



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:33 PM BST

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 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)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

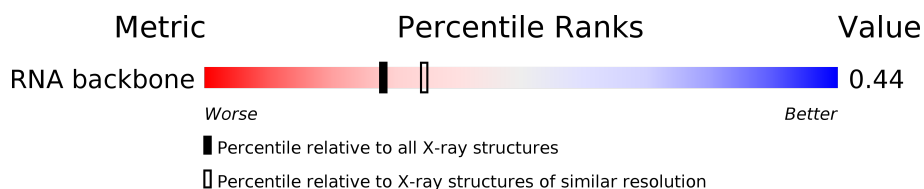
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AB	235	98% .
1	CB	235	99% .
2	AC	207	100%
2	CC	207	100%
3	AD	208	100%
3	CD	208	100%
4	AE	151	99% .
4	CE	151	99% .
5	AF	101	100%
5	CF	101	99% .

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Mol	Chain	Length	Quality of chain
6	AG	155	 100%
6	CG	155	 100%
7	AH	138	 100%
7	CH	138	 100%
8	AI	127	 100%
8	CI	127	 100%
9	AJ	99	 100%
9	CJ	99	 99% .
10	AK	119	 100%
10	CK	119	 100%
11	AL	125	 98% .
11	CL	125	 98% .
12	AM	125	 99% .
12	CM	125	 100%
13	AN	60	 100%
13	CN	60	 100%
14	AO	88	 100%
14	CO	88	 100%
15	AP	84	 100%
15	CP	84	 100%
16	AQ	100	 100%
16	CQ	100	 100%
17	AR	70	 100%
17	CR	70	 100%
18	AS	79	 100%

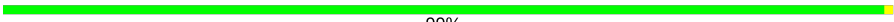














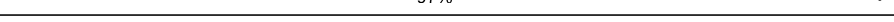
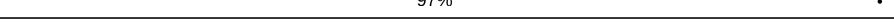
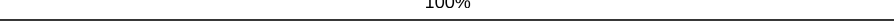
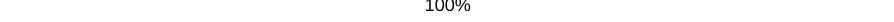
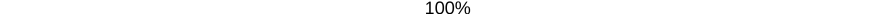
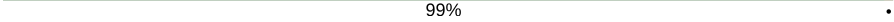
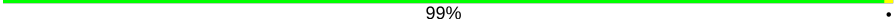

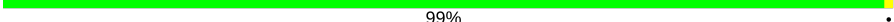
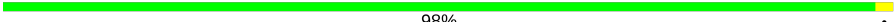
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Mol	Chain	Length	Quality of chain
18	CS	79	100%
19	AT	99	100%
19	CT	99	100%
20	AA	1511	79% 21%
20	CA	1511	80% 19%
21	AW	77	70% 30%
21	CW	77	70% 27%
22	AV	23	65% 35%
22	CV	23	65% 35%
23	AY	687	97%
23	CY	687	96%
24	AU	6	50% 50%
24	CU	6	50% 50%
25	BC	228	99%
25	DC	228	98%
26	BD	275	99%
26	DD	275	99%
27	BE	205	100%
27	DE	205	100%
28	BF	208	98%
28	DF	208	98%
29	BG	181	98%
29	DG	181	98%
30	BH	167	100%
30	DH	167	100%

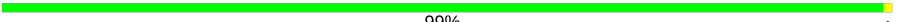














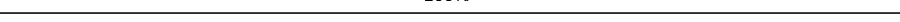
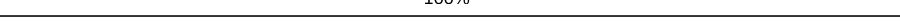
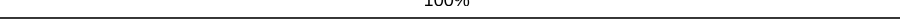
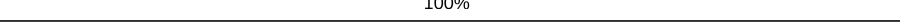
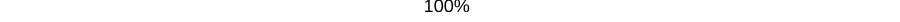
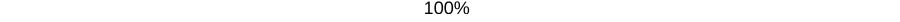
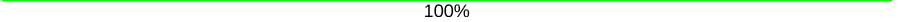
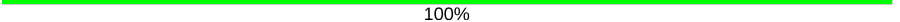


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Mol	Chain	Length	Quality of chain
31	BJ	170	 99%
31	DJ	170	 99%
32	BK	140	 100%
32	DK	140	 100%
33	BN	138	 100%
33	DN	138	 100%
34	BO	122	 100%
34	DO	122	 100%
35	BP	146	 100%
35	DP	146	 99%
36	BQ	141	 100%
36	DQ	141	 100%
37	BR	117	 100%
37	DR	117	 100%
38	BS	99	 97%
38	DS	99	 97%
39	BT	138	 100%
39	DT	138	 100%
40	BU	117	 100%
40	DU	117	 99%
41	BV	101	 99%
41	DV	101	 100%
42	BW	113	 99%
42	DW	113	 98%
43	BX	93	 100%













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Mol	Chain	Length	Quality of chain
43	DX	93	 99%
44	BY	107	 100%
44	DY	107	 100%
45	BZ	185	 100%
45	DZ	185	 100%
46	B0	84	 100%
46	D0	84	 100%
47	B2	71	 100%
47	D2	71	 100%
48	B3	60	 100%
48	D3	60	 100%
49	B5	59	 100%
49	D5	59	 100%
50	B6	50	 98%
50	D6	50	 100%
51	B7	49	 100%
51	D7	49	 100%
52	B8	64	 100%
52	D8	64	 100%
53	B9	37	 100%
53	D9	37	 100%
54	Be	102	 100%
54	De	102	 100%
55	Bf	31	 100%
55	Bg	31	 100%

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Mol	Chain	Length	Quality of chain
55	Df	31	 100%
55	Dg	31	 100%
56	Bh	30	 100%
56	Dh	30	 100%
57	B1	93	 98% .
57	D1	93	 98% ..
58	B4	35	 100%
58	D4	35	 100%
59	BA	2879	 75% 24% .
59	DA	2879	 75% 23% .
60	BB	119	 78% 22%
60	DB	119	 83% 17%

2 Entry composition

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
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

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

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

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

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

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

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

- 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
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
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
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
31	BJ	170	Total	C	N	O	0	0	0
			851	510	170	171			
31	DJ	170	Total	C	N	O	0	0	0
			851	510	170	171			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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
35	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

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

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

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
37	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
37	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

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

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

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

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
44	DY	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

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

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

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

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

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
47	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
47	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

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

- 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			

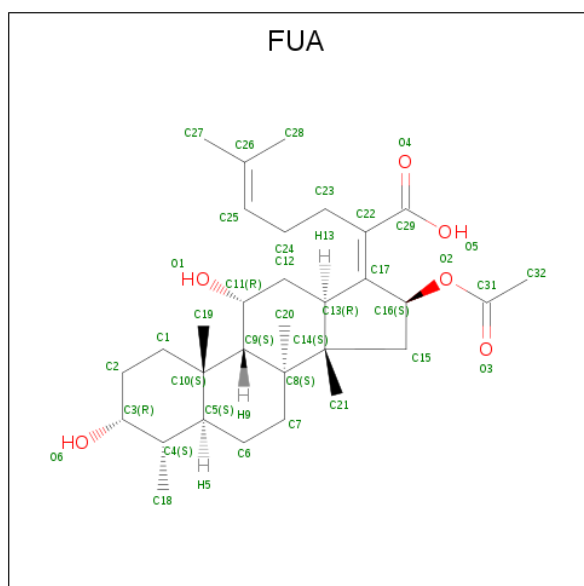
- Molecule 59 is a RNA chain called 23S ribosomal RNA.

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.

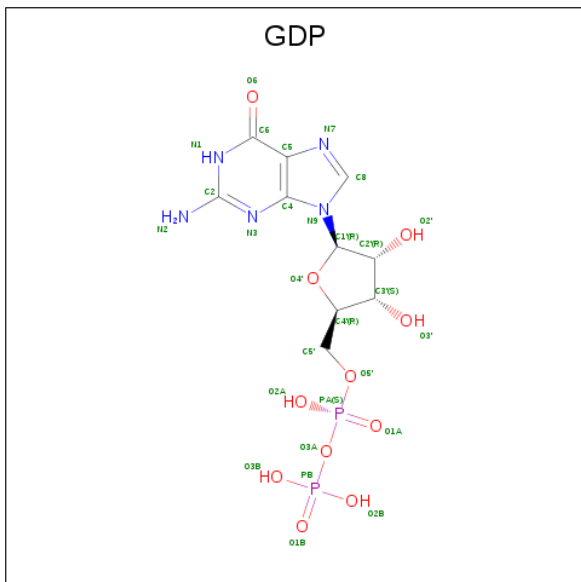
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



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			

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: 30S ribosomal protein S2

Chain AB:  98%



- Molecule 1: 30S ribosomal protein S2

Chain CB:  99%



- Molecule 2: 30S ribosomal protein S3

Chain AC:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 30S ribosomal protein S3

Chain CC:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: 30S ribosomal protein S4

Chain AD:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: 30S ribosomal protein S4

Chain CD:  100%



- Molecule 4: 30S ribosomal protein S5

Chain AE:  99%



- Molecule 4: 30S ribosomal protein S5

Chain CE:  99%



- Molecule 5: 30S ribosomal protein S6

Chain AF:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: 30S ribosomal protein S6

Chain CF:  99%



- Molecule 6: 30S ribosomal protein S7

Chain AG:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: 30S ribosomal protein S7

Chain CG:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S ribosomal protein S8

Chain AH:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 30S ribosomal protein S8

Chain CH:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 30S ribosomal protein S9

Chain AI:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 30S ribosomal protein S9

Chain CI:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: 30S ribosomal protein S10

Chain AJ:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: 30S ribosomal protein S10

Chain CJ:  99%



- Molecule 10: 30S ribosomal protein S11

Chain AK:  100%

There are no outlier residues recorded for this chain.

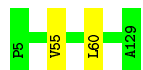
- Molecule 10: 30S ribosomal protein S11

Chain CK:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 30S ribosomal protein S12

Chain AL:  98%



- Molecule 11: 30S ribosomal protein S12

Chain CL:  98%



- Molecule 12: 30S ribosomal protein S13

Chain AM:  99%



- Molecule 12: 30S ribosomal protein S13

Chain CM:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 30S ribosomal protein S15

Chain AO:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 30S ribosomal protein S15

Chain CO:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 30S ribosomal protein S16

Chain AP:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 30S ribosomal protein S16

Chain CP:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 30S ribosomal protein S17

Chain AQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 30S ribosomal protein S17

Chain CQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S ribosomal protein S18

Chain AR:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 30S ribosomal protein S18

Chain CR:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 30S ribosomal protein S19

Chain AS:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 30S ribosomal protein S19

Chain CS:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 30S ribosomal protein S20

Chain AT:  100%


There are no outlier residues recorded for this chain.

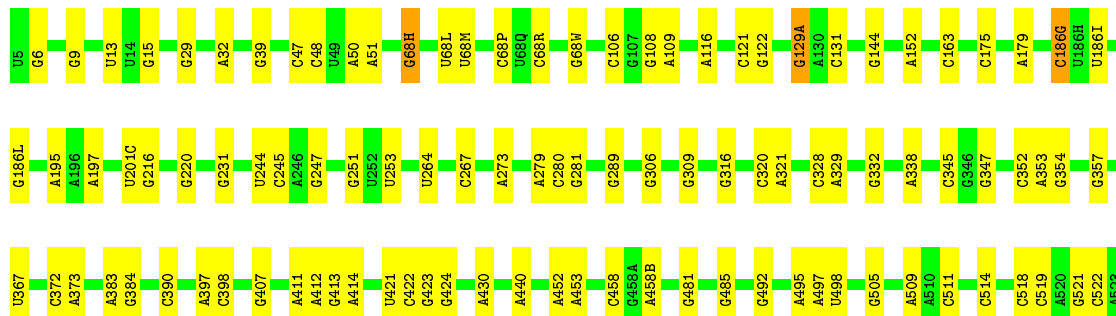
- Molecule 19: 30S ribosomal protein S20

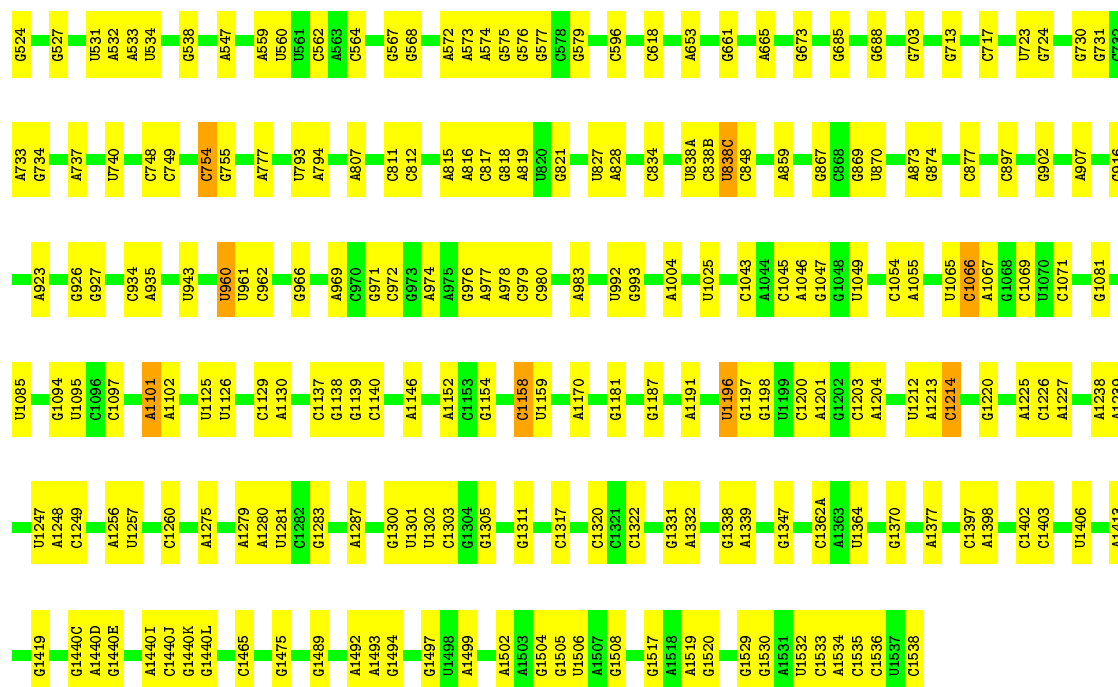
Chain CT:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: ribosomal RNA 16S

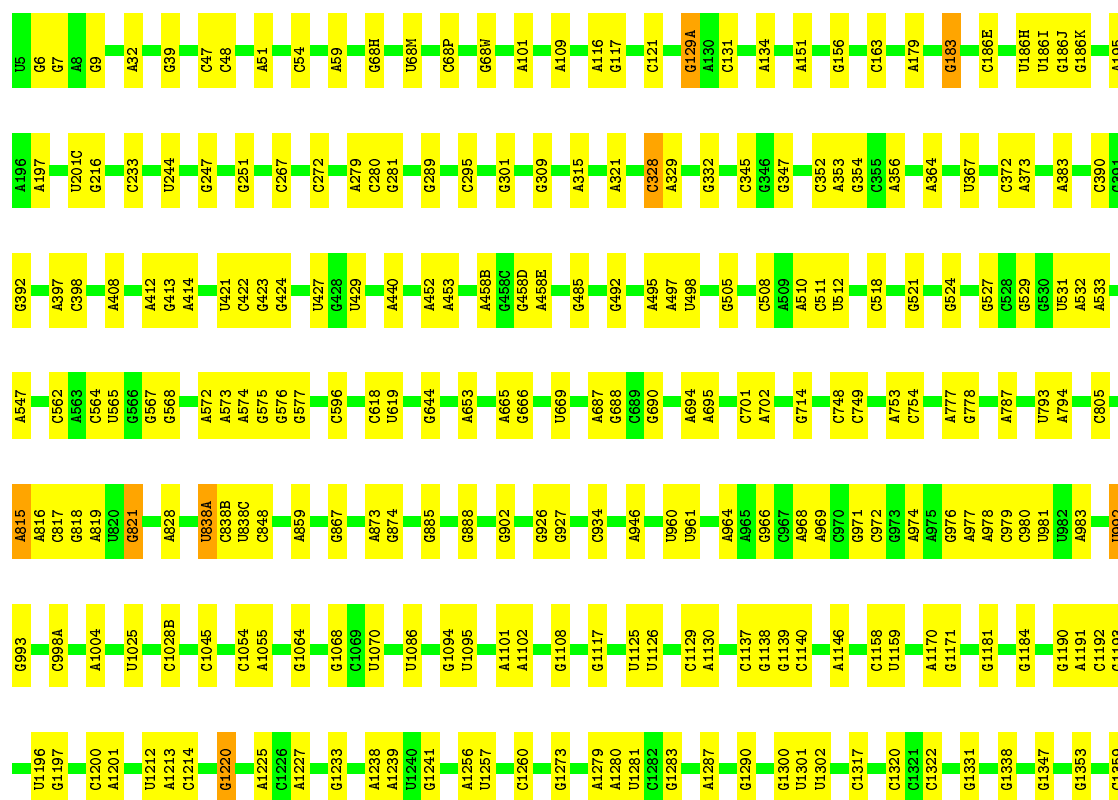
Chain AA:  79% 21%

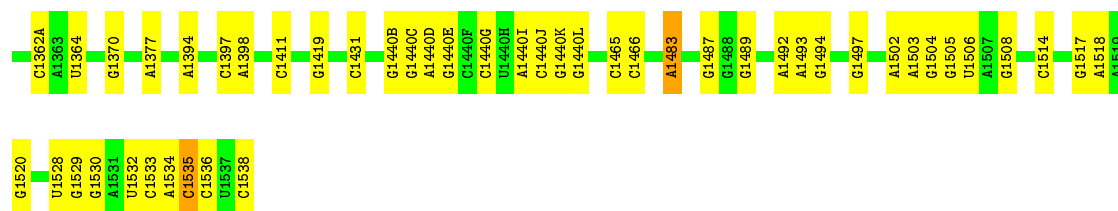




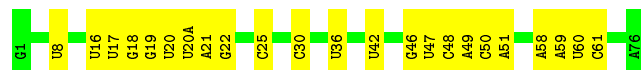
• Molecule 20: ribosomal RNA 16S

Chain CA: 80% 19%





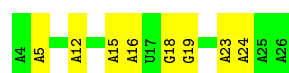
- Molecule 21: transfer RNA



- Molecule 21: transfer RNA



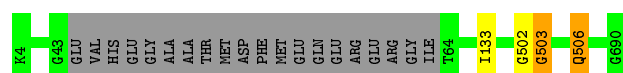
- Molecule 22: messenger RNA



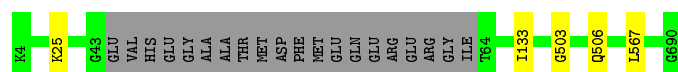
- Molecule 22: messenger RNA



- Molecule 23: Elongation factor G



- Molecule 23: Elongation factor G



- Molecule 24: VIOMYCIN

Chain AU:  50% 50%



- Molecule 24: VIOMYCIN

Chain CU:  50% 50%



- Molecule 25: 50S ribosomal protein L1

Chain BC:  99% .



- Molecule 25: 50S ribosomal protein L1

Chain DC:  98% .



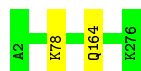
- Molecule 26: 50S ribosomal protein L2

Chain BD:  99% .



- Molecule 26: 50S ribosomal protein L2

Chain DD:  99% .



- Molecule 27: 50S ribosomal protein L3

Chain BE:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L3

Chain DE:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L4

Chain BF:  98%



- Molecule 28: 50S ribosomal protein L4

Chain DF:  98%



- Molecule 29: 50S ribosomal protein L5

Chain BG:  98%



- Molecule 29: 50S ribosomal protein L5

Chain DG:  98%



- Molecule 30: 50S ribosomal protein L6

Chain BH:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L6

Chain DH:  100%

There are no outlier residues recorded for this chain.

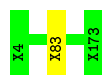
- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain BJ:  99%



- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain DJ:  99% .



- Molecule 32: 50S ribosomal protein L11

Chain BK:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L11

Chain DK:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L13

Chain BN:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L13

Chain DN:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L14

Chain BO:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L14

Chain DO:  100%

There are no outlier residues recorded for this chain.

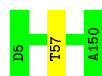
- Molecule 35: 50S ribosomal protein L15

Chain BP:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: 50S ribosomal protein L15

Chain DP:  99% .



- Molecule 36: 50S ribosomal protein L16

Chain BQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L16

Chain DQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L17

Chain BR:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L17

Chain DR:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 50S ribosomal protein L18

Chain BS:  97%



- Molecule 38: 50S ribosomal protein L18

Chain DS:  97%



- Molecule 39: 50S ribosomal protein L19

Chain BT:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 50S ribosomal protein L19

Chain DT:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L20

Chain BU:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L20

Chain DU:  99%



- Molecule 41: 50S ribosomal protein L21

Chain BV:  99%



- Molecule 41: 50S ribosomal protein L21

Chain DV:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 50S ribosomal protein L22

Chain BW:  99%



- Molecule 42: 50S ribosomal protein L22

Chain DW:  98%



- Molecule 43: 50S ribosomal protein L23

Chain BX:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 50S ribosomal protein L23

Chain DX:  99%



- Molecule 44: 50S ribosomal protein L24

Chain BY:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L24

Chain DY:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L25

Chain BZ:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L25

Chain DZ:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L27

Chain B0:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L27

Chain D0:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L29

Chain B2:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L29

Chain D2:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L30

Chain B3:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L30

Chain D3:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L32

Chain B5:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L32

Chain D5:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 50S ribosomal protein L33

Chain B6:  98%



- Molecule 50: 50S ribosomal protein L33

Chain D6:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 50S ribosomal protein L34

Chain B7:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 50S ribosomal protein L34

Chain D7:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L35

Chain B8:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L35

Chain D8:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 50S ribosomal protein L36

Chain B9:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 50S ribosomal protein L36

Chain D9:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

Chain Be:  100%

There are no outlier residues recorded for this chain.

- Molecule 54: 50S ribosomal protein L7/L12

Chain De:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf:  100%

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:  98%



- Molecule 57: 50S ribosomal protein L28

Chain D1:  98%



- Molecule 58: 50S ribosomal protein L31

Chain B4:  100%


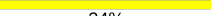
There are no outlier residues recorded for this chain.

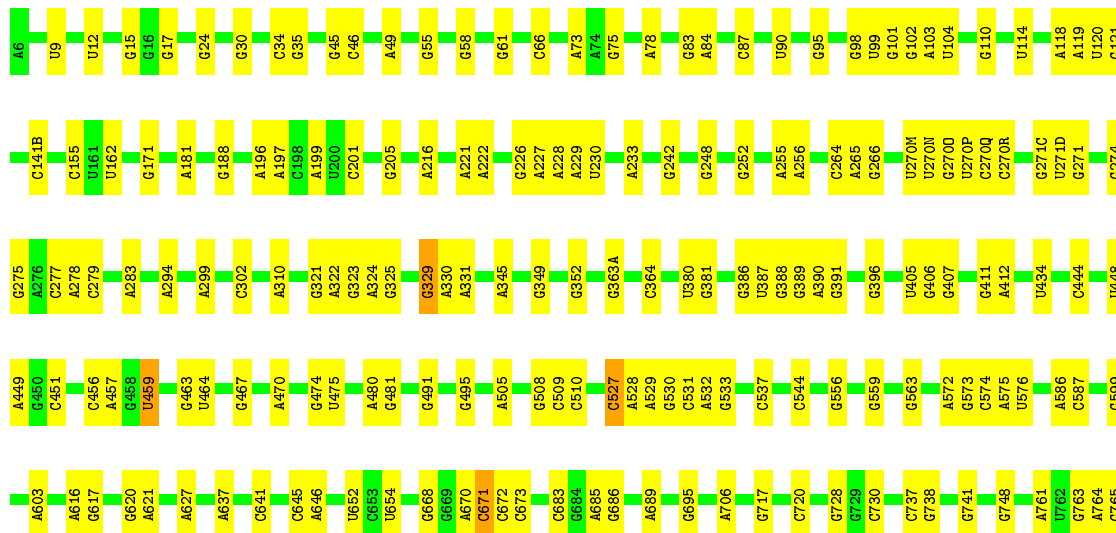
- Molecule 58: 50S ribosomal protein L31

Chain D4:  100%

There are no outlier residues recorded for this chain.

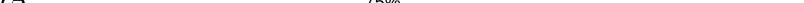
- Molecule 59: 23S ribosomal RNA

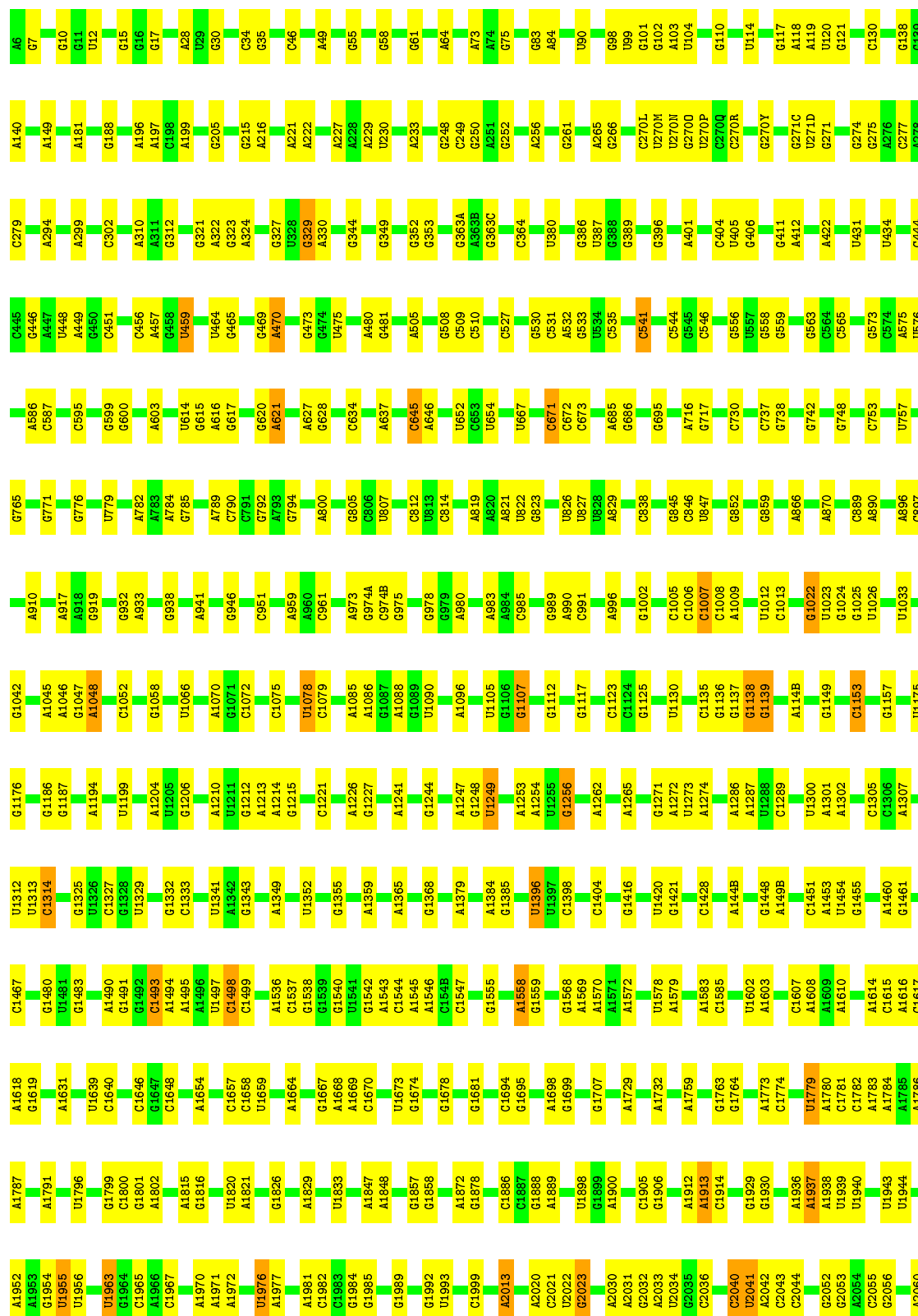
Chain BA:  75%  24%

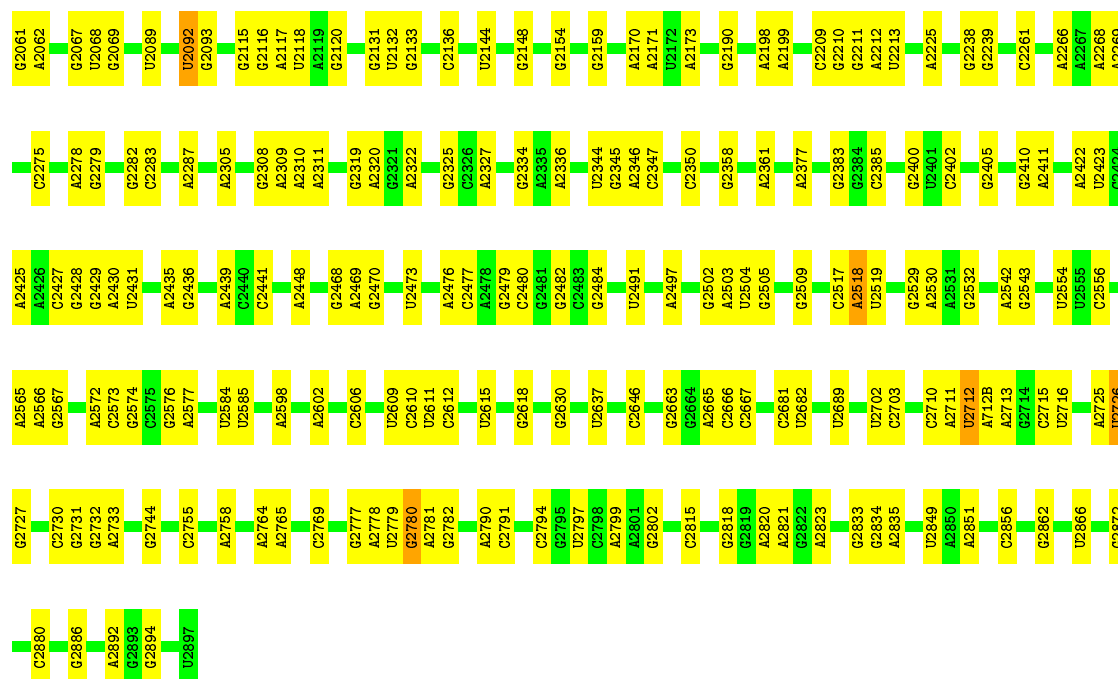


G2872	G2751	A2602	G2470	G2325	C2136	A1981	U1820	G1674	A1536	A1349	C1221	A1070	C935	G776
C2879	C2755	G2603	C2475	A2327	U2144	C1982	A1821	C1675	C1537	A1359	G1231	C1071	G939	U779
C2880	A2757	U2609	A2476	G2334	G2148	G1985	A1829	G1681	G1542	A1365	G1236	C1075	A941	A782
C2881	C2478	G2610	A2478	A2336	G2154	G1992	G1831	A1690	C1544	A1379	A1237	C1076	G946	A783
G2886	C2479	C2612	C2480	G2343	G2154	C2006	C1838	C1691	A1546	A1379	A1241	A1077	G959	A784
A2892	C2483	U2615	C2483	G2344	A2158	A2013	G1839	G1694	A1554	A1384	A1242	A1078	A960	G785
G2893	G2487	G2618	G2487	G2345	G2159	G2022	G1840	G1695	A1544	G1385	G1243	A1085	G962	A788
G2894	U2491	A2621	U2491	G2346	G2166	C2021	A1847	G1696	A1558	G1387	G1244	A1086	U963	G792
A2897	G2622	G2622	G2622	C2350	U2187	C2022	A1848	A1698	G1559	G1388	A1247	G1087	G971	A793
G2898	U2779	G2623	G2502	G2350	G2188	G2023	U1851	G1699	A1569	A1395	U1249	A1088	G974	G794
G2899	G2505	G2630	G2505	A2361	U2172	G2024	G1860	G1702	A1572	U1397	U1253	U1090	A800	A800
G2900	G2509	G2371	G2509	G2371	A2173	A2031	G1872	G1705	A1576	C1398	A1254	A1098	G974A	G805
G2901	A2518	A2377	A2518	A2377	A2198	G2032	A1872	U1706	U1576	G1416	U1255	G1106	A980	C812
G2902	G2529	G2378	G2529	G2378	G2210	A2033	G1888	U1707	G1581	U1420	G1256	G1107	A983	A819
G2903	A2530	G2379	G2530	G2379	G2211	G2035	A1889	A1729	C1585	G1421	A1265	G1112	C986	A820
G2904	A2531	G2383	A2531	G2383	G2212	C2039	G1896	A1732	A1586	G1422	G1271	C1123	A996	A821
G2905	G2532	G2385	G2532	G2385	U2213	U2041	A1900	C1742	A1587	G1423	A1272	C1127	U827	U827
G2906	U2546	G2391	U2546	G2391	G2215	G2055	A1901	G1743	C1598	C1428	U1273	A1127	G1002	U828
G2907	U2554	G2402	U2554	G2402	A2225	G2056	G1906	G1756	A1602	A1448	A1286	G1131	C1006	A829
G2908	C2555	C2402	C2555	C2402	G2239	A2060	G1929	A1762	A1603	C1451	U1287	G1132	C1007	G845
G2909	C2556	C2403	C2556	C2403	U2245	G2061	G1930	G1763	A1614	A1460	U1288	U1133	C1008	C846
G2910	A2567	G2426	A2567	G2426	G2251	A2062	U1931	G1781	A1615	G1461	C1289	C1135	A1009	U847
G2911	G2572	G2427	G2572	G2427	G2275	G2067	A1936	C1782	A1616	C1462	U1300	G1136	U1012	G852
G2912	C2573	G2428	C2573	G2428	A2278	U2068	A1937	A1783	C1617	C1463	U1312	A1155	U1013	G859
G2913	G2574	A2430	G2574	A2430	G2279	G2069	A1938	A1787	C163B	C1467	C1314	A1156	U1014	G859
G2914	C2575	A2434	C2575	A2434	G2282	G2093	U1940	A1791	A1631	G1483	A1321	G1157	G1024	G859
G2915	G2576	A2435	G2576	A2435	C2283	C2111	U1955	U1796	C1640	A1490	U1325	U1175	G1025	A896
G2916	G2577	G2436	G2577	G2436	A2287	G2115	U1956	U1956	G1643	G1491	C1327	G1176	A1027	C897
G2917	G2578	A2439	G2578	A2439	A2305	G2116	U1963	C1800	C1648	C1492	G1328	G1186	U1033	G906
G2918	C2582	C2440	C2582	C2440	G2308	A2117	C1967	G1801	C1689	G1491	U1329	U1199	U1033	A910
G2919	U2584	C2441	U2584	C2441	G2309	U2118	C1967	A1802	A1652	C1493	G1332	A1204	C1041	A917
G2920	G2585	G2447	G2585	G2447	A2310	G2120	A1970	A1803	A1664	A1494	G1338	A1205	G1042	A918
G2921	C2586	A2448	C2586	A2448	G2319	G2130	A1971	G1811	A1664	U1497	G1338	G1206	A1045	G919
G2922	G2586	U2460	G2586	U2460	A2320	G2131	A1972	G1814	A1668	C1498	U1341	G1212	A1046	G929
G2923	A2598	A2469	A2598	A2469	G2330	G2132	A1977	A1815	A1669	A1529	A1342	G1215	A1048	G932
G2924	G2598		G2598			G2133	A1978	G1816	U1673	U1535	G1343		U1061	

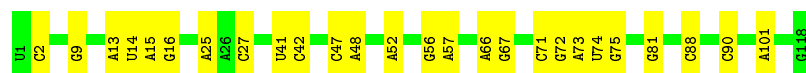
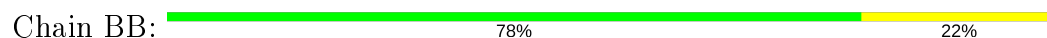
- Molecule 59: 23S ribosomal RNA

Chain DA:  75% 23%

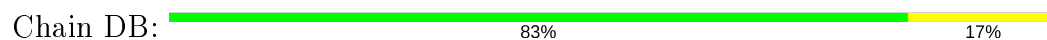




- Molecule 60: 5S ribosomal RNA



- Molecule 60: 5S ribosomal RNA



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.96 Å 670.66 Å 347.77 Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.58 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.328	Depositor
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.660	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.258 for h,-k,-l	Xtriage
Total number of atoms	308166	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, DPP, KBE, UAL, FUA, 5OH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	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

Continued on next page...

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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](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1510/1511 (99%)	305 (20%)	0
20	CA	1510/1511 (99%)	285 (18%)	0
21	AW	76/77 (98%)	23 (30%)	0
21	CW	76/77 (98%)	22 (28%)	0
22	AV	22/23 (95%)	8 (36%)	0
22	CV	22/23 (95%)	8 (36%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
59	BA	2878/2879 (99%)	665 (23%)	0
59	DA	2878/2879 (99%)	666 (23%)	0
60	BB	118/119 (99%)	21 (17%)	0
60	DB	118/119 (99%)	17 (14%)	0
All	All	9208/9218 (99%)	2020 (21%)	0

All (2020) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

There are no RNA pucker outliers to report.

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

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

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

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

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	UAL	AU	5	24	-	0/3/7/9	-
24	DPP	AU	2	24	-	0/2/4/6	-
24	KBE	AU	1	24	-	2/7/7/8	-
24	KBE	CU	1	24	-	4/7/7/8	-
24	DPP	CU	2	24	-	0/2/4/6	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	5OH	CU	6	24	-	1/2/18/20	0/1/1/1
24	UAL	CU	5	24	-	0/3/7/9	-

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
61	FUA	AY	701	-	36,40,40	1.78	6 (16%)	46,64,64	1.84	11 (23%)
62	GDP	CY	702	-	24,30,30	1.35	3 (12%)	31,47,47	1.99	8 (25%)
61	FUA	CY	701	-	36,40,40	1.70	5 (13%)	46,64,64	1.99	12 (26%)
62	GDP	AY	702	-	24,30,30	1.35	3 (12%)	31,47,47	1.99	8 (25%)

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
61	FUA	AY	701	-	-	6/11/92/92	0/4/4/4
62	GDP	CY	702	-	-	3/12/32/32	0/3/3/3
61	FUA	CY	701	-	-	5/11/92/92	0/4/4/4
62	GDP	AY	702	-	-	3/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	FUA	C23-C22	-6.43	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	701	FUA	C23-C22	-5.95	1.41	1.51
61	AY	701	FUA	C23-C24	-4.30	1.39	1.53
62	CY	702	GDP	C6-N1	4.14	1.40	1.33
61	CY	701	FUA	C23-C24	-4.11	1.39	1.53
62	AY	702	GDP	C6-N1	4.09	1.40	1.33
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
62	AY	702	GDP	C2-N1	2.95	1.40	1.35
62	CY	702	GDP	C2-N1	2.92	1.40	1.35
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 (39) 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
62	AY	702	GDP	C2-N3-C4	5.36	121.47	115.36
62	CY	702	GDP	C2-N3-C4	5.32	121.44	115.36
62	AY	702	GDP	N3-C2-N1	-5.26	120.21	127.22
62	CY	702	GDP	N3-C2-N1	-5.22	120.26	127.22
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
62	CY	702	GDP	C5-C6-N1	-3.54	118.59	123.43
62	AY	702	GDP	C5-C6-N1	-3.53	118.60	123.43
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
61	AY	701	FUA	C10-C9-C11	2.53	120.05	114.76
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
62	CY	702	GDP	C4-C5-N7	-2.20	107.11	109.40
61	AY	701	FUA	C20-C8-C14	-2.17	107.62	110.85
62	AY	702	GDP	C4-C5-N7	-2.15	107.16	109.40
61	CY	701	FUA	C23-C24-C25	2.13	118.86	111.88
62	AY	702	GDP	C6-N1-C2	2.11	119.28	115.93
62	CY	702	GDP	C6-N1-C2	2.10	119.27	115.93
62	AY	702	GDP	N2-C2-N1	2.04	120.43	117.25
62	CY	702	GDP	N2-C2-N1	2.03	120.41	117.25
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.

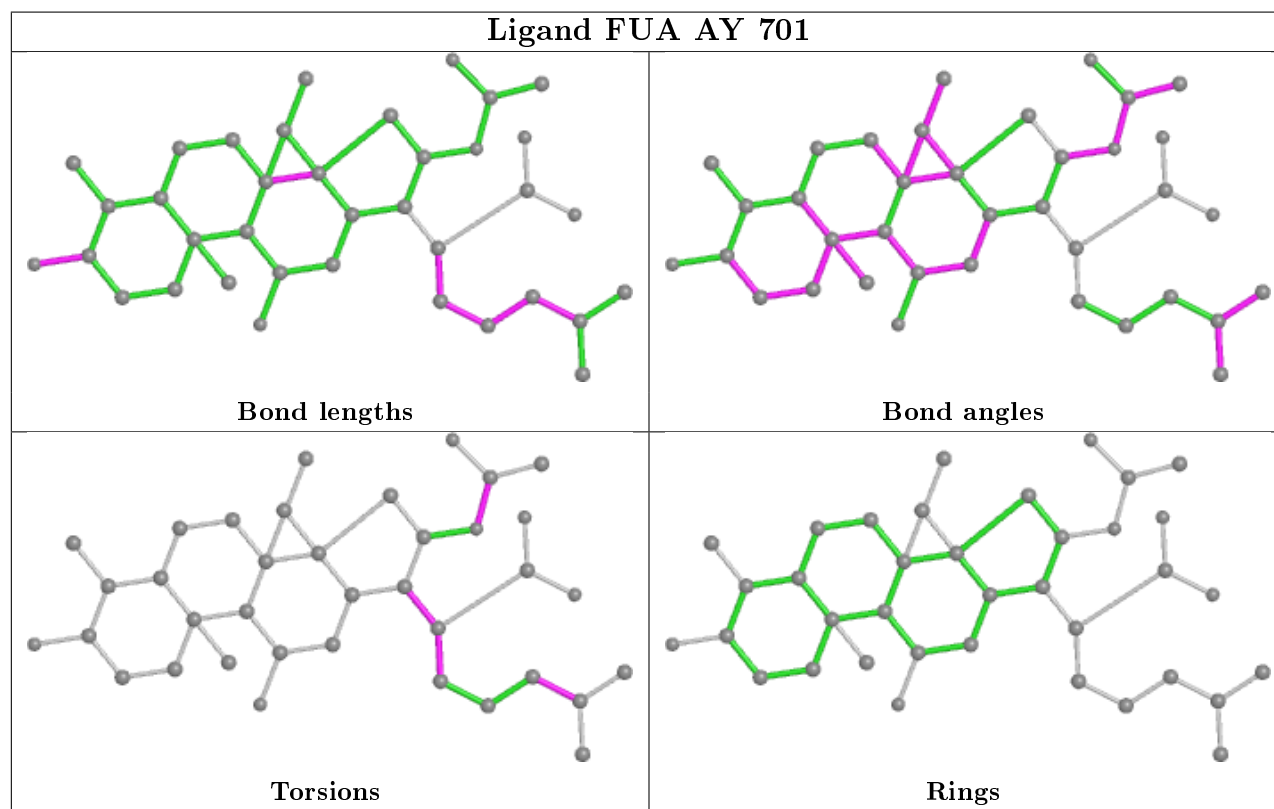
All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	CY	702	GDP	C5'-O5'-PA-O3A
62	CY	702	GDP	C5'-O5'-PA-O1A
62	AY	702	GDP	C5'-O5'-PA-O3A
62	AY	702	GDP	C5'-O5'-PA-O1A
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
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	CY	702	GDP	C5'-O5'-PA-O2A
62	AY	702	GDP	C5'-O5'-PA-O2A

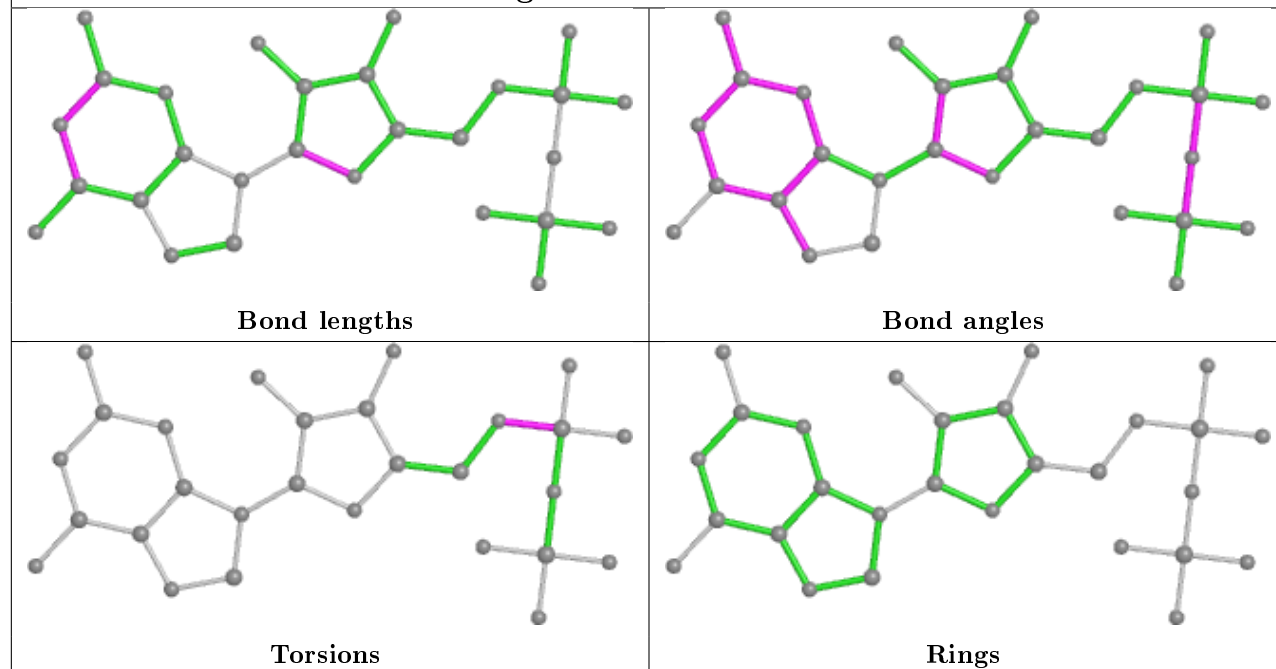
There are no ring outliers.

No monomer is involved in short contacts.

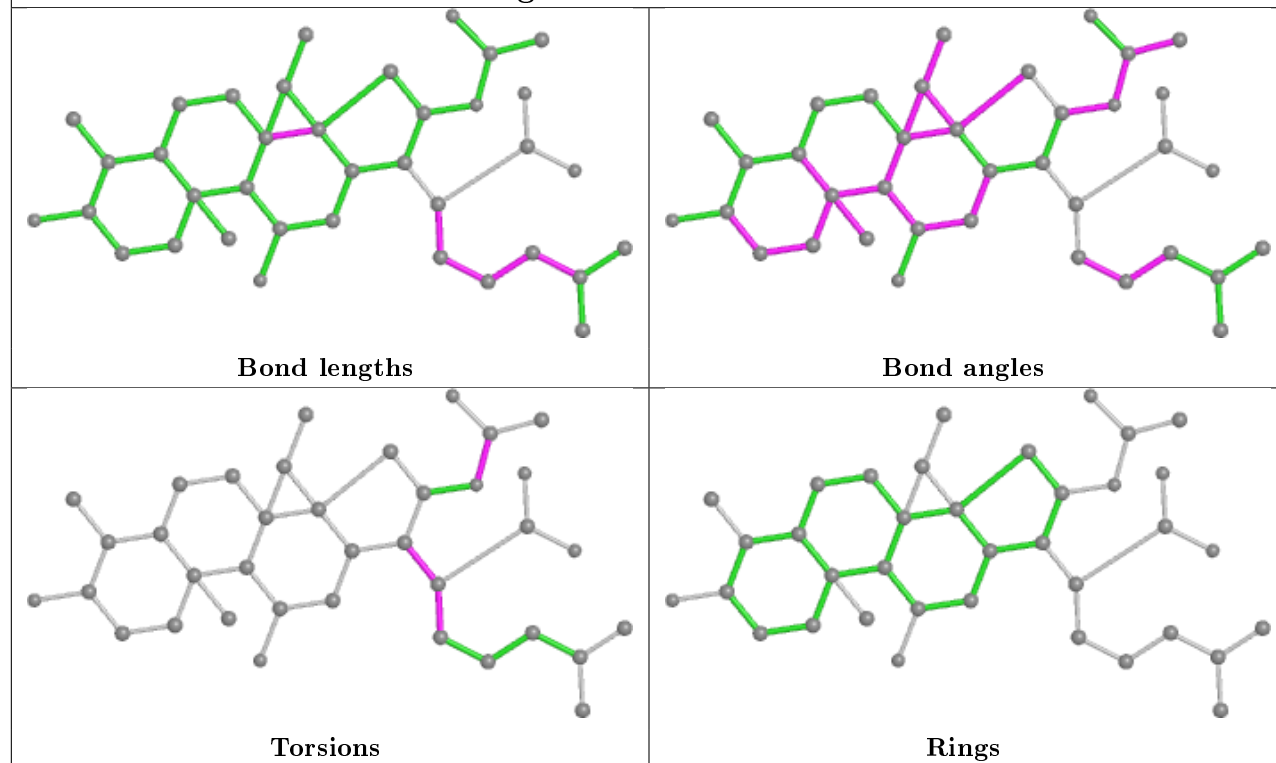
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

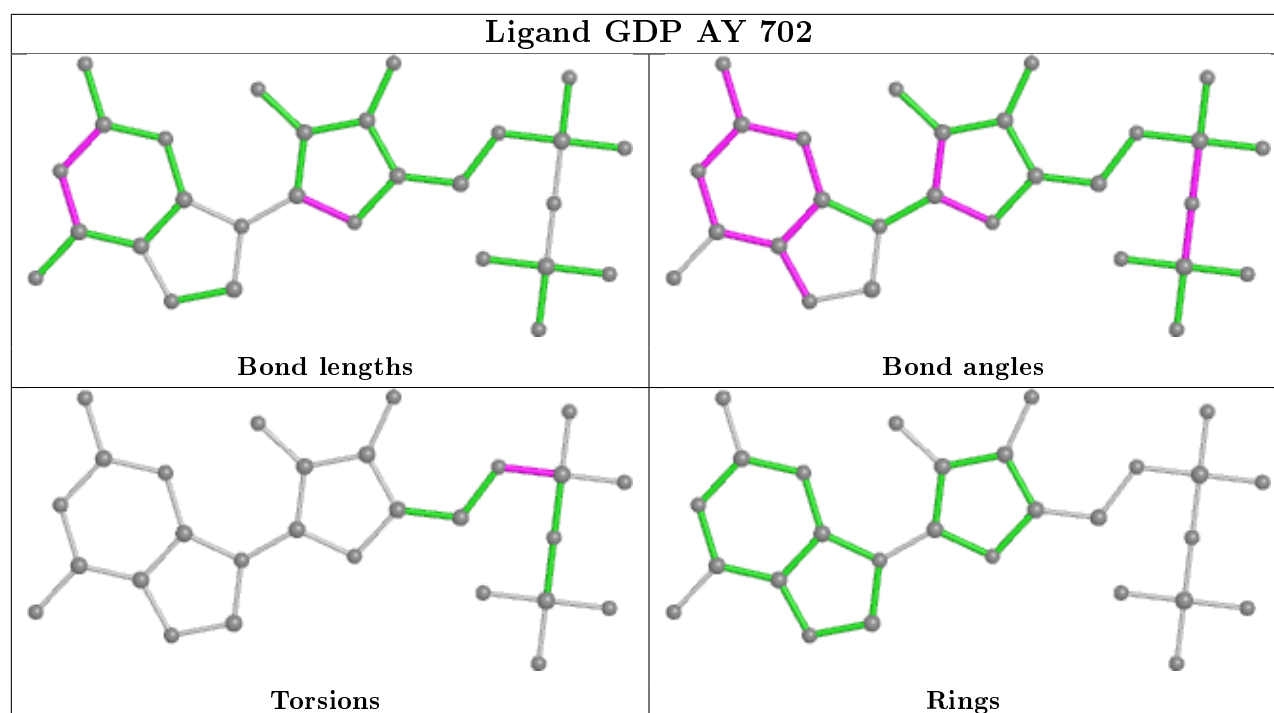


Ligand GDP CY 702



Ligand FUA CY 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	Be	1
54	De	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

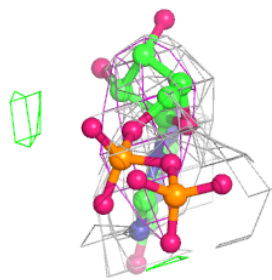
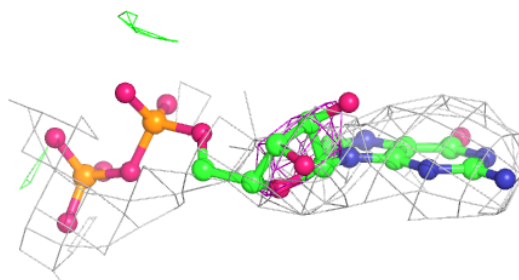
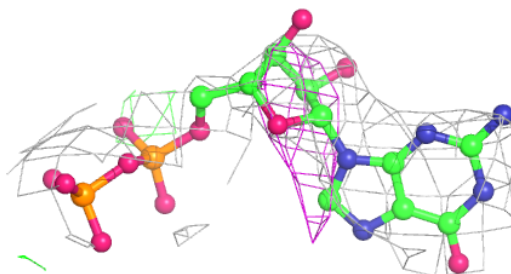
6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

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.

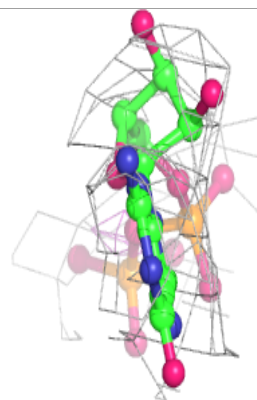
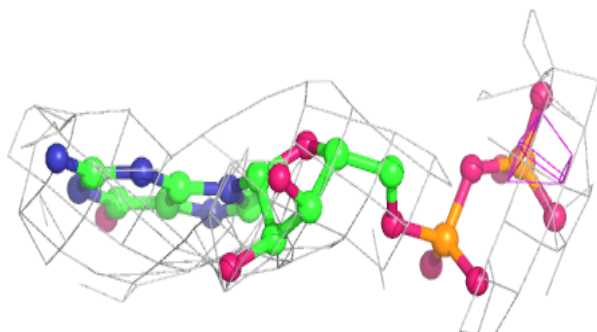
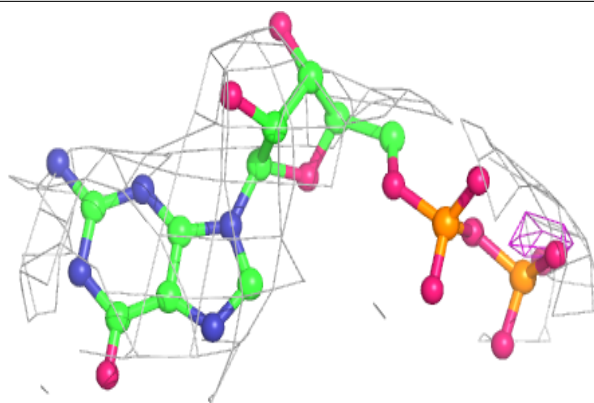
Electron density around GDP CY 702:

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



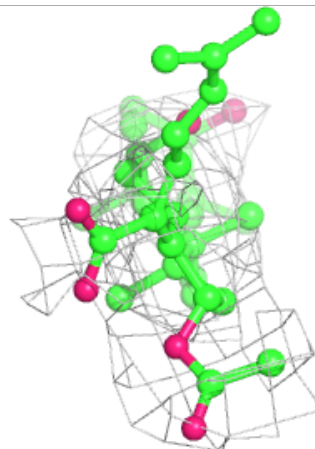
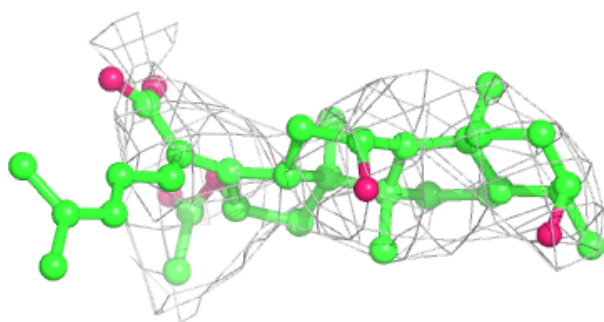
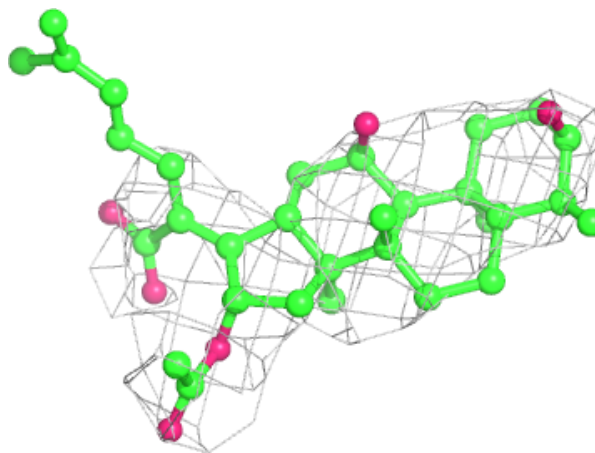
Electron density around GDP AY 702:

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



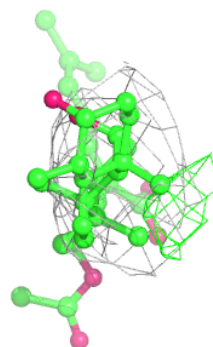
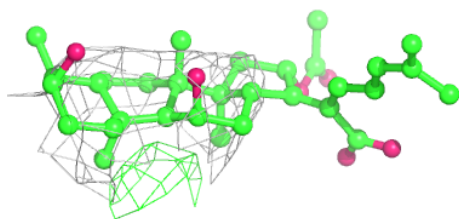
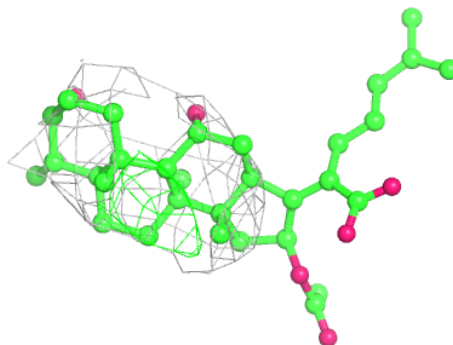
Electron density around FUA AY 701:

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



Electron density around 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)



6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.