/151 (99%)	117 (78%)	25 (17%)	7 (5%)	2	20
5	AF	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	8
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	8
6	AG	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	2	21
6	CG	153/155 (99%)	124 (81%)	22 (14%)	7 (5%)	2	21
7	AH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	8
7	CH	136/138 (99%)	97 (71%)	28 (21%)	11 (8%)	1	9
8	AI	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	3	24
8	CI	125/127 (98%)	99 (79%)	22 (18%)	4 (3%)	4	29
9	AJ	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	0	8
9	CJ	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	2	18
10	AK	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	0	5
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	6
11	AL	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	0
11	CL	123/125 (98%)	47 (38%)	43 (35%)	33 (27%)	0	0
12	AM	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	9
12	CM	123/125 (98%)	91 (74%)	25 (20%)	7 (6%)	1	16
13	AN	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	0	5
13	CN	58/60 (97%)	44 (76%)	10 (17%)	4 (7%)	1	12
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	9
14	CO	86/88 (98%)	60 (70%)	21 (24%)	5 (6%)	1	16
15	AP	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	13	50
15	CP	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	2	19
16	AQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	7
16	CQ	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	0	7
17	AR	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	0	7
17	CR	68/70 (97%)	48 (71%)	13 (19%)	7 (10%)	0	7
18	AS	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	2
18	CS	77/79 (98%)	46 (60%)	17 (22%)	14 (18%)	0	2
19	AT	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	23
19	CT	97/99 (98%)	79 (81%)	12 (12%)	6 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AY	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	0	6
23	CY	663/687 (96%)	461 (70%)	134 (20%)	68 (10%)	0	7
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
25	BC	226/228 (99%)	110 (49%)	66 (29%)	50 (22%)	0	1
25	DC	226/228 (99%)	123 (54%)	59 (26%)	44 (20%)	0	2
26	BD	273/275 (99%)	174 (64%)	47 (17%)	52 (19%)	0	2
26	DD	273/275 (99%)	165 (60%)	61 (22%)	47 (17%)	0	2
27	BE	203/205 (99%)	128 (63%)	40 (20%)	35 (17%)	0	2
27	DE	203/205 (99%)	122 (60%)	45 (22%)	36 (18%)	0	2
28	BF	206/208 (99%)	130 (63%)	46 (22%)	30 (15%)	0	3
28	DF	206/208 (99%)	128 (62%)	44 (21%)	34 (16%)	0	2
29	BG	179/181 (99%)	122 (68%)	48 (27%)	9 (5%)	2	19
29	DG	179/181 (99%)	134 (75%)	36 (20%)	9 (5%)	2	19
30	BH	165/167 (99%)	118 (72%)	27 (16%)	20 (12%)	0	5
30	DH	165/167 (99%)	111 (67%)	33 (20%)	21 (13%)	0	4
32	BK	138/140 (99%)	96 (70%)	30 (22%)	12 (9%)	1	9
32	DK	138/140 (99%)	97 (70%)	34 (25%)	7 (5%)	2	19
33	BN	136/138 (99%)	86 (63%)	28 (21%)	22 (16%)	0	2
33	DN	136/138 (99%)	88 (65%)	35 (26%)	13 (10%)	0	8
34	BO	120/122 (98%)	86 (72%)	24 (20%)	10 (8%)	1	9
34	DO	120/122 (98%)	87 (72%)	25 (21%)	8 (7%)	1	13
35	BP	144/146 (99%)	85 (59%)	39 (27%)	20 (14%)	0	3
35	DP	144/146 (99%)	81 (56%)	38 (26%)	25 (17%)	0	2
36	BQ	139/141 (99%)	96 (69%)	27 (19%)	16 (12%)	0	6
36	DQ	139/141 (99%)	97 (70%)	29 (21%)	13 (9%)	0	8
37	BR	115/117 (98%)	80 (70%)	27 (24%)	8 (7%)	1	12
37	DR	115/117 (98%)	83 (72%)	20 (17%)	12 (10%)	0	7
38	BS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
38	DS	97/99 (98%)	56 (58%)	21 (22%)	20 (21%)	0	1
39	BT	136/138 (99%)	80 (59%)	31 (23%)	25 (18%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	DT	136/138 (99%)	85 (62%)	29 (21%)	22 (16%)	0	2
40	BU	115/117 (98%)	84 (73%)	25 (22%)	6 (5%)	2	18
40	DU	115/117 (98%)	90 (78%)	16 (14%)	9 (8%)	1	10
41	BV	99/101 (98%)	66 (67%)	16 (16%)	17 (17%)	0	2
41	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
42	BW	111/113 (98%)	85 (77%)	11 (10%)	15 (14%)	0	4
42	DW	111/113 (98%)	85 (77%)	15 (14%)	11 (10%)	0	7
43	BX	91/93 (98%)	72 (79%)	15 (16%)	4 (4%)	2	21
43	DX	91/93 (98%)	72 (79%)	14 (15%)	5 (6%)	2	17
44	BY	105/107 (98%)	51 (49%)	30 (29%)	24 (23%)	0	1
44	DY	105/107 (98%)	46 (44%)	26 (25%)	33 (31%)	0	0
45	BZ	183/185 (99%)	132 (72%)	33 (18%)	18 (10%)	0	7
45	DZ	183/185 (99%)	132 (72%)	32 (18%)	19 (10%)	0	7
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	9
46	D0	82/84 (98%)	57 (70%)	15 (18%)	10 (12%)	0	5
47	B2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	1	16
47	D2	69/71 (97%)	56 (81%)	10 (14%)	3 (4%)	2	22
48	B3	58/60 (97%)	48 (83%)	6 (10%)	4 (7%)	1	12
48	D3	58/60 (97%)	42 (72%)	10 (17%)	6 (10%)	0	7
49	B5	57/59 (97%)	43 (75%)	11 (19%)	3 (5%)	2	17
49	D5	57/59 (97%)	41 (72%)	12 (21%)	4 (7%)	1	12
50	B6	48/50 (96%)	28 (58%)	13 (27%)	7 (15%)	0	3
50	D6	48/50 (96%)	29 (60%)	8 (17%)	11 (23%)	0	1
51	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	9
51	D7	47/49 (96%)	32 (68%)	9 (19%)	6 (13%)	0	4
52	B8	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	2
52	D8	62/64 (97%)	36 (58%)	18 (29%)	8 (13%)	0	4
53	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	3
53	D9	35/37 (95%)	24 (69%)	8 (23%)	3 (9%)	1	9
54	Be	70/102 (69%)	38 (54%)	24 (34%)	8 (11%)	0	6
54	De	70/102 (69%)	41 (59%)	23 (33%)	6 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	B1	91/93 (98%)	60 (66%)	19 (21%)	12 (13%)	0	4
57	D1	91/93 (98%)	56 (62%)	18 (20%)	17 (19%)	0	2
58	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	3
58	D4	33/35 (94%)	17 (52%)	9 (27%)	7 (21%)	0	1
All	All	13260/13576 (98%)	9009 (68%)	2708 (20%)	1543 (12%)	0	5

All (1543) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	9	GLU
1	AB	76	GLN
1	AB	165	VAL
1	AB	194	PRO
2	AC	4	LYS
2	AC	26	LYS
2	AC	49	SER
3	AD	4	TYR
3	AD	5	ILE
3	AD	24	GLU
3	AD	28	SER
3	AD	34	GLU
3	AD	43	HIS
3	AD	62	GLN
3	AD	63	LYS
3	AD	69	GLY
3	AD	113	SER
3	AD	156	GLU
4	AE	36	ASP
4	AE	125	SER
5	AF	69	GLU
5	AF	70	ASP
6	AG	37	ASN
7	AH	22	GLU
7	AH	103	VAL
7	AH	107	LEU
8	AI	58	HIS
9	AJ	88	LEU
9	AJ	92	THR
10	AK	42	TRP
10	AK	109	VAL
10	AK	120	ARG

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Mol	Chain	Res	Type
11	AL	6	THR
11	AL	7	ILE
11	AL	13	LYS
11	AL	39	VAL
11	AL	43	VAL
11	AL	48	PRO
11	AL	55	VAL
11	AL	78	GLN
11	AL	94	PRO
11	AL	102	ARG
11	AL	104	VAL
11	AL	107	ALA
11	AL	115	LYS
11	AL	123	LYS
12	AM	3	ARG
12	AM	6	GLY
12	AM	113	PRO
13	AN	3	ARG
14	AO	19	PRO
15	AP	28	ARG
16	AQ	28	PRO
16	AQ	55	ASP
16	AQ	69	LYS
17	AR	36	ASN
17	AR	37	VAL
17	AR	45	SER
18	AS	37	ARG
18	AS	38	SER
18	AS	53	ASN
18	AS	70	LYS
19	AT	74	LYS
23	AY	22	ASP
23	AY	84	THR
23	AY	87	HIS
23	AY	92	ILE
23	AY	171	GLU
23	AY	224	ASP
23	AY	244	ALA
23	AY	266	ASN
23	AY	330	VAL
23	AY	331	TYR
23	AY	384	ILE

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Mol	Chain	Res	Type
23	AY	395	PRO
23	AY	448	GLN
23	AY	518	PRO
23	AY	527	ASN
23	AY	565	VAL
23	AY	568	TYR
23	AY	628	ARG
23	AY	659	LEU
23	AY	681	LYS
25	BC	17	PRO
25	BC	42	VAL
25	BC	52	PRO
25	BC	66	PRO
25	BC	96	GLY
25	BC	109	MET
25	BC	114	VAL
25	BC	115	VAL
25	BC	139	PRO
25	BC	141	PRO
25	BC	142	LYS
25	BC	162	ILE
25	BC	167	ASP
25	BC	182	PRO
25	BC	210	LEU
25	BC	223	VAL
25	BC	227	PRO
26	BD	24	ILE
26	BD	36	PRO
26	BD	43	ARG
26	BD	79	VAL
26	BD	87	ASN
26	BD	89	SER
26	BD	98	VAL
26	BD	99	ASP
26	BD	118	VAL
26	BD	123	ALA
26	BD	166	GLN
26	BD	226	MET
26	BD	242	ARG
26	BD	273	ARG
27	BE	12	THR
27	BE	14	ILE

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Mol	Chain	Res	Type
27	BE	45	THR
27	BE	54	GLN
27	BE	56	PRO
27	BE	61	ARG
27	BE	66	HIS
27	BE	67	PHE
27	BE	68	ALA
27	BE	72	VAL
27	BE	74	PRO
27	BE	75	VAL
27	BE	126	PRO
27	BE	144	ARG
27	BE	147	PRO
27	BE	162	ALA
28	BF	3	GLU
28	BF	8	GLN
28	BF	10	PRO
28	BF	11	VAL
28	BF	66	PRO
28	BF	67	GLN
28	BF	84	VAL
28	BF	90	PHE
28	BF	134	GLY
28	BF	149	ASP
29	BG	87	PRO
29	BG	96	ARG
30	BH	41	MET
30	BH	84	SER
30	BH	123	PHE
30	BH	124	GLU
30	BH	156	ALA
30	BH	170	ARG
32	BK	5	VAL
32	BK	116	ASN
33	BN	17	ASP
33	BN	18	ALA
33	BN	56	ASN
33	BN	69	GLN
33	BN	111	PRO
33	BN	126	PRO
33	BN	130	HIS
33	BN	133	GLN

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Mol	Chain	Res	Type
34	BO	48	PRO
34	BO	80	ASP
35	BP	9	ASN
35	BP	57	THR
35	BP	110	TYR
35	BP	149	GLU
36	BQ	2	LEU
36	BQ	20	ALA
36	BQ	52	VAL
36	BQ	90	VAL
36	BQ	140	ALA
37	BR	5	LYS
38	BS	13	ARG
38	BS	32	LEU
38	BS	48	LEU
38	BS	53	SER
38	BS	98	VAL
38	BS	100	ALA
38	BS	106	ARG
39	BT	28	VAL
39	BT	30	VAL
39	BT	38	ASN
39	BT	49	VAL
39	BT	68	TYR
39	BT	78	LEU
39	BT	86	ILE
39	BT	90	GLN
40	BU	9	VAL
41	BV	15	GLU
41	BV	46	VAL
41	BV	49	THR
41	BV	50	PRO
41	BV	96	ILE
41	BV	97	LYS
42	BW	15	ARG
42	BW	73	ALA
42	BW	77	ASP
44	BY	32	PRO
44	BY	53	PRO
44	BY	56	PRO
44	BY	66	PRO
44	BY	78	ALA

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Mol	Chain	Res	Type
44	BY	97	ARG
44	BY	102	CYS
45	BZ	71	VAL
45	BZ	72	ARG
45	BZ	73	GLN
45	BZ	81	ARG
47	B2	47	ASN
47	B2	48	HIS
48	B3	51	ALA
49	B5	56	LYS
50	B6	7	ILE
50	B6	9	LEU
50	B6	31	PRO
52	B8	3	LYS
52	B8	30	ARG
52	B8	49	VAL
52	B8	62	LEU
53	B9	10	ILE
53	B9	20	HIS
57	B1	20	ARG
57	B1	87	PRO
1	CB	35	GLU
1	CB	165	VAL
1	CB	194	PRO
1	CB	195	ASP
1	CB	235	SER
2	CC	12	LEU
2	CC	49	SER
2	CC	130	VAL
2	CC	207	VAL
3	CD	4	TYR
3	CD	5	ILE
3	CD	28	SER
3	CD	34	GLU
3	CD	43	HIS
3	CD	113	SER
5	CF	38	GLU
5	CF	70	ASP
6	CG	12	LEU
6	CG	15	ASP
7	CH	22	GLU
10	CK	42	TRP

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Mol	Chain	Res	Type
10	CK	43	SER
10	CK	109	VAL
10	CK	111	ASP
10	CK	120	ARG
11	CL	7	ILE
11	CL	36	VAL
11	CL	37	CYS
11	CL	39	VAL
11	CL	43	VAL
11	CL	78	GLN
11	CL	81	SER
11	CL	94	PRO
11	CL	96	VAL
11	CL	104	VAL
11	CL	108	ALA
11	CL	115	LYS
11	CL	116	SER
11	CL	122	THR
11	CL	123	LYS
12	CM	6	GLY
12	CM	12	ASN
12	CM	107	ALA
12	CM	113	PRO
15	CP	66	PRO
16	CQ	14	LYS
16	CQ	49	GLU
16	CQ	55	ASP
16	CQ	69	LYS
17	CR	36	ASN
18	CS	37	ARG
18	CS	38	SER
18	CS	41	VAL
18	CS	70	LYS
19	CT	46	GLU
23	CY	9	LEU
23	CY	84	THR
23	CY	87	HIS
23	CY	92	ILE
23	CY	111	SER
23	CY	128	TYR
23	CY	129	LYS
23	CY	171	GLU

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Mol	Chain	Res	Type
23	CY	301	ILE
23	CY	330	VAL
23	CY	331	TYR
23	CY	384	ILE
23	CY	395	PRO
23	CY	436	PRO
23	CY	448	GLN
23	CY	498	ILE
23	CY	501	THR
23	CY	555	LEU
23	CY	565	VAL
23	CY	568	TYR
23	CY	614	GLU
23	CY	649	LEU
23	CY	681	LYS
25	DC	17	PRO
25	DC	52	PRO
25	DC	54	ARG
25	DC	66	PRO
25	DC	80	LYS
25	DC	96	GLY
25	DC	109	MET
25	DC	114	VAL
25	DC	139	PRO
25	DC	141	PRO
25	DC	142	LYS
25	DC	162	ILE
25	DC	167	ASP
25	DC	177	GLY
25	DC	182	PRO
25	DC	212	SER
25	DC	223	VAL
25	DC	227	PRO
26	DD	9	TYR
26	DD	24	ILE
26	DD	36	PRO
26	DD	52	ARG
26	DD	79	VAL
26	DD	99	ASP
26	DD	118	VAL
26	DD	123	ALA
26	DD	166	GLN

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Mol	Chain	Res	Type
26	DD	236	GLY
26	DD	246	PRO
26	DD	273	ARG
27	DE	12	THR
27	DE	13	ARG
27	DE	56	PRO
27	DE	60	ASN
27	DE	61	ARG
27	DE	66	HIS
27	DE	68	ALA
27	DE	72	VAL
27	DE	74	PRO
27	DE	75	VAL
27	DE	77	ILE
27	DE	126	PRO
27	DE	143	ASN
27	DE	144	ARG
27	DE	155	LYS
28	DF	3	GLU
28	DF	9	ILE
28	DF	10	PRO
28	DF	52	LYS
28	DF	66	PRO
28	DF	149	ASP
28	DF	153	SER
28	DF	192	LEU
29	DG	43	LEU
29	DG	96	ARG
29	DG	117	PHE
30	DH	40	GLU
30	DH	42	ARG
30	DH	108	GLY
30	DH	170	ARG
30	DH	176	ALA
32	DK	5	VAL
33	DN	17	ASP
33	DN	18	ALA
33	DN	126	PRO
33	DN	133	GLN
34	DO	28	SER
35	DP	13	ASN
35	DP	31	ALA

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Mol	Chain	Res	Type
35	DP	49	ARG
35	DP	50	ARG
35	DP	57	THR
35	DP	65	ARG
35	DP	71	VAL
36	DQ	14	ARG
36	DQ	52	VAL
36	DQ	90	VAL
37	DR	4	LEU
37	DR	8	ARG
38	DS	43	GLU
38	DS	47	THR
38	DS	98	VAL
38	DS	100	ALA
38	DS	101	LEU
38	DS	106	ARG
38	DS	108	GLY
39	DT	28	VAL
39	DT	30	VAL
39	DT	35	LYS
39	DT	36	GLU
39	DT	50	ILE
39	DT	86	ILE
39	DT	91	ARG
40	DU	116	ALA
41	DV	16	PRO
41	DV	29	PRO
41	DV	46	VAL
41	DV	50	PRO
41	DV	96	ILE
42	DW	11	ARG
42	DW	12	ILE
42	DW	73	ALA
42	DW	77	ASP
44	DY	28	LYS
44	DY	32	PRO
44	DY	38	ILE
44	DY	50	ARG
44	DY	56	PRO
44	DY	66	PRO
44	DY	77	PRO
44	DY	78	ALA

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Mol	Chain	Res	Type
44	DY	97	ARG
44	DY	107	ASP
45	DZ	71	VAL
45	DZ	72	ARG
45	DZ	73	GLN
45	DZ	81	ARG
45	DZ	95	PRO
45	DZ	152	ALA
46	D0	56	ASP
48	D3	41	PRO
48	D3	52	HIS
49	D5	56	LYS
50	D6	9	LEU
50	D6	16	CYS
50	D6	33	LYS
51	D7	9	ARG
51	D7	18	PHE
51	D7	45	ALA
52	D8	18	ALA
52	D8	30	ARG
52	D8	49	VAL
52	D8	62	LEU
54	De	65	LYS
57	D1	21	ARG
57	D1	52	ARG
1	AB	15	VAL
1	AB	34	ALA
1	AB	129	GLU
1	AB	186	ALA
1	AB	195	ASP
1	AB	229	VAL
2	AC	44	GLU
2	AC	48	TYR
2	AC	51	GLY
2	AC	60	ALA
2	AC	73	PRO
2	AC	76	VAL
2	AC	130	VAL
2	AC	161	GLU
3	AD	27	TYR
3	AD	44	GLY
3	AD	134	ASP

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Mol	Chain	Res	Type
3	AD	186	LEU
4	AE	6	PHE
4	AE	85	GLY
4	AE	104	ALA
5	AF	85	VAL
6	AG	15	ASP
6	AG	80	VAL
7	AH	27	PRO
7	AH	92	ARG
7	AH	134	ILE
9	AJ	51	ARG
9	AJ	55	LYS
9	AJ	59	SER
10	AK	12	ARG
10	AK	36	ASP
10	AK	43	SER
10	AK	90	GLY
10	AK	91	ARG
11	AL	19	ARG
11	AL	31	PRO
11	AL	34	ARG
11	AL	35	GLY
11	AL	37	CYS
11	AL	50	SER
11	AL	66	VAL
11	AL	80	HIS
11	AL	116	SER
11	AL	121	GLY
11	AL	125	PRO
12	AM	12	ASN
12	AM	101	GLN
16	AQ	12	SER
16	AQ	34	LYS
16	AQ	53	LEU
18	AS	45	VAL
18	AS	66	MET
18	AS	67	VAL
19	AT	71	THR
19	AT	94	ALA
23	AY	20	HIS
23	AY	21	ILE
23	AY	25	LYS

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Mol	Chain	Res	Type
23	AY	39	ILE
23	AY	40	HIS
23	AY	66	THR
23	AY	86	GLY
23	AY	129	LYS
23	AY	205	TYR
23	AY	258	VAL
23	AY	297	GLU
23	AY	436	PRO
23	AY	471	LYS
23	AY	475	ASN
23	AY	476	VAL
23	AY	521	SER
23	AY	555	LEU
23	AY	615	GLU
23	AY	631	ILE
23	AY	658	ASP
23	AY	661	SER
23	AY	668	SER
25	BC	33	LEU
25	BC	43	GLU
25	BC	59	VAL
25	BC	60	ARG
25	BC	71	LYS
25	BC	80	LYS
25	BC	94	TYR
25	BC	113	ALA
25	BC	119	ASP
25	BC	175	PRO
25	BC	177	GLY
25	BC	212	SER
25	BC	214	TYR
25	BC	218	THR
26	BD	23	GLU
26	BD	42	GLY
26	BD	45	ASN
26	BD	53	PHE
26	BD	165	ILE
26	BD	197	GLY
26	BD	222	ARG
26	BD	223	GLY
26	BD	224	ALA

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Mol	Chain	Res	Type
26	BD	232	PRO
26	BD	239	ARG
26	BD	244	ARG
26	BD	246	PRO
27	BE	11	MET
27	BE	13	ARG
27	BE	60	ASN
27	BE	63	LEU
27	BE	119	ARG
27	BE	121	ASN
27	BE	185	LYS
27	BE	186	GLY
28	BF	103	LYS
28	BF	192	LEU
30	BH	13	LYS
30	BH	15	VAL
30	BH	171	LEU
30	BH	173	PRO
30	BH	174	GLY
32	BK	30	HIS
32	BK	78	ILE
32	BK	96	VAL
33	BN	8	GLN
33	BN	64	GLY
33	BN	70	LYS
34	BO	28	SER
34	BO	49	ARG
34	BO	96	THR
35	BP	31	ALA
35	BP	50	ARG
35	BP	54	GLY
35	BP	103	ALA
36	BQ	109	VAL
36	BQ	115	MET
36	BQ	127	ILE
37	BR	6	SER
37	BR	57	ARG
37	BR	93	GLY
38	BS	15	ARG
38	BS	43	GLU
38	BS	47	THR
38	BS	101	LEU

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Mol	Chain	Res	Type
38	BS	104	GLY
38	BS	108	GLY
39	BT	3	ARG
39	BT	36	GLU
39	BT	50	ILE
39	BT	83	ILE
40	BU	88	ILE
40	BU	90	VAL
40	BU	97	ASP
41	BV	29	PRO
41	BV	48	GLY
41	BV	78	LYS
41	BV	80	GLN
42	BW	11	ARG
42	BW	12	ILE
42	BW	61	ASN
42	BW	63	ASP
43	BX	12	VAL
44	BY	38	ILE
44	BY	60	PHE
44	BY	74	PRO
44	BY	80	GLY
45	BZ	78	LYS
45	BZ	142	SER
45	BZ	168	GLU
46	B0	11	ARG
46	B0	49	LYS
46	B0	83	PRO
47	B2	50	ILE
48	B3	52	HIS
49	B5	23	HIS
50	B6	27	LYS
50	B6	33	LYS
50	B6	49	HIS
51	B7	44	PRO
52	B8	19	SER
52	B8	48	PHE
53	B9	2	LYS
53	B9	33	LYS
54	Be	62	VAL
54	Be	100	LYS
57	B1	23	LYS

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Mol	Chain	Res	Type
57	B1	34	THR
57	B1	36	GLY
57	B1	52	ARG
57	B1	53	VAL
57	B1	94	LEU
58	B4	14	ILE
58	B4	33	VAL
1	CB	9	GLU
1	CB	17	PHE
1	CB	20	GLU
1	CB	94	ASN
1	CB	128	GLU
1	CB	230	VAL
2	CC	51	GLY
2	CC	96	GLY
2	CC	161	GLU
3	CD	3	ARG
3	CD	21	LEU
3	CD	27	TYR
3	CD	30	LYS
3	CD	84	LYS
4	CE	85	GLY
6	CG	3	ARG
6	CG	8	GLU
6	CG	80	VAL
7	CH	27	PRO
7	CH	29	SER
7	CH	80	ILE
7	CH	100	ILE
7	CH	134	ILE
8	CI	127	LYS
9	CJ	51	ARG
9	CJ	88	LEU
10	CK	36	ASP
10	CK	41	THR
10	CK	107	SER
10	CK	121	PRO
11	CL	34	ARG
11	CL	35	GLY
11	CL	55	VAL
11	CL	66	VAL
11	CL	69	TYR

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Mol	Chain	Res	Type
11	CL	91	LYS
12	CM	99	ARG
12	CM	118	ALA
13	CN	14	PRO
14	CO	19	PRO
14	CO	44	LYS
16	CQ	12	SER
16	CQ	28	PRO
16	CQ	53	LEU
17	CR	37	VAL
18	CS	29	ARG
18	CS	45	VAL
18	CS	63	THR
18	CS	67	VAL
18	CS	77	THR
18	CS	78	ARG
19	CT	71	THR
23	CY	148	LEU
23	CY	205	TYR
23	CY	206	LEU
23	CY	333	GLY
23	CY	393	ASP
23	CY	401	SER
23	CY	554	PRO
23	CY	631	ILE
23	CY	652	MET
23	CY	668	SER
25	DC	20	VAL
25	DC	42	VAL
25	DC	43	GLU
25	DC	53	ARG
25	DC	55	SER
25	DC	59	VAL
25	DC	60	ARG
25	DC	81	GLY
25	DC	176	VAL
25	DC	210	LEU
25	DC	214	TYR
25	DC	218	THR
25	DC	228	HIS
26	DD	23	GLU
26	DD	43	ARG

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Mol	Chain	Res	Type
26	DD	45	ASN
26	DD	53	PHE
26	DD	89	SER
26	DD	127	VAL
26	DD	158	ALA
26	DD	163	ALA
26	DD	165	ILE
26	DD	197	GLY
26	DD	226	MET
26	DD	232	PRO
26	DD	237	GLU
26	DD	239	ARG
27	DE	14	ILE
27	DE	18	ASP
27	DE	54	GLN
27	DE	67	PHE
27	DE	90	THR
27	DE	119	ARG
27	DE	162	ALA
27	DE	186	GLY
28	DF	5	ALA
28	DF	7	TYR
28	DF	11	VAL
28	DF	16	GLY
28	DF	22	ALA
28	DF	46	ARG
28	DF	48	THR
28	DF	67	GLN
28	DF	69	HIS
28	DF	84	VAL
28	DF	105	VAL
28	DF	134	GLY
28	DF	158	THR
28	DF	172	TRP
28	DF	179	GLU
29	DG	142	PRO
30	DH	13	LYS
30	DH	41	MET
32	DK	51	ALA
33	DN	23	LEU
33	DN	28	THR
33	DN	56	ASN

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Mol	Chain	Res	Type
33	DN	130	HIS
34	DO	5	GLN
34	DO	26	LYS
34	DO	29	ASN
35	DP	25	SER
35	DP	28	GLY
35	DP	54	GLY
35	DP	103	ALA
36	DQ	18	LYS
36	DQ	53	ALA
36	DQ	135	ASP
37	DR	5	LYS
37	DR	12	ARG
37	DR	88	ARG
38	DS	14	VAL
38	DS	15	ARG
38	DS	32	LEU
38	DS	48	LEU
38	DS	93	LYS
38	DS	104	GLY
39	DT	3	ARG
39	DT	29	ARG
39	DT	31	SER
39	DT	49	VAL
39	DT	90	GLN
39	DT	104	ASN
40	DU	86	ALA
40	DU	90	VAL
40	DU	97	ASP
41	DV	8	GLY
41	DV	67	GLY
42	DW	61	ASN
42	DW	75	TYR
44	DY	41	GLY
44	DY	53	PRO
44	DY	60	PHE
44	DY	74	PRO
44	DY	80	GLY
44	DY	88	LYS
44	DY	89	PHE
44	DY	91	GLU
44	DY	101	LYS

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Mol	Chain	Res	Type
44	DY	102	CYS
45	DZ	108	PRO
45	DZ	168	GLU
45	DZ	186	GLU
46	D0	13	GLY
47	D2	48	HIS
48	D3	29	ARG
49	D5	23	HIS
50	D6	7	ILE
50	D6	17	LYS
50	D6	31	PRO
50	D6	37	ARG
52	D8	19	SER
52	D8	64	TYR
53	D9	33	LYS
57	D1	12	PRO
57	D1	22	GLY
57	D1	23	LYS
57	D1	34	THR
57	D1	85	LEU
57	D1	87	PRO
57	D1	94	LEU
58	D4	4	GLY
1	AB	17	PHE
1	AB	20	GLU
1	AB	94	ASN
1	AB	95	GLN
1	AB	100	GLY
1	AB	175	ARG
1	AB	183	PRO
1	AB	235	SER
2	AC	112	SER
2	AC	162	GLN
3	AD	21	LEU
3	AD	88	VAL
3	AD	89	THR
3	AD	197	PRO
4	AE	126	ARG
5	AF	14	LEU
5	AF	96	PRO
6	AG	10	ARG
6	AG	100	ALA

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Mol	Chain	Res	Type
7	AH	90	GLY
7	AH	99	GLU
8	AI	24	GLY
9	AJ	14	LYS
9	AJ	37	PRO
9	AJ	57	LYS
11	AL	18	VAL
11	AL	64	TYR
11	AL	69	TYR
11	AL	96	VAL
12	AM	99	ARG
12	AM	107	ALA
13	AN	58	LYS
18	AS	65	ASN
18	AS	77	THR
18	AS	80	TYR
23	AY	6	GLU
23	AY	91	THR
23	AY	111	SER
23	AY	128	TYR
23	AY	148	LEU
23	AY	203	GLU
23	AY	245	ALA
23	AY	257	PRO
23	AY	320	PRO
23	AY	437	THR
23	AY	498	ILE
23	AY	574	GLU
23	AY	660	ARG
25	BC	11	LEU
25	BC	53	ARG
25	BC	67	HIS
25	BC	81	GLY
25	BC	164	PHE
25	BC	176	VAL
25	BC	179	ALA
25	BC	222	SER
25	BC	228	HIS
26	BD	25	THR
26	BD	119	ALA
26	BD	127	VAL
26	BD	178	PRO

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Mol	Chain	Res	Type
26	BD	247	ALA
26	BD	260	ARG
26	BD	272	ALA
27	BE	39	PRO
27	BE	77	ILE
27	BE	129	HIS
27	BE	130	GLY
28	BF	5	ALA
28	BF	14	PRO
28	BF	48	THR
28	BF	52	LYS
28	BF	72	ARG
28	BF	150	GLY
29	BG	48	GLU
29	BG	84	LYS
30	BH	16	SER
30	BH	126	PRO
30	BH	137	ASP
32	BK	89	HIS
32	BK	122	ALA
33	BN	42	TRP
33	BN	51	PHE
33	BN	58	ASP
34	BO	14	THR
34	BO	23	ARG
35	BP	21	ARG
35	BP	23	PRO
35	BP	29	LYS
35	BP	43	GLY
35	BP	141	ALA
35	BP	145	PRO
36	BQ	54	MET
36	BQ	111	GLU
37	BR	11	ASN
37	BR	58	GLY
37	BR	108	GLY
38	BS	14	VAL
38	BS	24	LEU
38	BS	93	LYS
38	BS	105	ALA
39	BT	29	ARG
39	BT	35	LYS

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Mol	Chain	Res	Type
39	BT	46	GLU
39	BT	80	SER
39	BT	91	ARG
41	BV	16	PRO
41	BV	18	LEU
41	BV	55	ALA
42	BW	14	PRO
42	BW	42	ARG
42	BW	65	LEU
42	BW	75	TYR
42	BW	110	LYS
43	BX	4	ALA
44	BY	67	LEU
44	BY	77	PRO
45	BZ	92	SER
45	BZ	93	ASP
45	BZ	108	PRO
45	BZ	152	ALA
45	BZ	166	SER
46	B0	3	HIS
47	B2	17	SER
48	B3	29	ARG
51	B7	45	ALA
52	B8	64	TYR
54	Be	68	GLY
54	Be	81	ILE
57	B1	12	PRO
57	B1	35	THR
57	B1	40	ARG
1	CB	70	PHE
1	CB	191	ASP
1	CB	229	VAL
2	CC	112	SER
3	CD	24	GLU
3	CD	32	ALA
3	CD	33	MET
3	CD	197	PRO
4	CE	6	PHE
4	CE	126	ARG
5	CF	34	GLY
7	CH	72	PRO
7	CH	74	PRO

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Mol	Chain	Res	Type
10	CK	35	PRO
10	CK	37	GLY
11	CL	6	THR
11	CL	19	ARG
11	CL	77	LEU
11	CL	102	ARG
11	CL	125	PRO
13	CN	27	CYS
14	CO	23	GLY
14	CO	47	LYS
16	CQ	33	GLY
17	CR	21	LYS
17	CR	33	ASP
18	CS	71	LEU
18	CS	72	GLY
19	CT	74	LYS
23	CY	8	ASP
23	CY	20	HIS
23	CY	21	ILE
23	CY	23	ALA
23	CY	158	GLY
23	CY	188	TYR
23	CY	257	PRO
23	CY	258	VAL
23	CY	444	PRO
23	CY	532	GLY
23	CY	533	VAL
23	CY	559	PRO
23	CY	560	VAL
23	CY	566	THR
23	CY	664	GLN
24	CU	3	SER
25	DC	61	GLY
25	DC	115	VAL
25	DC	116	ALA
25	DC	119	ASP
25	DC	222	SER
26	DD	28	GLU
26	DD	39	LYS
26	DD	48	ARG
26	DD	51	VAL
26	DD	59	LYS

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Mol	Chain	Res	Type
26	DD	87	ASN
26	DD	98	VAL
26	DD	100	GLY
26	DD	109	ASP
26	DD	260	ARG
27	DE	11	MET
27	DE	160	TYR
28	DF	14	PRO
28	DF	178	PRO
29	DG	50	ALA
29	DG	87	PRO
30	DH	47	GLU
30	DH	61	HIS
30	DH	155	SER
30	DH	160	LYS
30	DH	164	TYR
30	DH	165	ALA
30	DH	173	PRO
32	DK	63	ARG
33	DN	128	HIS
34	DO	23	ARG
34	DO	119	PRO
35	DP	9	ASN
35	DP	76	LYS
35	DP	110	TYR
35	DP	149	GLU
36	DQ	20	ALA
36	DQ	80	GLU
37	DR	6	SER
37	DR	83	ILE
38	DS	13	ARG
38	DS	24	LEU
39	DT	68	TYR
39	DT	70	VAL
39	DT	80	SER
39	DT	107	ASP
40	DU	35	ALA
41	DV	48	GLY
41	DV	53	GLU
41	DV	80	GLN
41	DV	81	TYR
41	DV	97	LYS

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Mol	Chain	Res	Type
42	DW	15	ARG
42	DW	63	ASP
42	DW	65	LEU
43	DX	4	ALA
44	DY	29	GLU
44	DY	48	ALA
44	DY	70	SER
45	DZ	21	ALA
45	DZ	146	ILE
45	DZ	151	HIS
46	D0	3	HIS
46	D0	11	ARG
46	D0	33	ALA
46	D0	41	ARG
46	D0	49	LYS
47	D2	50	ILE
50	D6	20	ASN
50	D6	44	ARG
51	D7	42	LEU
52	D8	48	PHE
54	De	62	VAL
54	De	81	ILE
57	D1	20	ARG
57	D1	40	ARG
57	D1	65	SER
58	D4	2	LYS
1	AB	54	THR
1	AB	157	ARG
1	AB	184	VAL
1	AB	215	LEU
1	AB	237	ALA
2	AC	85	ARG
2	AC	96	GLY
3	AD	30	LYS
3	AD	33	MET
5	AF	34	GLY
6	AG	12	LEU
6	AG	33	ASP
7	AH	2	LEU
7	AH	100	ILE
8	AI	12	GLU
8	AI	119	ALA

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Mol	Chain	Res	Type
10	AK	15	ALA
10	AK	35	PRO
11	AL	127	GLU
12	AM	10	PRO
12	AM	21	TYR
12	AM	117	VAL
13	AN	13	THR
13	AN	27	CYS
14	AO	20	GLY
14	AO	24	SER
14	AO	47	LYS
16	AQ	33	GLY
16	AQ	71	PHE
17	AR	55	ARG
18	AS	40	ILE
23	AY	304	ASP
23	AY	341	VAL
23	AY	381	LYS
23	AY	531	GLY
23	AY	567	LEU
23	AY	600	VAL
25	BC	69	LEU
25	BC	76	LEU
26	BD	69	ARG
26	BD	100	GLY
26	BD	158	ALA
26	BD	207	GLY
26	BD	219	PRO
27	BE	17	ASP
27	BE	51	PHE
27	BE	90	THR
27	BE	123	ALA
27	BE	155	LYS
28	BF	7	TYR
28	BF	73	ALA
28	BF	133	ASN
28	BF	172	TRP
28	BF	178	PRO
28	BF	206	ILE
29	BG	82	LEU
29	BG	85	GLY
30	BH	118	PRO

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Mol	Chain	Res	Type
30	BH	138	LYS
30	BH	160	LYS
32	BK	61	ALA
32	BK	90	LYS
32	BK	102	GLU
32	BK	113	PRO
33	BN	3	THR
33	BN	47	ALA
33	BN	88	GLU
34	BO	34	THR
34	BO	72	PRO
35	BP	20	GLY
35	BP	106	LEU
36	BQ	139	GLU
37	BR	28	LEU
38	BS	20	ARG
38	BS	67	ARG
38	BS	85	VAL
39	BT	27	THR
39	BT	31	SER
39	BT	107	ASP
39	BT	128	GLU
40	BU	22	LYS
43	BX	24	GLY
44	BY	26	LYS
44	BY	29	GLU
44	BY	39	VAL
44	BY	70	SER
44	BY	103	GLY
45	BZ	22	GLY
45	BZ	32	HIS
45	BZ	51	ALA
45	BZ	95	PRO
45	BZ	179	ASP
46	B0	17	GLN
46	B0	33	ALA
48	B3	28	LEU
51	B7	42	LEU
52	B8	53	PRO
54	Be	53	PRO
54	Be	65	LYS
58	B4	4	GLY

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Mol	Chain	Res	Type
58	B4	7	PRO
1	CB	34	ALA
1	CB	51	LEU
1	CB	76	GLN
1	CB	100	GLY
1	CB	104	ASN
1	CB	153	ARG
2	CC	20	SER
2	CC	60	ALA
3	CD	47	ARG
3	CD	186	LEU
4	CE	125	SER
5	CF	14	LEU
5	CF	69	GLU
6	CG	10	ARG
7	CH	2	LEU
7	CH	97	VAL
8	CI	24	GLY
8	CI	104	ARG
9	CJ	41	PRO
10	CK	14	VAL
11	CL	79	GLU
13	CN	13	THR
14	CO	15	PHE
17	CR	53	ARG
17	CR	60	ALA
18	CS	80	TYR
19	CT	47	GLY
23	CY	6	GLU
23	CY	39	ILE
23	CY	40	HIS
23	CY	244	ALA
23	CY	288	PRO
23	CY	320	PRO
23	CY	447	GLY
23	CY	615	GLU
25	DC	67	HIS
25	DC	175	PRO
25	DC	215	VAL
26	DD	241	PRO
26	DD	245	PRO
26	DD	272	ALA

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Mol	Chain	Res	Type
27	DE	63	LEU
27	DE	86	PRO
27	DE	121	ASN
27	DE	123	ALA
27	DE	147	PRO
27	DE	193	GLY
28	DF	58	ALA
30	DH	124	GLU
30	DH	137	ASP
30	DH	171	LEU
32	DK	13	PRO
32	DK	122	ALA
33	DN	42	TRP
34	DO	14	THR
35	DP	17	LYS
35	DP	29	LYS
37	DR	107	ASP
38	DS	66	ALA
38	DS	94	TYR
38	DS	105	ALA
39	DT	2	ASN
39	DT	34	VAL
40	DU	32	PHE
40	DU	92	ARG
42	DW	14	PRO
43	DX	12	VAL
44	DY	5	MET
44	DY	75	ILE
44	DY	81	LYS
44	DY	106	LEU
45	DZ	32	HIS
45	DZ	78	LYS
46	D0	17	GLN
46	D0	83	PRO
47	D2	17	SER
50	D6	18	ARG
57	D1	10	LYS
57	D1	53	VAL
58	D4	33	VAL
1	AB	67	THR
1	AB	103	THR
2	AC	75	VAL

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Mol	Chain	Res	Type
3	AD	84	LYS
3	AD	204	ILE
4	AE	100	VAL
4	AE	106	PRO
5	AF	38	GLU
8	AI	101	PHE
9	AJ	32	ALA
10	AK	111	ASP
11	AL	79	GLU
13	AN	15	LYS
14	AO	18	PHE
17	AR	33	ASP
17	AR	87	ARG
23	AY	206	LEU
23	AY	225	GLU
23	AY	347	GLY
23	AY	532	GLY
23	AY	533	VAL
23	AY	688	ILE
25	BC	24	ASP
26	BD	3	VAL
26	BD	9	TYR
26	BD	26	LYS
26	BD	28	GLU
26	BD	76	PRO
26	BD	137	PRO
26	BD	147	LEU
26	BD	200	ASP
26	BD	225	ALA
27	BE	94	GLU
28	BF	46	ARG
28	BF	155	LEU
29	BG	17	PRO
29	BG	24	GLY
29	BG	106	LEU
30	BH	59	ARG
30	BH	107	VAL
30	BH	165	ALA
34	BO	119	PRO
35	BP	60	MET
36	BQ	53	ALA
39	BT	2	ASN

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Mol	Chain	Res	Type
39	BT	34	VAL
39	BT	136	GLN
42	BW	31	GLU
42	BW	80	PRO
42	BW	89	ALA
44	BY	76	CYS
44	BY	81	LYS
44	BY	88	LYS
44	BY	100	ALA
44	BY	101	LYS
46	B0	47	PRO
51	B7	23	ARG
52	B8	60	LEU
53	B9	3	VAL
1	CB	101	MET
1	CB	129	GLU
3	CD	62	GLN
3	CD	135	LEU
4	CE	39	GLY
4	CE	100	VAL
5	CF	13	ASN
5	CF	96	PRO
8	CI	35	GLU
9	CJ	90	LEU
11	CL	47	LYS
11	CL	48	PRO
11	CL	56	ALA
11	CL	67	THR
16	CQ	61	GLU
17	CR	34	TYR
19	CT	99	LEU
23	CY	360	ALA
25	DC	3	LYS
26	DD	3	VAL
26	DD	41	GLY
26	DD	178	PRO
27	DE	17	ASP
27	DE	51	PHE
27	DE	187	ALA
28	DF	45	ARG
28	DF	78	ILE
28	DF	132	VAL

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Mol	Chain	Res	Type
28	DF	133	ASN
28	DF	155	LEU
30	DH	62	LYS
33	DN	111	PRO
34	DO	34	THR
35	DP	23	PRO
35	DP	106	LEU
35	DP	141	ALA
35	DP	145	PRO
36	DQ	85	LYS
36	DQ	115	MET
37	DR	91	GLN
38	DS	85	VAL
39	DT	56	GLY
39	DT	85	LYS
41	DV	24	LYS
41	DV	40	LEU
42	DW	46	PHE
43	DX	13	LEU
43	DX	24	GLY
44	DY	18	GLY
45	DZ	92	SER
45	DZ	166	SER
48	D3	28	LEU
49	D5	28	PRO
50	D6	49	HIS
51	D7	39	ARG
52	D8	53	PRO
53	D9	3	VAL
54	De	68	GLY
57	D1	35	THR
57	D1	64	ALA
58	D4	5	ILE
1	AB	230	VAL
2	AC	13	GLY
3	AD	7	PRO
3	AD	47	ARG
4	AE	65	ASN
7	AH	72	PRO
11	AL	93	LEU
14	AO	5	LYS
23	AY	360	ALA

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Mol	Chain	Res	Type
23	AY	361	ASN
25	BC	37	LYS
25	BC	104	ILE
26	BD	121	PRO
26	BD	243	GLY
26	BD	250	TRP
28	BF	9	ILE
32	BK	51	ALA
33	BN	119	ARG
33	BN	127	ASP
33	BN	128	HIS
35	BP	48	PRO
35	BP	107	LYS
36	BQ	24	GLY
41	BV	19	LYS
44	BY	51	VAL
49	B5	54	GLY
54	Be	60	PHE
57	B1	37	ILE
1	CB	13	ALA
1	CB	26	PRO
2	CC	129	ALA
2	CC	181	ASN
3	CD	40	PRO
9	CJ	37	PRO
11	CL	88	GLY
11	CL	95	GLY
15	CP	43	LYS
16	CQ	31	LEU
23	CY	519	ARG
23	CY	574	GLU
23	CY	598	ASP
23	CY	628	ARG
25	DC	169	THR
26	DD	180	GLY
27	DE	53	PRO
28	DF	150	GLY
28	DF	159	GLY
29	DG	27	ASN
30	DH	15	VAL
30	DH	48	GLY
33	DN	46	VAL

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Mol	Chain	Res	Type
35	DP	20	GLY
35	DP	26	GLY
37	DR	103	ARG
39	DT	83	ILE
40	DU	9	VAL
44	DY	76	CYS
46	D0	74	ARG
57	D1	24	ALA
2	AC	109	PRO
2	AC	174	PRO
3	AD	23	GLY
4	AE	74	GLY
5	AF	37	VAL
7	AH	97	VAL
10	AK	113	PRO
14	AO	23	GLY
16	AQ	30	PRO
18	AS	46	GLY
23	AY	116	PRO
23	AY	638	GLY
23	AY	680	PRO
33	BN	46	VAL
35	BP	71	VAL
41	BV	67	GLY
41	BV	79	VAL
45	BZ	53	ILE
52	B8	45	GLY
4	CE	67	VAL
7	CH	103	VAL
12	CM	85	GLY
15	CP	33	ILE
15	CP	63	GLY
23	CY	202	PRO
23	CY	638	GLY
25	DC	136	GLY
25	DC	221	PRO
26	DD	238	GLY
28	DF	91	GLY
29	DG	85	GLY
35	DP	104	GLY
37	DR	32	GLY
43	DX	7	VAL

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Mol	Chain	Res	Type
44	DY	39	VAL
45	DZ	53	ILE
48	D3	16	PRO
48	D3	27	GLY
54	De	63	ILE
10	AK	14	VAL
23	AY	65	ILE
23	AY	301	ILE
36	BQ	27	VAL
39	BT	70	VAL
5	CF	85	VAL
10	CK	90	GLY
23	CY	341	VAL
26	DD	110	GLY
27	DE	30	PRO
30	DH	154	PRO
36	DQ	127	ILE
37	DR	117	VAL
40	DU	88	ILE
49	D5	7	PRO
51	D7	38	GLY
1	AB	164	VAL
1	AB	174	VAL
5	AF	51	PRO
13	AN	14	PRO
18	AS	59	PRO
25	BC	215	VAL
28	BF	92	PRO
28	BF	105	VAL
33	BN	129	PRO
36	BQ	62	GLY
36	BQ	81	VAL
41	BV	51	VAL
50	B6	48	VAL
2	CC	13	GLY
3	CD	44	GLY
5	CF	72	VAL
6	CG	14	PRO
18	CS	46	GLY
23	CY	69	VAL
23	CY	557	GLY
25	DC	181	PHE

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Mol	Chain	Res	Type
26	DD	235	GLY
29	DG	68	PRO
33	DN	14	VAL
36	DQ	27	VAL
38	DS	81	GLY
44	DY	49	VAL
53	D9	30	PRO
58	D4	10	VAL
58	D4	29	PRO
10	AK	48	ILE
11	AL	95	GLY
13	AN	18	VAL
16	AQ	64	PRO
17	AR	39	VAL
19	AT	47	GLY
25	BC	20	VAL
26	BD	238	GLY
27	BE	175	VAL
28	BF	61	GLY
54	Be	63	ILE
58	B4	10	VAL
13	CN	18	VAL
19	CT	98	PRO
26	DD	137	PRO
32	DK	90	LYS
44	DY	82	PRO
44	DY	98	VAL
45	DZ	39	VAL
45	DZ	165	VAL
54	De	53	PRO
58	D4	15	ILE
25	BC	65	LEU
25	BC	75	VAL
25	BC	181	PHE
40	BU	102	GLU
43	BX	49	VAL
23	CY	531	GLY
23	CY	600	VAL
36	DQ	109	VAL
35	DP	48	PRO
32	DK	22	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%)	164 (81%)	39 (19%)	1	7
1	CB	203/203 (100%)	167 (82%)	36 (18%)	2	10
2	AC	161/161 (100%)	132 (82%)	29 (18%)	1	9
2	CC	161/161 (100%)	136 (84%)	25 (16%)	2	16
3	AD	180/180 (100%)	145 (81%)	35 (19%)	1	7
3	CD	180/180 (100%)	150 (83%)	30 (17%)	2	12
4	AE	116/116 (100%)	93 (80%)	23 (20%)	1	7
4	CE	116/116 (100%)	98 (84%)	18 (16%)	2	16
5	AF	90/90 (100%)	78 (87%)	12 (13%)	4	21
5	CF	90/90 (100%)	82 (91%)	8 (9%)	9	37
6	AG	126/126 (100%)	113 (90%)	13 (10%)	7	32
6	CG	126/126 (100%)	115 (91%)	11 (9%)	10	38
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	10
7	CH	119/119 (100%)	105 (88%)	14 (12%)	5	25
8	AI	98/98 (100%)	82 (84%)	16 (16%)	2	13
8	CI	98/98 (100%)	84 (86%)	14 (14%)	3	19
9	AJ	89/89 (100%)	75 (84%)	14 (16%)	2	15
9	CJ	89/89 (100%)	72 (81%)	17 (19%)	1	8
10	AK	90/90 (100%)	71 (79%)	19 (21%)	1	5
10	CK	90/90 (100%)	73 (81%)	17 (19%)	1	8
11	AL	104/104 (100%)	77 (74%)	27 (26%)	0	3
11	CL	104/104 (100%)	72 (69%)	32 (31%)	0	2
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	12
12	CM	100/100 (100%)	89 (89%)	11 (11%)	6	29
13	AN	49/49 (100%)	43 (88%)	6 (12%)	5	23
13	CN	49/49 (100%)	43 (88%)	6 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	71 (90%)	8 (10%)	7	32
14	CO	79/79 (100%)	65 (82%)	14 (18%)	2	10
15	AP	72/72 (100%)	66 (92%)	6 (8%)	11	40
15	CP	72/72 (100%)	62 (86%)	10 (14%)	3	20
16	AQ	95/95 (100%)	81 (85%)	14 (15%)	3	18
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	12
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	13
17	CR	61/61 (100%)	53 (87%)	8 (13%)	4	21
18	AS	69/69 (100%)	55 (80%)	14 (20%)	1	6
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	5
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	15
19	CT	76/76 (100%)	67 (88%)	9 (12%)	5	25
23	AY	563/579 (97%)	470 (84%)	93 (16%)	2	13
23	CY	563/579 (97%)	463 (82%)	100 (18%)	2	10
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	140 (78%)	40 (22%)	1	5
25	DC	180/180 (100%)	138 (77%)	42 (23%)	1	4
26	BD	217/217 (100%)	169 (78%)	48 (22%)	1	5
26	DD	217/217 (100%)	164 (76%)	53 (24%)	0	4
27	BE	165/165 (100%)	134 (81%)	31 (19%)	1	8
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	4
28	BF	165/165 (100%)	133 (81%)	32 (19%)	1	7
28	DF	165/165 (100%)	135 (82%)	30 (18%)	1	9
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	14
29	DG	155/155 (100%)	127 (82%)	28 (18%)	1	9
30	BH	136/136 (100%)	116 (85%)	20 (15%)	3	18
30	DH	136/136 (100%)	125 (92%)	11 (8%)	11	41
32	BK	105/105 (100%)	90 (86%)	15 (14%)	3	19
32	DK	105/105 (100%)	89 (85%)	16 (15%)	3	17
33	BN	117/117 (100%)	95 (81%)	22 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DN	117/117 (100%)	94 (80%)	23 (20%)	1	7
34	BO	100/100 (100%)	80 (80%)	20 (20%)	1	7
34	DO	100/100 (100%)	81 (81%)	19 (19%)	1	8
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	4
35	DP	112/112 (100%)	94 (84%)	18 (16%)	2	14
36	BQ	111/111 (100%)	82 (74%)	29 (26%)	0	3
36	DQ	111/111 (100%)	86 (78%)	25 (22%)	1	4
37	BR	100/100 (100%)	87 (87%)	13 (13%)	4	21
37	DR	100/100 (100%)	82 (82%)	18 (18%)	1	9
38	BS	77/77 (100%)	62 (80%)	15 (20%)	1	7
38	DS	77/77 (100%)	58 (75%)	19 (25%)	0	4
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	5
39	DT	120/120 (100%)	92 (77%)	28 (23%)	1	4
40	BU	93/93 (100%)	72 (77%)	21 (23%)	1	4
40	DU	93/93 (100%)	73 (78%)	20 (22%)	1	5
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	3
41	DV	82/82 (100%)	59 (72%)	23 (28%)	0	3
42	BW	92/92 (100%)	68 (74%)	24 (26%)	0	3
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	5
43	BX	75/75 (100%)	64 (85%)	11 (15%)	3	18
43	DX	75/75 (100%)	60 (80%)	15 (20%)	1	7
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	5
44	DY	88/88 (100%)	72 (82%)	16 (18%)	1	9
45	BZ	162/162 (100%)	133 (82%)	29 (18%)	2	9
45	DZ	162/162 (100%)	134 (83%)	28 (17%)	2	11
46	B0	66/66 (100%)	54 (82%)	12 (18%)	1	9
46	D0	66/66 (100%)	51 (77%)	15 (23%)	1	4
47	B2	66/66 (100%)	62 (94%)	4 (6%)	18	51
47	D2	66/66 (100%)	60 (91%)	6 (9%)	9	36
48	B3	52/52 (100%)	45 (86%)	7 (14%)	4	21
48	D3	52/52 (100%)	45 (86%)	7 (14%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B5	51/51 (100%)	44 (86%)	7 (14%)	3	20
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	7
50	B6	49/49 (100%)	38 (78%)	11 (22%)	1	4
50	D6	49/49 (100%)	37 (76%)	12 (24%)	0	4
51	B7	42/42 (100%)	35 (83%)	7 (17%)	2	12
51	D7	42/42 (100%)	38 (90%)	4 (10%)	8	34
52	B8	54/54 (100%)	39 (72%)	15 (28%)	0	3
52	D8	54/54 (100%)	37 (68%)	17 (32%)	0	2
53	B9	34/34 (100%)	28 (82%)	6 (18%)	2	10
53	D9	34/34 (100%)	32 (94%)	2 (6%)	19	53
54	Be	54/54 (100%)	47 (87%)	7 (13%)	4	21
54	De	54/54 (100%)	46 (85%)	8 (15%)	3	17
57	B1	78/78 (100%)	59 (76%)	19 (24%)	0	4
57	D1	78/78 (100%)	58 (74%)	20 (26%)	0	3
58	B4	31/31 (100%)	23 (74%)	8 (26%)	0	3
58	D4	31/31 (100%)	26 (84%)	5 (16%)	2	14
All	All	11142/11174 (100%)	9117 (82%)	2025 (18%)	1	9

All (2025) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	7	VAL
1	AB	9	GLU
1	AB	12	GLU
1	AB	15	VAL
1	AB	17	PHE
1	AB	36	ARG
1	AB	40	HIS
1	AB	42	ILE
1	AB	49	GLU
1	AB	69	LEU
1	AB	70	PHE
1	AB	74	LYS
1	AB	96	ARG
1	AB	103	THR
1	AB	115	LEU

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Mol	Chain	Res	Type
1	AB	128	GLU
1	AB	134	GLU
1	AB	137	ARG
1	AB	140	HIS
1	AB	141	GLU
1	AB	142	LEU
1	AB	145	LEU
1	AB	157	ARG
1	AB	160	ASP
1	AB	162	ILE
1	AB	163	PHE
1	AB	168	THR
1	AB	172	ILE
1	AB	175	ARG
1	AB	185	ILE
1	AB	187	LEU
1	AB	190	THR
1	AB	191	ASP
1	AB	198	ASP
1	AB	212	GLN
1	AB	213	LEU
1	AB	226	ARG
1	AB	230	VAL
1	AB	239	VAL
2	AC	4	LYS
2	AC	5	ILE
2	AC	6	HIS
2	AC	10	PHE
2	AC	15	THR
2	AC	22	TRP
2	AC	32	LEU
2	AC	38	ARG
2	AC	57	ILE
2	AC	67	THR
2	AC	76	VAL
2	AC	83	ARG
2	AC	84	ILE
2	AC	101	LEU
2	AC	110	ASN
2	AC	124	ILE
2	AC	125	GLU
2	AC	128	PHE

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Mol	Chain	Res	Type
2	AC	132	ARG
2	AC	134	ILE
2	AC	136	GLN
2	AC	153	VAL
2	AC	167	TRP
2	AC	175	LEU
2	AC	176	HIS
2	AC	184	TYR
2	AC	196	LEU
2	AC	204	LEU
2	AC	208	ILE
3	AD	3	ARG
3	AD	5	ILE
3	AD	10	ARG
3	AD	19	LEU
3	AD	30	LYS
3	AD	53	ASP
3	AD	54	TYR
3	AD	57	ARG
3	AD	61	LYS
3	AD	66	ARG
3	AD	72	GLU
3	AD	80	GLU
3	AD	86	LYS
3	AD	89	THR
3	AD	96	LEU
3	AD	102	ASP
3	AD	107	ARG
3	AD	127	THR
3	AD	131	ARG
3	AD	132	ARG
3	AD	134	ASP
3	AD	138	TYR
3	AD	140	VAL
3	AD	141	ARG
3	AD	150	GLU
3	AD	156	GLU
3	AD	170	VAL
3	AD	177	ASP
3	AD	178	VAL
3	AD	181	MET
3	AD	187	ARG

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Mol	Chain	Res	Type
3	AD	191	ARG
3	AD	193	ASP
3	AD	196	LEU
3	AD	200	GLU
4	AE	11	ILE
4	AE	12	LEU
4	AE	26	PHE
4	AE	31	LEU
4	AE	34	VAL
4	AE	36	ASP
4	AE	41	VAL
4	AE	47	LYS
4	AE	51	VAL
4	AE	63	ARG
4	AE	64	ARG
4	AE	72	GLN
4	AE	75	THR
4	AE	78	HIS
4	AE	80	ILE
4	AE	91	LEU
4	AE	98	THR
4	AE	100	VAL
4	AE	107	ARG
4	AE	119	LEU
4	AE	125	SER
4	AE	139	LEU
4	AE	145	LYS
5	AF	2	ARG
5	AF	13	ASN
5	AF	16	GLN
5	AF	31	GLU
5	AF	33	TYR
5	AF	61	LEU
5	AF	63	TYR
5	AF	64	GLN
5	AF	67	MET
5	AF	80	ARG
5	AF	89	MET
5	AF	98	LEU
6	AG	5	ARG
6	AG	11	GLN
6	AG	13	GLN

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Mol	Chain	Res	Type
6	AG	24	THR
6	AG	32	ARG
6	AG	56	GLN
6	AG	68	ASN
6	AG	79	ARG
6	AG	80	VAL
6	AG	94	ARG
6	AG	97	GLN
6	AG	122	HIS
6	AG	149	ARG
7	AH	21	LYS
7	AH	31	PHE
7	AH	37	ARG
7	AH	44	PHE
7	AH	48	TYR
7	AH	51	VAL
7	AH	59	LEU
7	AH	62	TYR
7	AH	63	LEU
7	AH	69	ARG
7	AH	73	ASP
7	AH	82	HIS
7	AH	92	ARG
7	AH	95	VAL
7	AH	102	ARG
7	AH	103	VAL
7	AH	107	LEU
7	AH	111	ILE
7	AH	112	LEU
7	AH	120	THR
7	AH	138	TRP
8	AI	25	LYS
8	AI	28	VAL
8	AI	40	LEU
8	AI	66	ARG
8	AI	79	LEU
8	AI	85	LEU
8	AI	88	TYR
8	AI	95	LYS
8	AI	97	LYS
8	AI	99	LEU
8	AI	102	LEU

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Mol	Chain	Res	Type
8	AI	104	ARG
8	AI	111	ARG
8	AI	113	LYS
8	AI	121	ARG
8	AI	128	ARG
9	AJ	6	ILE
9	AJ	15	THR
9	AJ	16	LEU
9	AJ	38	ILE
9	AJ	43	ARG
9	AJ	55	LYS
9	AJ	70	ARG
9	AJ	73	ASP
9	AJ	75	ILE
9	AJ	78	ASN
9	AJ	79	ARG
9	AJ	83	GLU
9	AJ	96	ILE
9	AJ	101	VAL
10	AK	25	TYR
10	AK	29	ILE
10	AK	31	THR
10	AK	34	ASP
10	AK	40	ILE
10	AK	41	THR
10	AK	48	ILE
10	AK	57	THR
10	AK	73	MET
10	AK	77	MET
10	AK	80	VAL
10	AK	81	ASP
10	AK	84	VAL
10	AK	98	LEU
10	AK	110	ASP
10	AK	116	HIS
10	AK	117	ASN
10	AK	120	ARG
10	AK	124	LYS
11	AL	18	VAL
11	AL	20	LYS
11	AL	24	VAL
11	AL	33	ARG

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Mol	Chain	Res	Type
11	AL	38	THR
11	AL	42	THR
11	AL	43	VAL
11	AL	44	THR
11	AL	53	ARG
11	AL	54	LYS
11	AL	55	VAL
11	AL	59	ARG
11	AL	61	THR
11	AL	67	THR
11	AL	70	ILE
11	AL	75	HIS
11	AL	76	ASN
11	AL	79	GLU
11	AL	85	ILE
11	AL	90	VAL
11	AL	92	ASP
11	AL	96	VAL
11	AL	102	ARG
11	AL	105	TYR
11	AL	116	SER
11	AL	120	TYR
11	AL	127	GLU
12	AM	8	GLU
12	AM	16	ASP
12	AM	21	TYR
12	AM	27	LYS
12	AM	56	LEU
12	AM	61	GLU
12	AM	67	GLU
12	AM	71	ARG
12	AM	73	GLU
12	AM	82	MET
12	AM	83	ASP
12	AM	108	ARG
12	AM	110	ARG
12	AM	115	LYS
12	AM	120	LYS
12	AM	121	LYS
12	AM	125	ARG
13	AN	7	ILE
13	AN	21	TYR

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Mol	Chain	Res	Type
13	AN	35	ARG
13	AN	40	CYS
13	AN	41	ARG
13	AN	61	TRP
14	AO	5	LYS
14	AO	10	LYS
14	AO	31	LEU
14	AO	38	ARG
14	AO	41	GLU
14	AO	82	ILE
14	AO	85	LEU
14	AO	88	ARG
15	AP	28	ARG
15	AP	29	ASP
15	AP	57	ARG
15	AP	67	THR
15	AP	69	THR
15	AP	71	ARG
16	AQ	5	VAL
16	AQ	6	LEU
16	AQ	7	THR
16	AQ	16	GLN
16	AQ	24	GLU
16	AQ	32	TYR
16	AQ	48	GLU
16	AQ	52	LYS
16	AQ	59	ILE
16	AQ	63	ARG
16	AQ	66	SER
16	AQ	69	LYS
16	AQ	74	LEU
16	AQ	93	GLN
17	AR	19	LYS
17	AR	29	PHE
17	AR	32	ARG
17	AR	37	VAL
17	AR	43	PHE
17	AR	47	THR
17	AR	53	ARG
17	AR	54	ARG
17	AR	69	THR
17	AR	83	GLU

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Mol	Chain	Res	Type
18	AS	5	LEU
18	AS	6	LYS
18	AS	7	LYS
18	AS	23	ASN
18	AS	25	LYS
18	AS	28	LYS
18	AS	32	LYS
18	AS	47	HIS
18	AS	51	VAL
18	AS	58	VAL
18	AS	61	TYR
18	AS	62	ILE
18	AS	79	THR
18	AS	81	ARG
19	AT	13	LEU
19	AT	25	ARG
19	AT	35	THR
19	AT	36	LEU
19	AT	50	GLU
19	AT	54	LYS
19	AT	56	MET
19	AT	57	ARG
19	AT	71	THR
19	AT	73	HIS
19	AT	74	LYS
19	AT	80	ARG
23	AY	20	HIS
23	AY	29	THR
23	AY	30	GLU
23	AY	35	TYR
23	AY	36	THR
23	AY	72	CYS
23	AY	73	PHE
23	AY	87	HIS
23	AY	92	ILE
23	AY	93	GLU
23	AY	112	GLN
23	AY	119	GLU
23	AY	121	VAL
23	AY	126	GLU
23	AY	132	ARG
23	AY	133	ILE

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Mol	Chain	Res	Type
23	AY	137	ASN
23	AY	139	MET
23	AY	140	ASP
23	AY	146	LEU
23	AY	157	LEU
23	AY	165	GLN
23	AY	170	ARG
23	AY	174	PHE
23	AY	178	ILE
23	AY	186	TYR
23	AY	188	TYR
23	AY	191	ASP
23	AY	197	ARG
23	AY	199	ILE
23	AY	210	ARG
23	AY	227	ILE
23	AY	229	LEU
23	AY	240	GLU
23	AY	252	ASP
23	AY	255	ILE
23	AY	260	LEU
23	AY	264	LEU
23	AY	266	ASN
23	AY	271	LEU
23	AY	273	LEU
23	AY	282	SER
23	AY	299	VAL
23	AY	302	HIS
23	AY	312	LEU
23	AY	314	PHE
23	AY	319	ASP
23	AY	321	TYR
23	AY	328	ILE
23	AY	340	TYR
23	AY	341	VAL
23	AY	342	TYR
23	AY	344	THR
23	AY	352	VAL
23	AY	358	MET
23	AY	364	GLU
23	AY	368	GLU
23	AY	393	ASP

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Mol	Chain	Res	Type
23	AY	404	VAL
23	AY	406	GLU
23	AY	428	LEU
23	AY	440	VAL
23	AY	454	MET
23	AY	456	GLU
23	AY	460	GLU
23	AY	464	ASP
23	AY	468	ARG
23	AY	475	ASN
23	AY	487	ILE
23	AY	488	THR
23	AY	498	ILE
23	AY	499	ARG
23	AY	504	ARG
23	AY	506	GLN
23	AY	507	TYR
23	AY	512	ILE
23	AY	517	LEU
23	AY	525	PHE
23	AY	526	VAL
23	AY	529	ILE
23	AY	556	ILE
23	AY	563	ILE
23	AY	572	TYR
23	AY	574	GLU
23	AY	580	MET
23	AY	603	GLU
23	AY	610	VAL
23	AY	614	GLU
23	AY	617	MET
23	AY	641	GLN
23	AY	647	VAL
23	AY	666	ARG
23	AY	676	TYR
25	BC	7	ARG
25	BC	15	VAL
25	BC	19	LYS
25	BC	28	ARG
25	BC	31	LYS
25	BC	32	GLU
25	BC	41	THR

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Mol	Chain	Res	Type
25	BC	42	VAL
25	BC	47	LYS
25	BC	48	LEU
25	BC	50	ILE
25	BC	53	ARG
25	BC	59	VAL
25	BC	60	ARG
25	BC	62	THR
25	BC	63	VAL
25	BC	64	SER
25	BC	73	VAL
25	BC	74	ARG
25	BC	82	GLU
25	BC	94	TYR
25	BC	106	ASP
25	BC	112	ASP
25	BC	115	VAL
25	BC	119	ASP
25	BC	130	ARG
25	BC	131	ILE
25	BC	145	THR
25	BC	148	PHE
25	BC	150	ILE
25	BC	161	ARG
25	BC	164	PHE
25	BC	166	ASN
25	BC	169	THR
25	BC	172	ILE
25	BC	176	VAL
25	BC	185	LYS
25	BC	198	GLU
25	BC	215	VAL
25	BC	224	ARG
26	BD	4	LYS
26	BD	5	LYS
26	BD	9	TYR
26	BD	10	THR
26	BD	12	SER
26	BD	20	ASP
26	BD	23	GLU
26	BD	25	THR
26	BD	26	LYS

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Mol	Chain	Res	Type
26	BD	30	GLU
26	BD	33	LEU
26	BD	34	VAL
26	BD	40	THR
26	BD	64	ILE
26	BD	65	ILE
26	BD	67	PHE
26	BD	78	LYS
26	BD	82	ILE
26	BD	87	ASN
26	BD	94	LEU
26	BD	95	LEU
26	BD	96	HIS
26	BD	97	TYR
26	BD	105	ILE
26	BD	106	ILE
26	BD	112	GLN
26	BD	113	VAL
26	BD	115	GLN
26	BD	117	VAL
26	BD	122	ASP
26	BD	131	LEU
26	BD	140	THR
26	BD	142	VAL
26	BD	148	GLU
26	BD	165	ILE
26	BD	169	GLU
26	BD	171	ASP
26	BD	183	ARG
26	BD	190	TYR
26	BD	203	ASN
26	BD	221	VAL
26	BD	233	HIS
26	BD	239	ARG
26	BD	250	TRP
26	BD	254	THR
26	BD	257	LEU
26	BD	259	THR
26	BD	268	ARG
27	BE	4	ILE
27	BE	26	ILE
27	BE	27	LEU

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Mol	Chain	Res	Type
27	BE	33	VAL
27	BE	34	VAL
27	BE	38	THR
27	BE	44	TYR
27	BE	49	LEU
27	BE	51	PHE
27	BE	61	ARG
27	BE	63	LEU
27	BE	72	VAL
27	BE	78	LEU
27	BE	79	ARG
27	BE	85	ASN
27	BE	87	GLU
27	BE	113	PHE
27	BE	119	ARG
27	BE	120	TRP
27	BE	121	ASN
27	BE	122	PHE
27	BE	134	ILE
27	BE	140	SER
27	BE	144	ARG
27	BE	145	LYS
27	BE	146	THR
27	BE	154	LYS
27	BE	164	ARG
27	BE	184	VAL
27	BE	197	ILE
27	BE	200	GLU
28	BF	10	PRO
28	BF	12	LEU
28	BF	17	ARG
28	BF	18	ARG
28	BF	19	GLU
28	BF	28	ILE
28	BF	33	LEU
28	BF	38	ARG
28	BF	40	GLN
28	BF	43	LYS
28	BF	45	ARG
28	BF	46	ARG
28	BF	53	THR
28	BF	62	ARG

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Mol	Chain	Res	Type
28	BF	68	LYS
28	BF	72	ARG
28	BF	74	ARG
28	BF	78	ILE
28	BF	82	ILE
28	BF	90	PHE
28	BF	116	ASP
28	BF	124	LEU
28	BF	136	THR
28	BF	149	ASP
28	BF	152	GLU
28	BF	154	VAL
28	BF	170	LEU
28	BF	175	THR
28	BF	183	VAL
28	BF	186	ILE
28	BF	190	GLU
28	BF	194	MET
29	BG	5	VAL
29	BG	11	TYR
29	BG	15	VAL
29	BG	16	ARG
29	BG	33	ARG
29	BG	35	GLU
29	BG	48	GLU
29	BG	54	GLU
29	BG	55	LYS
29	BG	59	GLU
29	BG	63	ILE
29	BG	67	LYS
29	BG	80	PHE
29	BG	86	MET
29	BG	92	VAL
29	BG	103	LEU
29	BG	107	LEU
29	BG	109	VAL
29	BG	113	ARG
29	BG	133	LEU
29	BG	139	LEU
29	BG	146	TYR
29	BG	161	THR
29	BG	167	GLU

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Mol	Chain	Res	Type
29	BG	170	ARG
30	BH	17	VAL
30	BH	34	GLU
30	BH	37	VAL
30	BH	41	MET
30	BH	43	VAL
30	BH	44	VAL
30	BH	65	HIS
30	BH	71	LEU
30	BH	85	LYS
30	BH	86	GLU
30	BH	95	ARG
30	BH	103	LEU
30	BH	114	VAL
30	BH	116	GLU
30	BH	121	ILE
30	BH	124	GLU
30	BH	157	TYR
30	BH	159	GLU
30	BH	160	LYS
30	BH	171	LEU
32	BK	2	LYS
32	BK	9	LYS
32	BK	37	PHE
32	BK	41	PHE
32	BK	57	ILE
32	BK	59	ILE
32	BK	65	PHE
32	BK	66	THR
32	BK	69	THR
32	BK	78	ILE
32	BK	105	LEU
32	BK	117	THR
32	BK	119	ASP
32	BK	125	ARG
32	BK	132	ARG
33	BN	1	MET
33	BN	28	THR
33	BN	29	LYS
33	BN	32	THR
33	BN	48	MET
33	BN	62	VAL

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Mol	Chain	Res	Type
33	BN	63	THR
33	BN	71	ILE
33	BN	73	THR
33	BN	84	LYS
33	BN	85	ILE
33	BN	87	LEU
33	BN	90	MET
33	BN	99	LEU
33	BN	109	LYS
33	BN	112	LEU
33	BN	114	ARG
33	BN	119	ARG
33	BN	127	ASP
33	BN	134	ARG
33	BN	137	LYS
33	BN	138	LEU
34	BO	3	GLN
34	BO	8	LEU
34	BO	9	GLU
34	BO	14	THR
34	BO	17	ARG
34	BO	28	SER
34	BO	29	ASN
34	BO	34	THR
34	BO	37	ASP
34	BO	38	VAL
34	BO	39	ILE
34	BO	52	VAL
34	BO	82	ASN
34	BO	86	ILE
34	BO	89	ASN
34	BO	91	LEU
34	BO	98	VAL
34	BO	107	ARG
34	BO	112	MET
34	BO	117	LEU
35	BP	5	ASP
35	BP	7	ARG
35	BP	16	ARG
35	BP	18	ARG
35	BP	27	HIS
35	BP	30	THR

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Mol	Chain	Res	Type
35	BP	35	HIS
35	BP	39	LYS
35	BP	42	SER
35	BP	46	LYS
35	BP	55	ARG
35	BP	60	MET
35	BP	61	ARG
35	BP	68	GLN
35	BP	85	LEU
35	BP	87	ASP
35	BP	90	ARG
35	BP	98	GLU
35	BP	100	LEU
35	BP	106	LEU
35	BP	107	LYS
35	BP	115	LEU
35	BP	125	VAL
35	BP	131	SER
35	BP	135	LEU
36	BQ	1	MET
36	BQ	3	MET
36	BQ	7	MET
36	BQ	8	LYS
36	BQ	10	ARG
36	BQ	14	ARG
36	BQ	17	LEU
36	BQ	25	ASP
36	BQ	31	ASP
36	BQ	42	ILE
36	BQ	46	GLN
36	BQ	56	ARG
36	BQ	60	ARG
36	BQ	65	PHE
36	BQ	66	ILE
36	BQ	68	ILE
36	BQ	75	THR
36	BQ	79	LEU
36	BQ	80	GLU
36	BQ	90	VAL
36	BQ	91	GLU
36	BQ	93	TYR
36	BQ	96	VAL

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Mol	Chain	Res	Type
36	BQ	105	GLU
36	BQ	109	VAL
36	BQ	128	LYS
36	BQ	131	ILE
36	BQ	137	TYR
36	BQ	141	GLN
37	BR	3	HIS
37	BR	5	LYS
37	BR	8	ARG
37	BR	23	ASN
37	BR	43	GLU
37	BR	44	LEU
37	BR	45	ARG
37	BR	71	GLN
37	BR	79	LEU
37	BR	82	GLU
37	BR	99	LYS
37	BR	113	LEU
37	BR	115	GLU
38	BS	12	PHE
38	BS	13	ARG
38	BS	16	ASN
38	BS	18	ILE
38	BS	30	ARG
38	BS	41	ASP
38	BS	47	THR
38	BS	54	LEU
38	BS	71	ARG
38	BS	98	VAL
38	BS	99	LYS
38	BS	101	LEU
38	BS	103	GLU
38	BS	106	ARG
38	BS	107	GLU
39	BT	13	ARG
39	BT	15	VAL
39	BT	27	THR
39	BT	30	VAL
39	BT	33	LYS
39	BT	42	ILE
39	BT	44	ASP
39	BT	48	ILE

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Mol	Chain	Res	Type
39	BT	49	VAL
39	BT	57	PHE
39	BT	58	ASN
39	BT	59	THR
39	BT	65	LYS
39	BT	70	VAL
39	BT	72	VAL
39	BT	74	ARG
39	BT	75	ILE
39	BT	78	LEU
39	BT	80	SER
39	BT	82	LEU
39	BT	84	GLN
39	BT	95	ARG
39	BT	96	ARG
39	BT	101	PHE
39	BT	103	ARG
39	BT	115	ARG
40	BU	14	HIS
40	BU	16	LYS
40	BU	17	ILE
40	BU	18	LEU
40	BU	20	LEU
40	BU	29	SER
40	BU	51	LYS
40	BU	52	ARG
40	BU	53	ARG
40	BU	54	LYS
40	BU	55	ARG
40	BU	60	LEU
40	BU	64	ARG
40	BU	74	LEU
40	BU	79	PHE
40	BU	90	VAL
40	BU	91	ASP
40	BU	98	LEU
40	BU	101	ARG
40	BU	104	GLN
40	BU	108	GLU
41	BV	1	MET
41	BV	5	VAL
41	BV	6	LYS

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Mol	Chain	Res	Type
41	BV	15	GLU
41	BV	18	LEU
41	BV	19	LYS
41	BV	21	ARG
41	BV	25	LEU
41	BV	33	VAL
41	BV	37	VAL
41	BV	40	LEU
41	BV	47	VAL
41	BV	57	VAL
41	BV	61	VAL
41	BV	70	ILE
41	BV	74	LYS
41	BV	75	PHE
41	BV	83	ARG
41	BV	95	LEU
41	BV	97	LYS
41	BV	98	GLU
41	BV	99	ILE
42	BW	8	ARG
42	BW	9	TYR
42	BW	15	ARG
42	BW	17	VAL
42	BW	19	LEU
42	BW	28	SER
42	BW	30	GLU
42	BW	37	ARG
42	BW	39	THR
42	BW	40	ASN
42	BW	51	LEU
42	BW	61	ASN
42	BW	66	GLU
42	BW	68	ARG
42	BW	72	LYS
42	BW	75	TYR
42	BW	77	ASP
42	BW	88	ARG
42	BW	95	ILE
42	BW	99	ARG
42	BW	105	VAL
42	BW	107	LEU
42	BW	109	GLU

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Mol	Chain	Res	Type
42	BW	113	LYS
43	BX	5	TYR
43	BX	6	ASP
43	BX	35	THR
43	BX	54	VAL
43	BX	57	LEU
43	BX	58	HIS
43	BX	59	VAL
43	BX	68	ARG
43	BX	76	ARG
43	BX	78	LYS
43	BX	80	ILE
44	BY	2	ARG
44	BY	5	MET
44	BY	6	HIS
44	BY	8	LYS
44	BY	9	LYS
44	BY	13	VAL
44	BY	28	LYS
44	BY	33	LYS
44	BY	35	TYR
44	BY	39	VAL
44	BY	47	LYS
44	BY	49	VAL
44	BY	50	ARG
44	BY	60	PHE
44	BY	72	VAL
44	BY	75	ILE
44	BY	85	VAL
44	BY	89	PHE
44	BY	90	LEU
45	BZ	5	LEU
45	BZ	8	TYR
45	BZ	9	TYR
45	BZ	11	GLU
45	BZ	28	MET
45	BZ	29	TYR
45	BZ	43	GLU
45	BZ	46	LYS
45	BZ	56	VAL
45	BZ	59	LEU
45	BZ	71	VAL

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Mol	Chain	Res	Type
45	BZ	81	ARG
45	BZ	86	VAL
45	BZ	98	MET
45	BZ	112	ARG
45	BZ	119	GLU
45	BZ	122	ARG
45	BZ	123	ASP
45	BZ	124	ILE
45	BZ	127	LYS
45	BZ	136	PHE
45	BZ	150	LEU
45	BZ	154	ASP
45	BZ	155	LEU
45	BZ	162	GLU
45	BZ	165	VAL
45	BZ	166	SER
45	BZ	181	GLU
45	BZ	186	GLU
46	B0	10	THR
46	B0	27	GLU
46	B0	29	GLN
46	B0	31	VAL
46	B0	32	ARG
46	B0	35	ASN
46	B0	36	ILE
46	B0	37	LEU
46	B0	39	ARG
46	B0	43	THR
46	B0	55	ARG
46	B0	84	LEU
47	B2	8	LYS
47	B2	35	LEU
47	B2	47	ASN
47	B2	65	ASN
48	B3	9	VAL
48	B3	17	LYS
48	B3	18	ASP
48	B3	28	LEU
48	B3	31	LEU
48	B3	37	LEU
48	B3	52	HIS
49	B5	3	LYS

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Mol	Chain	Res	Type
49	B5	23	HIS
49	B5	25	LEU
49	B5	36	CYS
49	B5	46	CYS
49	B5	55	ARG
49	B5	58	LEU
50	B6	6	ARG
50	B6	7	ILE
50	B6	9	LEU
50	B6	11	LEU
50	B6	13	CYS
50	B6	18	ARG
50	B6	27	LYS
50	B6	39	TYR
50	B6	47	THR
50	B6	48	VAL
50	B6	51	GLU
51	B7	1	MET
51	B7	15	THR
51	B7	24	THR
51	B7	40	TRP
51	B7	41	ARG
51	B7	47	ARG
51	B7	49	ARG
52	B8	4	MET
52	B8	14	VAL
52	B8	15	LYS
52	B8	16	ILE
52	B8	30	ARG
52	B8	31	HIS
52	B8	32	LEU
52	B8	40	GLU
52	B8	42	ARG
52	B8	46	ARG
52	B8	53	PRO
52	B8	54	GLU
52	B8	56	GLU
52	B8	59	LYS
52	B8	61	LEU
53	B9	1	MET
53	B9	2	LYS
53	B9	17	ILE

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Mol	Chain	Res	Type
53	B9	18	ARG
53	B9	29	ASN
53	B9	32	HIS
54	Be	62	VAL
54	Be	78	LEU
54	Be	86	LEU
54	Be	90	LYS
54	Be	94	GLU
54	Be	106	GLN
54	Be	118	VAL
57	B1	4	VAL
57	B1	5	CYS
57	B1	10	LYS
57	B1	11	ARG
57	B1	14	VAL
57	B1	18	ILE
57	B1	27	GLU
57	B1	32	LYS
57	B1	39	LYS
57	B1	41	ARG
57	B1	43	TYR
57	B1	46	LEU
57	B1	47	GLN
57	B1	50	ARG
57	B1	58	ILE
57	B1	61	ARG
57	B1	67	ILE
57	B1	73	LEU
57	B1	88	LYS
58	B4	1	MET
58	B4	6	HIS
58	B4	8	LYS
58	B4	9	LEU
58	B4	14	ILE
58	B4	23	GLU
58	B4	30	GLU
58	B4	32	TYR
1	CB	7	VAL
1	CB	8	LYS
1	CB	9	GLU
1	CB	12	GLU
1	CB	17	PHE

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Mol	Chain	Res	Type
1	CB	21	ARG
1	CB	36	ARG
1	CB	42	ILE
1	CB	49	GLU
1	CB	56	ARG
1	CB	68	ILE
1	CB	74	LYS
1	CB	76	GLN
1	CB	96	ARG
1	CB	103	THR
1	CB	106	LYS
1	CB	108	ILE
1	CB	141	GLU
1	CB	145	LEU
1	CB	146	GLN
1	CB	152	PHE
1	CB	155	LEU
1	CB	163	PHE
1	CB	168	THR
1	CB	172	ILE
1	CB	175	ARG
1	CB	180	LEU
1	CB	185	ILE
1	CB	187	LEU
1	CB	190	THR
1	CB	210	SER
1	CB	212	GLN
1	CB	213	LEU
1	CB	226	ARG
1	CB	230	VAL
1	CB	239	VAL
2	CC	4	LYS
2	CC	5	ILE
2	CC	10	PHE
2	CC	15	THR
2	CC	22	TRP
2	CC	33	LEU
2	CC	40	ARG
2	CC	52	LEU
2	CC	62	ASP
2	CC	67	THR
2	CC	84	ILE

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Mol	Chain	Res	Type
2	CC	101	LEU
2	CC	110	ASN
2	CC	124	ILE
2	CC	128	PHE
2	CC	132	ARG
2	CC	134	ILE
2	CC	152	ILE
2	CC	157	ILE
2	CC	176	HIS
2	CC	178	LEU
2	CC	201	TYR
2	CC	204	LEU
2	CC	206	GLU
2	CC	208	ILE
3	CD	3	ARG
3	CD	8	VAL
3	CD	9	CYS
3	CD	12	CYS
3	CD	30	LYS
3	CD	50	ARG
3	CD	53	ASP
3	CD	54	TYR
3	CD	61	LYS
3	CD	65	ARG
3	CD	67	ILE
3	CD	72	GLU
3	CD	86	LYS
3	CD	101	LEU
3	CD	114	ARG
3	CD	127	THR
3	CD	131	ARG
3	CD	134	ASP
3	CD	135	LEU
3	CD	140	VAL
3	CD	141	ARG
3	CD	148	VAL
3	CD	150	GLU
3	CD	156	GLU
3	CD	165	MET
3	CD	170	VAL
3	CD	177	ASP
3	CD	193	ASP

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Mol	Chain	Res	Type
3	CD	196	LEU
3	CD	198	VAL
4	CE	10	MET
4	CE	11	ILE
4	CE	12	LEU
4	CE	31	LEU
4	CE	41	VAL
4	CE	45	PHE
4	CE	47	LYS
4	CE	51	VAL
4	CE	57	LYS
4	CE	64	ARG
4	CE	75	THR
4	CE	78	HIS
4	CE	120	THR
4	CE	126	ARG
4	CE	137	GLU
4	CE	139	LEU
4	CE	144	THR
4	CE	147	ASP
5	CF	2	ARG
5	CF	14	LEU
5	CF	22	GLU
5	CF	55	ASP
5	CF	57	GLN
5	CF	65	VAL
5	CF	67	MET
5	CF	80	ARG
6	CG	3	ARG
6	CG	11	GLN
6	CG	20	ASP
6	CG	35	LYS
6	CG	68	ASN
6	CG	79	ARG
6	CG	80	VAL
6	CG	89	MET
6	CG	94	ARG
6	CG	104	LEU
6	CG	149	ARG
7	CH	37	ARG
7	CH	39	LEU
7	CH	49	GLU

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Mol	Chain	Res	Type
7	CH	63	LEU
7	CH	69	ARG
7	CH	73	ASP
7	CH	83	ILE
7	CH	102	ARG
7	CH	107	LEU
7	CH	111	ILE
7	CH	112	LEU
7	CH	120	THR
7	CH	136	GLU
7	CH	138	TRP
8	CI	25	LYS
8	CI	32	ASP
8	CI	33	PHE
8	CI	34	ASN
8	CI	40	LEU
8	CI	85	LEU
8	CI	88	TYR
8	CI	95	LYS
8	CI	97	LYS
8	CI	99	LEU
8	CI	104	ARG
8	CI	121	ARG
8	CI	125	TYR
8	CI	128	ARG
9	CJ	3	LYS
9	CJ	8	LEU
9	CJ	11	PHE
9	CJ	16	LEU
9	CJ	35	SER
9	CJ	38	ILE
9	CJ	46	ARG
9	CJ	48	THR
9	CJ	50	ILE
9	CJ	65	LEU
9	CJ	74	ILE
9	CJ	75	ILE
9	CJ	78	ASN
9	CJ	79	ARG
9	CJ	81	THR
9	CJ	89	ASP
9	CJ	96	ILE

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Mol	Chain	Res	Type
10	CK	14	VAL
10	CK	29	ILE
10	CK	31	THR
10	CK	33	THR
10	CK	34	ASP
10	CK	48	ILE
10	CK	57	THR
10	CK	66	LEU
10	CK	67	ASP
10	CK	75	TYR
10	CK	80	VAL
10	CK	105	VAL
10	CK	107	SER
10	CK	120	ARG
10	CK	122	LYS
10	CK	124	LYS
10	CK	126	ARG
11	CL	9	GLN
11	CL	15	ARG
11	CL	18	VAL
11	CL	20	LYS
11	CL	24	VAL
11	CL	33	ARG
11	CL	34	ARG
11	CL	38	THR
11	CL	42	THR
11	CL	46	LYS
11	CL	49	ASN
11	CL	52	LEU
11	CL	53	ARG
11	CL	54	LYS
11	CL	55	VAL
11	CL	59	ARG
11	CL	67	THR
11	CL	70	ILE
11	CL	77	LEU
11	CL	79	GLU
11	CL	84	LEU
11	CL	85	ILE
11	CL	89	ARG
11	CL	92	ASP
11	CL	93	LEU

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Mol	Chain	Res	Type
11	CL	96	VAL
11	CL	97	ARG
11	CL	98	TYR
11	CL	104	VAL
11	CL	105	TYR
11	CL	119	LYS
11	CL	127	GLU
12	CM	8	GLU
12	CM	21	TYR
12	CM	27	LYS
12	CM	31	LYS
12	CM	48	LEU
12	CM	61	GLU
12	CM	65	LYS
12	CM	82	MET
12	CM	108	ARG
12	CM	110	ARG
12	CM	121	LYS
13	CN	9	LYS
13	CN	18	VAL
13	CN	21	TYR
13	CN	35	ARG
13	CN	40	CYS
13	CN	61	TRP
14	CO	5	LYS
14	CO	6	GLU
14	CO	10	LYS
14	CO	12	ILE
14	CO	15	PHE
14	CO	38	ARG
14	CO	41	GLU
14	CO	42	HIS
14	CO	47	LYS
14	CO	54	ARG
14	CO	62	GLN
14	CO	64	ARG
14	CO	83	GLU
14	CO	87	ILE
15	CP	14	ASN
15	CP	20	VAL
15	CP	23	ASP
15	CP	28	ARG

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Mol	Chain	Res	Type
15	CP	36	ILE
15	CP	54	GLU
15	CP	57	ARG
15	CP	58	TYR
15	CP	67	THR
15	CP	69	THR
16	CQ	6	LEU
16	CQ	10	VAL
16	CQ	16	GLN
16	CQ	19	VAL
16	CQ	24	GLU
16	CQ	52	LYS
16	CQ	59	ILE
16	CQ	63	ARG
16	CQ	68	ARG
16	CQ	69	LYS
16	CQ	70	ARG
16	CQ	74	LEU
16	CQ	75	ARG
16	CQ	76	LEU
16	CQ	89	LEU
16	CQ	93	GLN
17	CR	23	LYS
17	CR	32	ARG
17	CR	37	VAL
17	CR	43	PHE
17	CR	51	LEU
17	CR	53	ARG
17	CR	79	LEU
17	CR	85	LEU
18	CS	5	LEU
18	CS	6	LYS
18	CS	11	VAL
18	CS	14	HIS
18	CS	30	LEU
18	CS	31	ILE
18	CS	37	ARG
18	CS	38	SER
18	CS	39	THR
18	CS	47	HIS
18	CS	58	VAL
18	CS	61	TYR

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Mol	Chain	Res	Type
18	CS	62	ILE
18	CS	66	MET
18	CS	79	THR
19	CT	13	LEU
19	CT	23	ARG
19	CT	41	ILE
19	CT	50	GLU
19	CT	54	LYS
19	CT	57	ARG
19	CT	64	ASP
19	CT	74	LYS
19	CT	80	ARG
23	CY	8	ASP
23	CY	14	ASN
23	CY	15	ILE
23	CY	20	HIS
23	CY	22	ASP
23	CY	30	GLU
23	CY	35	TYR
23	CY	72	CYS
23	CY	80	ASN
23	CY	84	THR
23	CY	87	HIS
23	CY	92	ILE
23	CY	119	GLU
23	CY	126	GLU
23	CY	132	ARG
23	CY	133	ILE
23	CY	137	ASN
23	CY	139	MET
23	CY	140	ASP
23	CY	146	LEU
23	CY	147	TRP
23	CY	153	MET
23	CY	157	LEU
23	CY	170	ARG
23	CY	171	GLU
23	CY	172	ASP
23	CY	175	SER
23	CY	177	ILE
23	CY	178	ILE
23	CY	187	THR

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Mol	Chain	Res	Type
23	CY	197	ARG
23	CY	199	ILE
23	CY	211	GLU
23	CY	224	ASP
23	CY	225	GLU
23	CY	226	ASN
23	CY	227	ILE
23	CY	228	MET
23	CY	229	LEU
23	CY	235	GLU
23	CY	240	GLU
23	CY	260	LEU
23	CY	270	GLN
23	CY	273	LEU
23	CY	285	ASP
23	CY	299	VAL
23	CY	300	GLU
23	CY	301	ILE
23	CY	302	HIS
23	CY	314	PHE
23	CY	316	ILE
23	CY	328	ILE
23	CY	336	THR
23	CY	340	TYR
23	CY	341	VAL
23	CY	348	ARG
23	CY	352	VAL
23	CY	355	LEU
23	CY	357	ARG
23	CY	358	MET
23	CY	364	GLU
23	CY	390	VAL
23	CY	393	ASP
23	CY	397	VAL
23	CY	406	GLU
23	CY	422	GLU
23	CY	428	LEU
23	CY	431	LEU
23	CY	440	VAL
23	CY	454	MET
23	CY	456	GLU
23	CY	464	ASP

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Mol	Chain	Res	Type
23	CY	471	LYS
23	CY	487	ILE
23	CY	488	THR
23	CY	504	ARG
23	CY	506	GLN
23	CY	512	ILE
23	CY	514	VAL
23	CY	529	ILE
23	CY	555	LEU
23	CY	556	ILE
23	CY	563	ILE
23	CY	572	TYR
23	CY	580	MET
23	CY	584	ILE
23	CY	598	ASP
23	CY	600	VAL
23	CY	603	GLU
23	CY	607	ARG
23	CY	610	VAL
23	CY	614	GLU
23	CY	615	GLU
23	CY	617	MET
23	CY	635	GLU
23	CY	649	LEU
23	CY	658	ASP
23	CY	666	ARG
23	CY	676	TYR
23	CY	685	GLU
25	DC	7	ARG
25	DC	9	ARG
25	DC	15	VAL
25	DC	19	LYS
25	DC	20	VAL
25	DC	24	ASP
25	DC	28	ARG
25	DC	32	GLU
25	DC	37	LYS
25	DC	39	ASP
25	DC	41	THR
25	DC	42	VAL
25	DC	47	LYS
25	DC	48	LEU

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Mol	Chain	Res	Type
25	DC	53	ARG
25	DC	60	ARG
25	DC	73	VAL
25	DC	74	ARG
25	DC	83	LYS
25	DC	94	TYR
25	DC	104	ILE
25	DC	106	ASP
25	DC	114	VAL
25	DC	119	ASP
25	DC	131	ILE
25	DC	138	LEU
25	DC	148	PHE
25	DC	161	ARG
25	DC	164	PHE
25	DC	166	ASN
25	DC	169	THR
25	DC	172	ILE
25	DC	176	VAL
25	DC	185	LYS
25	DC	189	ASN
25	DC	198	GLU
25	DC	201	LYS
25	DC	211	ARG
25	DC	213	VAL
25	DC	215	VAL
25	DC	216	THR
25	DC	224	ARG
26	DD	4	LYS
26	DD	5	LYS
26	DD	9	TYR
26	DD	13	ARG
26	DD	23	GLU
26	DD	25	THR
26	DD	26	LYS
26	DD	30	GLU
26	DD	33	LEU
26	DD	34	VAL
26	DD	35	LYS
26	DD	38	LYS
26	DD	40	THR
26	DD	43	ARG

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Mol	Chain	Res	Type
26	DD	44	ASN
26	DD	60	ARG
26	DD	63	ARG
26	DD	64	ILE
26	DD	65	ILE
26	DD	69	ARG
26	DD	71	ASP
26	DD	78	LYS
26	DD	82	ILE
26	DD	87	ASN
26	DD	88	ARG
26	DD	95	LEU
26	DD	97	TYR
26	DD	101	GLU
26	DD	105	ILE
26	DD	106	ILE
26	DD	113	VAL
26	DD	115	GLN
26	DD	117	VAL
26	DD	140	THR
26	DD	142	VAL
26	DD	147	LEU
26	DD	148	GLU
26	DD	150	LYS
26	DD	161	THR
26	DD	164	GLN
26	DD	165	ILE
26	DD	171	ASP
26	DD	173	VAL
26	DD	175	LEU
26	DD	190	TYR
26	DD	212	SER
26	DD	226	MET
26	DD	233	HIS
26	DD	242	ARG
26	DD	250	TRP
26	DD	254	THR
26	DD	257	LEU
26	DD	259	THR
27	DE	4	ILE
27	DE	21	VAL
27	DE	24	THR

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Mol	Chain	Res	Type
27	DE	27	LEU
27	DE	33	VAL
27	DE	36	ARG
27	DE	38	THR
27	DE	45	THR
27	DE	48	GLN
27	DE	49	LEU
27	DE	51	PHE
27	DE	55	ASN
27	DE	61	ARG
27	DE	63	LEU
27	DE	73	GLU
27	DE	78	LEU
27	DE	79	ARG
27	DE	84	PHE
27	DE	87	GLU
27	DE	91	VAL
27	DE	109	LYS
27	DE	113	PHE
27	DE	119	ARG
27	DE	120	TRP
27	DE	127	ASP
27	DE	132	HIS
27	DE	133	LYS
27	DE	134	ILE
27	DE	144	ARG
27	DE	154	LYS
27	DE	164	ARG
27	DE	174	ASP
27	DE	175	VAL
27	DE	184	VAL
27	DE	191	PRO
27	DE	196	VAL
27	DE	197	ILE
27	DE	202	LYS
28	DF	8	GLN
28	DF	9	ILE
28	DF	18	ARG
28	DF	19	GLU
28	DF	28	ILE
28	DF	33	LEU
28	DF	35	GLU

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Mol	Chain	Res	Type
28	DF	40	GLN
28	DF	43	LYS
28	DF	45	ARG
28	DF	46	ARG
28	DF	53	THR
28	DF	62	ARG
28	DF	68	LYS
28	DF	72	ARG
28	DF	74	ARG
28	DF	75	HIS
28	DF	78	ILE
28	DF	82	ILE
28	DF	90	PHE
28	DF	106	ARG
28	DF	124	LEU
28	DF	136	THR
28	DF	149	ASP
28	DF	154	VAL
28	DF	175	THR
28	DF	179	GLU
28	DF	185	ASP
28	DF	186	ILE
28	DF	204	ASN
29	DG	5	VAL
29	DG	11	TYR
29	DG	27	ASN
29	DG	33	ARG
29	DG	34	LEU
29	DG	35	GLU
29	DG	45	GLU
29	DG	48	GLU
29	DG	53	LEU
29	DG	54	GLU
29	DG	55	LYS
29	DG	59	GLU
29	DG	63	ILE
29	DG	67	LYS
29	DG	80	PHE
29	DG	86	MET
29	DG	92	VAL
29	DG	98	ARG
29	DG	99	MET

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Mol	Chain	Res	Type
29	DG	109	VAL
29	DG	113	ARG
29	DG	120	LEU
29	DG	121	ASN
29	DG	143	GLU
29	DG	144	ILE
29	DG	152	LEU
29	DG	153	ARG
29	DG	168	GLU
30	DH	18	GLU
30	DH	34	GLU
30	DH	41	MET
30	DH	43	VAL
30	DH	71	LEU
30	DH	83	TYR
30	DH	85	LYS
30	DH	122	THR
30	DH	157	TYR
30	DH	158	HIS
30	DH	171	LEU
32	DK	2	LYS
32	DK	9	LYS
32	DK	11	GLN
32	DK	37	PHE
32	DK	41	PHE
32	DK	42	ASN
32	DK	57	ILE
32	DK	59	ILE
32	DK	65	PHE
32	DK	66	THR
32	DK	78	ILE
32	DK	114	ASP
32	DK	117	THR
32	DK	120	LEU
32	DK	125	ARG
32	DK	132	ARG
33	DN	1	MET
33	DN	32	THR
33	DN	33	LEU
33	DN	35	ARG
33	DN	48	MET
33	DN	58	ASP

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Mol	Chain	Res	Type
33	DN	63	THR
33	DN	69	GLN
33	DN	71	ILE
33	DN	74	ARG
33	DN	76	SER
33	DN	85	ILE
33	DN	87	LEU
33	DN	88	GLU
33	DN	90	MET
33	DN	99	LEU
33	DN	112	LEU
33	DN	114	ARG
33	DN	119	ARG
33	DN	127	ASP
33	DN	130	HIS
33	DN	134	ARG
33	DN	137	LYS
34	DO	9	GLU
34	DO	17	ARG
34	DO	24	VAL
34	DO	28	SER
34	DO	31	LYS
34	DO	34	THR
34	DO	38	VAL
34	DO	39	ILE
34	DO	47	ILE
34	DO	52	VAL
34	DO	66	LYS
34	DO	78	ARG
34	DO	82	ASN
34	DO	87	ILE
34	DO	91	LEU
34	DO	92	GLU
34	DO	98	VAL
34	DO	108	GLU
34	DO	112	MET
35	DP	7	ARG
35	DP	16	ARG
35	DP	18	ARG
35	DP	32	THR
35	DP	39	LYS
35	DP	41	ARG

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Mol	Chain	Res	Type
35	DP	42	SER
35	DP	55	ARG
35	DP	60	MET
35	DP	61	ARG
35	DP	62	LEU
35	DP	79	ARG
35	DP	84	ASN
35	DP	85	LEU
35	DP	100	LEU
35	DP	107	LYS
35	DP	123	LEU
35	DP	135	LEU
36	DQ	1	MET
36	DQ	2	LEU
36	DQ	3	MET
36	DQ	6	ARG
36	DQ	7	MET
36	DQ	10	ARG
36	DQ	12	GLN
36	DQ	31	ASP
36	DQ	35	VAL
36	DQ	46	GLN
36	DQ	60	ARG
36	DQ	66	ILE
36	DQ	68	ILE
36	DQ	74	TYR
36	DQ	76	LYS
36	DQ	77	LYS
36	DQ	79	LEU
36	DQ	90	VAL
36	DQ	91	GLU
36	DQ	93	TYR
36	DQ	96	VAL
36	DQ	125	LEU
36	DQ	128	LYS
36	DQ	135	ASP
36	DQ	137	TYR
37	DR	3	HIS
37	DR	4	LEU
37	DR	6	SER
37	DR	8	ARG
37	DR	14	SER

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Mol	Chain	Res	Type
37	DR	36	THR
37	DR	43	GLU
37	DR	44	LEU
37	DR	45	ARG
37	DR	56	LYS
37	DR	65	LEU
37	DR	67	LEU
37	DR	72	ASP
37	DR	79	LEU
37	DR	88	ARG
37	DR	99	LYS
37	DR	102	GLU
37	DR	115	GLU
38	DS	12	PHE
38	DS	13	ARG
38	DS	29	PHE
38	DS	41	ASP
38	DS	42	ASP
38	DS	47	THR
38	DS	52	SER
38	DS	54	LEU
38	DS	69	VAL
38	DS	84	GLN
38	DS	87	PHE
38	DS	88	ASP
38	DS	97	ARG
38	DS	98	VAL
38	DS	99	LYS
38	DS	101	LEU
38	DS	103	GLU
38	DS	106	ARG
38	DS	107	GLU
39	DT	1	MET
39	DT	13	ARG
39	DT	22	PHE
39	DT	23	ARG
39	DT	27	THR
39	DT	29	ARG
39	DT	30	VAL
39	DT	33	LYS
39	DT	44	ASP
39	DT	48	ILE

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Mol	Chain	Res	Type
39	DT	50	ILE
39	DT	53	ARG
39	DT	57	PHE
39	DT	58	ASN
39	DT	59	THR
39	DT	65	LYS
39	DT	70	VAL
39	DT	73	GLU
39	DT	74	ARG
39	DT	82	LEU
39	DT	84	GLN
39	DT	85	LYS
39	DT	90	GLN
39	DT	95	ARG
39	DT	101	PHE
39	DT	102	ILE
39	DT	115	ARG
39	DT	134	GLU
40	DU	8	VAL
40	DU	11	ARG
40	DU	14	HIS
40	DU	18	LEU
40	DU	20	LEU
40	DU	28	ARG
40	DU	49	HIS
40	DU	51	LYS
40	DU	52	ARG
40	DU	54	LYS
40	DU	55	ARG
40	DU	60	LEU
40	DU	64	ARG
40	DU	74	LEU
40	DU	76	TYR
40	DU	90	VAL
40	DU	95	LEU
40	DU	101	ARG
40	DU	104	GLN
40	DU	114	LYS
41	DV	1	MET
41	DV	2	PHE
41	DV	7	THR
41	DV	11	GLN

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Mol	Chain	Res	Type
41	DV	14	VAL
41	DV	19	LYS
41	DV	20	LEU
41	DV	21	ARG
41	DV	33	VAL
41	DV	37	VAL
41	DV	39	LEU
41	DV	40	LEU
41	DV	49	THR
41	DV	57	VAL
41	DV	61	VAL
41	DV	62	LEU
41	DV	70	ILE
41	DV	74	LYS
41	DV	78	LYS
41	DV	80	GLN
41	DV	92	THR
41	DV	98	GLU
41	DV	99	ILE
42	DW	9	TYR
42	DW	11	ARG
42	DW	15	ARG
42	DW	17	VAL
42	DW	19	LEU
42	DW	30	GLU
42	DW	34	ASN
42	DW	37	ARG
42	DW	51	LEU
42	DW	66	GLU
42	DW	76	VAL
42	DW	88	ARG
42	DW	92	ARG
42	DW	95	ILE
42	DW	100	THR
42	DW	103	ILE
42	DW	105	VAL
42	DW	107	LEU
42	DW	109	GLU
42	DW	113	LYS
43	DX	5	TYR
43	DX	6	ASP
43	DX	8	ILE

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Mol	Chain	Res	Type
43	DX	9	LEU
43	DX	27	THR
43	DX	45	THR
43	DX	54	VAL
43	DX	57	LEU
43	DX	59	VAL
43	DX	63	LYS
43	DX	68	ARG
43	DX	76	ARG
43	DX	78	LYS
43	DX	80	ILE
43	DX	87	GLN
44	DY	2	ARG
44	DY	5	MET
44	DY	7	VAL
44	DY	9	LYS
44	DY	28	LYS
44	DY	31	LEU
44	DY	35	TYR
44	DY	39	VAL
44	DY	47	LYS
44	DY	50	ARG
44	DY	60	PHE
44	DY	76	CYS
44	DY	84	ARG
44	DY	89	PHE
44	DY	90	LEU
44	DY	97	ARG
45	DZ	6	LYS
45	DZ	9	TYR
45	DZ	11	GLU
45	DZ	28	MET
45	DZ	29	TYR
45	DZ	32	HIS
45	DZ	52	SER
45	DZ	59	LEU
45	DZ	66	SER
45	DZ	70	LEU
45	DZ	71	VAL
45	DZ	81	ARG
45	DZ	86	VAL
45	DZ	87	ASP

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Mol	Chain	Res	Type
45	DZ	94	GLU
45	DZ	96	VAL
45	DZ	98	MET
45	DZ	112	ARG
45	DZ	119	GLU
45	DZ	123	ASP
45	DZ	124	ILE
45	DZ	126	VAL
45	DZ	127	LYS
45	DZ	150	LEU
45	DZ	162	GLU
45	DZ	165	VAL
45	DZ	175	VAL
45	DZ	185	GLU
46	D0	3	HIS
46	D0	10	THR
46	D0	27	GLU
46	D0	29	GLN
46	D0	31	VAL
46	D0	32	ARG
46	D0	36	ILE
46	D0	37	LEU
46	D0	41	ARG
46	D0	44	ARG
46	D0	50	ASN
46	D0	55	ARG
46	D0	64	ASP
46	D0	75	LEU
46	D0	84	LEU
47	D2	8	LYS
47	D2	35	LEU
47	D2	37	PHE
47	D2	40	SER
47	D2	64	LEU
47	D2	70	GLN
48	D3	11	SER
48	D3	17	LYS
48	D3	24	LYS
48	D3	31	LEU
48	D3	37	LEU
48	D3	54	VAL
48	D3	59	VAL

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Mol	Chain	Res	Type
49	D5	3	LYS
49	D5	8	LYS
49	D5	25	LEU
49	D5	26	THR
49	D5	29	THR
49	D5	30	LEU
49	D5	44	THR
49	D5	51	TYR
49	D5	55	ARG
49	D5	58	LEU
50	D6	6	ARG
50	D6	9	LEU
50	D6	10	LEU
50	D6	11	LEU
50	D6	18	ARG
50	D6	19	ARG
50	D6	27	LYS
50	D6	30	THR
50	D6	39	TYR
50	D6	42	TRP
50	D6	43	CYS
50	D6	48	VAL
51	D7	1	MET
51	D7	22	MET
51	D7	40	TRP
51	D7	42	LEU
52	D8	4	MET
52	D8	6	THR
52	D8	16	ILE
52	D8	17	THR
52	D8	30	ARG
52	D8	31	HIS
52	D8	34	TRP
52	D8	36	LYS
52	D8	42	ARG
52	D8	44	LYS
52	D8	48	PHE
52	D8	49	VAL
52	D8	50	LEU
52	D8	54	GLU
52	D8	56	GLU
52	D8	59	LYS

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Mol	Chain	Res	Type
52	D8	61	LEU
53	D9	22	ARG
53	D9	28	GLU
54	De	62	VAL
54	De	73	GLU
54	De	75	ILE
54	De	78	LEU
54	De	81	ILE
54	De	86	LEU
54	De	94	GLU
54	De	118	VAL
57	D1	3	LYS
57	D1	5	CYS
57	D1	17	SER
57	D1	20	ARG
57	D1	32	LYS
57	D1	34	THR
57	D1	37	ILE
57	D1	39	LYS
57	D1	41	ARG
57	D1	43	TYR
57	D1	46	LEU
57	D1	51	VAL
57	D1	56	GLN
57	D1	58	ILE
57	D1	60	PHE
57	D1	61	ARG
57	D1	62	VAL
57	D1	67	ILE
57	D1	82	LEU
57	D1	94	LEU
58	D4	1	MET
58	D4	9	LEU
58	D4	10	VAL
58	D4	30	GLU
58	D4	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
2	AC	69	HIS
2	AC	102	ASN

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Mol	Chain	Res	Type
3	AD	77	ASN
5	AF	100	ASN
6	AG	97	GLN
7	AH	78	GLN
8	AI	117	HIS
10	AK	62	GLN
10	AK	93	GLN
10	AK	116	HIS
11	AL	49	ASN
11	AL	76	ASN
15	AP	16	HIS
17	AR	63	GLN
23	AY	20	HIS
23	AY	117	GLN
23	AY	137	ASN
23	AY	190	ASN
25	BC	58	ASN
26	BD	115	GLN
26	BD	198	ASN
28	BF	8	GLN
28	BF	40	GLN
28	BF	67	GLN
32	BK	30	HIS
33	BN	69	GLN
34	BO	82	ASN
35	BP	128	HIS
36	BQ	46	GLN
38	BS	16	ASN
39	BT	55	ASN
39	BT	58	ASN
39	BT	84	GLN
40	BU	71	GLN
57	B1	45	ASN
3	CD	119	GLN
7	CH	15	ASN
10	CK	26	ASN
10	CK	62	GLN
10	CK	93	GLN
10	CK	116	HIS
11	CL	8	ASN
16	CQ	16	GLN
17	CR	36	ASN

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Mol	Chain	Res	Type
23	CY	14	ASN
23	CY	137	ASN
23	CY	165	GLN
23	CY	421	GLN
23	CY	595	GLN
26	DD	115	GLN
27	DE	48	GLN
28	DF	40	GLN
28	DF	67	GLN
28	DF	169	ASN
29	DG	40	ASN
29	DG	121	ASN
32	DK	116	ASN
33	DN	131	GLN
34	DO	82	ASN
35	DP	13	ASN
36	DQ	45	GLN
37	DR	53	HIS
39	DT	58	ASN
40	DU	49	HIS
40	DU	71	GLN
42	DW	57	ASN
46	D0	35	ASN
46	D0	70	GLN
47	D2	48	HIS
49	D5	22	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	305 (20%)	17 (1%)
20	CA	1510/1511 (99%)	285 (18%)	16 (1%)
21	AW	76/77 (98%)	23 (30%)	1 (1%)
21	CW	76/77 (98%)	22 (28%)	1 (1%)
22	AV	22/23 (95%)	8 (36%)	1 (4%)
22	CV	22/23 (95%)	8 (36%)	2 (9%)
59	BA	2878/2879 (99%)	665 (23%)	27 (0%)
59	DA	2878/2879 (99%)	666 (23%)	21 (0%)
60	BB	118/119 (99%)	21 (17%)	1 (0%)
60	DB	118/119 (99%)	17 (14%)	1 (0%)
All	All	9208/9218 (99%)	2020 (21%)	88 (0%)

All (20Z) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	9	G
20	AA	13	U
20	AA	15	G
20	AA	29	G
20	AA	32	A
20	AA	39	G
20	AA	47	C
20	AA	48	C
20	AA	50	A
20	AA	51	A
20	AA	68(H)	G
20	AA	68(L)	U
20	AA	68(M)	U
20	AA	68(P)	C
20	AA	68(W)	G
20	AA	106	C
20	AA	108	G
20	AA	109	A
20	AA	116	A
20	AA	121	C
20	AA	122	G
20	AA	129(A)	G
20	AA	131	C
20	AA	144	G
20	AA	152	A
20	AA	163	C
20	AA	175	C
20	AA	179	A
20	AA	186(G)	C
20	AA	186(I)	U
20	AA	186(L)	G
20	AA	195	A
20	AA	197	A
20	AA	201(C)	U
20	AA	216	G
20	AA	220	G
20	AA	231	G
20	AA	244	U
20	AA	245	C
20	AA	247	G
20	AA	251	G

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Mol	Chain	Res	Type
20	AA	253	U
20	AA	264	U
20	AA	267	C
20	AA	273	A
20	AA	279	A
20	AA	280	C
20	AA	281	G
20	AA	289	G
20	AA	306	G
20	AA	309	G
20	AA	316	G
20	AA	321	A
20	AA	328	C
20	AA	329	A
20	AA	332	G
20	AA	338	A
20	AA	345	C
20	AA	347	G
20	AA	352	C
20	AA	353	A
20	AA	354	G
20	AA	357	G
20	AA	367	U
20	AA	372	C
20	AA	373	A
20	AA	384	G
20	AA	390	C
20	AA	397	A
20	AA	398	C
20	AA	407	G
20	AA	411	A
20	AA	412	A
20	AA	413	G
20	AA	414	A
20	AA	422	C
20	AA	423	G
20	AA	424	G
20	AA	430	A
20	AA	440	A
20	AA	452	A
20	AA	453	A
20	AA	458	C

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Mol	Chain	Res	Type
20	AA	458(B)	A
20	AA	481	G
20	AA	485	G
20	AA	492	G
20	AA	495	A
20	AA	497	A
20	AA	498	U
20	AA	505	G
20	AA	509	A
20	AA	511	C
20	AA	514	C
20	AA	518	C
20	AA	519	C
20	AA	521	G
20	AA	522	C
20	AA	524	G
20	AA	527	G
20	AA	531	U
20	AA	532	A
20	AA	533	A
20	AA	534	U
20	AA	538	G
20	AA	547	A
20	AA	559	A
20	AA	560	U
20	AA	562	C
20	AA	564	C
20	AA	567	G
20	AA	568	G
20	AA	572	A
20	AA	573	A
20	AA	574	A
20	AA	575	G
20	AA	576	G
20	AA	577	G
20	AA	579	G
20	AA	596	C
20	AA	653	A
20	AA	661	G
20	AA	665	A
20	AA	673	G
20	AA	685	G

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Mol	Chain	Res	Type
20	AA	688	G
20	AA	703	G
20	AA	713	G
20	AA	723	U
20	AA	724	G
20	AA	730	G
20	AA	731	G
20	AA	733	A
20	AA	734	G
20	AA	737	A
20	AA	740	U
20	AA	749	C
20	AA	754	C
20	AA	755	G
20	AA	777	A
20	AA	793	U
20	AA	794	A
20	AA	807	A
20	AA	811	C
20	AA	812	C
20	AA	816	A
20	AA	817	C
20	AA	818	G
20	AA	819	A
20	AA	821	G
20	AA	827	U
20	AA	828	A
20	AA	834	C
20	AA	838(A)	U
20	AA	838(B)	C
20	AA	838(C)	U
20	AA	848	C
20	AA	859	A
20	AA	867	G
20	AA	869	G
20	AA	870	U
20	AA	873	A
20	AA	874	G
20	AA	877	C
20	AA	897	C
20	AA	902	G
20	AA	907	A

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Mol	Chain	Res	Type
20	AA	916	G
20	AA	923	A
20	AA	926	G
20	AA	927	G
20	AA	934	C
20	AA	935	A
20	AA	960	U
20	AA	961	U
20	AA	962	C
20	AA	966	G
20	AA	969	A
20	AA	971	G
20	AA	972	C
20	AA	974	A
20	AA	976	G
20	AA	977	A
20	AA	978	A
20	AA	979	C
20	AA	980	C
20	AA	983	A
20	AA	992	U
20	AA	993	G
20	AA	1004	A
20	AA	1025	U
20	AA	1045	C
20	AA	1046	A
20	AA	1047	G
20	AA	1049	U
20	AA	1054	C
20	AA	1055	A
20	AA	1065	U
20	AA	1066	C
20	AA	1067	A
20	AA	1069	C
20	AA	1081	G
20	AA	1085	U
20	AA	1094	G
20	AA	1095	U
20	AA	1097	C
20	AA	1101	A
20	AA	1102	A
20	AA	1125	U

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Mol	Chain	Res	Type
20	AA	1126	U
20	AA	1129	C
20	AA	1130	A
20	AA	1137	C
20	AA	1138	G
20	AA	1139	G
20	AA	1140	C
20	AA	1146	A
20	AA	1152	A
20	AA	1154	G
20	AA	1158	C
20	AA	1159	U
20	AA	1181	G
20	AA	1187	G
20	AA	1191	A
20	AA	1196	U
20	AA	1197	G
20	AA	1198	G
20	AA	1200	C
20	AA	1201	A
20	AA	1203	C
20	AA	1204	A
20	AA	1212	U
20	AA	1213	A
20	AA	1214	C
20	AA	1220	G
20	AA	1225	A
20	AA	1226	C
20	AA	1227	A
20	AA	1238	A
20	AA	1239	A
20	AA	1247	U
20	AA	1249	C
20	AA	1256	A
20	AA	1257	U
20	AA	1260	C
20	AA	1275	A
20	AA	1279	A
20	AA	1280	A
20	AA	1281	U
20	AA	1283	G
20	AA	1287	A

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Mol	Chain	Res	Type
20	AA	1300	G
20	AA	1301	U
20	AA	1302	U
20	AA	1303	C
20	AA	1305	G
20	AA	1311	G
20	AA	1317	C
20	AA	1320	C
20	AA	1322	C
20	AA	1331	G
20	AA	1338	G
20	AA	1339	A
20	AA	1347	G
20	AA	1362(A)	C
20	AA	1364	U
20	AA	1370	G
20	AA	1377	A
20	AA	1397	C
20	AA	1398	A
20	AA	1402	C
20	AA	1403	C
20	AA	1406	U
20	AA	1413	A
20	AA	1419	G
20	AA	1440(C)	G
20	AA	1440(D)	A
20	AA	1440(E)	G
20	AA	1440(I)	A
20	AA	1440(J)	C
20	AA	1440(K)	G
20	AA	1440(L)	G
20	AA	1475	G
20	AA	1489	G
20	AA	1492	A
20	AA	1493	A
20	AA	1494	G
20	AA	1497	G
20	AA	1499	A
20	AA	1502	A
20	AA	1504	G
20	AA	1505	G
20	AA	1506	U

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Mol	Chain	Res	Type
20	AA	1517	G
20	AA	1519	A
20	AA	1520	G
20	AA	1529	G
20	AA	1530	G
20	AA	1532	U
20	AA	1533	C
20	AA	1534	A
20	AA	1535	C
20	AA	1536	C
20	AA	1538	C
21	AW	8	U
21	AW	16	U
21	AW	17	U
21	AW	18	G
21	AW	19	G
21	AW	20	U
21	AW	20(A)	U
21	AW	21	A
21	AW	22	G
21	AW	25	C
21	AW	30	C
21	AW	36	U
21	AW	42	U
21	AW	46	G
21	AW	47	U
21	AW	48	C
21	AW	49	A
21	AW	50	C
21	AW	51	A
21	AW	58	A
21	AW	59	A
21	AW	60	U
21	AW	61	C
22	AV	5	A
22	AV	12	A
22	AV	15	A
22	AV	16	A
22	AV	18	G
22	AV	19	G
22	AV	23	A
22	AV	24	A

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Mol	Chain	Res	Type
59	BA	12	U
59	BA	15	G
59	BA	17	G
59	BA	34	C
59	BA	35	G
59	BA	46	C
59	BA	49	A
59	BA	55	G
59	BA	58	G
59	BA	61	G
59	BA	66	C
59	BA	73	A
59	BA	75	G
59	BA	78	A
59	BA	84	A
59	BA	87	C
59	BA	90	U
59	BA	98	G
59	BA	99	U
59	BA	101	G
59	BA	102	G
59	BA	104	U
59	BA	110	G
59	BA	118	A
59	BA	119	A
59	BA	120	U
59	BA	141(B)	C
59	BA	155	C
59	BA	162	U
59	BA	171	G
59	BA	181	A
59	BA	188	G
59	BA	196	A
59	BA	197	A
59	BA	199	A
59	BA	201	C
59	BA	205	G
59	BA	216	A
59	BA	221	A
59	BA	222	A
59	BA	227	A
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	242	G
59	BA	248	G
59	BA	252	G
59	BA	255	A
59	BA	256	A
59	BA	264	C
59	BA	265	A
59	BA	266	G
59	BA	270(M)	U
59	BA	270(N)	U
59	BA	270(O)	G
59	BA	270(P)	U
59	BA	270(Q)	C
59	BA	270(R)	C
59	BA	271(C)	G
59	BA	271(D)	U
59	BA	271	G
59	BA	274	G
59	BA	275	G
59	BA	277	C
59	BA	279	C
59	BA	283	A
59	BA	299	A
59	BA	302	C
59	BA	310	A
59	BA	321	G
59	BA	322	A
59	BA	323	G
59	BA	324	A
59	BA	325	G
59	BA	329	G
59	BA	330	A
59	BA	331	A
59	BA	345	A
59	BA	349	G
59	BA	352	G
59	BA	363(A)	G
59	BA	364	C
59	BA	380	U

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Mol	Chain	Res	Type
59	BA	381	G
59	BA	386	G
59	BA	387	U
59	BA	388	G
59	BA	389	G
59	BA	390	A
59	BA	391	G
59	BA	396	G
59	BA	405	U
59	BA	406	G
59	BA	407	G
59	BA	411	G
59	BA	412	A
59	BA	434	U
59	BA	444	C
59	BA	448	U
59	BA	449	A
59	BA	451	C
59	BA	456	C
59	BA	457	A
59	BA	459	U
59	BA	464	U
59	BA	467	G
59	BA	470	A
59	BA	475	U
59	BA	480	A
59	BA	481	G
59	BA	491	G
59	BA	495	G
59	BA	505	A
59	BA	508	G
59	BA	509	C
59	BA	527	C
59	BA	528	A
59	BA	529	A
59	BA	530	G
59	BA	531	C
59	BA	532	A
59	BA	533	G
59	BA	537	C
59	BA	544	C
59	BA	556	G

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Mol	Chain	Res	Type
59	BA	559	G
59	BA	563	G
59	BA	572	A
59	BA	573	G
59	BA	574	C
59	BA	575	A
59	BA	586	A
59	BA	587	C
59	BA	599	G
59	BA	603	A
59	BA	616	A
59	BA	617	G
59	BA	620	G
59	BA	627	A
59	BA	637	A
59	BA	641	C
59	BA	645	C
59	BA	646	A
59	BA	652	U
59	BA	654	U
59	BA	668	G
59	BA	670	A
59	BA	671	C
59	BA	672	C
59	BA	683	C
59	BA	685	A
59	BA	686	G
59	BA	689	A
59	BA	695	G
59	BA	706	A
59	BA	717	G
59	BA	720	C
59	BA	728	G
59	BA	730	C
59	BA	738	G
59	BA	741	G
59	BA	748	G
59	BA	761	A
59	BA	763	G
59	BA	764	A
59	BA	765	G
59	BA	776	G

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Mol	Chain	Res	Type
59	BA	779	U
59	BA	782	A
59	BA	784	A
59	BA	785	G
59	BA	788	A
59	BA	792	G
59	BA	794	G
59	BA	800	A
59	BA	805	G
59	BA	812	C
59	BA	819	A
59	BA	821	A
59	BA	827	U
59	BA	829	A
59	BA	845	G
59	BA	846	C
59	BA	847	U
59	BA	852	G
59	BA	859	G
59	BA	866	A
59	BA	869	G
59	BA	870	A
59	BA	890	A
59	BA	896	A
59	BA	897	C
59	BA	906	G
59	BA	910	A
59	BA	917	A
59	BA	919	G
59	BA	929	G
59	BA	932	G
59	BA	935	C
59	BA	939	G
59	BA	941	A
59	BA	946	G
59	BA	959	A
59	BA	961	C
59	BA	962	G
59	BA	971	C
59	BA	974(A)	G
59	BA	974(B)	C
59	BA	980	A

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Mol	Chain	Res	Type
59	BA	983	A
59	BA	986	C
59	BA	996	A
59	BA	1002	G
59	BA	1007	C
59	BA	1008	C
59	BA	1009	A
59	BA	1012	U
59	BA	1013	C
59	BA	1020	A
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	1041	C
59	BA	1042	G
59	BA	1045	A
59	BA	1046	A
59	BA	1047	G
59	BA	1048	A
59	BA	1061	U
59	BA	1070	A
59	BA	1072	C
59	BA	1075	C
59	BA	1077	A
59	BA	1078	U
59	BA	1079	C
59	BA	1085	A
59	BA	1086	A
59	BA	1088	A
59	BA	1090	U
59	BA	1098	A
59	BA	1106	G
59	BA	1107	G
59	BA	1112	G
59	BA	1123	C
59	BA	1127	A
59	BA	1131	G
59	BA	1135	C
59	BA	1136	G

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Mol	Chain	Res	Type
59	BA	1139	G
59	BA	1155	A
59	BA	1157	G
59	BA	1175	U
59	BA	1176	G
59	BA	1186	G
59	BA	1199	U
59	BA	1204	A
59	BA	1206	G
59	BA	1212	G
59	BA	1215	G
59	BA	1221	C
59	BA	1231	G
59	BA	1236	G
59	BA	1237	A
59	BA	1241	A
59	BA	1242	A
59	BA	1244	G
59	BA	1247	A
59	BA	1248	G
59	BA	1249	U
59	BA	1253	A
59	BA	1255	U
59	BA	1256	G
59	BA	1265	A
59	BA	1271	G
59	BA	1272	A
59	BA	1273	U
59	BA	1274	A
59	BA	1286	A
59	BA	1288	U
59	BA	1289	C
59	BA	1300	U
59	BA	1301	A
59	BA	1302	A
59	BA	1306	C
59	BA	1307	A
59	BA	1312	U
59	BA	1314	C
59	BA	1321	A
59	BA	1325	G
59	BA	1328	G

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Mol	Chain	Res	Type
59	BA	1329	U
59	BA	1332	G
59	BA	1338	G
59	BA	1341	U
59	BA	1343	G
59	BA	1349	A
59	BA	1359	A
59	BA	1365	A
59	BA	1379	A
59	BA	1384	A
59	BA	1385	G
59	BA	1387	C
59	BA	1388	G
59	BA	1395	A
59	BA	1396	U
59	BA	1398	C
59	BA	1416	G
59	BA	1420	U
59	BA	1421	G
59	BA	1423	G
59	BA	1428	C
59	BA	144(B)	A
59	BA	1451	C
59	BA	1453	A
59	BA	1454	U
59	BA	1455	G
59	BA	1458	C
59	BA	1460	A
59	BA	1461	G
59	BA	1463	C
59	BA	1467	C
59	BA	1483	G
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	1529	A
59	BA	1535	U
59	BA	1536	A

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Mol	Chain	Res	Type
59	BA	1538	G
59	BA	1542	G
59	BA	1543	A
59	BA	1544	C
59	BA	1545	A
59	BA	1546	A
59	BA	1554	A
59	BA	1558	A
59	BA	1559	G
59	BA	1569	A
59	BA	1572	A
59	BA	1576	U
59	BA	1581	G
59	BA	1585	C
59	BA	1587	A
59	BA	1598	C
59	BA	1602	U
59	BA	1603	A
59	BA	1607	C
59	BA	1608	A
59	BA	1610	A
59	BA	1613	G
59	BA	1614	A
59	BA	1615	C
59	BA	1616	A
59	BA	1617	C
59	BA	163(B)	C
59	BA	1631	A
59	BA	1640	C
59	BA	1643	G
59	BA	1648	C
59	BA	1652	A
59	BA	1664	A
59	BA	1668	A
59	BA	1669	A
59	BA	1674	G
59	BA	1675	C
59	BA	1681	G
59	BA	1682	G
59	BA	1690	A
59	BA	1691	C
59	BA	1694	C

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Mol	Chain	Res	Type
59	BA	1696	G
59	BA	1698	A
59	BA	1699	G
59	BA	1702	G
59	BA	1705	G
59	BA	1707	G
59	BA	1729	A
59	BA	1732	A
59	BA	1742	C
59	BA	1756	G
59	BA	1762	A
59	BA	1763	G
59	BA	1764	G
59	BA	1773	A
59	BA	1780	A
59	BA	1781	C
59	BA	1783	A
59	BA	1787	A
59	BA	1791	A
59	BA	1796	U
59	BA	1800	C
59	BA	1802	A
59	BA	1803	A
59	BA	1810	A
59	BA	1811	G
59	BA	1814	G
59	BA	1815	A
59	BA	1816	G
59	BA	1820	U
59	BA	1821	A
59	BA	1829	A
59	BA	1831	G
59	BA	1838	C
59	BA	1840	G
59	BA	1847	A
59	BA	1848	A
59	BA	1851	U
59	BA	1860	G
59	BA	1888	G
59	BA	1889	A
59	BA	1896	G
59	BA	1900	A

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Mol	Chain	Res	Type
59	BA	1901	A
59	BA	1906	G
59	BA	1912	A
59	BA	1913	A
59	BA	1914	C
59	BA	1920	C
59	BA	1929	G
59	BA	1930	G
59	BA	1931	U
59	BA	1936	A
59	BA	1937	A
59	BA	1938	A
59	BA	1939	U
59	BA	1940	U
59	BA	1955	U
59	BA	1956	U
59	BA	1963	U
59	BA	1967	C
59	BA	1970	A
59	BA	1971	A
59	BA	1972	A
59	BA	1977	A
59	BA	1978	A
59	BA	1981	A
59	BA	1982	C
59	BA	1992	G
59	BA	2006	C
59	BA	2013	A
59	BA	2020	A
59	BA	2021	C
59	BA	2022	U
59	BA	2023	G
59	BA	2024	G
59	BA	2031	A
59	BA	2032	G
59	BA	2033	A
59	BA	2034	U
59	BA	2036	C
59	BA	2039	C
59	BA	2040	C
59	BA	2041	U
59	BA	2043	C

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Mol	Chain	Res	Type
59	BA	2044	C
59	BA	2052	G
59	BA	2055	C
59	BA	2056	G
59	BA	2060	A
59	BA	2061	G
59	BA	2062	A
59	BA	2067	G
59	BA	2068	U
59	BA	2069	G
59	BA	2093	G
59	BA	2111	C
59	BA	2115	G
59	BA	2116	G
59	BA	2117	A
59	BA	2118	U
59	BA	2120	G
59	BA	2130	U
59	BA	2132	U
59	BA	2133	G
59	BA	2136	C
59	BA	2144	U
59	BA	2148	G
59	BA	2154	G
59	BA	2158	A
59	BA	2159	G
59	BA	2166	G
59	BA	2168	G
59	BA	2171	A
59	BA	2172	U
59	BA	2173	A
59	BA	2198	A
59	BA	2210	G
59	BA	2211	G
59	BA	2212	A
59	BA	2213	U
59	BA	2215	G
59	BA	2225	A
59	BA	2239	G
59	BA	2245	U
59	BA	2251	G
59	BA	2266	A

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Mol	Chain	Res	Type
59	BA	2268	A
59	BA	2269	A
59	BA	2275	C
59	BA	2278	A
59	BA	2279	G
59	BA	2282	G
59	BA	2283	C
59	BA	2287	A
59	BA	2305	A
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	2327	A
59	BA	2334	G
59	BA	2336	A
59	BA	2343	C
59	BA	2345	G
59	BA	2346	A
59	BA	2347	C
59	BA	2350	C
59	BA	2361	A
59	BA	2371	G
59	BA	2377	A
59	BA	2378	A
59	BA	2379	G
59	BA	2383	G
59	BA	2385	C
59	BA	2391	G
59	BA	2402	C
59	BA	2403	C
59	BA	2406	U
59	BA	2407	G
59	BA	2422	A
59	BA	2423	U
59	BA	2425	A
59	BA	2426	A
59	BA	2427	C
59	BA	2428	G
59	BA	2429	G

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Mol	Chain	Res	Type
59	BA	2430	A
59	BA	2434	A
59	BA	2435	A
59	BA	2436	G
59	BA	2439	A
59	BA	2440	C
59	BA	2441	C
59	BA	2448	A
59	BA	2460	U
59	BA	2469	A
59	BA	2470	G
59	BA	2475	C
59	BA	2476	A
59	BA	2477	C
59	BA	2479	G
59	BA	2480	C
59	BA	2483	C
59	BA	2487	G
59	BA	2491	U
59	BA	2502	G
59	BA	2505	G
59	BA	2509	G
59	BA	2518	A
59	BA	2529	G
59	BA	2530	A
59	BA	2532	G
59	BA	2539	C
59	BA	2542	A
59	BA	2543	G
59	BA	2546	U
59	BA	2554	U
59	BA	2555	U
59	BA	2556	C
59	BA	2566	A
59	BA	2567	G
59	BA	2572	A
59	BA	2573	C
59	BA	2574	G
59	BA	2577	A
59	BA	2578	G
59	BA	2582	G
59	BA	2584	U

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Mol	Chain	Res	Type
59	BA	2585	U
59	BA	2586	C
59	BA	2597	G
59	BA	2602	A
59	BA	2603	G
59	BA	2609	U
59	BA	2610	C
59	BA	2611	U
59	BA	2612	C
59	BA	2615	U
59	BA	2618	G
59	BA	2621	A
59	BA	2623	G
59	BA	2630	G
59	BA	2645	G
59	BA	2646	C
59	BA	2663	G
59	BA	2665	A
59	BA	2667	C
59	BA	2672	G
59	BA	2682	U
59	BA	2689	U
59	BA	2690	C
59	BA	2702	U
59	BA	2703	C
59	BA	2711	A
59	BA	2712	U
59	BA	712(B)	A
59	BA	2713	A
59	BA	2715	C
59	BA	2726	U
59	BA	2727	G
59	BA	2730	C
59	BA	2731	G
59	BA	2733	A
59	BA	2740	A
59	BA	2748	A
59	BA	2751	G
59	BA	2755	C
59	BA	2757	A
59	BA	2764	A
59	BA	2765	A

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Mol	Chain	Res	Type
59	BA	2774	C
59	BA	2777	G
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	2791	C
59	BA	2792	G
59	BA	2793	G
59	BA	2797	U
59	BA	2799	A
59	BA	2805	G
59	BA	2811	G
59	BA	2818	G
59	BA	2820	A
59	BA	2821	A
59	BA	2823	A
59	BA	2827	C
59	BA	2833	G
59	BA	2834	G
59	BA	2835	A
59	BA	2849	U
59	BA	2851	A
59	BA	2856	C
59	BA	2862	G
59	BA	2866	U
59	BA	2872	G
59	BA	2879	C
59	BA	2880	C
59	BA	2881	C
59	BA	2886	G
59	BA	2892	A
59	BA	2894	G
60	BB	2	C
60	BB	13	A
60	BB	14	U
60	BB	15	A
60	BB	16	G
60	BB	25	A
60	BB	27	C

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Mol	Chain	Res	Type
60	BB	41	U
60	BB	42	C
60	BB	47	C
60	BB	48	A
60	BB	52	A
60	BB	56	G
60	BB	57	A
60	BB	66	A
60	BB	67	G
60	BB	71	C
60	BB	72	G
60	BB	73	A
60	BB	74	U
60	BB	90	C
20	CA	6	G
20	CA	7	G
20	CA	9	G
20	CA	32	A
20	CA	39	G
20	CA	47	C
20	CA	48	C
20	CA	51	A
20	CA	54	C
20	CA	59	A
20	CA	68(H)	G
20	CA	68(M)	U
20	CA	68(P)	C
20	CA	68(W)	G
20	CA	101	A
20	CA	109	A
20	CA	116	A
20	CA	117	G
20	CA	121	C
20	CA	129(A)	G
20	CA	131	C
20	CA	134	A
20	CA	151	A
20	CA	156	G
20	CA	163	C
20	CA	179	A
20	CA	183	G
20	CA	186(E)	C

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Mol	Chain	Res	Type
20	CA	186(H)	U
20	CA	186(I)	U
20	CA	186(K)	G
20	CA	195	A
20	CA	197	A
20	CA	201(C)	U
20	CA	216	G
20	CA	233	C
20	CA	244	U
20	CA	247	G
20	CA	251	G
20	CA	267	C
20	CA	272	C
20	CA	279	A
20	CA	280	C
20	CA	281	G
20	CA	289	G
20	CA	295	C
20	CA	301	G
20	CA	309	G
20	CA	315	A
20	CA	321	A
20	CA	328	C
20	CA	329	A
20	CA	332	G
20	CA	345	C
20	CA	347	G
20	CA	352	C
20	CA	353	A
20	CA	354	G
20	CA	356	A
20	CA	364	A
20	CA	367	U
20	CA	372	C
20	CA	373	A
20	CA	390	C
20	CA	392	G
20	CA	397	A
20	CA	398	C
20	CA	408	A
20	CA	412	A
20	CA	413	G

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Mol	Chain	Res	Type
20	CA	414	A
20	CA	422	C
20	CA	423	G
20	CA	424	G
20	CA	427	U
20	CA	429	U
20	CA	440	A
20	CA	452	A
20	CA	453	A
20	CA	458(B)	A
20	CA	458(D)	G
20	CA	458(E)	A
20	CA	485	G
20	CA	492	G
20	CA	495	A
20	CA	497	A
20	CA	498	U
20	CA	505	G
20	CA	508	C
20	CA	510	A
20	CA	511	C
20	CA	512	U
20	CA	518	C
20	CA	521	G
20	CA	524	G
20	CA	527	G
20	CA	529	G
20	CA	531	U
20	CA	532	A
20	CA	533	A
20	CA	547	A
20	CA	562	C
20	CA	564	C
20	CA	565	U
20	CA	567	G
20	CA	568	G
20	CA	572	A
20	CA	573	A
20	CA	574	A
20	CA	575	G
20	CA	576	G
20	CA	577	G

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Mol	Chain	Res	Type
20	CA	596	C
20	CA	619	U
20	CA	644	G
20	CA	653	A
20	CA	665	A
20	CA	666	G
20	CA	669	U
20	CA	688	G
20	CA	690	G
20	CA	694	A
20	CA	695	A
20	CA	701	C
20	CA	702	A
20	CA	714	G
20	CA	749	C
20	CA	753	A
20	CA	777	A
20	CA	778	G
20	CA	787	A
20	CA	793	U
20	CA	794	A
20	CA	805	C
20	CA	815	A
20	CA	816	A
20	CA	817	C
20	CA	818	G
20	CA	819	A
20	CA	821	G
20	CA	828	A
20	CA	838(A)	U
20	CA	838(B)	C
20	CA	848	C
20	CA	859	A
20	CA	867	G
20	CA	873	A
20	CA	874	G
20	CA	885	G
20	CA	888	G
20	CA	902	G
20	CA	926	G
20	CA	927	G
20	CA	934	C

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Mol	Chain	Res	Type
20	CA	946	A
20	CA	960	U
20	CA	961	U
20	CA	964	A
20	CA	966	G
20	CA	968	A
20	CA	969	A
20	CA	971	G
20	CA	972	C
20	CA	974	A
20	CA	976	G
20	CA	977	A
20	CA	978	A
20	CA	979	C
20	CA	980	C
20	CA	981	U
20	CA	983	A
20	CA	992	U
20	CA	993	G
20	CA	998(A)	C
20	CA	1004	A
20	CA	1025	U
20	CA	1028(B)	C
20	CA	1045	C
20	CA	1054	C
20	CA	1055	A
20	CA	1064	G
20	CA	1068	G
20	CA	1070	U
20	CA	1086	U
20	CA	1094	G
20	CA	1095	U
20	CA	1101	A
20	CA	1102	A
20	CA	1108	G
20	CA	1117	G
20	CA	1125	U
20	CA	1126	U
20	CA	1129	C
20	CA	1130	A
20	CA	1137	C
20	CA	1138	G

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Mol	Chain	Res	Type
20	CA	1139	G
20	CA	1140	C
20	CA	1146	A
20	CA	1159	U
20	CA	1171	G
20	CA	1181	G
20	CA	1184	G
20	CA	1190	G
20	CA	1191	A
20	CA	1192	C
20	CA	1193	G
20	CA	1196	U
20	CA	1197	G
20	CA	1200	C
20	CA	1201	A
20	CA	1212	U
20	CA	1213	A
20	CA	1214	C
20	CA	1220	G
20	CA	1225	A
20	CA	1227	A
20	CA	1233	G
20	CA	1238	A
20	CA	1239	A
20	CA	1241	G
20	CA	1256	A
20	CA	1257	U
20	CA	1260	C
20	CA	1273	G
20	CA	1279	A
20	CA	1280	A
20	CA	1281	U
20	CA	1283	G
20	CA	1287	A
20	CA	1300	G
20	CA	1301	U
20	CA	1302	U
20	CA	1317	C
20	CA	1320	C
20	CA	1322	C
20	CA	1331	G
20	CA	1338	G

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Mol	Chain	Res	Type
20	CA	1347	G
20	CA	1353	G
20	CA	1359	C
20	CA	1362(A)	C
20	CA	1364	U
20	CA	1370	G
20	CA	1377	A
20	CA	1394	A
20	CA	1397	C
20	CA	1398	A
20	CA	1411	C
20	CA	1419	G
20	CA	1431	C
20	CA	1440(B)	G
20	CA	1440(C)	G
20	CA	1440(D)	A
20	CA	1440(E)	G
20	CA	1440(G)	C
20	CA	1440(I)	A
20	CA	1440(J)	C
20	CA	1440(K)	G
20	CA	1440(L)	G
20	CA	1466	C
20	CA	1483	A
20	CA	1487	G
20	CA	1489	G
20	CA	1492	A
20	CA	1493	A
20	CA	1494	G
20	CA	1497	G
20	CA	1502	A
20	CA	1503	A
20	CA	1504	G
20	CA	1505	G
20	CA	1506	U
20	CA	1517	G
20	CA	1518	A
20	CA	1520	G
20	CA	1528	U
20	CA	1529	G
20	CA	1530	G
20	CA	1532	U

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Mol	Chain	Res	Type
20	CA	1533	C
20	CA	1534	A
20	CA	1535	C
20	CA	1536	C
20	CA	1538	C
21	CW	8	U
21	CW	16	U
21	CW	17	U
21	CW	18	G
21	CW	19	G
21	CW	20	U
21	CW	20(A)	U
21	CW	21	A
21	CW	22	G
21	CW	25	C
21	CW	36	U
21	CW	42	U
21	CW	46	G
21	CW	47	U
21	CW	48	C
21	CW	50	C
21	CW	51	A
21	CW	58	A
21	CW	59	A
21	CW	60	U
21	CW	61	C
21	CW	68	U
22	CV	9	G
22	CV	12	A
22	CV	16	A
22	CV	18	G
22	CV	19	G
22	CV	21	A
22	CV	23	A
22	CV	24	A
59	DA	7	G
59	DA	10	G
59	DA	12	U
59	DA	15	G
59	DA	17	G
59	DA	28	A
59	DA	34	C

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Mol	Chain	Res	Type
59	DA	35	G
59	DA	46	C
59	DA	49	A
59	DA	55	G
59	DA	58	G
59	DA	61	G
59	DA	64	A
59	DA	73	A
59	DA	75	G
59	DA	84	A
59	DA	90	U
59	DA	98	G
59	DA	99	U
59	DA	101	G
59	DA	102	G
59	DA	104	U
59	DA	110	G
59	DA	117	G
59	DA	118	A
59	DA	119	A
59	DA	120	U
59	DA	138	G
59	DA	140	A
59	DA	149	A
59	DA	181	A
59	DA	188	G
59	DA	196	A
59	DA	197	A
59	DA	199	A
59	DA	205	G
59	DA	215	G
59	DA	216	A
59	DA	221	A
59	DA	222	A
59	DA	227	A
59	DA	229	A
59	DA	230	U
59	DA	233	A
59	DA	248	G
59	DA	249	C
59	DA	250	G
59	DA	252	G

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Mol	Chain	Res	Type
59	DA	256	A
59	DA	261	G
59	DA	265	A
59	DA	266	G
59	DA	270(M)	U
59	DA	270(N)	U
59	DA	270(O)	G
59	DA	270(P)	U
59	DA	270(R)	C
59	DA	270(Y)	G
59	DA	271(C)	G
59	DA	271(D)	U
59	DA	271	G
59	DA	274	G
59	DA	275	G
59	DA	277	C
59	DA	279	C
59	DA	299	A
59	DA	302	C
59	DA	310	A
59	DA	312	G
59	DA	321	G
59	DA	322	A
59	DA	323	G
59	DA	324	A
59	DA	327	G
59	DA	329	G
59	DA	330	A
59	DA	349	G
59	DA	352	G
59	DA	353	G
59	DA	363(A)	G
59	DA	363(C)	G
59	DA	364	C
59	DA	380	U
59	DA	386	G
59	DA	387	U
59	DA	389	G
59	DA	396	G
59	DA	404	C
59	DA	405	U
59	DA	406	G

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Mol	Chain	Res	Type
59	DA	411	G
59	DA	412	A
59	DA	431	U
59	DA	434	U
59	DA	444	C
59	DA	446	G
59	DA	448	U
59	DA	449	A
59	DA	451	C
59	DA	456	C
59	DA	457	A
59	DA	459	U
59	DA	464	U
59	DA	465	G
59	DA	469	G
59	DA	470	A
59	DA	473	G
59	DA	475	U
59	DA	480	A
59	DA	481	G
59	DA	505	A
59	DA	508	G
59	DA	509	C
59	DA	527	C
59	DA	530	G
59	DA	531	C
59	DA	532	A
59	DA	533	G
59	DA	535	C
59	DA	541	C
59	DA	546	C
59	DA	556	G
59	DA	558	G
59	DA	559	G
59	DA	563	G
59	DA	573	G
59	DA	575	A
59	DA	586	A
59	DA	587	C
59	DA	595	C
59	DA	599	G
59	DA	600	G

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Mol	Chain	Res	Type
59	DA	603	A
59	DA	614	U
59	DA	615	G
59	DA	616	A
59	DA	617	G
59	DA	620	G
59	DA	621	A
59	DA	627	A
59	DA	628	G
59	DA	634	C
59	DA	637	A
59	DA	645	C
59	DA	646	A
59	DA	652	U
59	DA	654	U
59	DA	667	U
59	DA	671	C
59	DA	672	C
59	DA	685	A
59	DA	686	G
59	DA	695	G
59	DA	716	A
59	DA	717	G
59	DA	730	C
59	DA	738	G
59	DA	742	G
59	DA	748	G
59	DA	753	C
59	DA	765	G
59	DA	771	G
59	DA	776	G
59	DA	779	U
59	DA	782	A
59	DA	784	A
59	DA	785	G
59	DA	789	A
59	DA	790	C
59	DA	792	G
59	DA	794	G
59	DA	800	A
59	DA	805	G
59	DA	812	C

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Mol	Chain	Res	Type
59	DA	814	C
59	DA	819	A
59	DA	821	A
59	DA	822	U
59	DA	823	G
59	DA	826	U
59	DA	827	U
59	DA	829	A
59	DA	838	C
59	DA	845	G
59	DA	846	C
59	DA	847	U
59	DA	852	G
59	DA	859	G
59	DA	866	A
59	DA	870	A
59	DA	889	C
59	DA	890	A
59	DA	896	A
59	DA	897	C
59	DA	910	A
59	DA	917	A
59	DA	919	G
59	DA	932	G
59	DA	933	A
59	DA	938	G
59	DA	941	A
59	DA	946	G
59	DA	951	C
59	DA	959	A
59	DA	961	C
59	DA	973	A
59	DA	974(A)	G
59	DA	974(B)	C
59	DA	975	G
59	DA	978	G
59	DA	980	A
59	DA	983	A
59	DA	989	G
59	DA	990	A
59	DA	991	C
59	DA	996	A

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Mol	Chain	Res	Type
59	DA	1002	G
59	DA	1005	C
59	DA	1007	C
59	DA	1008	C
59	DA	1009	A
59	DA	1012	U
59	DA	1013	C
59	DA	1022	G
59	DA	1023	U
59	DA	1024	G
59	DA	1025	G
59	DA	1026	U
59	DA	1033	U
59	DA	1042	G
59	DA	1045	A
59	DA	1046	A
59	DA	1047	G
59	DA	1048	A
59	DA	1058	G
59	DA	1066	U
59	DA	1070	A
59	DA	1072	C
59	DA	1075	C
59	DA	1078	U
59	DA	1079	C
59	DA	1085	A
59	DA	1086	A
59	DA	1088	A
59	DA	1090	U
59	DA	1096	A
59	DA	1105	U
59	DA	1107	G
59	DA	1112	G
59	DA	1117	G
59	DA	1123	C
59	DA	1125	G
59	DA	1130	U
59	DA	1135	C
59	DA	1136	G
59	DA	1138	G
59	DA	1139	G
59	DA	114(B)	A

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Mol	Chain	Res	Type
59	DA	1153	C
59	DA	1175	U
59	DA	1176	G
59	DA	1186	G
59	DA	1187	G
59	DA	1194	A
59	DA	1199	U
59	DA	1204	A
59	DA	1206	G
59	DA	1210	A
59	DA	1212	G
59	DA	1214	A
59	DA	1215	G
59	DA	1221	C
59	DA	1226	A
59	DA	1227	G
59	DA	1241	A
59	DA	1244	G
59	DA	1247	A
59	DA	1248	G
59	DA	1249	U
59	DA	1253	A
59	DA	1254	A
59	DA	1256	G
59	DA	1262	A
59	DA	1265	A
59	DA	1271	G
59	DA	1272	A
59	DA	1273	U
59	DA	1274	A
59	DA	1286	A
59	DA	1289	C
59	DA	1300	U
59	DA	1301	A
59	DA	1302	A
59	DA	1305	C
59	DA	1307	A
59	DA	1312	U
59	DA	1314	C
59	DA	1325	G
59	DA	1329	U
59	DA	1332	G

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Mol	Chain	Res	Type
59	DA	1333	C
59	DA	1341	U
59	DA	1343	G
59	DA	1349	A
59	DA	1352	U
59	DA	1355	G
59	DA	1359	A
59	DA	1365	A
59	DA	1368	G
59	DA	1379	A
59	DA	1384	A
59	DA	1385	G
59	DA	1396	U
59	DA	1398	C
59	DA	1404	C
59	DA	1416	G
59	DA	1420	U
59	DA	1421	G
59	DA	1428	C
59	DA	144(B)	A
59	DA	149(B)	A
59	DA	1451	C
59	DA	1453	A
59	DA	1454	U
59	DA	1455	G
59	DA	1460	A
59	DA	1461	G
59	DA	1467	C
59	DA	1480	G
59	DA	1483	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	1499	C
59	DA	1536	A
59	DA	1537	C
59	DA	1538	G
59	DA	1540	G

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Mol	Chain	Res	Type
59	DA	1542	G
59	DA	1543	A
59	DA	1544	C
59	DA	1545	A
59	DA	1546	A
59	DA	1547	C
59	DA	1555	G
59	DA	1558	A
59	DA	1559	G
59	DA	1568	G
59	DA	1569	A
59	DA	1572	A
59	DA	1578	U
59	DA	1579	A
59	DA	1583	A
59	DA	1585	C
59	DA	1602	U
59	DA	1603	A
59	DA	1607	C
59	DA	1608	A
59	DA	1610	A
59	DA	1614	A
59	DA	1615	C
59	DA	1616	A
59	DA	1617	C
59	DA	1618	A
59	DA	1619	G
59	DA	1631	A
59	DA	1639	U
59	DA	1640	C
59	DA	1646	C
59	DA	1648	C
59	DA	1654	A
59	DA	1657	C
59	DA	1659	U
59	DA	1664	A
59	DA	1667	G
59	DA	1668	A
59	DA	1669	A
59	DA	1670	C
59	DA	1674	G
59	DA	1678	G

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Mol	Chain	Res	Type
59	DA	1681	G
59	DA	1694	C
59	DA	1695	G
59	DA	1698	A
59	DA	1699	G
59	DA	1707	G
59	DA	1729	A
59	DA	1732	A
59	DA	1759	A
59	DA	1763	G
59	DA	1764	G
59	DA	1773	A
59	DA	1779	U
59	DA	1780	A
59	DA	1781	C
59	DA	1782	C
59	DA	1783	A
59	DA	1784	A
59	DA	1786	A
59	DA	1787	A
59	DA	1791	A
59	DA	1796	U
59	DA	1799	G
59	DA	1800	C
59	DA	1801	G
59	DA	1802	A
59	DA	1815	A
59	DA	1816	G
59	DA	1820	U
59	DA	1821	A
59	DA	1826	G
59	DA	1829	A
59	DA	1833	U
59	DA	1847	A
59	DA	1848	A
59	DA	1857	G
59	DA	1858	G
59	DA	1878	G
59	DA	1886	C
59	DA	1888	G
59	DA	1889	A
59	DA	1898	U

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Mol	Chain	Res	Type
59	DA	1900	A
59	DA	1905	C
59	DA	1906	G
59	DA	1912	A
59	DA	1913	A
59	DA	1914	C
59	DA	1929	G
59	DA	1930	G
59	DA	1936	A
59	DA	1937	A
59	DA	1938	A
59	DA	1939	U
59	DA	1940	U
59	DA	1943	U
59	DA	1944	U
59	DA	1952	A
59	DA	1954	G
59	DA	1955	U
59	DA	1956	U
59	DA	1963	U
59	DA	1965	C
59	DA	1967	C
59	DA	1970	A
59	DA	1971	A
59	DA	1972	A
59	DA	1976	U
59	DA	1977	A
59	DA	1981	A
59	DA	1982	C
59	DA	1984	G
59	DA	1989	G
59	DA	1992	G
59	DA	1993	U
59	DA	1999	C
59	DA	2013	A
59	DA	2020	A
59	DA	2021	C
59	DA	2022	U
59	DA	2023	G
59	DA	2030	A
59	DA	2031	A
59	DA	2032	G

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Mol	Chain	Res	Type
59	DA	2033	A
59	DA	2034	U
59	DA	2036	C
59	DA	2040	C
59	DA	2041	U
59	DA	2042	A
59	DA	2043	C
59	DA	2044	C
59	DA	2052	G
59	DA	2055	C
59	DA	2056	G
59	DA	2060	A
59	DA	2061	G
59	DA	2062	A
59	DA	2067	G
59	DA	2068	U
59	DA	2069	G
59	DA	2089	U
59	DA	2092	U
59	DA	2093	G
59	DA	2115	G
59	DA	2116	G
59	DA	2117	A
59	DA	2118	U
59	DA	2120	G
59	DA	2131	G
59	DA	2132	U
59	DA	2133	G
59	DA	2136	C
59	DA	2144	U
59	DA	2148	G
59	DA	2154	G
59	DA	2159	G
59	DA	2170	A
59	DA	2171	A
59	DA	2173	A
59	DA	2190	G
59	DA	2198	A
59	DA	2199	A
59	DA	2209	C
59	DA	2210	G
59	DA	2211	G

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Mol	Chain	Res	Type
59	DA	2212	A
59	DA	2213	U
59	DA	2225	A
59	DA	2238	G
59	DA	2239	G
59	DA	2261	C
59	DA	2266	A
59	DA	2268	A
59	DA	2269	A
59	DA	2275	C
59	DA	2278	A
59	DA	2279	G
59	DA	2282	G
59	DA	2283	C
59	DA	2287	A
59	DA	2305	A
59	DA	2308	G
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	2325	G
59	DA	2327	A
59	DA	2334	G
59	DA	2336	A
59	DA	2345	G
59	DA	2346	A
59	DA	2347	C
59	DA	2350	C
59	DA	2358	G
59	DA	2361	A
59	DA	2377	A
59	DA	2383	G
59	DA	2385	C
59	DA	2400	G
59	DA	2402	C
59	DA	2405	G
59	DA	2410	G
59	DA	2411	A
59	DA	2422	A

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Mol	Chain	Res	Type
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	2448	A
59	DA	2468	G
59	DA	2469	A
59	DA	2470	G
59	DA	2476	A
59	DA	2477	C
59	DA	2479	G
59	DA	2480	C
59	DA	2482	G
59	DA	2484	G
59	DA	2491	U
59	DA	2497	A
59	DA	2502	G
59	DA	2503	A
59	DA	2504	U
59	DA	2505	G
59	DA	2509	G
59	DA	2517	C
59	DA	2518	A
59	DA	2519	U
59	DA	2529	G
59	DA	2530	A
59	DA	2532	G
59	DA	2542	A
59	DA	2543	G
59	DA	2554	U
59	DA	2556	C
59	DA	2565	A
59	DA	2566	A
59	DA	2567	G
59	DA	2572	A

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Mol	Chain	Res	Type
59	DA	2573	C
59	DA	2574	G
59	DA	2576	G
59	DA	2577	A
59	DA	2584	U
59	DA	2602	A
59	DA	2606	C
59	DA	2609	U
59	DA	2610	C
59	DA	2611	U
59	DA	2612	C
59	DA	2615	U
59	DA	2618	G
59	DA	2630	G
59	DA	2637	U
59	DA	2646	C
59	DA	2663	G
59	DA	2665	A
59	DA	2666	C
59	DA	2667	C
59	DA	2682	U
59	DA	2689	U
59	DA	2702	U
59	DA	2703	C
59	DA	2711	A
59	DA	2712	U
59	DA	712(B)	A
59	DA	2713	A
59	DA	2715	C
59	DA	2716	U
59	DA	2725	A
59	DA	2726	U
59	DA	2727	G
59	DA	2730	C
59	DA	2731	G
59	DA	2732	G
59	DA	2733	A
59	DA	2744	G
59	DA	2755	C
59	DA	2758	A
59	DA	2764	A
59	DA	2765	A

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Mol	Chain	Res	Type
59	DA	2769	C
59	DA	2777	G
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	2797	U
59	DA	2799	A
59	DA	2815	C
59	DA	2818	G
59	DA	2820	A
59	DA	2821	A
59	DA	2823	A
59	DA	2833	G
59	DA	2834	G
59	DA	2835	A
59	DA	2849	U
59	DA	2851	A
59	DA	2856	C
59	DA	2862	G
59	DA	2866	U
59	DA	2872	G
59	DA	2880	C
59	DA	2886	G
59	DA	2892	A
59	DA	2894	G
60	DB	2	C
60	DB	13	A
60	DB	15	A
60	DB	16	G
60	DB	25	A
60	DB	35	U
60	DB	41	U
60	DB	45	A
60	DB	46	A
60	DB	48	A
60	DB	52	A
60	DB	67	G
60	DB	73	A

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Mol	Chain	Res	Type
60	DB	74	U
60	DB	85	G
60	DB	90	C
60	DB	108	C

All (88) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	AA	115	G
20	AA	243	A
20	AA	266	G
20	AA	281	G
20	AA	328	C
20	AA	429	U
20	AA	484	G
20	AA	687	A
20	AA	739	C
20	AA	748	C
20	AA	992	U
20	AA	1064	G
20	AA	1101	A
20	AA	1145	C
20	AA	1504	G
20	AA	1532	U
20	AA	1537	U
21	AW	41	A
22	AV	18	G
59	BA	221	A
59	BA	241	A
59	BA	271(C)	G
59	BA	278	A
59	BA	363(G)	A
59	BA	474	G
59	BA	479	A
59	BA	586	A
59	BA	1007	C
59	BA	1022	G
59	BA	1240	U
59	BA	1542	G
59	BA	1558	A
59	BA	1786	A
59	BA	1912	A

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Mol	Chain	Res	Type
59	BA	1913	A
59	BA	1937	A
59	BA	2039	C
59	BA	2040	C
59	BA	2092	U
59	BA	2171	A
59	BA	2447	G
59	BA	2688	U
59	BA	2750	A
59	BA	2780	G
59	BA	2781	A
59	BA	2791	C
60	BB	66	A
20	CA	115	G
20	CA	186(J)	G
20	CA	243	A
20	CA	266	G
20	CA	328	C
20	CA	484	G
20	CA	687	A
20	CA	748	C
20	CA	992	U
20	CA	1101	A
20	CA	1145	C
20	CA	1200	C
20	CA	1504	G
20	CA	1532	U
20	CA	1535	C
20	CA	1537	U
21	CW	41	A
22	CV	8	A
22	CV	18	G
59	DA	221	A
59	DA	271(C)	G
59	DA	363(G)	A
59	DA	464	U
59	DA	474	G
59	DA	479	A
59	DA	1022	G
59	DA	1240	U
59	DA	1542	G
59	DA	1558	A

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Mol	Chain	Res	Type
59	DA	1786	A
59	DA	1912	A
59	DA	1913	A
59	DA	1937	A
59	DA	2040	C
59	DA	2092	U
59	DA	2212	A
59	DA	2447	G
59	DA	2481	G
59	DA	2518	A
59	DA	2780	G
60	DB	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	KBE	CU	1	24	8,8,9	0.65	0	7,8,10	1.86	1 (14%)
24	5OH	AU	6	24	8,12,13	0.67	0	3,16,18	2.90	1 (33%)
24	UAL	CU	5	24	7,8,9	2.56	2 (28%)	5,9,11	1.78	1 (20%)
24	KBE	AU	1	24	8,8,9	0.62	0	7,8,10	1.53	1 (14%)
24	UAL	AU	5	24	7,8,9	2.47	2 (28%)	5,9,11	1.38	1 (20%)
24	DPP	CU	2	24	3,5,6	0.39	0	1,5,7	0.49	0
24	5OH	CU	6	24	8,12,13	0.72	0	3,16,18	2.00	2 (66%)
24	DPP	AU	2	24	3,5,6	0.35	0	1,5,7	1.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	CU	1	24	-	4/7/7/8	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	UAL	CU	5	24	-	0/3/7/9	-
24	KBE	AU	1	24	-	2/7/7/8	-
24	UAL	AU	5	24	-	0/3/7/9	-
24	DPP	CU	2	24	-	0/2/4/6	-
24	5OH	CU	6	24	-	1/2/18/20	0/1/1/1
24	DPP	AU	2	24	-	0/2/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C-CA	5.30	1.53	1.45
24	AU	5	UAL	C-CA	5.29	1.53	1.45
24	CU	5	UAL	C1-N1	-3.25	1.35	1.40
24	AU	5	UAL	C1-N1	-2.86	1.35	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AU	6	5OH	CR-CB-CA	4.67	117.65	112.61
24	CU	1	KBE	CB-CA-C	4.61	119.03	112.25
24	CU	5	UAL	O-C-CA	-3.63	120.78	125.39
24	AU	1	KBE	CB-CA-C	3.39	117.24	112.25
24	AU	5	UAL	O-C-CA	-2.74	121.90	125.39
24	CU	6	5OH	CR-CB-CA	2.62	115.44	112.61
24	CU	6	5OH	O-C-CA	-2.25	118.88	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	C-CA-CB-N
24	CU	1	KBE	C-CA-CB-N
24	CU	1	KBE	C-CA-CB-CG
24	CU	6	5OH	C-CA-CB-CR
24	CU	1	KBE	N-CB-CG-CD
24	CU	1	KBE	CA-CB-CG-CD
24	AU	1	KBE	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	AY	702	-	24,30,30	1.28	2 (8%)	30,47,47	1.57	6 (20%)
61	FUA	AY	701	-	39,40,40	1.70	7 (17%)	49,64,64	1.83	12 (24%)
62	GDP	CY	702	-	24,30,30	1.28	2 (8%)	30,47,47	1.57	6 (20%)
61	FUA	CY	701	-	39,40,40	1.68	6 (15%)	49,64,64	1.98	13 (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
62	GDP	AY	702	-	-	3/12/32/32	0/3/3/3
61	FUA	AY	701	-	-	6/15/92/92	0/4/4/4
62	GDP	CY	702	-	-	3/12/32/32	0/3/3/3
61	FUA	CY	701	-	-	5/15/92/92	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	701	FUA	C29-C22	4.68	1.54	1.47
61	AY	701	FUA	C23-C22	-4.31	1.40	1.51
61	AY	701	FUA	C23-C24	-4.30	1.39	1.53
61	AY	701	FUA	C29-C22	4.17	1.53	1.47
61	CY	701	FUA	C23-C24	-4.11	1.39	1.53
61	CY	701	FUA	C23-C22	-3.99	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	GDP	C5-C6	-3.91	1.39	1.47
62	AY	702	GDP	C5-C6	-3.90	1.39	1.47
61	CY	701	FUA	C14-C8	-3.40	1.53	1.59
61	AY	701	FUA	C24-C25	-3.28	1.39	1.50
61	CY	701	FUA	C24-C25	-3.01	1.40	1.50
61	AY	701	FUA	C14-C8	-2.96	1.53	1.59
61	CY	701	FUA	C25-C26	2.65	1.40	1.32
61	AY	701	FUA	O6-C3	-2.55	1.38	1.43
61	AY	701	FUA	C25-C26	2.36	1.39	1.32
62	CY	702	GDP	O4'-C1'	2.25	1.44	1.41
62	AY	702	GDP	O4'-C1'	2.23	1.44	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	FUA	C13-C12-C11	-6.40	102.94	111.90
61	AY	701	FUA	C13-C12-C11	-5.83	103.73	111.90
61	CY	701	FUA	C1-C10-C5	4.41	114.02	107.76
61	AY	701	FUA	C16-O2-C31	-3.99	110.99	117.06
62	CY	702	GDP	PA-O3A-PB	-3.93	119.33	132.83
62	AY	702	GDP	PA-O3A-PB	-3.93	119.34	132.83
61	CY	701	FUA	C15-C14-C8	-3.61	112.99	116.84
61	CY	701	FUA	O2-C31-C32	3.57	117.66	111.09
61	CY	701	FUA	C16-O2-C31	-3.21	112.18	117.06
61	AY	701	FUA	C1-C10-C5	3.20	112.30	107.76
62	CY	702	GDP	C2-N1-C6	-3.17	119.27	125.10
62	AY	702	GDP	C2-N1-C6	-3.16	119.28	125.10
61	AY	701	FUA	O2-C31-C32	3.07	116.73	111.09
61	AY	701	FUA	C21-C14-C8	-2.97	109.53	112.27
61	CY	701	FUA	C10-C9-C11	2.94	120.90	114.76
62	CY	702	GDP	C8-N7-C5	2.87	108.47	102.99
62	AY	702	GDP	C8-N7-C5	2.83	108.39	102.99
61	CY	701	FUA	C21-C14-C8	-2.80	109.69	112.27
61	CY	701	FUA	C20-C8-C14	-2.78	106.72	110.85
61	AY	701	FUA	C1-C2-C3	-2.68	106.51	111.72
62	AY	702	GDP	O4'-C1'-C2'	-2.65	103.05	106.93
61	CY	701	FUA	C1-C2-C3	-2.64	106.60	111.72
62	CY	702	GDP	O4'-C1'-C2'	-2.64	103.07	106.93
62	AY	702	GDP	C5-C6-N1	2.63	118.60	113.95
62	CY	702	GDP	C5-C6-N1	2.63	118.59	113.95
61	AY	701	FUA	C10-C9-C11	2.53	120.05	114.76
61	CY	701	FUA	O5-C29-O4	-2.46	117.98	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	FUA	C7-C8-C14	-2.28	108.71	110.77
61	AY	701	FUA	C28-C26-C27	2.28	119.64	114.60
61	CY	701	FUA	C14-C8-C9	-2.22	105.06	109.40
61	AY	701	FUA	O5-C29-O4	-2.20	118.57	123.61
61	AY	701	FUA	C20-C8-C14	-2.17	107.62	110.85
61	CY	701	FUA	C23-C24-C25	2.13	118.86	111.88
62	AY	702	GDP	O6-C6-C5	-2.11	120.24	124.37
62	CY	702	GDP	O6-C6-C5	-2.10	120.27	124.37
61	AY	701	FUA	C19-C10-C9	-2.02	108.22	113.09
61	CY	701	FUA	C19-C10-C9	-2.00	108.26	113.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

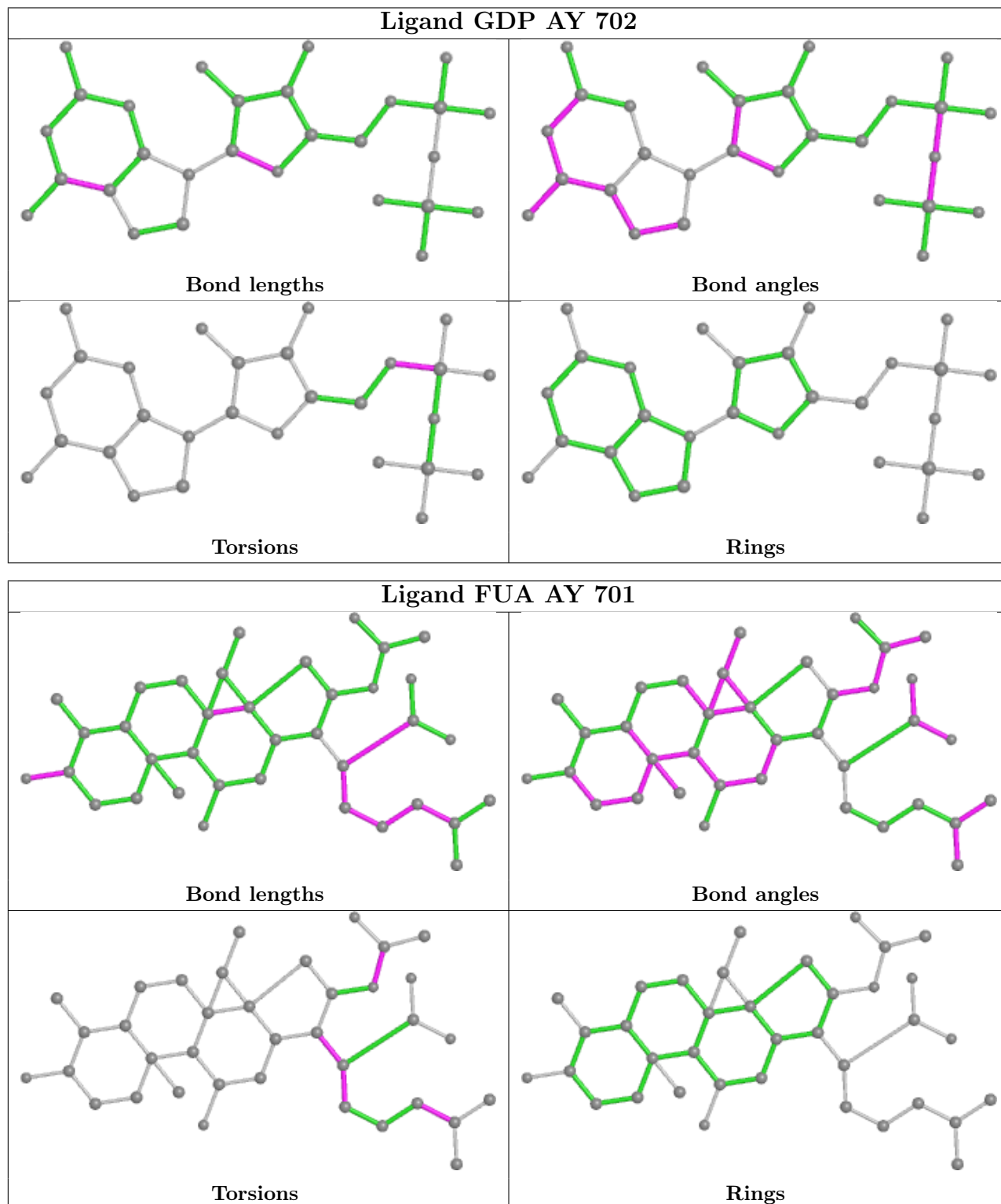
Mol	Chain	Res	Type	Atoms
61	AY	701	FUA	C13-C17-C22-C29
61	AY	701	FUA	C17-C22-C23-C24
61	AY	701	FUA	C29-C22-C23-C24
61	CY	701	FUA	C13-C17-C22-C29
61	CY	701	FUA	C17-C22-C23-C24
61	CY	701	FUA	C29-C22-C23-C24
62	AY	702	GDP	C5'-O5'-PA-O3A
62	AY	702	GDP	C5'-O5'-PA-O1A
62	CY	702	GDP	C5'-O5'-PA-O3A
62	CY	702	GDP	C5'-O5'-PA-O1A
61	CY	701	FUA	C32-C31-O2-C16
61	AY	701	FUA	C32-C31-O2-C16
61	AY	701	FUA	O3-C31-O2-C16
61	CY	701	FUA	O3-C31-O2-C16
61	AY	701	FUA	C24-C25-C26-C27
62	AY	702	GDP	C5'-O5'-PA-O2A
62	CY	702	GDP	C5'-O5'-PA-O2A

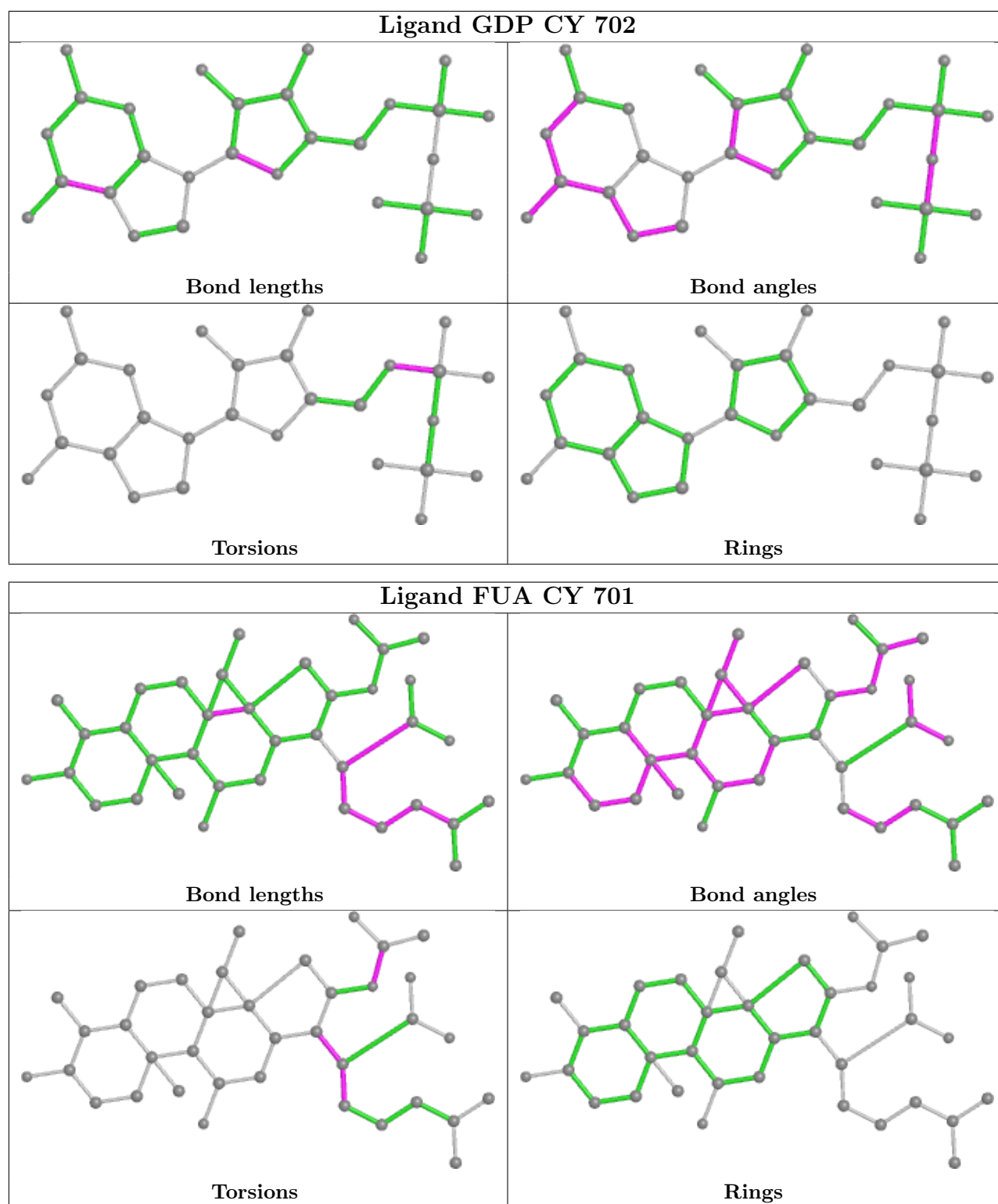
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	De	1
54	Be	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	37.69
1	Be	30:UNK	C	51:ALA	N	36.65

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%)	0.48	32 (13%) 3 4	4, 59, 144, 223	0
1	CB	235/235 (100%)	0.48	29 (12%) 4 5	5, 60, 155, 214	0
2	AC	207/207 (100%)	0.27	23 (11%) 5 6	4, 63, 136, 190	0
2	CC	207/207 (100%)	0.42	22 (10%) 6 7	3, 57, 130, 186	0
3	AD	208/208 (100%)	-0.54	4 (1%) 66 61	4, 57, 142, 206	0
3	CD	208/208 (100%)	-0.42	3 (1%) 75 69	14, 72, 144, 196	0
4	AE	151/151 (100%)	0.43	21 (13%) 2 3	5, 34, 122, 151	0
4	CE	151/151 (100%)	0.17	16 (10%) 6 7	4, 35, 133, 165	0
5	AF	101/101 (100%)	-0.86	0 100 100	4, 27, 93, 145	0
5	CF	101/101 (100%)	-0.87	0 100 100	5, 37, 115, 163	0
6	AG	155/155 (100%)	0.58	24 (15%) 2 2	10, 78, 153, 229	0
6	CG	155/155 (100%)	1.03	30 (19%) 1 1	3, 84, 172, 210	0
7	AH	138/138 (100%)	0.06	1 (0%) 87 83	3, 31, 89, 166	0
7	CH	138/138 (100%)	0.21	10 (7%) 15 15	1, 37, 130, 199	0
8	AI	127/127 (100%)	1.06	33 (25%) 0 0	6, 72, 140, 199	0
8	CI	127/127 (100%)	0.61	16 (12%) 3 5	14, 84, 152, 237	0
9	AJ	99/99 (100%)	-0.12	10 (10%) 7 7	9, 68, 136, 163	0
9	CJ	99/99 (100%)	-0.28	4 (4%) 38 33	13, 65, 154, 217	0
10	AK	119/119 (100%)	-0.13	4 (3%) 45 40	7, 56, 137, 180	0
10	CK	119/119 (100%)	0.09	11 (9%) 9 9	8, 55, 145, 175	0
11	AL	125/125 (100%)	0.48	20 (16%) 1 2	5, 39, 105, 171	0
11	CL	125/125 (100%)	0.64	19 (15%) 2 2	8, 52, 134, 176	0
12	AM	125/125 (100%)	0.93	26 (20%) 1 1	23, 90, 167, 199	0
12	CM	125/125 (100%)	0.58	20 (16%) 1 2	14, 90, 166, 190	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	0.55	8 (13%) 3 4	8, 38, 114, 139	0
13	CN	60/60 (100%)	0.12	0 100 100	8, 42, 131, 166	0
14	AO	88/88 (100%)	-0.65	2 (2%) 60 54	5, 37, 108, 158	0
14	CO	88/88 (100%)	-0.50	0 100 100	8, 49, 130, 197	0
15	AP	84/84 (100%)	0.56	11 (13%) 3 4	18, 68, 131, 171	0
15	CP	84/84 (100%)	0.51	11 (13%) 3 4	8, 79, 159, 224	0
16	AQ	100/100 (100%)	0.12	6 (6%) 21 19	9, 43, 120, 169	0
16	CQ	100/100 (100%)	0.29	11 (11%) 5 6	5, 43, 118, 142	0
17	AR	70/70 (100%)	-0.53	1 (1%) 75 69	7, 30, 134, 185	0
17	CR	70/70 (100%)	-0.32	4 (5%) 23 21	7, 28, 130, 193	0
18	AS	79/79 (100%)	0.56	12 (15%) 2 2	15, 78, 159, 206	0
18	CS	79/79 (100%)	0.08	8 (10%) 7 7	10, 80, 154, 204	0
19	AT	99/99 (100%)	-0.11	4 (4%) 38 33	4, 64, 120, 186	0
19	CT	99/99 (100%)	0.09	8 (8%) 12 12	16, 71, 155, 187	0
20	AA	1511/1511 (100%)	-0.31	34 (2%) 60 54	3, 62, 163, 289	0
20	CA	1511/1511 (100%)	-0.34	28 (1%) 66 61	5, 63, 173, 323	0
21	AW	77/77 (100%)	-0.49	1 (1%) 77 71	21, 91, 179, 234	0
21	CW	77/77 (100%)	-0.10	6 (7%) 13 13	44, 97, 221, 273	0
22	AV	23/23 (100%)	0.88	5 (21%) 0 0	56, 136, 187, 205	0
22	CV	23/23 (100%)	2.08	9 (39%) 0 0	66, 119, 215, 230	0
23	AY	667/687 (97%)	-0.10	49 (7%) 15 15	5, 64, 147, 208	0
23	CY	667/687 (97%)	0.03	63 (9%) 8 9	4, 68, 150, 203	0
24	AU	2/6 (33%)	0.18	0 100 100	155, 155, 155, 155	0
24	CU	2/6 (33%)	-0.18	0 100 100	81, 81, 81, 88	0
25	BC	228/228 (100%)	0.85	50 (21%) 0 0	45, 128, 217, 259	0
25	DC	228/228 (100%)	1.69	78 (34%) 0 0	33, 153, 230, 287	0
26	BD	275/275 (100%)	-0.42	5 (1%) 68 62	4, 26, 103, 166	0
26	DD	275/275 (100%)	-0.53	7 (2%) 57 51	4, 25, 107, 210	0
27	BE	205/205 (100%)	-0.41	3 (1%) 73 68	1, 31, 135, 229	0
27	DE	205/205 (100%)	-0.28	7 (3%) 45 40	6, 41, 144, 221	0
28	BF	208/208 (100%)	0.49	27 (12%) 3 4	6, 49, 162, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	0.61	34 (16%) 1 2	10, 62, 162, 266	0
29	BG	181/181 (100%)	1.39	56 (30%) 0 0	11, 91, 152, 197	0
29	DG	181/181 (100%)	1.35	58 (32%) 0 0	33, 105, 176, 209	0
30	BH	167/167 (100%)	-0.50	1 (0%) 89 86	3, 47, 130, 224	0
30	DH	167/167 (100%)	-0.32	5 (2%) 50 44	6, 56, 141, 187	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	1.16	39 (27%) 0 0	17, 104, 194, 230	0
32	DK	140/140 (100%)	1.58	44 (31%) 0 0	37, 124, 205, 244	0
33	BN	138/138 (100%)	0.58	23 (16%) 1 2	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.49	20 (14%) 2 3	59, 81, 104, 111	0
34	BO	122/122 (100%)	-0.03	3 (2%) 57 51	5, 33, 94, 148	0
34	DO	122/122 (100%)	-0.17	4 (3%) 46 41	4, 30, 131, 183	0
35	BP	146/146 (100%)	0.20	13 (8%) 9 10	7, 55, 131, 173	0
35	DP	146/146 (100%)	0.01	11 (7%) 14 14	1, 60, 152, 204	0
36	BQ	141/141 (100%)	-0.65	2 (1%) 75 69	20, 43, 113, 170	0
36	DQ	141/141 (100%)	-0.49	6 (4%) 35 31	8, 32, 107, 219	0
37	BR	117/117 (100%)	-0.20	5 (4%) 35 31	7, 38, 125, 156	0
37	DR	117/117 (100%)	-0.25	6 (5%) 28 25	2, 38, 126, 213	0
38	BS	99/99 (100%)	1.01	23 (23%) 0 0	27, 104, 191, 225	0
38	DS	99/99 (100%)	2.04	40 (40%) 0 0	11, 106, 194, 248	0
39	BT	138/138 (100%)	-0.10	7 (5%) 28 25	6, 53, 139, 225	0
39	DT	138/138 (100%)	0.09	11 (7%) 12 12	3, 68, 141, 201	0
40	BU	117/117 (100%)	-0.07	5 (4%) 35 31	11, 22, 80, 175	0
40	DU	117/117 (100%)	-0.23	3 (2%) 56 49	6, 20, 94, 136	0
41	BV	101/101 (100%)	0.15	5 (4%) 28 25	0, 32, 104, 143	0
41	DV	101/101 (100%)	-0.21	3 (2%) 50 44	2, 32, 117, 147	0
42	BW	113/113 (100%)	-0.05	6 (5%) 26 24	8, 32, 103, 140	0
42	DW	113/113 (100%)	-0.05	5 (4%) 34 30	2, 31, 116, 157	0
43	BX	93/93 (100%)	-0.31	3 (3%) 47 42	5, 51, 118, 172	0
43	DX	93/93 (100%)	0.08	5 (5%) 25 23	7, 50, 136, 198	0
44	BY	107/107 (100%)	-0.27	7 (6%) 18 17	12, 69, 151, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DY	107/107 (100%)	-0.13	6 (5%) 24 22	6, 70, 150, 196	0
45	BZ	185/185 (100%)	-0.41	7 (3%) 40 36	13, 52, 123, 175	0
45	DZ	185/185 (100%)	-0.18	7 (3%) 40 36	10, 61, 135, 194	0
46	B0	84/84 (100%)	-0.51	2 (2%) 59 53	6, 53, 127, 163	0
46	D0	84/84 (100%)	-0.31	2 (2%) 59 53	7, 58, 132, 217	0
47	B2	71/71 (100%)	-0.70	0 100 100	12, 61, 137, 175	0
47	D2	71/71 (100%)	-0.70	0 100 100	9, 60, 127, 145	0
48	B3	60/60 (100%)	-0.44	0 100 100	8, 31, 96, 111	0
48	D3	60/60 (100%)	-0.25	0 100 100	13, 29, 101, 126	0
49	B5	59/59 (100%)	-0.52	1 (1%) 70 64	8, 37, 148, 208	0
49	D5	59/59 (100%)	-0.40	0 100 100	6, 44, 156, 223	0
50	B6	50/50 (100%)	0.06	4 (8%) 12 12	12, 92, 147, 163	0
50	D6	50/50 (100%)	0.84	10 (20%) 1 1	31, 89, 175, 242	0
51	B7	49/49 (100%)	1.04	11 (22%) 0 0	9, 16, 135, 218	0
51	D7	49/49 (100%)	1.54	13 (26%) 0 0	11, 32, 107, 180	0
52	B8	64/64 (100%)	-0.01	3 (4%) 31 28	5, 46, 98, 130	0
52	D8	64/64 (100%)	0.08	3 (4%) 31 28	7, 56, 123, 178	0
53	B9	37/37 (100%)	-0.52	0 100 100	10, 26, 148, 246	0
53	D9	37/37 (100%)	-0.59	0 100 100	8, 19, 104, 158	0
54	Be	72/102 (70%)	2.74	41 (56%) 0 0	24, 113, 183, 201	0
54	De	72/102 (70%)	2.77	29 (40%) 0 0	18, 114, 206, 259	0
55	Bf	0/31	-	-	-	-
55	Bg	0/31	-	-	-	-
55	Df	0/31	-	-	-	-
55	Dg	0/31	-	-	-	-
56	Bh	0/30	-	-	-	-
56	Dh	0/30	-	-	-	-
57	B1	93/93 (100%)	0.94	22 (23%) 0 0	1, 79, 187, 243	0
57	D1	93/93 (100%)	1.06	26 (27%) 0 0	8, 72, 174, 241	0
58	B4	35/35 (100%)	2.45	17 (48%) 0 0	74, 144, 233, 266	0
58	D4	35/35 (100%)	3.00	23 (65%) 0 0	64, 158, 226, 275	0
59	BA	2879/2879 (100%)	-0.50	17 (0%) 89 86	3, 43, 145, 276	0
59	DA	2879/2879 (100%)	-0.46	28 (0%) 82 77	0, 47, 163, 315	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BB	119/119 (100%)	-0.41	4 (3%) 45 40	21, 108, 175, 210	0
60	DB	119/119 (100%)	0.04	10 (8%) 11 11	23, 97, 186, 258	0
All	All	22686/23318 (97%)	-0.05	1575 (6%) 16 16	0, 57, 160, 323	0

All (1575) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	Be	58	THR	13.8
32	DK	67	PHE	12.3
54	De	99	VAL	12.3
54	De	59	GLU	12.3
32	DK	62	ASP	12.1
58	D4	4	GLY	11.9
38	DS	53	SER	11.8
57	D1	24	ALA	11.1
54	De	58	THR	11.1
54	Be	122	VAL	10.9
44	DY	107	ASP	10.9
25	DC	113	ALA	10.7
54	De	52	ALA	10.7
51	D7	48	LYS	10.7
54	Be	121	VAL	10.2
18	AS	48	THR	10.1
54	De	51	ALA	10.0
54	De	100	LYS	9.9
25	DC	107	GLY	9.6
38	DS	37	ALA	9.4
6	AG	80	VAL	9.3
58	D4	24	THR	9.3
25	DC	175	PRO	9.2
54	De	53	PRO	8.9
51	D7	47	ARG	8.9
22	CV	26	A	8.8
57	B1	16	ASN	8.7
12	AM	124	PRO	8.7
59	DA	2894	G	8.6
32	BK	14	ALA	8.5
25	DC	112	ASP	8.4
25	DC	48	LEU	8.4
25	DC	136	GLY	8.1
10	CK	41	THR	8.1

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Mol	Chain	Res	Type	RSRZ
54	De	122	VAL	8.0
25	DC	69	LEU	7.9
38	DS	55	ALA	7.9
32	DK	66	THR	7.9
54	De	82	THR	7.8
12	AM	20	THR	7.8
54	Be	119	GLY	7.8
38	DS	83	LYS	7.7
25	DC	106	ASP	7.7
57	B1	15	ALA	7.7
32	DK	10	LEU	7.6
58	B4	24	THR	7.6
7	CH	25	ASP	7.6
1	CB	29	ALA	7.5
54	De	54	ALA	7.5
38	DS	54	LEU	7.4
29	BG	117	PHE	7.4
28	DF	194	MET	7.4
29	BG	64	THR	7.3
54	Be	59	GLU	7.3
6	CG	80	VAL	7.3
25	DC	162	ILE	7.3
10	AK	128	ALA	7.3
28	BF	27	GLU	7.2
25	DC	125	GLY	7.2
1	CB	30	ARG	7.1
6	CG	47	CYS	7.1
58	B4	30	GLU	7.1
38	DS	57	LYS	7.0
6	CG	79	ARG	7.0
29	DG	22	ARG	6.8
32	BK	62	ASP	6.8
29	BG	66	GLN	6.8
17	CR	19	LYS	6.7
57	D1	38	SER	6.7
54	De	56	GLU	6.7
25	DC	49	GLY	6.7
32	DK	57	ILE	6.7
25	DC	210	LEU	6.7
2	CC	190	ARG	6.6
32	DK	60	TYR	6.6
2	CC	131	ARG	6.6

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Mol	Chain	Res	Type	RSRZ
25	BC	126	SER	6.6
57	D1	16	ASN	6.6
32	BK	10	LEU	6.6
54	De	55	GLU	6.5
54	Be	65	LYS	6.5
25	BC	128	LEU	6.5
38	DS	48	LEU	6.5
25	DC	127	LYS	6.5
50	D6	37	ARG	6.5
22	CV	25	A	6.5
38	BS	59	LYS	6.4
44	BY	107	ASP	6.4
2	CC	164	ARG	6.4
57	B1	35	THR	6.4
25	DC	75	VAL	6.4
58	D4	23	GLU	6.4
23	CY	231	TYR	6.3
38	DS	82	ILE	6.3
32	BK	57	ILE	6.3
10	CK	31	THR	6.3
16	CQ	38	ARG	6.3
25	DC	179	ALA	6.3
32	BK	21	PRO	6.3
58	D4	7	PRO	6.2
6	CG	81	GLY	6.2
25	DC	163	GLU	6.2
38	BS	53	SER	6.2
20	CA	1534	A	6.1
22	CV	4	A	6.1
11	AL	83	VAL	6.0
23	AY	385	THR	6.0
22	CV	12	A	6.0
51	B7	47	ARG	6.0
32	BK	23	VAL	6.0
57	D1	32	LYS	6.0
2	AC	3	ASN	6.0
38	DS	34	HIS	5.9
23	AY	5	VAL	5.9
38	BS	57	LYS	5.9
25	BC	162	ILE	5.9
58	B4	14	ILE	5.9
1	CB	131	PRO	5.8

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Mol	Chain	Res	Type	RSRZ
23	AY	4	LYS	5.8
6	CG	82	GLY	5.8
57	B1	28	GLY	5.8
32	BK	22	PRO	5.8
57	B1	25	LYS	5.8
6	CG	44	TYR	5.8
29	DG	66	GLN	5.8
29	DG	90	LEU	5.8
32	BK	9	LYS	5.8
59	DA	2799	A	5.8
20	CA	1028(D)	C	5.8
23	CY	311	ALA	5.7
51	D7	41	ARG	5.7
6	AG	22	LEU	5.7
57	D1	23	LYS	5.7
57	D1	19	GLN	5.7
25	DC	135	ARG	5.7
59	DA	2132	U	5.7
28	BF	193	VAL	5.7
25	DC	34	ALA	5.6
25	DC	108	TRP	5.6
6	CG	156	TRP	5.6
23	AY	231	TYR	5.6
25	DC	126	SER	5.6
57	D1	15	ALA	5.6
57	B1	14	VAL	5.6
25	BC	30	VAL	5.6
25	BC	101	ILE	5.6
8	CI	8	GLY	5.5
6	CG	32	ARG	5.5
4	AE	135	THR	5.5
38	DS	38	GLN	5.5
60	DB	25	A	5.5
58	B4	27	THR	5.5
25	BC	112	ASP	5.5
43	DX	34	ALA	5.5
23	CY	237	PRO	5.5
54	Be	112	LYS	5.5
33	BN	50	ASP	5.5
38	BS	68	GLN	5.4
20	AA	941	G	5.4
10	CK	127	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
8	CI	15	ALA	5.4
15	AP	19	ILE	5.4
28	DF	155	LEU	5.4
54	Be	120	ALA	5.4
29	DG	41	GLN	5.4
29	DG	92	VAL	5.4
10	AK	127	LYS	5.4
54	Be	63	ILE	5.4
16	AQ	39	SER	5.4
58	D4	6	HIS	5.4
54	De	83	GLY	5.4
58	D4	5	ILE	5.4
38	DS	33	LYS	5.3
58	B4	25	TYR	5.3
25	DC	176	VAL	5.3
38	BS	101	LEU	5.3
54	Be	102	GLY	5.3
11	CL	68	ALA	5.3
4	AE	120	THR	5.3
29	BG	134	GLY	5.3
57	D1	33	LYS	5.3
8	AI	88	TYR	5.3
6	CG	54	THR	5.3
10	CK	128	ALA	5.3
15	CP	39	TYR	5.2
28	DF	125	LEU	5.2
38	DS	39	ILE	5.2
29	DG	51	ARG	5.2
36	DQ	141	GLN	5.2
25	DC	101	ILE	5.2
58	D4	25	TYR	5.2
50	D6	54	ILE	5.2
54	De	104	SER	5.2
51	B7	48	LYS	5.2
60	BB	25	A	5.2
10	AK	129	SER	5.2
23	CY	531	GLY	5.2
8	AI	84	ALA	5.2
12	CM	124	PRO	5.2
23	AY	255	ILE	5.2
44	DY	34	LYS	5.2
28	DF	11	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
23	AY	232	LEU	5.2
25	DC	30	VAL	5.1
23	AY	237	PRO	5.1
29	BG	90	LEU	5.1
32	DK	21	PRO	5.1
54	De	101	GLU	5.1
1	CB	100	GLY	5.1
25	BC	41	THR	5.1
39	DT	138	ALA	5.1
20	CA	1099	G	5.1
32	DK	115	LEU	5.1
25	DC	124	VAL	5.1
38	DS	35	ILE	5.1
32	DK	61	ALA	5.1
12	AM	125	ARG	5.1
29	BG	118	ARG	5.1
25	BC	42	VAL	5.1
6	CG	53	LYS	5.1
50	D6	12	GLU	5.1
38	DS	88	ASP	5.0
51	B7	41	ARG	5.0
59	DA	2798	C	5.0
58	B4	17	GLY	5.0
57	D1	37	ILE	5.0
32	BK	20	ALA	5.0
58	B4	31	ILE	5.0
25	DC	153	ILE	5.0
54	De	57	LYS	5.0
9	CJ	58	ASP	5.0
12	CM	47	ASP	4.9
1	AB	16	HIS	4.9
22	CV	13	A	4.9
19	AT	19	SER	4.9
4	AE	49	PRO	4.9
57	B1	34	THR	4.9
1	AB	150	SER	4.9
38	DS	106	ARG	4.9
25	DC	70	GLY	4.8
22	CV	7	G	4.8
58	D4	31	ILE	4.8
32	DK	114	ASP	4.8
54	Be	99	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
8	AI	4	TYR	4.8
4	AE	106	PRO	4.8
44	DY	106	LEU	4.8
32	BK	66	THR	4.8
54	Be	92	LEU	4.8
4	CE	135	THR	4.8
15	CP	42	ARG	4.8
29	DG	135	LEU	4.8
59	BA	2897	U	4.8
23	AY	107	VAL	4.8
2	CC	184	TYR	4.7
28	DF	176	LEU	4.7
12	AM	66	LEU	4.7
29	BG	68	PRO	4.7
2	AC	45	LYS	4.7
32	DK	23	VAL	4.7
38	DS	101	LEU	4.7
6	AG	81	GLY	4.7
54	De	98	PRO	4.7
29	DG	54	GLU	4.7
8	AI	15	ALA	4.7
12	CM	113	PRO	4.7
23	AY	310	ALA	4.7
54	De	60	PHE	4.7
12	AM	23	TYR	4.6
12	CM	39	ILE	4.6
25	BC	33	LEU	4.6
58	D4	11	PRO	4.6
51	D7	49	ARG	4.6
40	DU	94	ASN	4.6
1	AB	148	TYR	4.6
1	AB	207	ALA	4.6
32	DK	65	PHE	4.6
54	Be	88	GLU	4.6
25	BC	124	VAL	4.6
1	AB	135	GLN	4.6
54	Be	118	VAL	4.6
38	BS	87	PHE	4.6
58	D4	3	GLU	4.6
4	CE	28	PHE	4.6
29	BG	75	LYS	4.6
1	CB	99	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
8	CI	77	ILE	4.6
29	BG	135	LEU	4.6
51	D7	42	LEU	4.6
15	AP	22	THR	4.6
9	AJ	59	SER	4.5
28	DF	172	TRP	4.5
28	BF	114	VAL	4.5
4	AE	29	GLY	4.5
40	BU	118	GLY	4.5
38	BS	65	VAL	4.5
50	D6	47	THR	4.5
54	Be	104	SER	4.5
12	AM	27	LYS	4.5
6	CG	153	HIS	4.5
25	BC	113	ALA	4.5
38	DS	59	LYS	4.5
2	AC	170	GLN	4.5
29	DG	102	PHE	4.5
18	CS	32	LYS	4.5
32	DK	9	LYS	4.5
45	DZ	165	VAL	4.4
33	BN	43	THR	4.4
39	DT	106	SER	4.4
32	DK	19	PRO	4.4
2	CC	207	VAL	4.4
28	DF	10	PRO	4.4
59	BA	2793	G	4.4
8	CI	117	HIS	4.4
9	AJ	58	ASP	4.4
25	DC	110	ASP	4.4
7	CH	49	GLU	4.4
8	CI	122	ALA	4.4
29	DG	6	ALA	4.4
17	CR	20	ALA	4.4
25	DC	132	LEU	4.4
8	AI	26	VAL	4.4
28	DF	134	GLY	4.4
29	DG	87	PRO	4.4
29	BG	115	ARG	4.4
23	CY	6	GLU	4.3
20	CA	1533	C	4.3
32	BK	8	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
26	BD	40	THR	4.3
57	D1	35	THR	4.3
12	CM	85	GLY	4.3
35	DP	5	ASP	4.3
51	B7	42	LEU	4.3
8	CI	121	ARG	4.3
43	BX	74	PRO	4.3
1	CB	101	MET	4.3
28	BF	157	VAL	4.3
25	DC	128	LEU	4.3
25	BC	63	VAL	4.3
28	BF	113	ALA	4.3
50	D6	24	GLU	4.3
54	Be	91	ASP	4.3
33	BN	49	GLY	4.3
23	AY	122	TRP	4.3
1	CB	151	GLY	4.3
1	CB	170	GLU	4.3
38	BS	105	ALA	4.3
29	BG	179	PRO	4.3
32	BK	24	GLY	4.2
20	AA	1028(D)	C	4.2
60	DB	30	C	4.2
25	DC	33	LEU	4.2
29	DG	106	LEU	4.2
32	BK	40	ALA	4.2
2	AC	129	ALA	4.2
20	AA	1367	C	4.2
2	CC	201	TYR	4.2
58	D4	29	PRO	4.2
11	AL	32	PHE	4.2
32	DK	12	LEU	4.2
8	AI	63	ILE	4.2
2	AC	190	ARG	4.2
8	AI	45	ALA	4.2
38	BS	41	ASP	4.2
23	CY	107	VAL	4.2
8	AI	62	TYR	4.2
11	AL	86	ARG	4.2
1	AB	124	SER	4.1
38	DS	65	VAL	4.1
38	BS	44	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
54	Be	94	GLU	4.1
20	CA	1098	C	4.1
32	BK	27	LEU	4.1
34	BO	11	ALA	4.1
25	DC	139	PRO	4.1
39	BT	106	SER	4.1
54	Be	73	GLU	4.1
57	B1	38	SER	4.1
23	CY	135	PHE	4.1
25	DC	47	LYS	4.1
37	DR	69	ASP	4.1
28	BF	57	VAL	4.1
23	AY	106	VAL	4.1
29	BG	6	ALA	4.1
29	DG	182	LYS	4.1
32	DK	76	TYR	4.1
29	BG	49	ASP	4.1
19	CT	71	THR	4.1
28	DF	193	VAL	4.1
29	BG	61	ALA	4.1
10	CK	32	ILE	4.1
23	CY	66	THR	4.1
57	D1	18	ILE	4.1
57	D1	39	LYS	4.1
1	CB	28	PHE	4.1
32	BK	85	GLU	4.0
54	De	117	ALA	4.0
6	CG	43	PHE	4.0
29	DG	155	MET	4.0
16	AQ	2	PRO	4.0
20	AA	942	G	4.0
32	BK	18	THR	4.0
23	CY	310	ALA	4.0
44	BY	3	VAL	4.0
44	BY	108	THR	4.0
29	BG	155	MET	4.0
25	BC	62	THR	4.0
12	AM	65	LYS	4.0
38	BS	33	LYS	4.0
57	B1	43	TYR	4.0
54	Be	55	GLU	4.0
1	CB	132	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
28	BF	125	LEU	4.0
58	B4	4	GLY	4.0
60	DB	28	C	4.0
38	DS	107	GLU	4.0
20	CA	1238	A	4.0
19	CT	10	LEU	4.0
23	CY	83	ASP	4.0
29	BG	119	GLY	4.0
38	DS	109	GLY	4.0
38	DS	41	ASP	4.0
32	DK	56	GLU	3.9
1	CB	27	LYS	3.9
20	CA	1367	C	3.9
22	AV	5	A	3.9
23	AY	181	LEU	3.9
7	CH	90	GLY	3.9
29	BG	74	LYS	3.9
1	AB	208	ILE	3.9
6	AG	26	PHE	3.9
20	AA	951	G	3.9
12	AM	123	ALA	3.9
38	BS	34	HIS	3.9
29	BG	63	ILE	3.9
25	DC	227	PRO	3.9
29	BG	60	LEU	3.9
26	BD	48	ARG	3.9
25	DC	215	VAL	3.9
29	DG	97	ASP	3.9
29	DG	109	VAL	3.9
44	BY	106	LEU	3.9
25	BC	74	ARG	3.9
29	DG	178	PHE	3.9
38	DS	56	LEU	3.8
33	BN	42	TRP	3.8
8	AI	17	VAL	3.8
23	CY	5	VAL	3.8
13	AN	2	ALA	3.8
8	CI	73	GLN	3.8
57	D1	40	ARG	3.8
25	DC	36	ALA	3.8
25	DC	104	ILE	3.8
28	BF	11	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	CB	144	ARG	3.8
2	CC	45	LYS	3.8
4	AE	48	ALA	3.8
25	BC	163	GLU	3.8
23	AY	384	ILE	3.8
28	BF	154	VAL	3.8
18	CS	33	THR	3.8
57	B1	19	GLN	3.8
29	BG	39	ILE	3.8
13	AN	61	TRP	3.8
57	B1	21	ARG	3.8
4	CE	8	GLU	3.8
32	DK	37	PHE	3.8
11	AL	93	LEU	3.8
23	CY	105	ILE	3.8
12	AM	122	LYS	3.8
2	CC	26	LYS	3.8
6	AG	152	ALA	3.8
11	CL	20	LYS	3.8
1	AB	170	GLU	3.8
51	B7	49	ARG	3.7
58	D4	13	ARG	3.7
7	CH	31	PHE	3.7
25	BC	79	ALA	3.7
38	BS	35	ILE	3.7
15	CP	14	ASN	3.7
12	AM	85	GLY	3.7
58	D4	21	VAL	3.7
25	DC	58	ASN	3.7
11	AL	31	PRO	3.7
38	BS	88	ASP	3.7
21	CW	20(A)	U	3.7
42	DW	113	LYS	3.7
32	DK	55	VAL	3.7
28	BF	116	ASP	3.7
23	AY	6	GLU	3.7
8	CI	113	LYS	3.7
9	CJ	59	SER	3.7
11	CL	83	VAL	3.7
23	CY	330	VAL	3.7
26	DD	48	ARG	3.7
59	BA	2794	C	3.7

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Mol	Chain	Res	Type	RSRZ
18	AS	66	MET	3.7
28	BF	111	ALA	3.7
20	AA	51	A	3.7
20	AA	353	A	3.7
4	AE	27	ARG	3.7
23	CY	122	TRP	3.7
28	BF	1	MET	3.7
32	DK	24	GLY	3.6
12	AM	22	ILE	3.6
35	BP	110	TYR	3.6
38	DS	30	ARG	3.6
33	BN	1	MET	3.6
32	BK	39	LYS	3.6
34	BO	99	PHE	3.6
39	BT	1	MET	3.6
12	CM	20	THR	3.6
58	D4	22	ILE	3.6
26	DD	267	SER	3.6
59	BA	2317	C	3.6
6	CG	50	ILE	3.6
23	CY	65	ILE	3.6
23	CY	391	GLY	3.6
29	DG	141	PHE	3.6
11	CL	19	ARG	3.6
26	BD	49	ILE	3.6
41	BV	12	TYR	3.6
57	D1	42	GLN	3.6
23	AY	134	ALA	3.6
39	DT	1	MET	3.6
29	DG	89	GLY	3.6
11	CL	21	LYS	3.6
25	DC	131	ILE	3.6
35	DP	65	ARG	3.6
23	CY	181	LEU	3.6
32	BK	119	ASP	3.6
18	CS	17	GLU	3.6
45	DZ	166	SER	3.6
28	DF	181	LEU	3.6
20	AA	934	C	3.6
29	DG	137	GLU	3.6
32	DK	79	ARG	3.6
28	DF	185	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	CC	163	ALA	3.5
8	AI	61	ALA	3.5
29	BG	151	ALA	3.5
57	D1	13	ILE	3.5
54	Be	64	LEU	3.5
25	DC	138	LEU	3.5
11	AL	85	ILE	3.5
12	CM	40	ASN	3.5
11	CL	18	VAL	3.5
57	D1	34	THR	3.5
25	DC	137	LEU	3.5
28	DF	111	ALA	3.5
29	BG	137	GLU	3.5
2	CC	165	THR	3.5
38	DS	40	ILE	3.5
6	AG	120	ILE	3.5
23	CY	571	SER	3.5
34	DO	99	PHE	3.5
25	BC	127	LYS	3.5
44	BY	36	ALA	3.5
23	AY	222	ASP	3.5
25	DC	169	THR	3.5
7	CH	70	GLN	3.5
29	DG	100	TRP	3.5
29	BG	121	ASN	3.5
37	BR	2	ARG	3.5
19	CT	9	ASN	3.5
38	BS	27	SER	3.5
16	CQ	20	THR	3.5
17	CR	22	VAL	3.5
1	CB	137	ARG	3.5
8	AI	19	LEU	3.5
2	AC	2	GLY	3.5
57	B1	13	ILE	3.4
1	AB	132	LYS	3.4
20	CA	1028(C)	G	3.4
12	CM	2	ALA	3.4
38	DS	51	ALA	3.4
43	DX	18	TYR	3.4
15	AP	31	LYS	3.4
45	DZ	127	LYS	3.4
8	AI	56	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
15	AP	71	ARG	3.4
18	AS	31	ILE	3.4
20	AA	1028(E)	G	3.4
13	AN	3	ARG	3.4
41	BV	75	PHE	3.4
33	DN	133	GLN	3.4
29	BG	116	ASP	3.4
23	AY	228	MET	3.4
18	AS	33	THR	3.4
57	B1	24	ALA	3.4
29	DG	14	GLU	3.4
29	DG	39	ILE	3.4
57	B1	29	GLY	3.4
9	AJ	57	LYS	3.4
32	BK	69	THR	3.4
1	CB	133	LYS	3.4
25	BC	104	ILE	3.4
25	DC	157	ILE	3.4
60	DB	60	C	3.4
8	AI	42	ARG	3.4
29	BG	51	ARG	3.4
2	CC	148	GLY	3.4
25	DC	109	MET	3.4
32	DK	64	SER	3.4
41	DV	7	THR	3.4
32	DK	27	LEU	3.4
37	BR	81	ASP	3.4
54	Be	76	LYS	3.4
6	AG	156	TRP	3.4
32	BK	56	GLU	3.4
38	BS	20	ARG	3.4
25	BC	105	LEU	3.4
28	DF	8	GLN	3.4
54	Be	101	GLU	3.4
20	AA	147	G	3.3
25	DC	114	VAL	3.3
20	AA	1349	A	3.3
21	CW	63	C	3.3
59	DA	2897	U	3.3
23	AY	233	GLU	3.3
4	CE	14	ARG	3.3
23	CY	18	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
27	DE	162	ALA	3.3
35	DP	7	ARG	3.3
28	BF	92	PRO	3.3
45	DZ	95	PRO	3.3
58	B4	7	PRO	3.3
58	D4	28	LYS	3.3
28	BF	176	LEU	3.3
29	DG	3	LEU	3.3
20	AA	971	G	3.3
60	DB	27	C	3.3
33	DN	58	ASP	3.3
25	DC	170	GLY	3.3
8	AI	50	LEU	3.3
28	DF	27	GLU	3.3
9	CJ	60	ARG	3.3
11	AL	56	ALA	3.3
12	AM	8	GLU	3.3
23	CY	635	GLU	3.3
60	DB	5	C	3.3
23	CY	104	ALA	3.3
32	DK	2	LYS	3.3
2	AC	185	GLY	3.3
32	BK	115	LEU	3.3
38	DS	60	GLY	3.3
20	AA	824	C	3.3
23	CY	106	VAL	3.3
23	CY	133	ILE	3.3
32	BK	112	MET	3.3
33	BN	38	HIS	3.3
10	CK	42	TRP	3.3
29	DG	88	ILE	3.3
57	B1	18	ILE	3.3
12	AM	83	ASP	3.3
33	BN	48	MET	3.3
35	DP	6	LEU	3.3
38	DS	31	SER	3.3
25	BC	32	GLU	3.3
25	DC	140	ASN	3.3
1	AB	152	PHE	3.3
1	AB	205	ASP	3.3
23	CY	259	PHE	3.3
11	AL	68	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
12	CM	123	ALA	3.3
45	BZ	117	LEU	3.3
34	DO	77	ILE	3.3
4	AE	43	LEU	3.3
11	CL	53	ARG	3.3
4	CE	48	ALA	3.2
27	DE	127	ASP	3.2
33	DN	4	TYR	3.2
29	DG	13	GLU	3.2
29	DG	42	GLY	3.2
59	BA	2802	G	3.2
23	CY	637	ARG	3.2
23	AY	82	ILE	3.2
11	AL	20	LYS	3.2
32	BK	37	PHE	3.2
57	D1	14	VAL	3.2
1	AB	144	ARG	3.2
58	B4	32	TYR	3.2
23	CY	227	ILE	3.2
27	DE	89	ASP	3.2
11	CL	22	SER	3.2
12	AM	49	THR	3.2
37	BR	50	HIS	3.2
58	B4	29	PRO	3.2
2	CC	46	GLU	3.2
26	DD	229	VAL	3.2
33	DN	1	MET	3.2
25	BC	3	LYS	3.2
38	DS	19	LYS	3.2
2	AC	164	ARG	3.2
34	DO	76	ALA	3.2
23	AY	531	GLY	3.2
23	CY	258	VAL	3.2
12	AM	15	VAL	3.2
36	BQ	140	ALA	3.2
16	CQ	26	GLN	3.2
29	BG	26	GLN	3.2
22	CV	11	U	3.2
38	DS	49	VAL	3.2
1	AB	134	GLU	3.2
1	CB	36	ARG	3.2
13	AN	7	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
8	AI	86	VAL	3.2
10	CK	38	ASN	3.2
18	CS	57	HIS	3.2
27	BE	73	GLU	3.2
32	DK	126	MET	3.2
54	De	120	ALA	3.2
59	DA	2612	C	3.2
32	DK	63	ARG	3.2
39	BT	20	PRO	3.2
25	DC	209	PHE	3.2
1	AB	29	ALA	3.1
60	DB	29	A	3.1
1	CB	102	LEU	3.1
25	BC	125	GLY	3.1
29	DG	180	PHE	3.1
37	DR	74	LYS	3.1
16	CQ	10	VAL	3.1
26	BD	36	PRO	3.1
54	De	91	ASP	3.1
22	AV	8	A	3.1
29	BG	136	ARG	3.1
1	AB	211	ILE	3.1
19	AT	9	ASN	3.1
37	BR	60	LEU	3.1
25	DC	35	THR	3.1
39	DT	25	GLY	3.1
4	AE	25	ARG	3.1
4	AE	20	GLN	3.1
57	D1	20	ARG	3.1
25	DC	174	ALA	3.1
32	BK	60	TYR	3.1
2	AC	186	PHE	3.1
8	CI	69	GLY	3.1
44	BY	104	GLY	3.1
28	DF	112	MET	3.1
32	DK	101	TRP	3.1
40	BU	94	ASN	3.1
59	BA	115	C	3.1
4	CE	132	ALA	3.1
3	AD	122	ARG	3.1
16	AQ	26	GLN	3.1
39	DT	20	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
12	CM	125	ARG	3.1
32	BK	5	VAL	3.1
29	DG	2	PRO	3.1
52	B8	33	ASN	3.1
59	DA	425	G	3.1
38	DS	20	ARG	3.1
51	B7	12	ARG	3.1
1	CB	135	GLN	3.1
25	BC	164	PHE	3.1
26	DD	231	HIS	3.1
29	BG	36	LYS	3.1
12	CM	122	LYS	3.1
1	AB	166	ASP	3.0
51	D7	46	VAL	3.0
54	De	121	VAL	3.0
59	DA	2146	C	3.0
57	D1	21	ARG	3.0
13	AN	15	LYS	3.0
11	AL	16	GLU	3.0
59	DA	400	G	3.0
29	BG	114	ILE	3.0
29	BG	140	ILE	3.0
11	CL	56	ALA	3.0
54	De	70	LYS	3.0
12	AM	19	LEU	3.0
15	AP	10	GLY	3.0
25	DC	129	GLY	3.0
59	DA	10	G	3.0
4	AE	28	PHE	3.0
11	AL	28	LYS	3.0
29	BG	41	GLN	3.0
29	BG	111	LEU	3.0
23	CY	382	GLU	3.0
15	CP	19	ILE	3.0
23	AY	123	ARG	3.0
29	BG	45	GLU	3.0
28	DF	157	VAL	3.0
28	DF	154	VAL	3.0
23	AY	383	THR	3.0
2	CC	166	GLU	3.0
29	BG	178	PHE	3.0
25	DC	20	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
43	DX	74	PRO	3.0
12	CM	56	LEU	3.0
6	AG	79	ARG	3.0
23	AY	118	SER	3.0
1	AB	118	LEU	3.0
12	CM	34	LEU	3.0
50	D6	34	LEU	3.0
29	BG	54	GLU	3.0
39	BT	50	ILE	3.0
45	DZ	97	GLU	3.0
23	AY	167	PRO	3.0
28	DF	192	LEU	3.0
20	CA	1062	U	3.0
25	DC	190	ILE	3.0
54	De	81	ILE	3.0
20	CA	353	A	3.0
35	BP	23	PRO	3.0
42	DW	92	ARG	3.0
57	B1	58	ILE	3.0
58	B4	22	ILE	3.0
58	D4	10	VAL	3.0
25	DC	31	LYS	3.0
29	BG	157	ILE	3.0
12	CM	21	TYR	3.0
23	AY	104	ALA	3.0
28	BF	80	ALA	3.0
23	AY	17	ILE	3.0
16	AQ	38	ARG	2.9
23	CY	242	LEU	2.9
36	BQ	97	VAL	2.9
38	DS	27	SER	2.9
19	AT	22	ARG	2.9
25	BC	83	LYS	2.9
4	CE	29	GLY	2.9
25	BC	174	ALA	2.9
4	AE	18	ARG	2.9
29	DG	96	ARG	2.9
33	BN	116	LEU	2.9
54	Be	54	ALA	2.9
11	CL	123	LYS	2.9
25	DC	197	LEU	2.9
38	DS	58	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
45	BZ	70	LEU	2.9
25	DC	102	GLN	2.9
50	B6	28	ARG	2.9
54	De	84	LEU	2.9
33	DN	11	PRO	2.9
12	AM	102	ARG	2.9
20	AA	112	G	2.9
42	DW	17	VAL	2.9
2	AC	4	LYS	2.9
6	CG	136	LYS	2.9
32	BK	65	PHE	2.9
25	BC	58	ASN	2.9
25	BC	110	ASP	2.9
9	AJ	49	VAL	2.9
29	DG	5	VAL	2.9
20	CA	643	C	2.9
21	CW	62	C	2.9
2	CC	149	ALA	2.9
4	CE	86	ALA	2.9
6	CG	20	ASP	2.9
10	CK	65	ALA	2.9
54	Be	97	GLY	2.9
20	CA	1239	A	2.9
1	CB	154	LEU	2.9
29	BG	2	PRO	2.9
33	BN	45	ASN	2.9
33	BN	19	GLU	2.9
54	Be	71	LYS	2.9
6	CG	85	TYR	2.9
34	DO	122	LEU	2.9
2	CC	25	GLY	2.9
20	AA	182	U	2.9
29	DG	116	ASP	2.9
35	BP	144	GLU	2.9
46	B0	77	ARG	2.9
51	D7	39	ARG	2.9
4	AE	132	ALA	2.9
41	DV	8	GLY	2.9
23	CY	230	LYS	2.9
20	CA	1195	C	2.9
23	CY	575	VAL	2.8
29	DG	64	THR	2.8

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Mol	Chain	Res	Type	RSRZ
51	D7	35	ARG	2.8
11	AL	119	LYS	2.8
33	DN	2	LYS	2.8
38	BS	38	GLN	2.8
59	DA	2790	A	2.8
1	AB	101	MET	2.8
58	B4	1	MET	2.8
12	AM	25	ILE	2.8
25	BC	59	VAL	2.8
11	CL	112	ASP	2.8
38	DS	52	SER	2.8
33	DN	134	ARG	2.8
2	CC	189	ALA	2.8
6	AG	46	ALA	2.8
36	DQ	27	VAL	2.8
32	BK	2	LYS	2.8
28	DF	133	ASN	2.8
2	CC	200	ALA	2.8
6	AG	155	ARG	2.8
2	AC	175	LEU	2.8
7	CH	35	ILE	2.8
32	DK	96	VAL	2.8
59	BA	790	C	2.8
28	BF	95	ARG	2.8
1	CB	114	ARG	2.8
33	BN	61	ARG	2.8
58	B4	11	PRO	2.8
20	CA	974	A	2.8
23	CY	287	PRO	2.8
35	DP	134	ALA	2.8
33	BN	51	PHE	2.8
28	DF	50	SER	2.8
12	CM	8	GLU	2.8
18	CS	65	ASN	2.8
25	BC	210	LEU	2.8
32	DK	59	ILE	2.8
54	Be	89	ALA	2.8
59	BA	1544	C	2.8
54	De	64	LEU	2.8
3	AD	84	LYS	2.8
39	BT	2	ASN	2.8
29	DG	57	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
25	BC	182	PRO	2.8
11	AL	19	ARG	2.8
32	DK	69	THR	2.8
1	AB	127	ILE	2.7
2	AC	166	GLU	2.7
39	DT	24	PRO	2.7
23	CY	228	MET	2.7
23	CY	389	LEU	2.7
59	DA	2334	G	2.7
12	AM	24	GLY	2.7
42	DW	93	ALA	2.7
4	CE	27	ARG	2.7
23	CY	290	LYS	2.7
28	DF	46	ARG	2.7
35	DP	57	THR	2.7
1	AB	12	GLU	2.7
18	AS	17	GLU	2.7
23	AY	369	LEU	2.7
28	BF	115	ALA	2.7
29	DG	34	LEU	2.7
36	DQ	28	ALA	2.7
17	CR	21	LYS	2.7
33	BN	84	LYS	2.7
19	CT	20	LEU	2.7
26	BD	38	LYS	2.7
59	DA	2144	U	2.7
20	AA	104	G	2.7
20	CA	942	G	2.7
1	AB	167	PRO	2.7
25	DC	2	PRO	2.7
37	DR	30	THR	2.7
57	D1	36	GLY	2.7
23	CY	369	LEU	2.7
60	DB	61	G	2.7
20	AA	49	U	2.7
29	DG	59	GLU	2.7
11	AL	53	ARG	2.7
38	DS	69	VAL	2.7
58	D4	1	MET	2.7
60	BB	26	A	2.7
23	CY	180	VAL	2.7
28	DF	115	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
39	DT	48	ILE	2.7
59	DA	383	U	2.7
4	CE	12	LEU	2.7
35	BP	136	GLU	2.7
23	AY	133	ILE	2.7
28	BF	78	ILE	2.7
23	CY	238	THR	2.7
25	DC	3	LYS	2.7
32	BK	118	THR	2.7
37	DR	47	PHE	2.7
42	BW	2	GLU	2.7
16	CQ	69	LYS	2.7
33	DN	43	THR	2.7
20	AA	1362(A)	C	2.7
28	DF	118	ALA	2.7
57	D1	26	ARG	2.7
29	BG	65	GLY	2.7
45	DZ	155	LEU	2.7
51	D7	31	LEU	2.7
23	CY	236	GLU	2.7
27	DE	73	GLU	2.7
39	BT	63	VAL	2.7
23	AY	529	ILE	2.7
12	AM	93	ARG	2.6
8	AI	41	VAL	2.6
2	CC	185	GLY	2.6
6	AG	65	ALA	2.6
25	BC	12	LEU	2.6
25	DC	160	GLY	2.6
29	BG	25	TYR	2.6
33	DN	19	GLU	2.6
57	D1	43	TYR	2.6
2	CC	157	ILE	2.6
1	AB	114	ARG	2.6
6	CG	55	GLY	2.6
19	CT	89	ARG	2.6
23	AY	311	ALA	2.6
29	BG	124	SER	2.6
57	D1	28	GLY	2.6
2	AC	192	THR	2.6
25	BC	52	PRO	2.6
4	AE	134	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
10	CK	129	SER	2.6
23	CY	233	GLU	2.6
1	AB	99	GLY	2.6
59	BA	1384	A	2.6
50	D6	39	TYR	2.6
6	AG	62	PHE	2.6
29	DG	107	LEU	2.6
10	CK	67	ASP	2.6
25	DC	133	GLY	2.6
57	B1	85	LEU	2.6
23	AY	510	VAL	2.6
18	AS	35	SER	2.6
15	CP	18	ARG	2.6
23	AY	387	ASP	2.6
44	DY	2	ARG	2.6
50	B6	40	CYS	2.6
11	CL	35	GLY	2.6
25	BC	69	LEU	2.6
32	DK	4	VAL	2.6
23	AY	132	ARG	2.6
23	CY	132	ARG	2.6
35	BP	148	LEU	2.6
59	DA	387	U	2.6
36	DQ	140	ALA	2.6
57	B1	32	LYS	2.6
15	AP	32	TYR	2.6
25	DC	121	MET	2.6
6	CG	83	ALA	2.6
32	BK	12	LEU	2.6
11	AL	55	VAL	2.6
29	DG	179	PRO	2.6
6	CG	86	GLN	2.6
59	DA	2803	C	2.6
7	CH	26	VAL	2.6
25	DC	77	ALA	2.6
8	AI	58	HIS	2.6
4	AE	144	THR	2.6
41	BV	36	PRO	2.6
35	DP	110	TYR	2.6
42	BW	103	ILE	2.6
57	B1	59	THR	2.6
58	D4	9	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
23	CY	123	ARG	2.6
25	DC	54	ARG	2.6
26	DD	262	ARG	2.6
21	CW	20	U	2.6
60	DB	16	G	2.6
28	DF	191	ARG	2.6
36	DQ	40	ALA	2.6
32	DK	41	PHE	2.6
21	AW	20(A)	U	2.5
34	BO	100	GLY	2.5
59	DA	2110	G	2.5
40	DU	20	LEU	2.5
1	AB	131	PRO	2.5
29	DG	40	ASN	2.5
8	AI	121	ARG	2.5
11	AL	33	ARG	2.5
18	CS	74	PHE	2.5
18	AS	16	LEU	2.5
51	D7	30	VAL	2.5
58	B4	34	GLU	2.5
28	DF	30	PRO	2.5
29	BG	102	PHE	2.5
29	DG	117	PHE	2.5
29	BG	131	TYR	2.5
42	DW	20	VAL	2.5
2	AC	169	ALA	2.5
8	AI	117	HIS	2.5
23	AY	103	GLY	2.5
25	BC	5	GLY	2.5
33	DN	12	ARG	2.5
20	CA	68(L)	U	2.5
23	AY	356	LEU	2.5
29	DG	7	LEU	2.5
38	BS	39	ILE	2.5
51	B7	24	THR	2.5
6	CG	135	VAL	2.5
1	AB	94	ASN	2.5
23	CY	124	GLN	2.5
38	BS	54	LEU	2.5
9	AJ	48	THR	2.5
23	AY	160	ARG	2.5
30	DH	55	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	AC	182	ILE	2.5
15	CP	33	ILE	2.5
23	CY	272	LEU	2.5
59	DA	426	C	2.5
28	BF	69	HIS	2.5
29	BG	5	VAL	2.5
11	AL	6	THR	2.5
8	AI	85	LEU	2.5
25	BC	227	PRO	2.5
25	DC	149	ASN	2.5
29	DG	177	GLY	2.5
1	AB	128	GLU	2.5
6	AG	85	TYR	2.5
6	CG	33	ASP	2.5
59	BA	382	G	2.5
11	AL	82	VAL	2.5
15	CP	2	VAL	2.5
32	DK	133	SER	2.5
50	B6	37	ARG	2.5
9	AJ	47	PHE	2.5
9	AJ	55	LYS	2.5
15	AP	59	TRP	2.5
4	CE	106	PRO	2.5
33	BN	44	PRO	2.5
32	DK	30	HIS	2.5
44	DY	102	CYS	2.5
23	AY	105	ILE	2.5
29	BG	31	VAL	2.5
20	AA	1066	C	2.5
33	BN	11	PRO	2.5
41	BV	74	LYS	2.5
54	Be	113	LYS	2.5
32	BK	61	ALA	2.5
57	D1	22	GLY	2.5
54	Be	70	LYS	2.5
1	AB	119	GLU	2.5
25	BC	221	PRO	2.5
12	CM	15	VAL	2.5
23	AY	275	ALA	2.5
29	BG	37	VAL	2.5
30	DH	65	HIS	2.5
58	D4	2	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
8	AI	87	GLN	2.5
16	CQ	44	ALA	2.5
18	AS	41	VAL	2.5
20	CA	1365	G	2.4
20	AA	47	C	2.4
20	AA	1344	C	2.4
35	BP	30	THR	2.4
29	DG	181	ARG	2.4
37	BR	58	GLY	2.4
43	DX	33	LYS	2.4
15	CP	16	HIS	2.4
35	BP	78	PRO	2.4
54	Be	53	PRO	2.4
20	CA	1362(A)	C	2.4
23	CY	202	PRO	2.4
3	AD	137	SER	2.4
23	AY	19	ALA	2.4
25	BC	129	GLY	2.4
32	DK	13	PRO	2.4
16	CQ	35	VAL	2.4
19	CT	16	HIS	2.4
28	DF	18	ARG	2.4
35	BP	36	LYS	2.4
8	CI	94	ALA	2.4
4	CE	85	GLY	2.4
12	AM	28	ALA	2.4
11	CL	122	THR	2.4
29	DG	176	LEU	2.4
32	BK	120	LEU	2.4
8	AI	119	ALA	2.4
28	BF	181	LEU	2.4
29	DG	103	LEU	2.4
51	B7	29	LYS	2.4
1	CB	129	GLU	2.4
29	BG	59	GLU	2.4
25	DC	100	ILE	2.4
8	AI	123	PRO	2.4
20	AA	201(C)	U	2.4
13	AN	47	LEU	2.4
23	CY	254	LYS	2.4
25	BC	161	ARG	2.4
38	BS	52	SER	2.4

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Mol	Chain	Res	Type	RSRZ
59	BA	1545	A	2.4
4	CE	131	ILE	2.4
18	CS	82	GLY	2.4
25	BC	109	MET	2.4
29	DG	101	ILE	2.4
39	DT	50	ILE	2.4
15	AP	35	LYS	2.4
51	D7	32	LYS	2.4
6	AG	44	TYR	2.4
17	AR	22	VAL	2.4
20	CA	239	U	2.4
9	CJ	52	GLY	2.4
11	AL	84	LEU	2.4
39	DT	63	VAL	2.4
39	DT	137	LYS	2.4
59	BA	10	G	2.4
23	CY	67	ALA	2.4
37	DR	70	LEU	2.4
32	DK	28	GLY	2.4
40	BU	13	LYS	2.4
25	DC	205	ALA	2.4
28	BF	58	ALA	2.4
59	BA	2799	A	2.4
32	BK	84	LEU	2.4
59	DA	1008	C	2.4
12	AM	45	VAL	2.4
7	CH	101	PRO	2.4
20	AA	1231	G	2.4
22	AV	7	G	2.4
25	DC	26	ALA	2.4
33	DN	124	ALA	2.4
3	CD	198	VAL	2.4
16	CQ	7	THR	2.4
23	CY	501	THR	2.4
12	CM	52	GLU	2.4
54	Be	111	ILE	2.4
59	DA	311	A	2.4
58	B4	16	CYS	2.4
25	DC	12	LEU	2.4
23	AY	89	ASP	2.4
12	AM	126	LYS	2.4
20	AA	306	G	2.4

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Mol	Chain	Res	Type	RSRZ
29	BG	69	ALA	2.4
8	CI	126	SER	2.4
8	AI	60	ASP	2.4
33	BN	41	ASP	2.4
43	BX	3	THR	2.4
6	CG	115	ARG	2.3
32	DK	22	PRO	2.3
45	DZ	163	LEU	2.3
46	D0	73	GLY	2.3
25	BC	111	PHE	2.3
29	BG	20	ILE	2.3
54	Be	87	LYS	2.3
6	AG	11	GLN	2.3
1	CB	197	VAL	2.3
6	AG	127	ALA	2.3
29	DG	110	ALA	2.3
58	D4	12	ALA	2.3
9	AJ	54	PHE	2.3
1	CB	96	ARG	2.3
54	De	77	GLU	2.3
12	AM	30	ALA	2.3
20	CA	1392	G	2.3
22	CV	14	A	2.3
2	AC	207	VAL	2.3
28	DF	156	LEU	2.3
38	BS	58	LEU	2.3
50	D6	36	LEU	2.3
11	CL	28	LYS	2.3
15	CP	84	ALA	2.3
32	BK	3	LYS	2.3
1	AB	204	ASN	2.3
3	CD	2	GLY	2.3
19	CT	24	LEU	2.3
33	DN	122	VAL	2.3
52	D8	46	ARG	2.3
59	BA	2807	G	2.3
25	BC	73	VAL	2.3
6	AG	116	ALA	2.3
33	DN	37	LYS	2.3
1	CB	179	LYS	2.3
11	CL	49	ASN	2.3
32	DK	80	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
51	B7	30	VAL	2.3
57	D1	25	LYS	2.3
20	CA	1167	A	2.3
20	CA	1235	U	2.3
45	BZ	118	GLN	2.3
32	DK	18	THR	2.3
8	CI	47	LEU	2.3
23	AY	537	GLU	2.3
46	D0	75	LEU	2.3
52	B8	39	LYS	2.3
8	AI	6	GLY	2.3
2	CC	3	ASN	2.3
23	AY	577	SER	2.3
45	BZ	149	SER	2.3
7	CH	5	PRO	2.3
35	DP	105	LEU	2.3
1	AB	210	SER	2.3
1	CB	104	ASN	2.3
20	CA	1386	G	2.3
25	DC	37	LYS	2.3
32	DK	77	LEU	2.3
30	DH	34	GLU	2.3
2	CC	186	PHE	2.3
38	BS	90	GLY	2.3
29	DG	151	ALA	2.3
8	AI	44	VAL	2.3
45	BZ	165	VAL	2.3
58	D4	8	LYS	2.3
25	BC	176	VAL	2.3
59	DA	2797	U	2.3
35	BP	53	GLY	2.3
33	BN	47	ALA	2.3
29	DG	55	LYS	2.3
9	AJ	53	PRO	2.3
20	CA	135	C	2.3
23	CY	163	VAL	2.3
25	BC	15	VAL	2.3
25	BC	175	PRO	2.3
15	AP	55	ARG	2.3
25	DC	164	PHE	2.3
29	BG	108	ASN	2.3
33	DN	44	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
20	AA	916	G	2.3
50	B6	29	ASN	2.3
30	DH	92	ILE	2.3
46	B0	18	ALA	2.3
54	Be	51	ALA	2.3
27	DE	15	PHE	2.3
33	DN	8	GLN	2.3
1	AB	123	ALA	2.3
27	DE	120	TRP	2.3
20	AA	1302	U	2.2
29	DG	21	ARG	2.2
54	Be	107	GLU	2.2
60	BB	24	G	2.2
4	AE	131	ILE	2.2
4	AE	138	ALA	2.2
23	CY	134	ALA	2.2
35	BP	39	LYS	2.2
23	CY	312	LEU	2.2
2	AC	131	ARG	2.2
28	DF	23	ASP	2.2
32	DK	58	THR	2.2
25	BC	68	GLY	2.2
32	DK	54	PRO	2.2
60	DB	62	C	2.2
15	CP	48	TRP	2.2
8	AI	110	GLU	2.2
40	DU	89	GLU	2.2
59	DA	2155	G	2.2
6	CG	39	ALA	2.2
28	BF	156	LEU	2.2
49	B5	2	ALA	2.2
29	DG	136	ARG	2.2
25	BC	39	ASP	2.2
4	CE	49	PRO	2.2
6	AG	61	VAL	2.2
37	DR	44	LEU	2.2
8	CI	114	TYR	2.2
39	DT	51	ARG	2.2
59	DA	125	G	2.2
15	CP	13	HIS	2.2
23	AY	404	VAL	2.2
32	BK	114	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
41	BV	38	LEU	2.2
23	CY	160	ARG	2.2
33	DN	116	LEU	2.2
12	AM	110	ARG	2.2
25	BC	56	ASP	2.2
59	DA	1862	G	2.2
20	AA	1183	A	2.2
1	AB	201	ILE	2.2
23	AY	272	LEU	2.2
25	DC	219	MET	2.2
28	BF	112	MET	2.2
8	AI	18	PHE	2.2
2	AC	201	TYR	2.2
33	BN	37	LYS	2.2
4	CE	81	GLU	2.2
25	BC	177	GLY	2.2
38	BS	82	ILE	2.2
8	AI	20	ARG	2.2
25	DC	19	LYS	2.2
13	AN	14	PRO	2.2
23	CY	161	PRO	2.2
32	BK	19	PRO	2.2
20	CA	1063	C	2.2
44	BY	102	CYS	2.2
2	AC	163	ALA	2.2
18	AS	32	LYS	2.2
42	BW	113	LYS	2.2
1	CB	78	GLN	2.2
23	CY	426	GLN	2.2
8	AI	21	PRO	2.2
38	DS	47	THR	2.2
29	DG	124	SER	2.2
59	BA	890	A	2.2
58	D4	32	TYR	2.2
28	DF	189	THR	2.2
43	BX	60	ARG	2.2
54	Be	77	GLU	2.2
25	DC	105	LEU	2.2
28	DF	124	LEU	2.2
6	AG	109	ASN	2.2
10	AK	57	THR	2.2
22	AV	4	A	2.2

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Mol	Chain	Res	Type	RSRZ
57	D1	41	ARG	2.2
32	BK	41	PHE	2.2
10	CK	69	ALA	2.2
23	CY	159	ALA	2.2
23	CY	401	SER	2.2
23	AY	321	TYR	2.2
4	AE	15	ARG	2.2
12	AM	60	VAL	2.2
29	BG	120	LEU	2.2
33	BN	59	LYS	2.2
54	Be	57	LYS	2.2
30	DH	100	GLY	2.2
12	CM	16	ASP	2.2
12	CM	49	THR	2.2
29	BG	46	ALA	2.2
35	BP	57	THR	2.2
54	Be	69	ALA	2.2
4	CE	11	ILE	2.2
38	DS	89	ARG	2.2
6	CG	112	PRO	2.2
25	DC	193	PHE	2.2
26	DD	36	PRO	2.2
35	BP	24	GLY	2.2
20	CA	1294	G	2.2
1	CB	73	THR	2.2
32	BK	33	ASN	2.2
51	D7	45	ALA	2.2
43	DX	16	LYS	2.2
58	B4	8	LYS	2.2
25	DC	32	GLU	2.2
29	DG	125	PHE	2.2
45	BZ	160	GLY	2.1
59	BA	2797	U	2.2
2	AC	11	ARG	2.1
14	AO	88	ARG	2.1
23	CY	430	ARG	2.1
28	BF	158	THR	2.1
28	DF	114	VAL	2.1
32	DK	7	VAL	2.1
33	DN	52	VAL	2.1
35	BP	95	VAL	2.1
38	DS	14	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
39	BT	88	ILE	2.1
20	AA	933	G	2.1
23	CY	85	PRO	2.1
16	AQ	70	ARG	2.1
20	AA	1341	U	2.1
27	BE	104	VAL	2.1
28	DF	174	VAL	2.1
32	DK	84	LEU	2.1
23	AY	419	ALA	2.1
23	CY	429	ALA	2.1
6	CG	104	LEU	2.1
20	AA	1320	C	2.1
29	DG	25	TYR	2.1
26	DD	49	ILE	2.1
20	CA	1440(B)	G	2.1
54	Be	82	THR	2.1
54	Be	109	GLU	2.1
25	BC	14	LYS	2.1
6	CG	22	LEU	2.1
45	BZ	161	VAL	2.1
54	Be	78	LEU	2.1
6	AG	153	HIS	2.1
32	BK	36	GLU	2.1
33	BN	36	GLY	2.1
33	BN	76	SER	2.1
16	CQ	25	ARG	2.1
23	AY	96	ARG	2.1
27	DE	25	VAL	2.1
38	DS	26	LEU	2.1
42	BW	76	VAL	2.1
11	CL	69	TYR	2.1
16	AQ	58	GLU	2.1
23	CY	400	GLU	2.1
12	CM	126	LYS	2.1
51	B7	26	GLY	2.1
57	B1	36	GLY	2.1
29	BG	83	ARG	2.1
25	DC	221	PRO	2.1
33	DN	21	LYS	2.1
40	BU	108	GLU	2.1
6	AG	69	VAL	2.1
6	CG	116	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
18	AS	44	MET	2.1
25	DC	63	VAL	2.1
35	DP	85	LEU	2.1
50	D6	49	HIS	2.1
57	B1	40	ARG	2.1
51	B7	25	PRO	2.1
44	DY	71	LYS	2.1
15	AP	84	ALA	2.1
16	CQ	11	VAL	2.1
35	DP	101	VAL	2.1
1	CB	122	PHE	2.1
16	CQ	39	SER	2.1
13	AN	53	LEU	2.1
29	DG	111	LEU	2.1
3	AD	126	ILE	2.1
29	BG	40	ASN	2.1
32	BK	113	PRO	2.1
54	De	105	LYS	2.1
14	AO	89	GLY	2.1
22	CV	5	A	2.1
25	BC	61	GLY	2.1
54	Be	66	GLU	2.1
8	CI	70	LYS	2.1
23	AY	87	HIS	2.1
59	BA	2161	C	2.1
59	DA	2804	C	2.1
7	CH	22	GLU	2.1
29	BG	141	PHE	2.1
1	AB	27	LYS	2.1
7	AH	70	GLN	2.1
38	DS	36	TYR	2.1
59	DA	2893	G	2.1
18	CS	51	VAL	2.1
23	CY	166	LEU	2.1
38	DS	108	GLY	2.1
20	AA	390	C	2.1
23	AY	108	PHE	2.1
25	DC	192	ALA	2.1
41	DV	75	PHE	2.1
3	CD	84	LYS	2.1
6	CG	137	LYS	2.1
11	CL	23	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
6	CG	56	GLN	2.1
27	BE	8	LYS	2.1
2	AC	184	TYR	2.1
23	CY	212	TYR	2.1
8	AI	73	GLN	2.1
9	AJ	8	LEU	2.1
11	AL	35	GLY	2.1
18	AS	63	THR	2.1
6	AG	42	ILE	2.1
54	De	75	ILE	2.1
33	BN	125	GLY	2.1
59	DA	1809	A	2.0
2	CC	24	ALA	2.0
4	AE	16	THR	2.0
6	CG	125	MET	2.0
21	CW	57	G	2.0
42	BW	3	ALA	2.0
18	AS	36	ARG	2.0
28	BF	155	LEU	2.0
57	B1	60	PHE	2.0
2	AC	154	SER	2.0
6	AG	93	PRO	2.0
15	AP	70	ALA	2.0
19	AT	16	HIS	2.0
20	AA	1235	U	2.0
28	BF	18	ARG	2.0
28	DF	186	ILE	2.0
29	BG	87	PRO	2.0
29	DG	157	ILE	2.0
50	D6	50	ARG	2.0
8	CI	41	VAL	2.0
22	AV	24	A	2.0
23	CY	216	LEU	2.0
8	CI	110	GLU	2.0
11	CL	124	LYS	2.0
2	AC	200	ALA	2.0
8	AI	76	ALA	2.0
59	DA	407	G	2.0
20	AA	1342	C	2.0
28	BF	194	MET	2.0
36	DQ	39	PRO	2.0
60	BB	60	C	2.0

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Mol	Chain	Res	Type	RSRZ
29	BG	176	LEU	2.0
35	DP	148	LEU	2.0
52	D8	14	VAL	2.0
42	BW	94	ASP	2.0
25	DC	152	GLU	2.0
4	AE	14	ARG	2.0
11	CL	89	ARG	2.0
29	DG	52	ILE	2.0
33	DN	40	PRO	2.0
58	D4	14	ILE	2.0
1	CB	152	PHE	2.0
19	CT	96	GLY	2.0
8	AI	55	ALA	2.0
20	CA	1071	C	2.0
40	BU	11	ARG	2.0
52	B8	43	GLN	2.0
4	AE	87	SER	2.0
33	BN	52	VAL	2.0
6	AG	24	THR	2.0
29	DG	63	ILE	2.0
51	D7	12	ARG	2.0
52	D8	24	ALA	2.0
28	DF	20	LEU	2.0
30	BH	33	LEU	2.0
54	Be	100	LYS	2.0
20	AA	31	G	2.0
21	CW	42	U	2.0
33	DN	47	ALA	2.0
1	CB	150	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
24	UAL	AU	5	9/10	0.52	0.37	149,151,153,154	0
24	DPP	AU	2	6/7	0.65	0.23	153,153,154,154	0
24	UAL	CU	5	9/10	0.74	0.34	89,90,91,91	0
24	5OH	CU	6	12/13	0.82	0.34	84,88,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	KBE	AU	1	9/10	0.84	0.21	154,155,156,156	0
24	5OH	AU	6	12/13	0.86	0.55	151,153,154,154	0
24	KBE	CU	1	9/10	0.90	0.30	69,74,77,77	0
24	DPP	CU	2	6/7	0.90	0.17	77,79,80,82	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

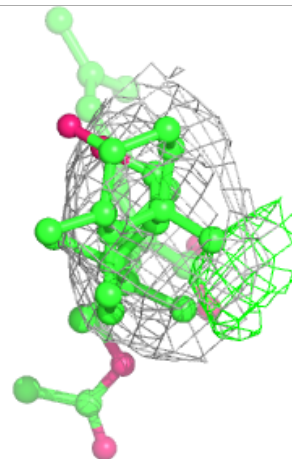
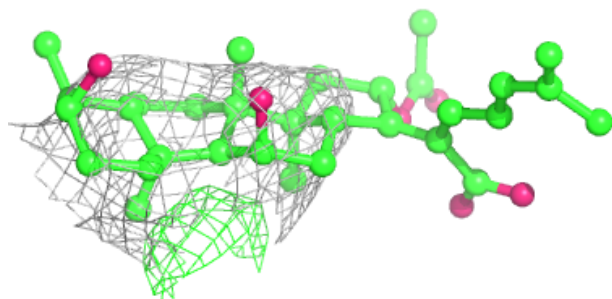
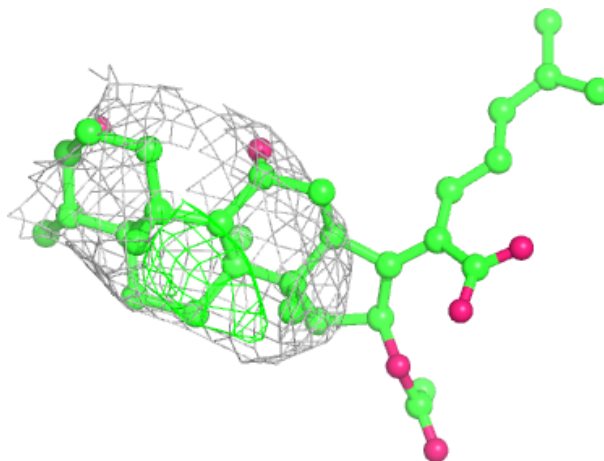
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	FUA	CY	701	37/37	0.65	0.67	199,200,202,202	0
61	FUA	AY	701	37/37	0.81	0.43	154,155,156,156	0
62	GDP	CY	702	28/28	0.84	0.29	78,82,83,84	0
62	GDP	AY	702	28/28	0.92	0.19	78,82,83,84	0
63	MG	BA	2901	1/1	0.98	0.28	5,5,5,5	0
63	MG	CY	703	1/1	0.98	0.18	1,1,1,1	0

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

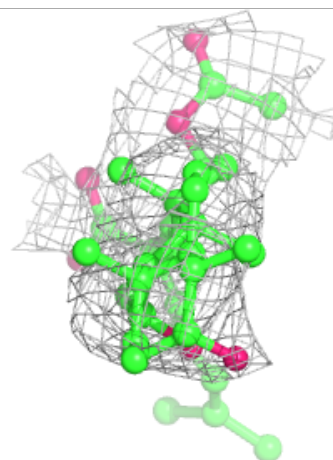
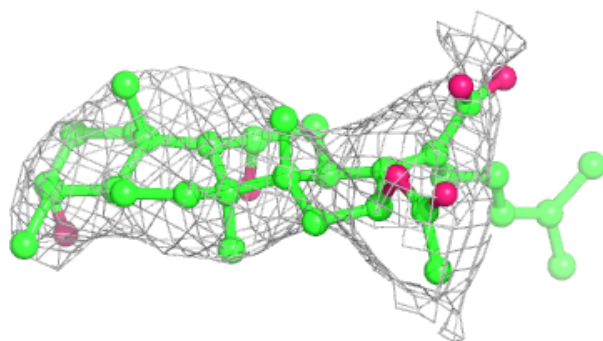
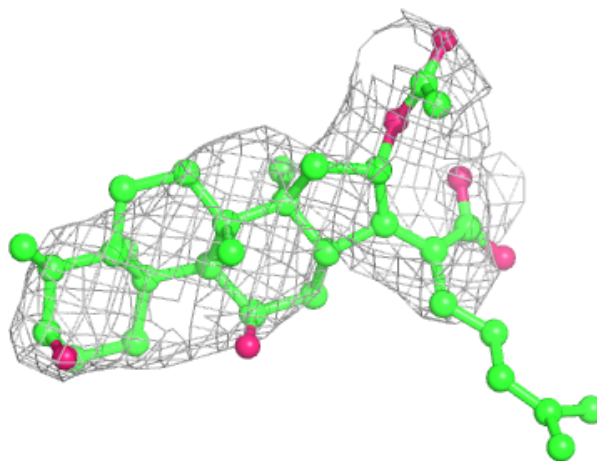
Electron density around FUA CY 701:

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



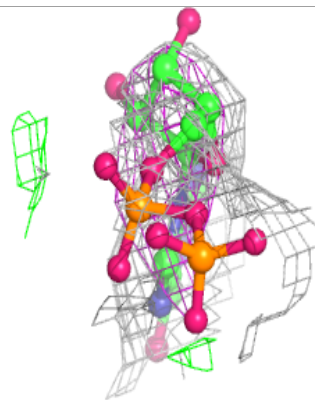
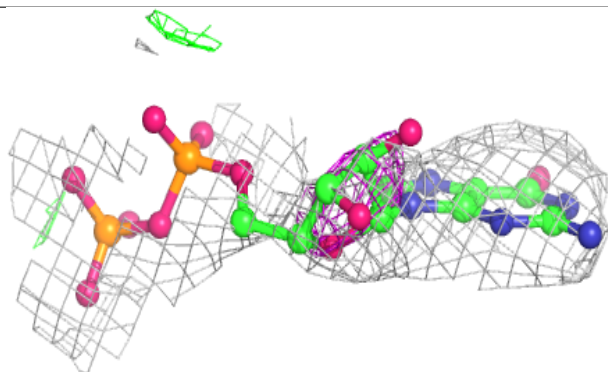
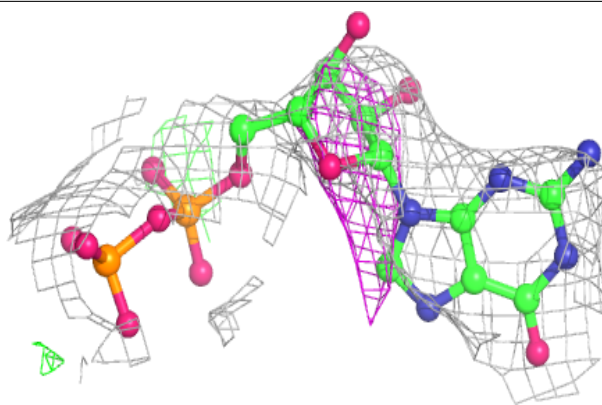
Electron density around FUA AY 701:

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

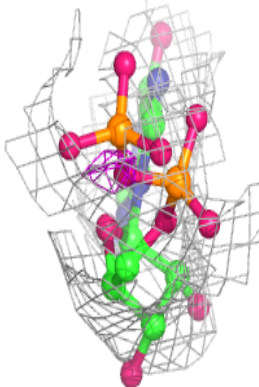
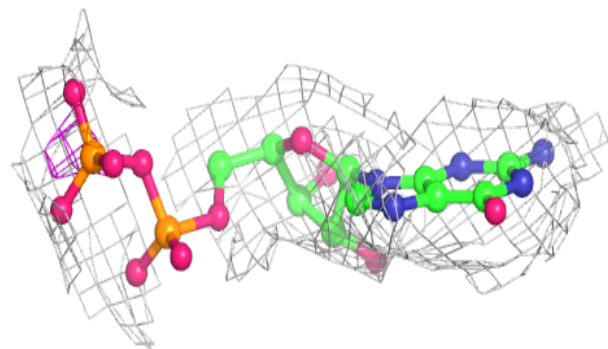
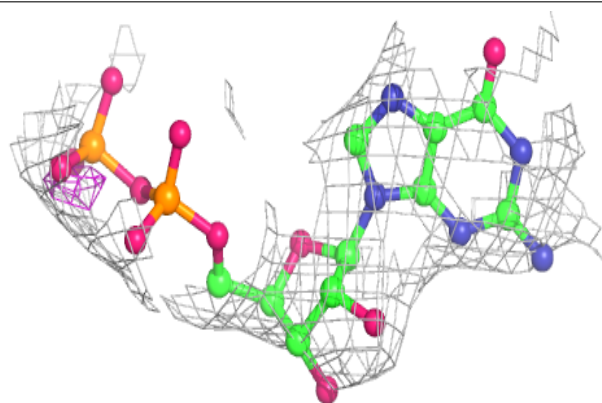


Electron density around GDP CY 702:

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

**Electron density around GDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.