Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 10:38 PM EDT

PDB ID	:	4XEJ
Title	:	IRES bound to bacterial Ribosome
Authors	:	Zhu, J.; Korostelev, A.; Noller, H.F.; Donohue, J.P.
Deposited on	:	2014-12-23
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

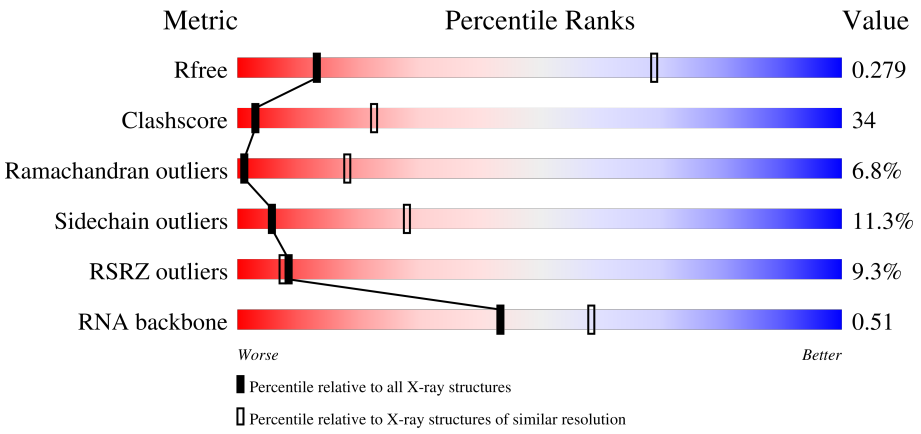
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	AL02	271	.% 82% 17% .
1	BL02	271	77% 21% .
2	AL03	204	3% 80% 19% .
2	BL03	204	3% 77% 21% .

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Mol	Chain	Length	Quality of chain
3	AL04	202	2%, 87%, 13%
3	BL04	202	%, 82%, 17%
4	AL05	181	30%, 83%, 15%
4	BL05	181	28%, 82%, 16%
5	AL06	159	38%, 91%, 9%
5	BL06	159	6%, 84%, 16%
6	AL09	145	30%, 80%, 19%
6	BL09	145	14%, 81%, 17%
7	AL11	147	80%, 90%, 10%
7	BL11	147	77%, 90%, 10%
8	AL13	137	6%, 77%, 21%
8	BL13	137	4%, 77%, 21%
9	AL14	122	84%, 15%
9	BL14	122	2%, 84%, 15%
10	AL15	146	5%, 64%, 28%, 8%
10	BL15	146	9%, 68%, 27%, 5%
11	AL16	134	7%, 86%, 13%
11	BL16	134	8%, 80%, 18%
12	AL17	117	7%, 81%, 19%
12	BL17	117	2%, 84%, 15%
13	AL18	98	27%, 81%, 18%
13	BL18	98	17%, 82%, 16%
14	AL19	137	5%, 76%, 23%
14	BL19	137	3%, 81%, 15%
15	AL20	117	2%, 84%, 15%

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Mol	Chain	Length	Quality of chain
15	BL20	117	87% 13%
16	AL21	101	2% 81% 18%
16	BL21	101	5% 76% 23%
17	AL22	112	4% 88% 12%
17	BL22	112	3% 88% 12%
18	AL23	92	90% 10%
18	BL23	92	2% 90% 10%
19	AL24	100	20% 73% 25%
19	BL24	100	10% 74% 22%
20	AL25	187	22% 90% 10%
20	BL25	187	7% 91% 9%
21	AL27	76	7% 87% 12%
21	BL27	76	7% 86% 12%
22	AL28	88	3% 72% 25%
22	BL28	88	5% 70% 28%
23	AL29	62	6% 87% 11%
23	BL29	62	10% 73% 26%
24	AL30	59	25% 90% 10%
24	BL30	59	8% 83% 14%
25	AL32	52	13% 83% 13%
25	BL32	52	4% 85% 15%
26	AL33	44	100% 77% 23%
26	BL33	44	89% 70% 30%
27	AL34	48	88% 12%
27	BL34	48	79% 19%

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Mol	Chain	Length	Quality of chain
28	AL35	63	2% 83% 14%
28	BL35	63	2% 81% 17%
29	AS02	234	9% 88% 12%
29	BS02	234	11% 91% 8%
30	AS03	206	7% 84% 14%
30	BS03	206	6% 88% 12%
31	AS04	208	2% 87% 12%
31	BS04	208	15% 85% 15%
32	AS05	151	3% 87% 12%
32	BS05	151	3% 89% 11%
33	AS06	101	5% 88% 11%
33	BS06	101	2% 87% 13%
34	AS07	155	21% 95% 5%
34	BS07	155	19% 95% 5%
35	AS08	138	9% 88% 11%
35	BS08	138	10% 91% 9%
36	AS09	127	30% 89% 10%
36	BS09	127	24% 91% 9%
37	AS10	98	50% 88% 11%
37	BS10	98	34% 90% 10%
38	AS11	114	11% 87% 13%
38	BS11	114	3% 89% 11%
39	AS12	122	10% 88% 12%
39	BS12	122	7% 89% 10%
40	AS13	117	35% 97%

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Mol	Chain	Length	Quality of chain
40	BS13	117	26% 92% 8%
41	AS14	60	18% 93% 5%
41	BS14	60	15% 92% 8%
42	AS15	88	6% 89% 11%
42	BS15	88	6% 86% 14%
43	AS16	83	14% 83% 17%
43	BS16	83	33% 93% 7%
44	AS17	99	3% 86% 14%
44	BS17	99	3% 89% 10%
45	AS18	70	13% 90% 10%
45	BS18	70	% 84% 16%
46	AS19	78	49% 87% 12%
46	BS19	78	36% 85% 14%
47	AS20	99	9% 86% 14%
47	BS20	99	22% 92% 8%
48	ATHX	24	4% 96%
48	BTHX	24	33% 92% 8%
49	AL31	30	43% 90% 10%
49	BL31	30	37% 87% 10%
50	A16S	1506	3% 83% 17%
50	B16S	1506	4% 83% 17%
51	A23S	2879	4% 81% 19%
51	B23S	2879	4% 80% 20%
52	A5S	119	% 27% 61% 13%
52	B5S	119	% 25% 66% 9%

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Mol	Chain	Length	Quality of chain
53	AIRE	196	5% 14% 84%
53	BIRE	196	% 14% 84%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 287293 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AL02	271	2105	1329	416	357	3	0	0	0
1	BL02	271	2105	1329	416	357	3	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AL03	204	1564	988	299	271	6	0	0	0
2	BL03	204	1564	988	299	271	6	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AL04	202	1587	1011	297	276	3	0	0	0
3	BL04	202	1587	1011	297	276	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AL05	181	1475	943	268	260	4	0	0	0
4	BL05	181	1475	943	268	260	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AL06	159	1223	773	228	221	1	0	0	0
5	BL06	159	1223	773	228	221	1	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AL09	145	1133	724	200	208	1	0	0	0
6	BL09	145	1133	724	200	208	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AL11	147	1088	692	191	199	6	0	0	0
7	BL11	147	1088	692	191	199	6	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	AL13	137	1097	707	205	182	3	0	0	0
8	BL13	137	1097	707	205	182	3	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AL14	122	932	587	171	170	4	0	0	0
9	BL14	122	932	587	171	170	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AL15	146	1114	692	227	193	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BL15	146	1114	692	227	193	2	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AL16	134	1065	680	201	179	5	0	0	0
11	BL16	134	1065	680	201	179	5	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	AL17	117	960	599	202	159	0	0	0
12	BL17	117	960	599	202	159	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	AL18	98	771	486	154	131	0	0	0
13	BL18	98	771	486	154	131	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AL19	137	1144	713	234	196	1	0	0	0
14	BL19	137	1144	713	234	196	1	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AL20	117	964	610	202	151	1	0	0	0
15	BL20	117	964	610	202	151	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AL21	101	779	501	142	135	1	0	0	0
16	BL21	101	779	501	142	135	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AL22	112	891	560	175	154	2	0	0	0
17	BL22	112	891	560	175	154	2	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AL23	92	726	471	131	124	0	0	0
18	BL23	92	726	471	131	124	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AL24	100	776	500	148	124	4	0	0	0
19	BL24	100	776	500	148	124	4	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AL25	187	1483	945	264	272	2	0	0	0
20	BL25	187	1483	945	264	272	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	AL27	76	605	376	126	102	1	0	0	0
21	BL27	76	605	376	126	102	1	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	AL28	88	695	435	141	119	0	0	0
22	BL28	88	695	435	141	119	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	AL29	62	521	325	102	92	2	0	0	0
23	BL29	62	521	325	102	92	2	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	AL30	59	468	298	90	79	1	0	0	0
24	BL30	59	468	298	90	79	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	AL32	52	405	255	79	66	5	0	0	0
25	BL32	52	405	255	79	66	5	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	AL33	44	381	235	77	65	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	BL33	44	381	235	77	65	4	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	AL34	48	419	257	104	56	2	0	0	0
27	BL34	48	419	257	104	56	2	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	AL35	63	508	326	101	79	2	0	0	0
28	BL35	63	508	326	101	79	2	0	0	0

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	AS02	234	1901	1213	341	342	5	0	0	0
29	BS02	234	1901	1213	341	342	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	AS03	206	1613	1016	314	282	1	0	0	0
30	BS03	206	1613	1016	314	282	1	0	0	0

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	AS04	208	1703	1066	339	291	7	0	0	0
31	BS04	208	1703	1066	339	291	7	0	0	0

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	AS05	151	1156	729	218	205	4	0	0	0
32	BS05	151	1156	729	218	205	4	0	0	0

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	AS06	101	843	531	155	154	3	0	0	0
33	BS06	101	843	531	155	154	3	0	0	0

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	AS07	155	1257	781	252	218	6	0	0	0
34	BS07	155	1257	781	252	218	6	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	AS08	138	1116	705	215	193	3	0	0	0
35	BS08	138	1116	705	215	193	3	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
36	AS09	127	1011	639	198	174	0	0	0
36	BS09	127	1011	639	198	174	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	AS10	98	795	499	156	139	1	0	0	0
37	BS10	98	795	499	156	139	1	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	AS11	114	843	522	159	159	3	0	0	0
38	BS11	114	843	522	159	159	3	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	AS12	122	957	603	193	160	1	0	0	0
39	BS12	122	957	603	193	160	1	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	AS13	117	934	577	192	163	2	0	0	0
40	BS13	117	934	577	192	163	2	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	AS14	60	492	312	104	72	4	0	0	0
41	BS14	60	492	312	104	72	4	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	AS15	88	734	459	147	126	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BS15	88	734	459	147	126	2	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	AS16	83	701	443	139	118	1	0	0	0
43	BS16	83	701	443	139	118	1	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	AS17	99	824	528	152	142	2	0	0	0
44	BS17	99	824	528	152	142	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	AS18	70	574	367	112	95	0	0	0
45	BS18	70	574	367	112	95	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	AS19	78	630	403	114	111	2	0	0	0
46	BS19	78	630	403	114	111	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	AS20	99	762	469	162	129	2	0	0	0
47	BS20	99	762	469	162	129	2	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	ATHX	24	209	128	50	31	0	0	0
48	BTHX	24	209	128	50	31	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	AL31	30	226	142	36	44	4	0	0	0
49	BL31	30	226	142	36	44	4	0	0	0

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
50	A16S	1504	32332	14391	5994	10444	1503	0	0	0
50	B16S	1504	32331	14391	5994	10443	1503	0	0	0

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
51	A23S	2876	61929	27563	11567	19924	2875	0	0	0
51	B23S	2876	61931	27565	11569	19922	2875	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A23S	1141A	U	C	conflict	GB 46197919
A23S	2825	U	G	conflict	GB 46197919
B23S	1141A	U	C	conflict	GB 46197919
B23S	2825	U	G	conflict	GB 46197919

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
52	A5S	119	2551	1136	471	826	118	0	0	0
52	B5S	119	2551	1136	471	826	118	0	0	0

- Molecule 53 is a RNA chain called IRES RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	AIRE	32	672	302	114	225	31	0	0	0
53	BIRE	32	672	302	114	225	31	0	0	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

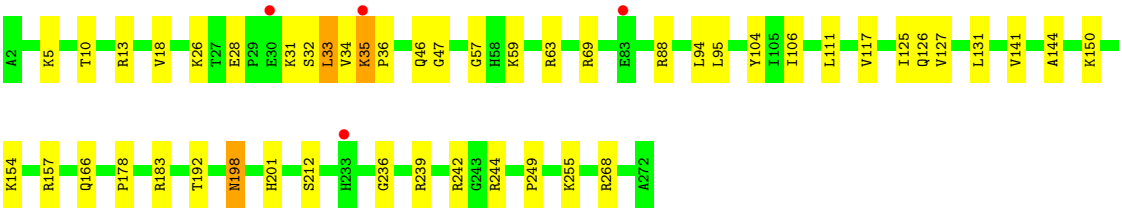
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
54	AS04	1	1	1	0	0
54	AS14	1	1	1	0	0
54	BS04	1	1	1	0	0
54	BS14	1	1	1	0	0

3 Residue-property plots (i)

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

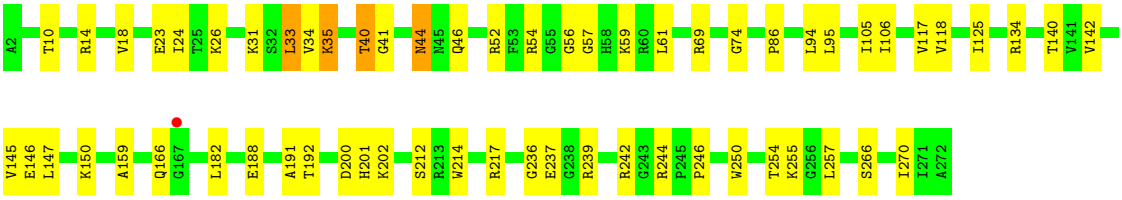
• Molecule 1: 50S ribosomal protein L2

Chain AL02:



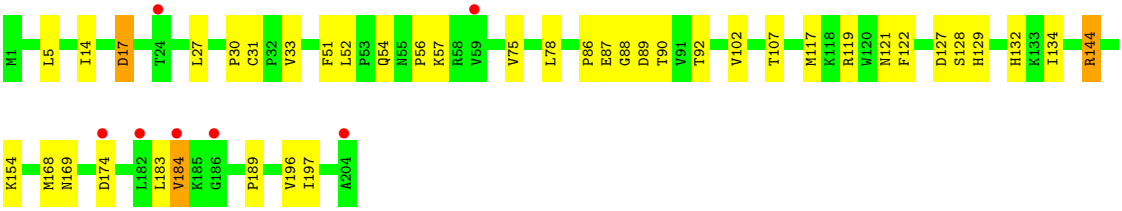
• Molecule 1: 50S ribosomal protein L2

Chain BL02:



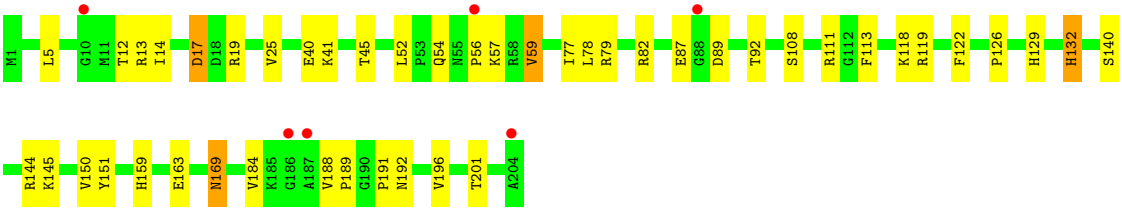
• Molecule 2: 50S ribosomal protein L3

Chain AL03:



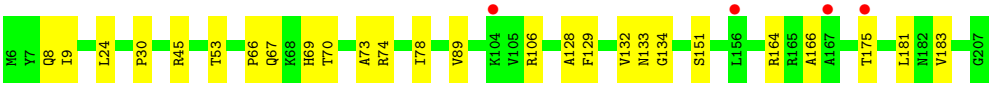
• Molecule 2: 50S ribosomal protein L3

Chain BL03:



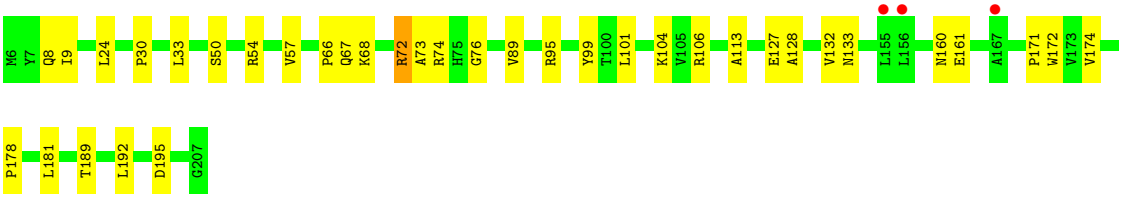
- Molecule 3: 50S ribosomal protein L4

Chain AL04:



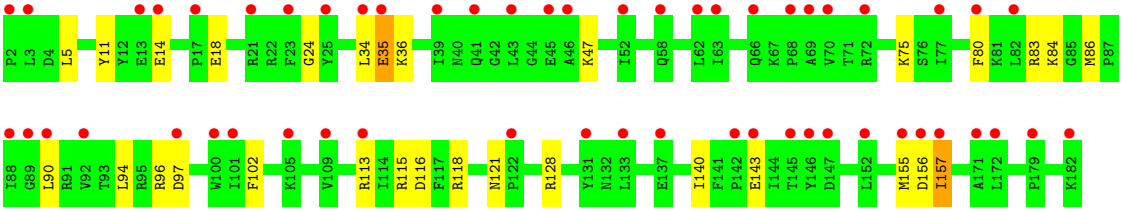
- Molecule 3: 50S ribosomal protein L4

Chain BL04:



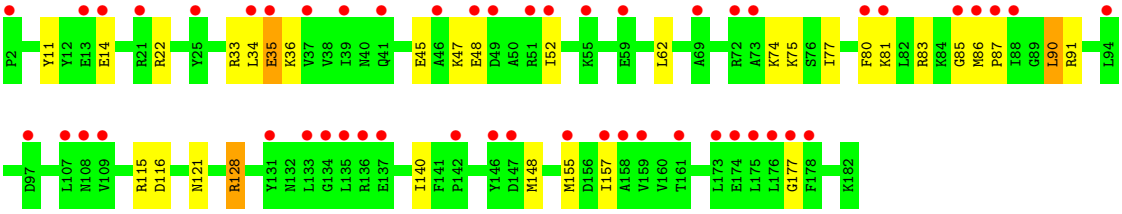
- Molecule 4: 50S ribosomal protein L5

Chain AL05:



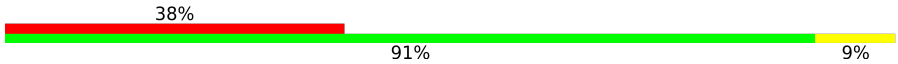
- Molecule 4: 50S ribosomal protein L5

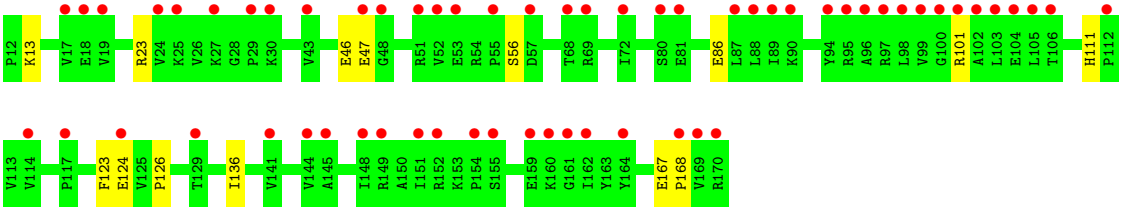
Chain BL05:



- Molecule 5: 50S ribosomal protein L6

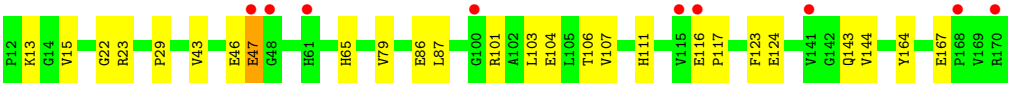
Chain AL06:





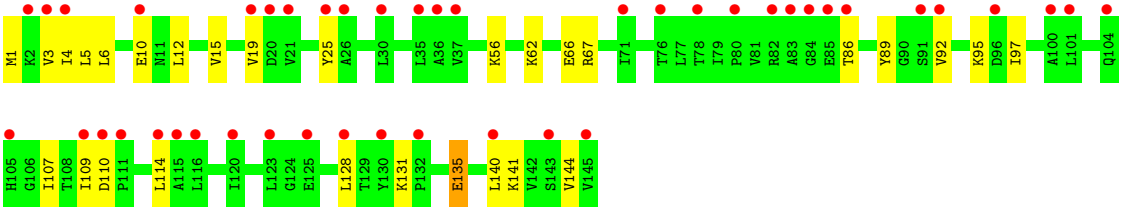
• Molecule 5: 50S ribosomal protein L6

Chain BL06:



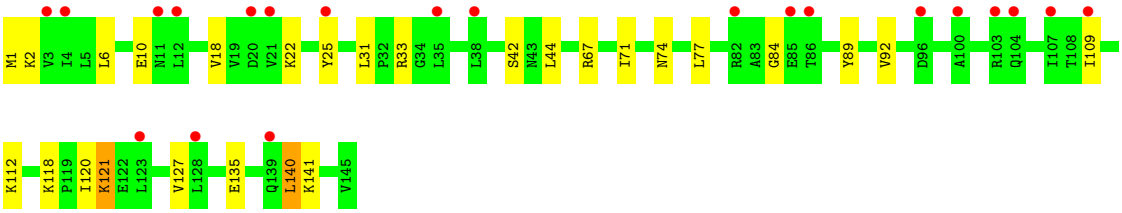
• Molecule 6: 50S ribosomal protein L9

Chain AL09:



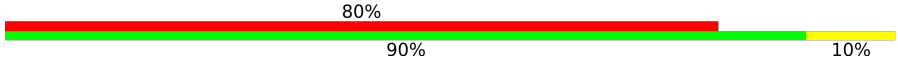
• Molecule 6: 50S ribosomal protein L9

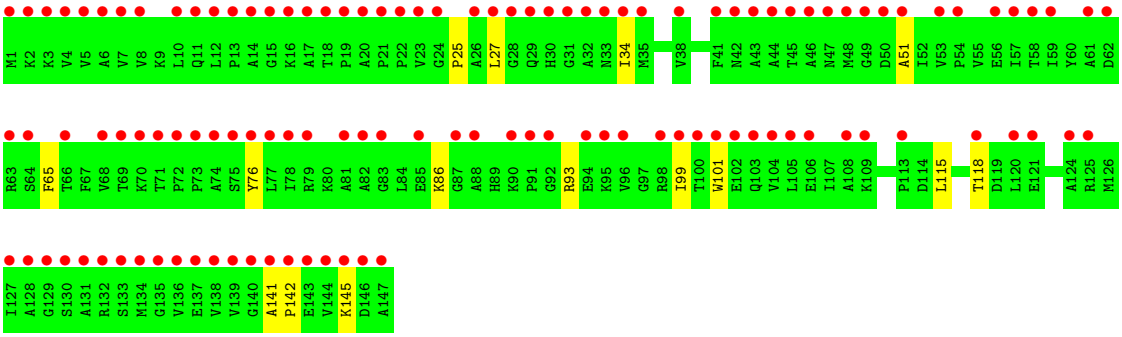
Chain BL09:



• Molecule 7: 50S ribosomal protein L11

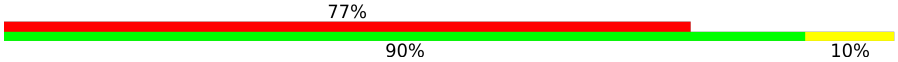
Chain AL11:

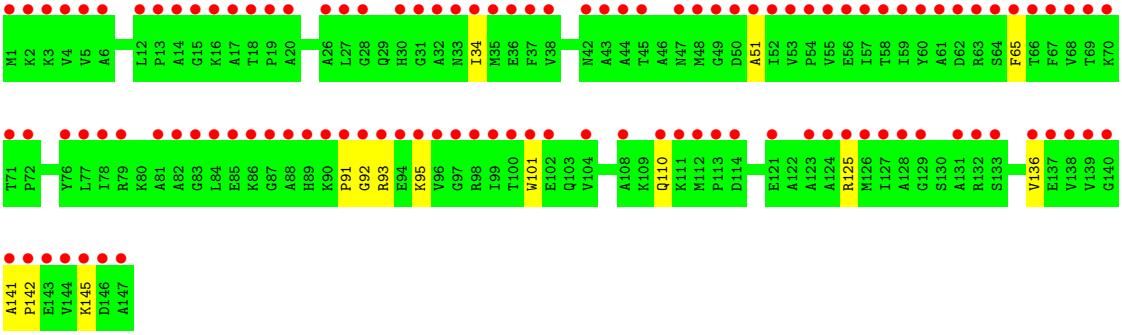




• Molecule 7: 50S ribosomal protein L11

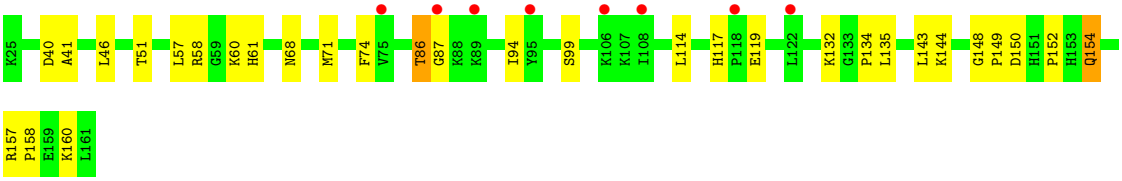
Chain BL11:





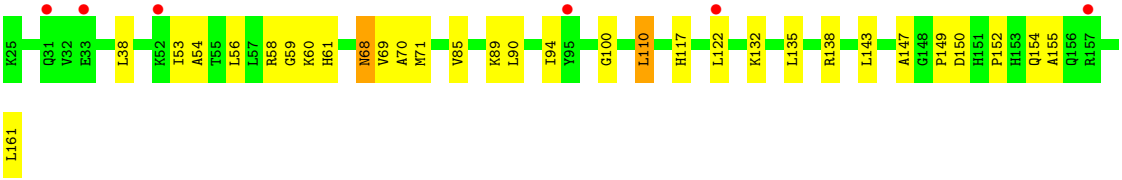
• Molecule 8: 50S ribosomal protein L13

Chain AL13:



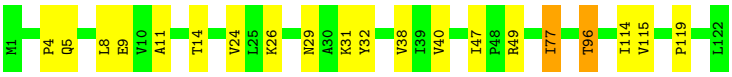
• Molecule 8: 50S ribosomal protein L13

Chain BL13:



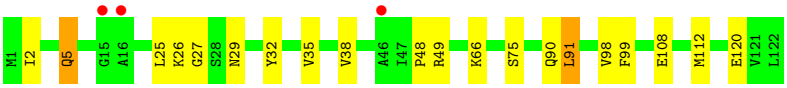
• Molecule 9: 50S ribosomal protein L14

Chain AL14:



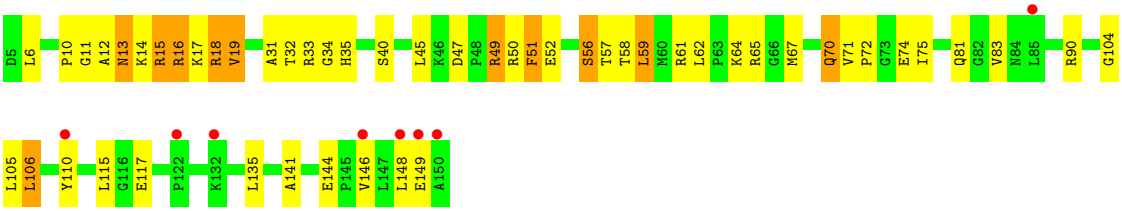
• Molecule 9: 50S ribosomal protein L14

Chain BL14:



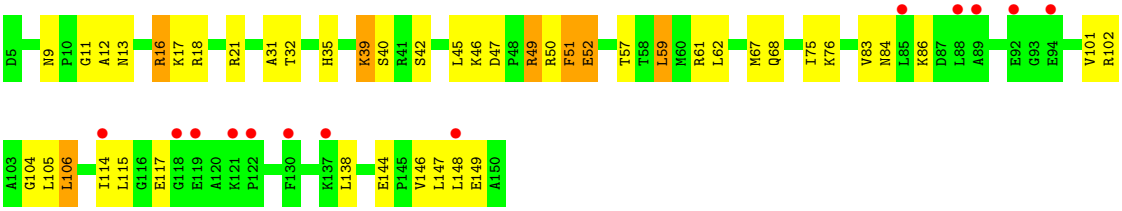
• Molecule 10: 50S ribosomal protein L15

Chain AL15: 5% 64% 28% 8%



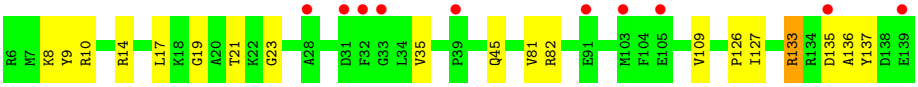
- Molecule 10: 50S ribosomal protein L15

Chain BL15: 9% 68% 27% 5%



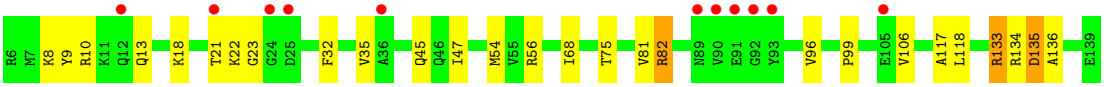
- Molecule 11: 50S ribosomal protein L16

Chain AL16: 7% 86% 13%



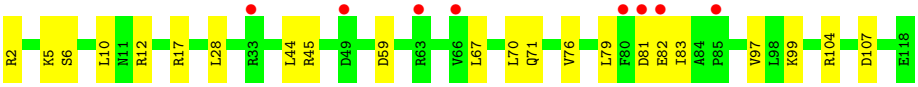
- Molecule 11: 50S ribosomal protein L16

Chain BL16: 8% 80% 18%



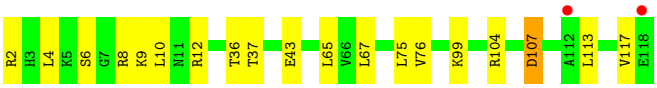
- Molecule 12: 50S ribosomal protein L17

Chain AL17: 7% 81% 19%



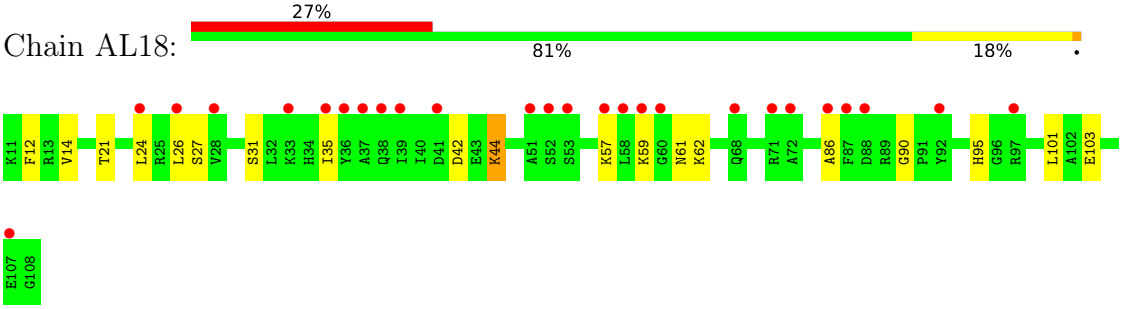
- Molecule 12: 50S ribosomal protein L17

Chain BL17: 2% 84% 15%



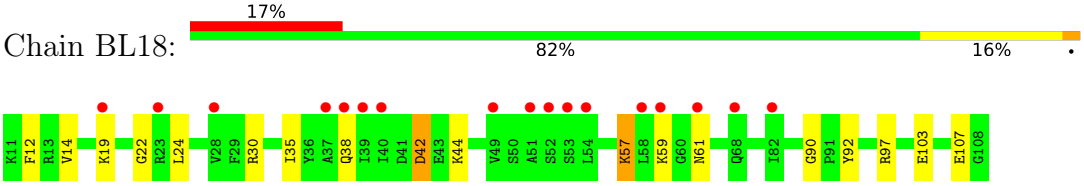
• Molecule 13: 50S ribosomal protein L18

Chain AL18:



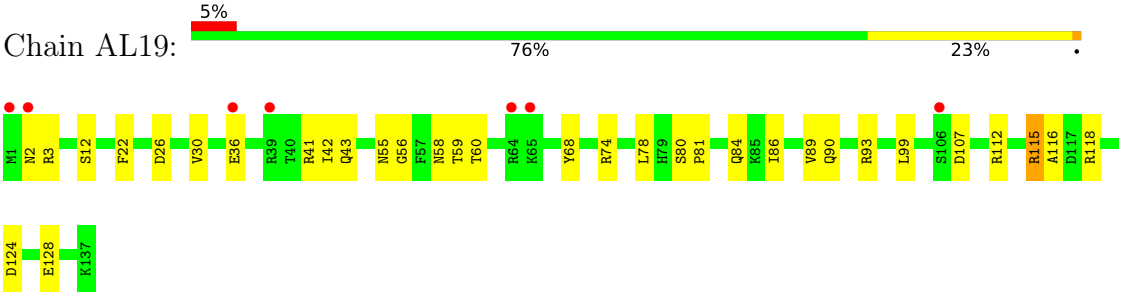
• Molecule 13: 50S ribosomal protein L18

Chain BL18:



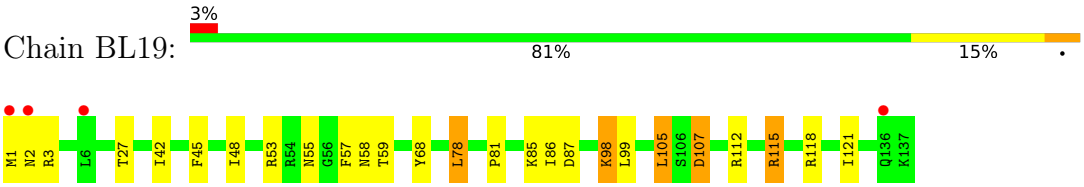
• Molecule 14: 50S ribosomal protein L19

Chain AL19:



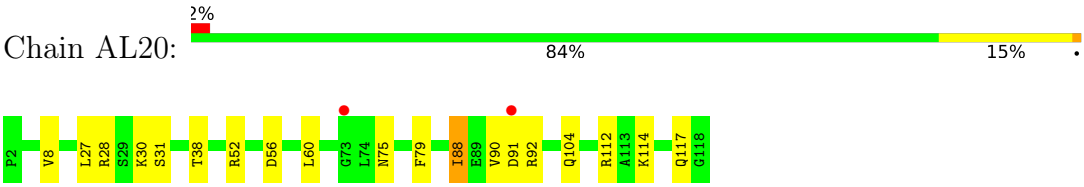
• Molecule 14: 50S ribosomal protein L19

Chain BL19:



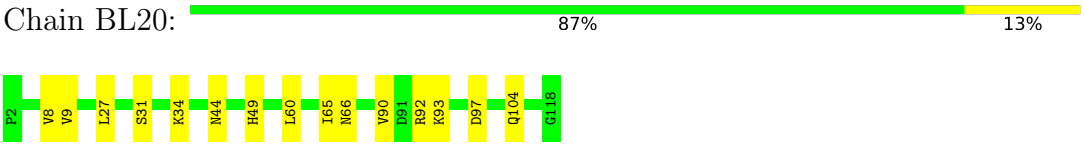
• Molecule 15: 50S ribosomal protein L20

Chain AL20:



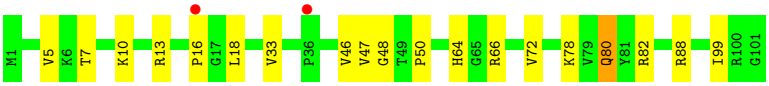
• Molecule 15: 50S ribosomal protein L20

Chain BL20:



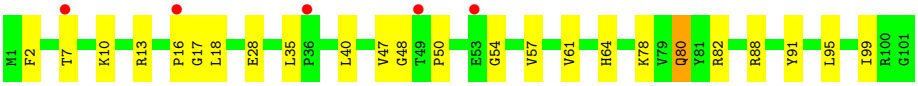
• Molecule 16: 50S ribosomal protein L21

Chain AL21:



• Molecule 16: 50S ribosomal protein L21

Chain BL21:

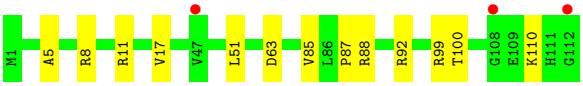


• Molecule 17: 50S ribosomal protein L22

Chain AL22:

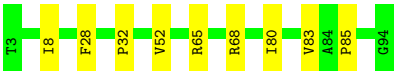
• Molecule 17: 50S ribosomal protein L22

Chain BL22:



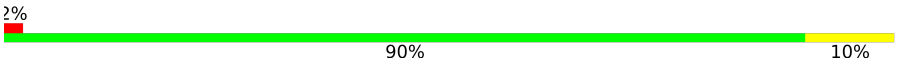
• Molecule 18: 50S ribosomal protein L23

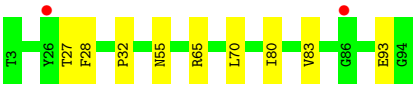
Chain AL23:



• Molecule 18: 50S ribosomal protein L23

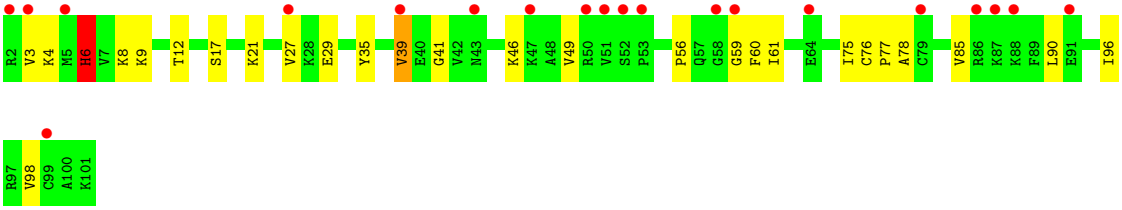
Chain BL23:





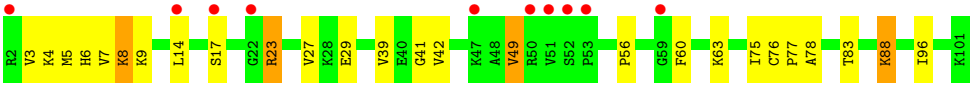
• Molecule 19: 50S ribosomal protein L24

Chain AL24:



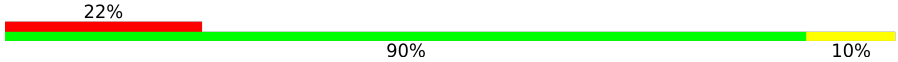
- Molecule 19: 50S ribosomal protein L24

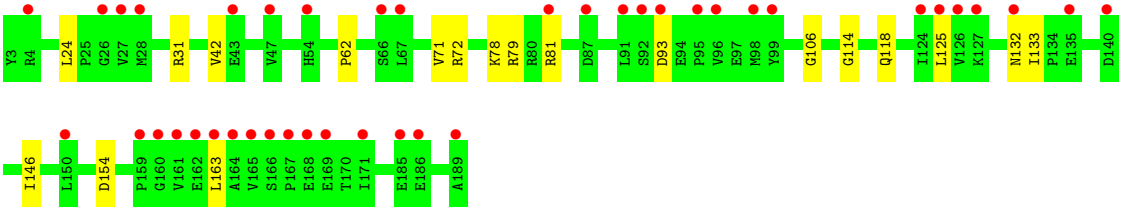
Chain BL24:



- Molecule 20: 50S ribosomal protein L25

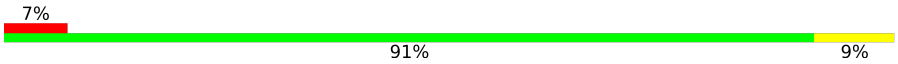
Chain AL25:





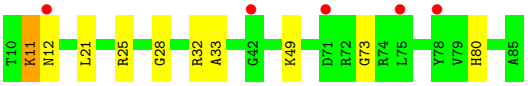
- Molecule 20: 50S ribosomal protein L25

Chain BL25:



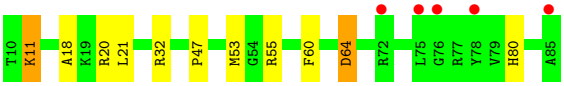
- Molecule 21: 50S ribosomal protein L27

Chain AL27:



- Molecule 21: 50S ribosomal protein L27

Chain BL27:



- Molecule 22: 50S ribosomal protein L28

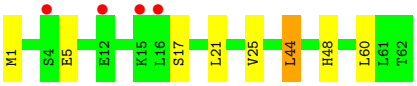
Chain AL28:

• Molecule 22: 50S ribosomal protein L28

Chain BL28:

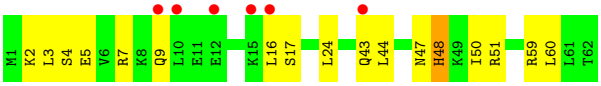
• Molecule 23: 50S ribosomal protein L29

Chain AL29:



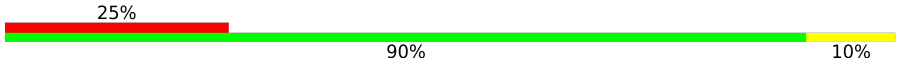
• Molecule 23: 50S ribosomal protein L29

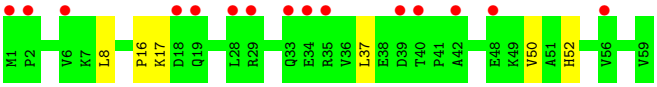
Chain BL29:



• Molecule 24: 50S ribosomal protein L30

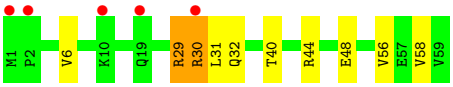
Chain AL30:





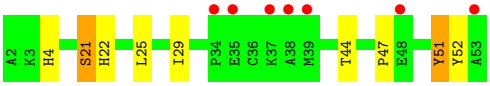
• Molecule 24: 50S ribosomal protein L30

Chain BL30:



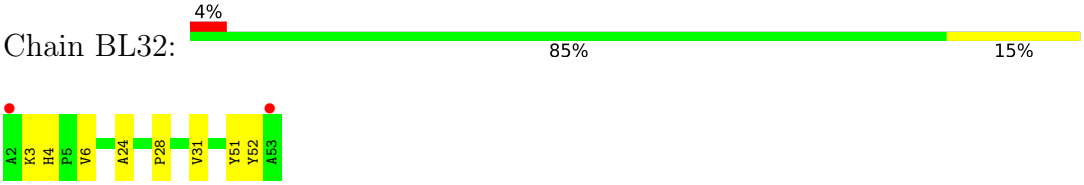
• Molecule 25: 50S ribosomal protein L32

Chain AL32:



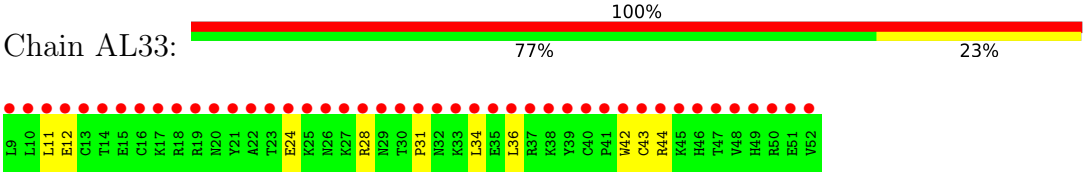
• Molecule 25: 50S ribosomal protein L32

Chain BL32:



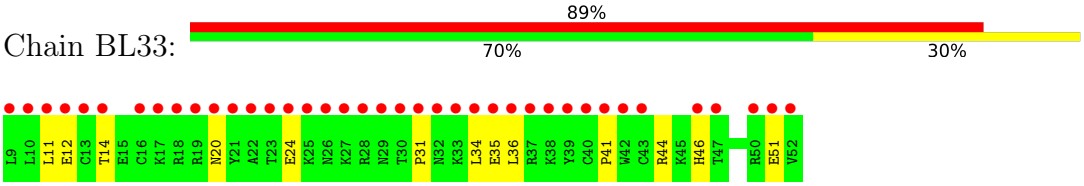
• Molecule 26: 50S ribosomal protein L33

Chain AL33:



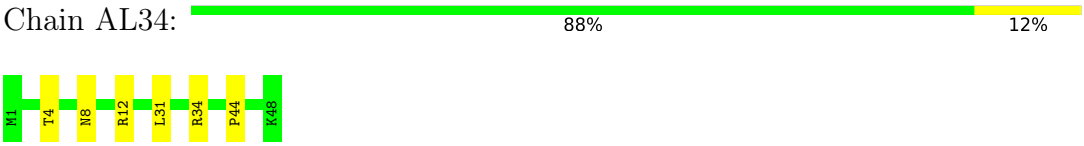
• Molecule 26: 50S ribosomal protein L33

Chain BL33:



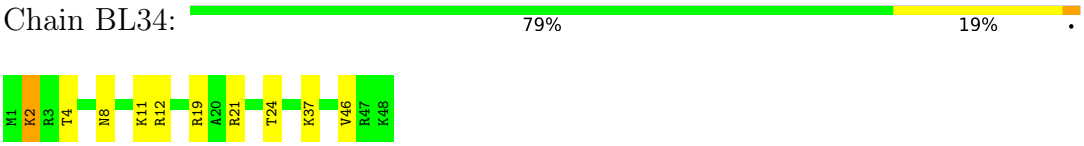
• Molecule 27: 50S ribosomal protein L34

Chain AL34:



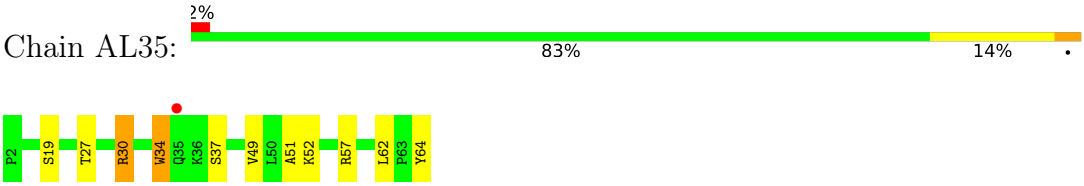
• Molecule 27: 50S ribosomal protein L34

Chain BL34:



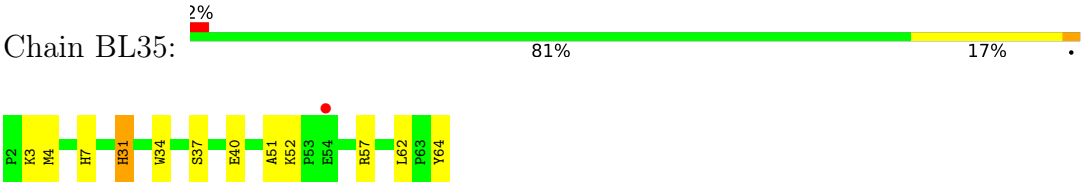
• Molecule 28: 50S ribosomal protein L35

Chain AL35:



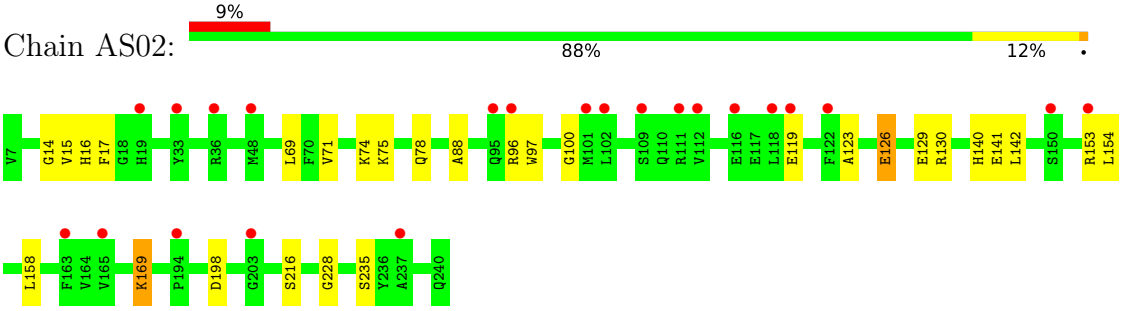
• Molecule 28: 50S ribosomal protein L35

Chain BL35:



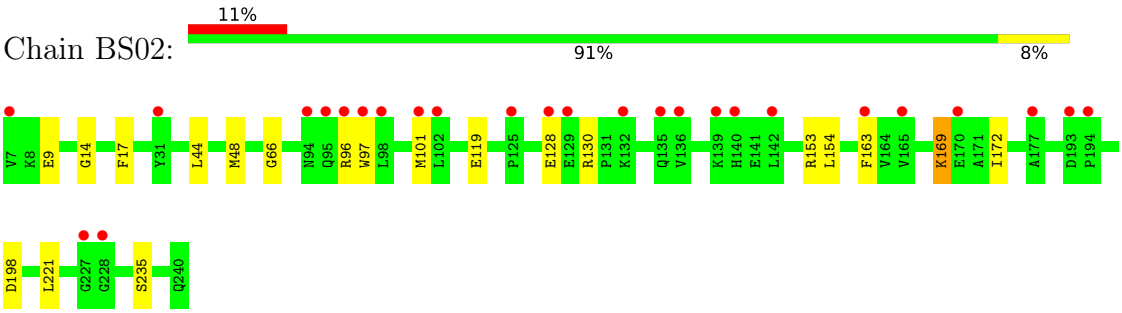
• Molecule 29: 30S ribosomal protein S2

Chain AS02:



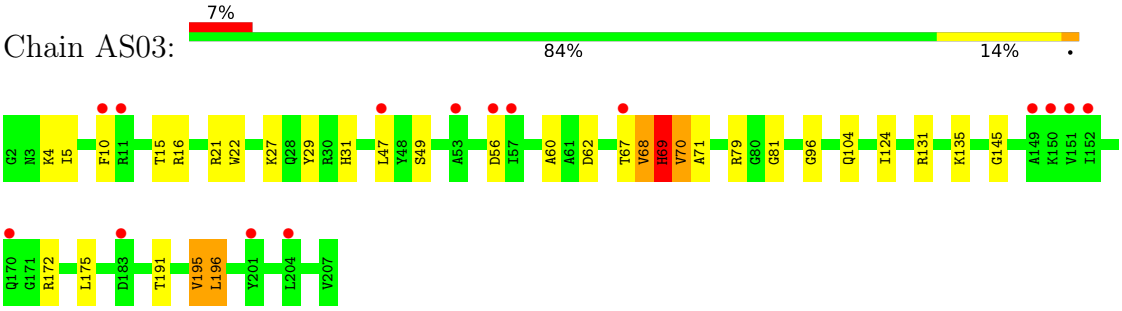
• Molecule 29: 30S ribosomal protein S2

Chain BS02:



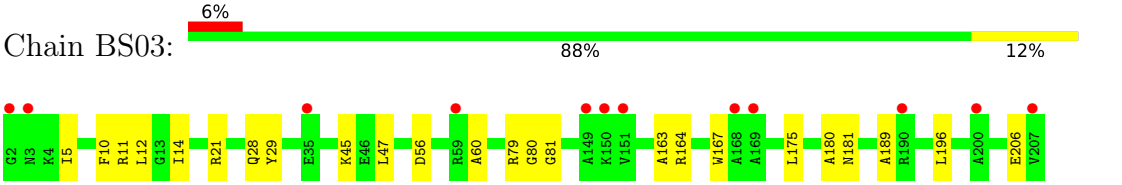
• Molecule 30: 30S ribosomal protein S3

Chain AS03:



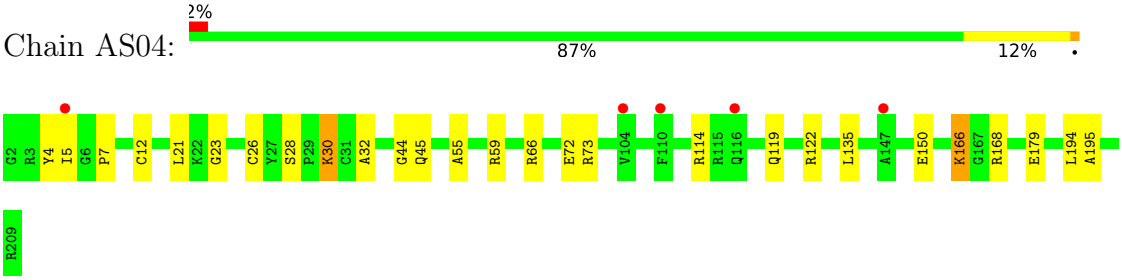
• Molecule 30: 30S ribosomal protein S3

Chain BS03:



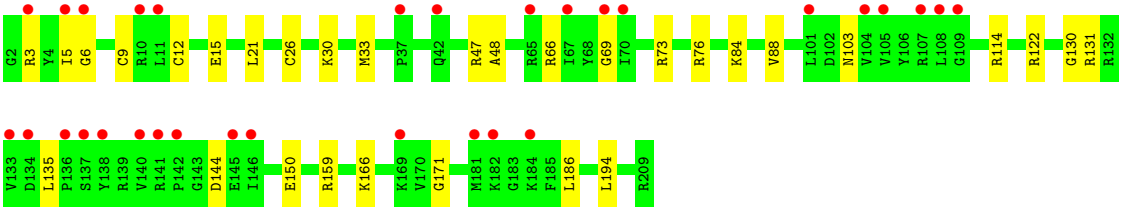
• Molecule 31: 30S ribosomal protein S4

Chain AS04:



• Molecule 31: 30S ribosomal protein S4

Chain BS04:

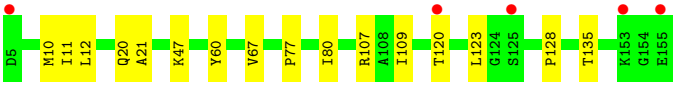


• Molecule 32: 30S ribosomal protein S5

Chain AS05:

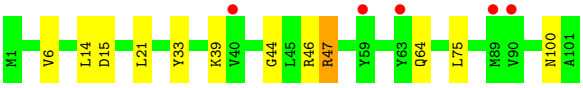
• Molecule 32: 30S ribosomal protein S5

Chain BS05:



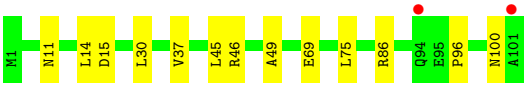
• Molecule 33: 30S ribosomal protein S6

Chain AS06:



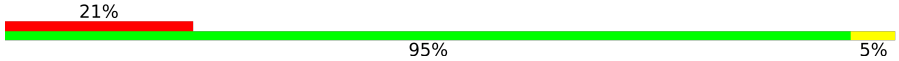
• Molecule 33: 30S ribosomal protein S6

Chain BS06:



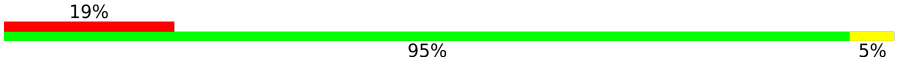
• Molecule 34: 30S ribosomal protein S7

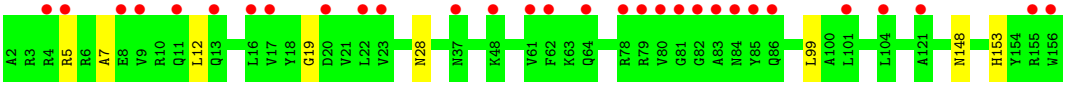
Chain AS07:



• Molecule 34: 30S ribosomal protein S7

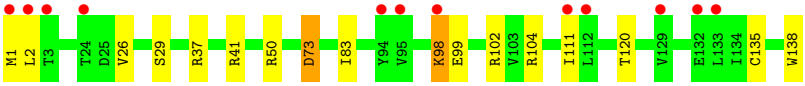
Chain BS07:





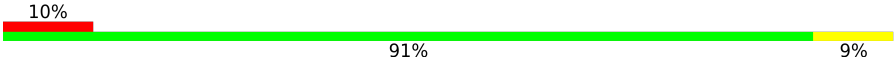
• Molecule 35: 30S ribosomal protein S8

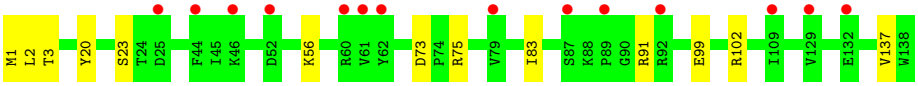
Chain AS08:



• Molecule 35: 30S ribosomal protein S8

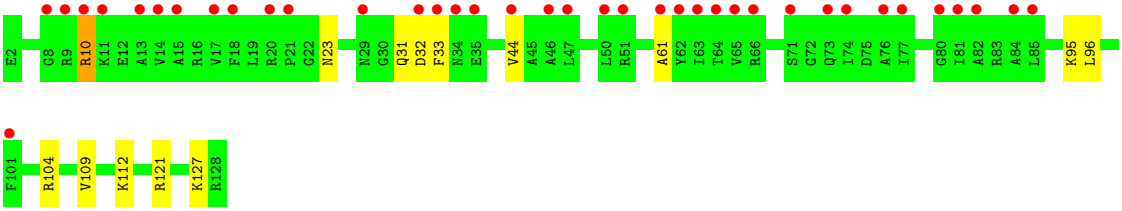
Chain BS08:





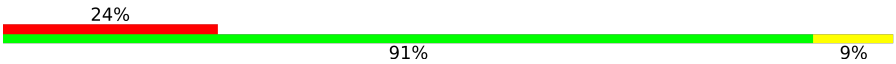
• Molecule 36: 30S ribosomal protein S9

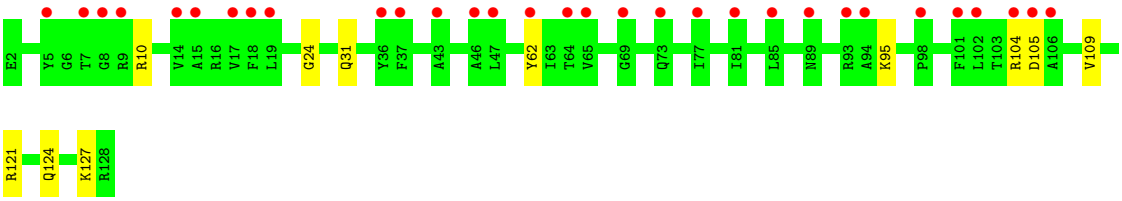
Chain AS09:



• Molecule 36: 30S ribosomal protein S9

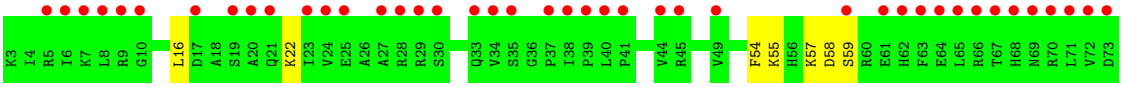
Chain BS09:

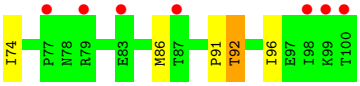




• Molecule 37: 30S ribosomal protein S10

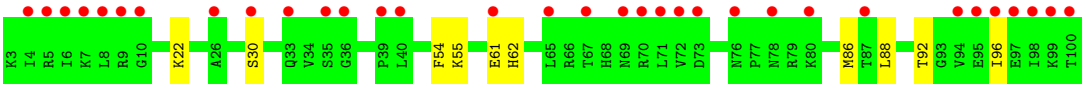
Chain AS10:





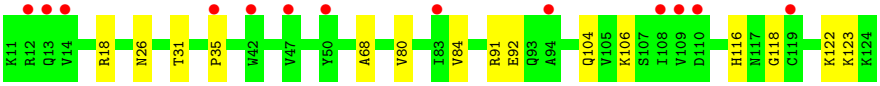
• Molecule 37: 30S ribosomal protein S10

Chain BS10:



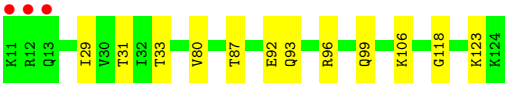
• Molecule 38: 30S ribosomal protein S11

Chain AS11:



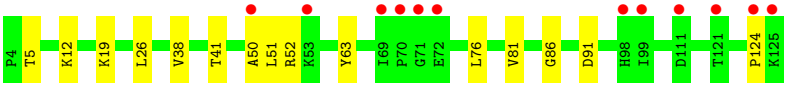
• Molecule 38: 30S ribosomal protein S11

Chain BS11:



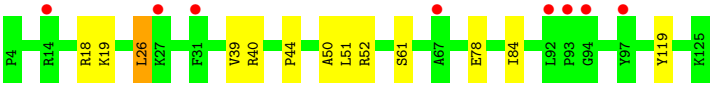
• Molecule 39: 30S ribosomal protein S12

Chain AS12:



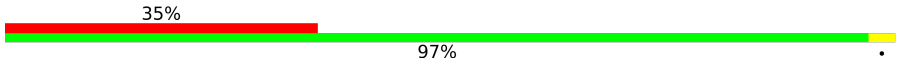
• Molecule 39: 30S ribosomal protein S12

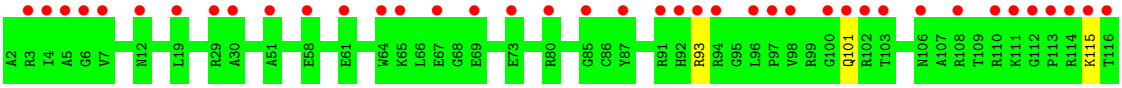
Chain BS12:



• Molecule 40: 30S ribosomal protein S13

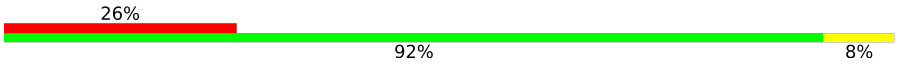
Chain AS13:

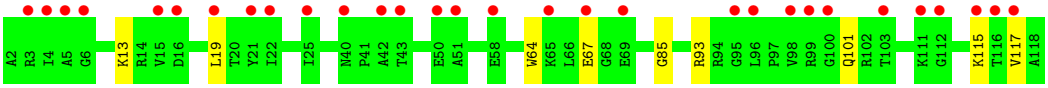




• Molecule 40: 30S ribosomal protein S13

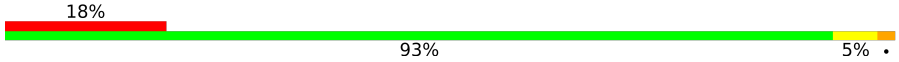
Chain BS13:

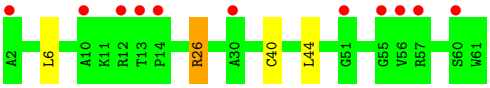




• Molecule 41: 30S ribosomal protein S14

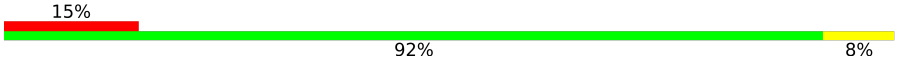
Chain AS14:

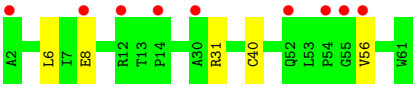




• Molecule 41: 30S ribosomal protein S14

Chain BS14:



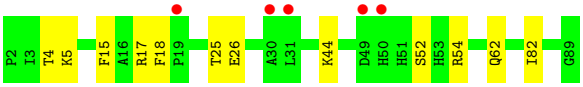


• Molecule 42: 30S ribosomal protein S15

Chain AS15:

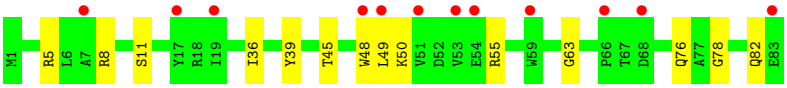
• Molecule 42: 30S ribosomal protein S15

Chain BS15:



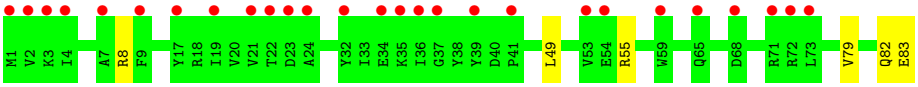
• Molecule 43: 30S ribosomal protein S16

Chain AS16:



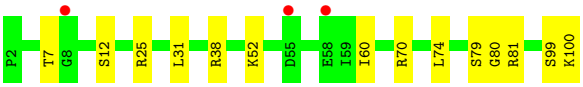
• Molecule 43: 30S ribosomal protein S16

Chain BS16: 33% 93% 7%



• Molecule 44: 30S ribosomal protein S17

Chain AS17: 3% 86% 14%

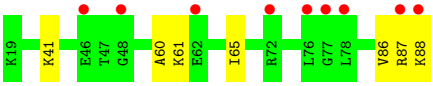


• Molecule 44: 30S ribosomal protein S17

Chain BS17: 3% 89% 10%

• Molecule 45: 30S ribosomal protein S18

Chain AS18: 13% 90% 10%

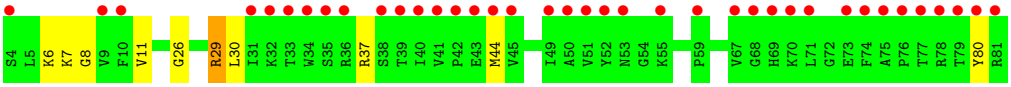


• Molecule 45: 30S ribosomal protein S18

Chain BS18: % 84% 16%

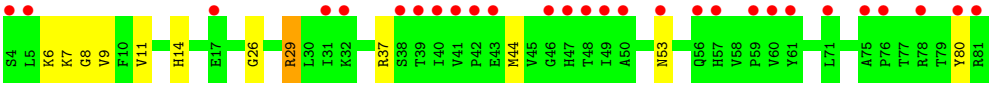
• Molecule 46: 30S ribosomal protein S19

Chain AS19: 49% 87% 12%



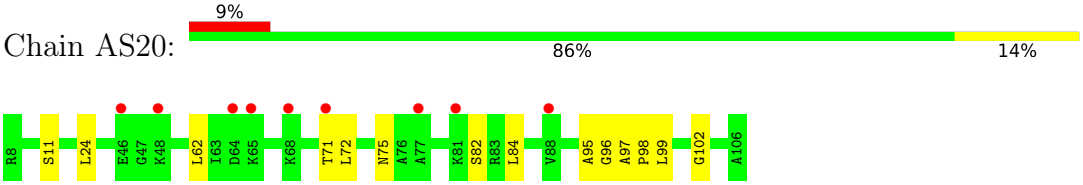
• Molecule 46: 30S ribosomal protein S19

Chain BS19: 36% 85% 14%



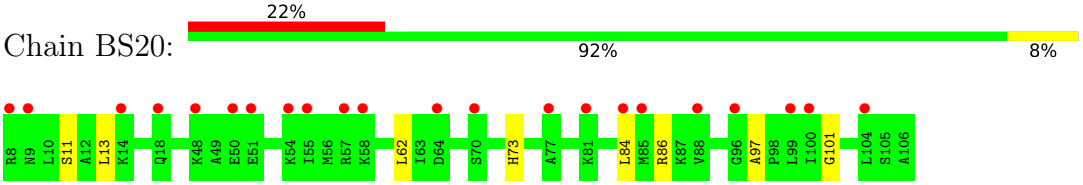
• Molecule 47: 30S ribosomal protein S20

Chain AS20:



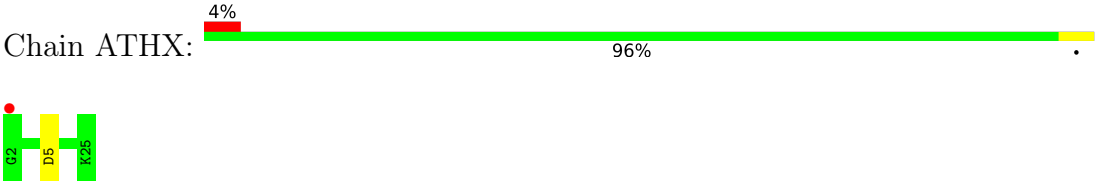
• Molecule 47: 30S ribosomal protein S20

Chain BS20:



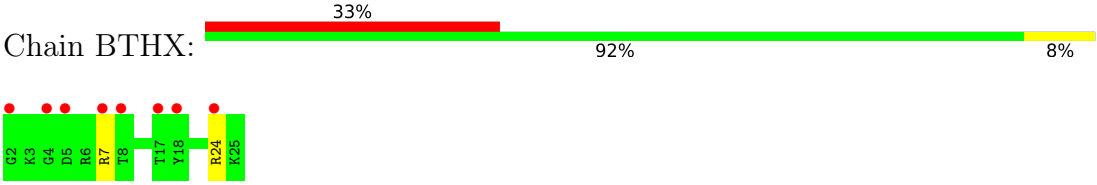
• Molecule 48: 30S ribosomal protein Thx

Chain ATHX:



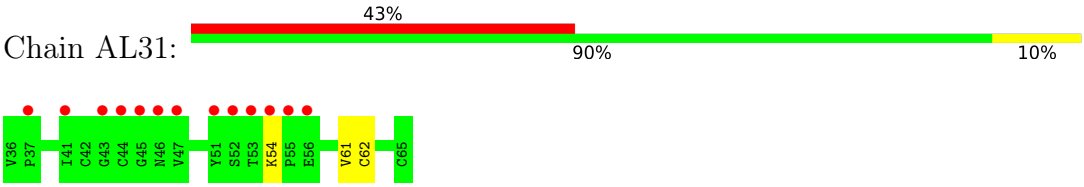
• Molecule 48: 30S ribosomal protein Thx

Chain BTHX:



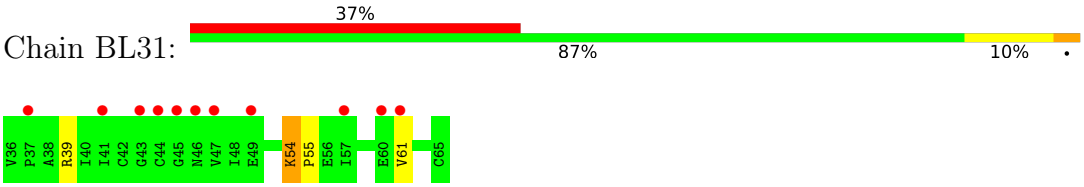
• Molecule 49: 50S ribosomal protein L31

Chain AL31:



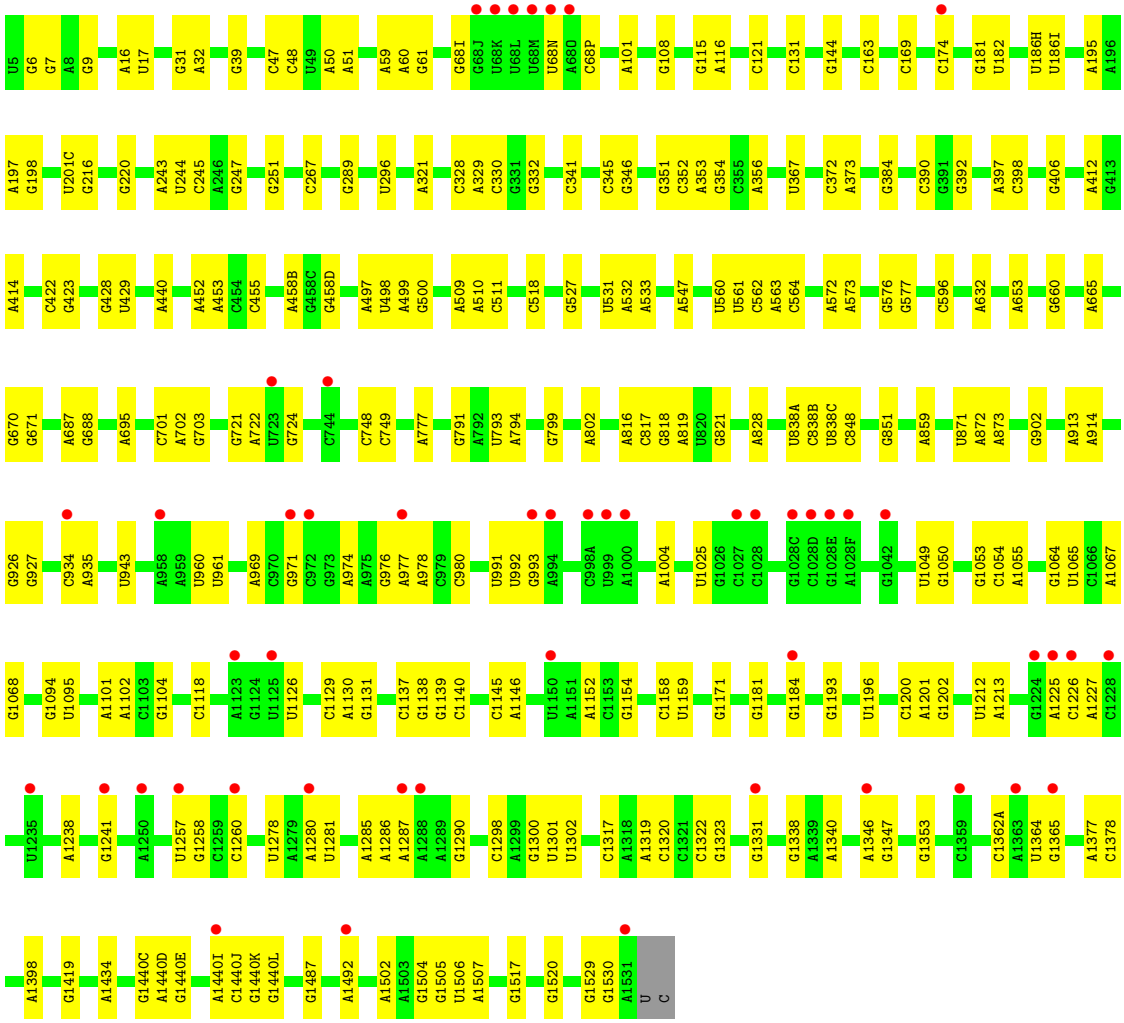
• Molecule 49: 50S ribosomal protein L31

Chain BL31:



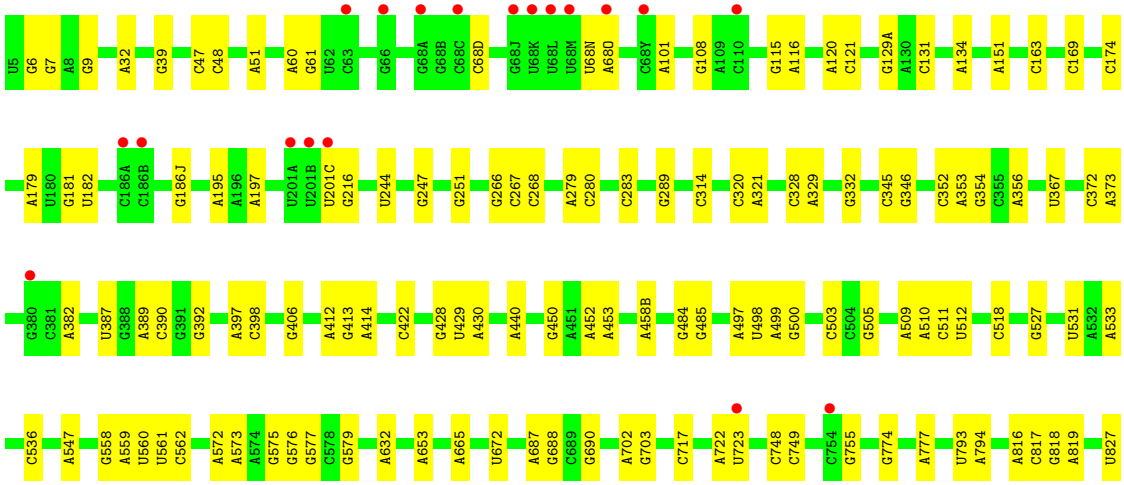
• Molecule 50: 16S ribosomal RNA

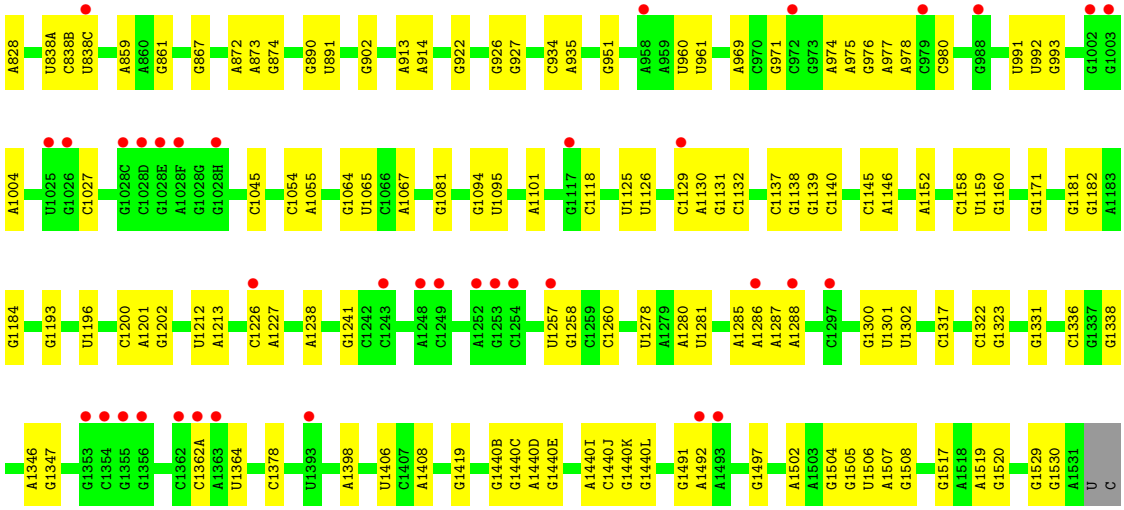
Chain A16S:



- Molecule 50: 16S ribosomal RNA

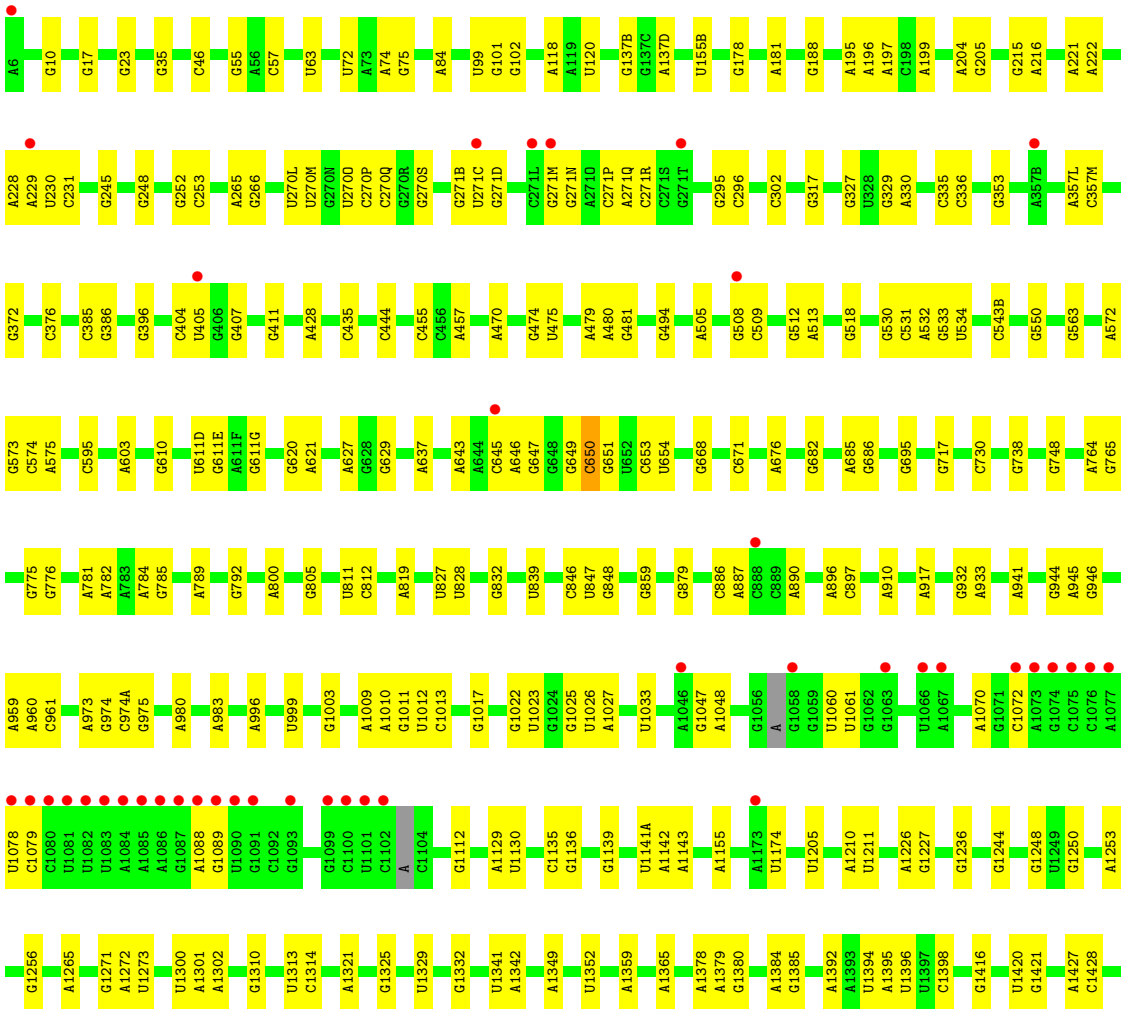
Chain B16S:

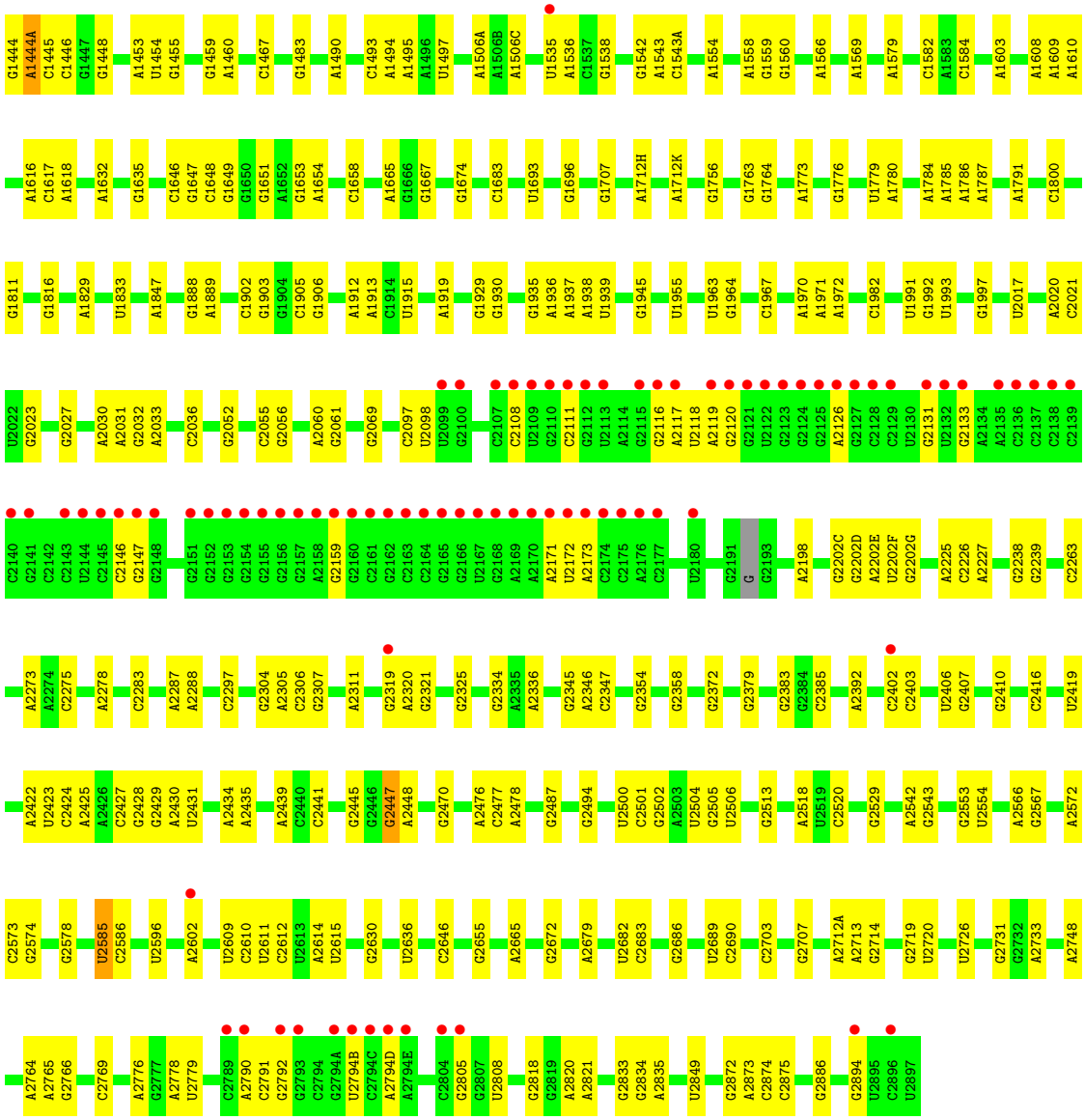




- Molecule 51: 23S ribosomal RNA

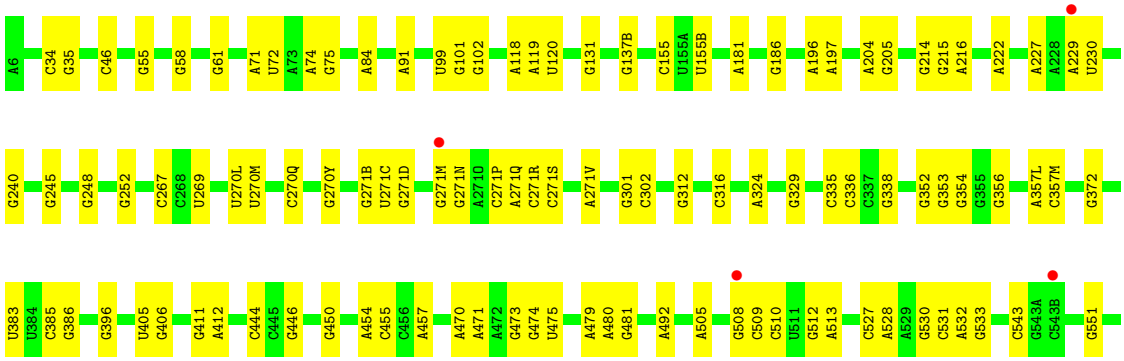
Chain A23S:





- Molecule 51: 23S ribosomal RNA

Chain B23S:



G563 G573 C574 A575 C587 G599 A603 U611D G611E A611F G611G G620 A621 G622 A627 A637 C645 A646 G647 C650 G651 U652 C653 U654 A655 G668 G669 A670 C671 A685 G686 C687 U688 G717 A722 C730 G733 A746 U747 G748 U762 G763

A764 G765 G769 A774 G775 G776 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 G805 C812 A819 A820 U827 U828 A829 G830 G831 G832 C846 U847 G848 A849 G859 G879 C884 C885 C886 A887 C888 C889 A890 A896 C897 C898 U907 A910

C914 C915 G916 A917 A918 G919 A926 G932 G938 A941 A945 G946 A953 A959 A960 C961 G962 G974 C974A G975 G979 A980 A983 A990 A996 U999 G1003 C1004 C1005 A1009 A1010 G1011 U1012 C1013 A1020 A1021 G1022 U1023 G1024 G1025 U1026 U1033

G1047 A1048 G1056 A G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 G1087 A1088 G1089 U1090 G1091 C1092 G1093 A1098 G1099 G1112 A1129 U1130 C1135 G1136 U1141A A1142 G1151 A1155 A1173

U1174 G1175 A1177 G1186 U1205 A1210 U1211 A1219A C1220 G1227 G1236 U1240 G1244 G1248 U1249 G1250 C1251 G1252 A1253 G1256 G1271 A1272 C1297 U1300 A1301 A1302 G1309 U1313 C1314 A1321 U1329 C1330 A1331 G1332 G1344 C1345 A1349 A1359 A1365

A1366 A1379 G1380 A1384 G1385 C1386 A1395 U1396 G1416 A1427 C1428 A1444A A1453 U1454 G1455 C1458 G1459 A1460 C1467 G1483 A1490 C1493 A1494 A1495 A1496 U1497 A1506C U1535 G1538 G1542 A1543 C1543A A1558 G1559 A1566 A1569 U1578 A1579 C1584

A1586 A1603 A1608 A1609 A1610 C1617 U1639 C1644 G1645 C1646 G1647 C1648 G1651 A1652 G1653 G1674 G1681 C1685 A1689 C1694 G1695 A1698 A1712H U1712I G1712J A1712K G1712Q G1750 C1754 A1755 G1756 G1763 G1764 A1773 A1785 A1786 A1787 C1788 A1791

C1800 G1801 G1811 G1816 U1833 C1838 G1839 G1840 A1847 G1858 A1859 G1860 G1878 A1889 G1903 G1904 C1905 G1906 A1913 C1914 A1919 G1929 C1934 G1935 A1936 A1937 A1938 U1939 G1945 U1955 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1973 C1974 A1981 C1982

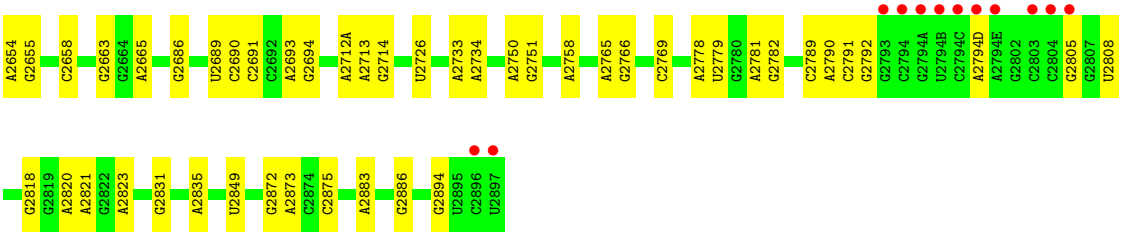
C1983 G1984 U1991 G1992 U1993 G1997 G2004 A2005 C2006 C2021 U2022 G2023 A2031 G2032 A2033 C2036 C2043 G2052 C2055 G2056 A2057 A2058 A2059 A2060 G2061 G2069 G2080 C2081 U2086 C2097 U U2099 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119

G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 G2142 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 G2184 G2190 G2191 G

G2193 A2198 G2202C G2202D A2202E U2202F G2202G A2225 C2226 G2238 G2239 U2243 G2251 A2266 A2269 A2273 A2274 C2275 A2278 C2283 A2287 U2296 G2304 A2305 C2306 G2307 A2310 C2317 G2318 G2319 A2320 G2321 G2325 G2334 A2335 A2336 U2344 G2345 A2346 C2347

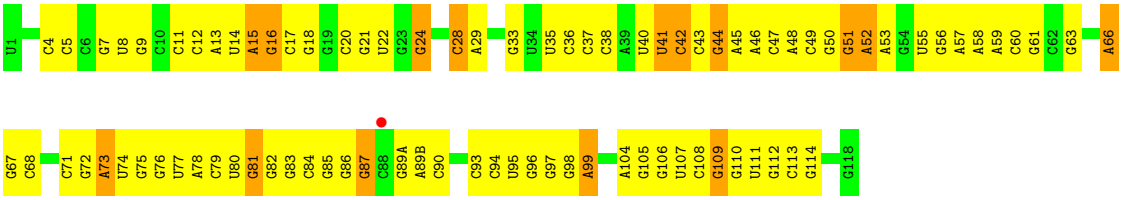
C2350 A2361 G2379 G2383 G2384 C2385 A2388 A2392 C2402 C2403 U2406 G2410 A2422 U2423 C2424 A2425 G2429 A2430 U2431 A2432 A2433 A2434 A2435 G2436 A2439 C2440 C2441 G2446 G2447 A2448 U2449 C2464 G2468 A2469 G2470 A2476 C2477 A2478 G2484 G2489 G2490 U2491

G2494 U2500 C2501 G2502 A2503 U2504 G2505 U2506 G2513 A2518 U2519 C2520 G2529 A2542 G2543 U2554 A2566 G2567 C2568 G2569 A2572 C2573 G2578 U2585 C2586 U2593 A2602 G2603 U2604 U2605 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 G2630 G2634 C2635 U2636 G2641



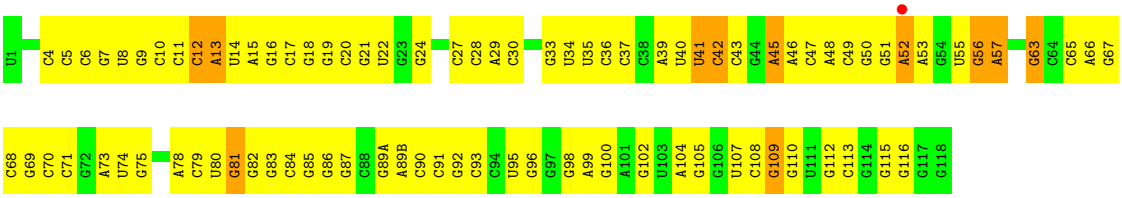
- Molecule 52: 5S ribosomal RNA

Chain A5S:



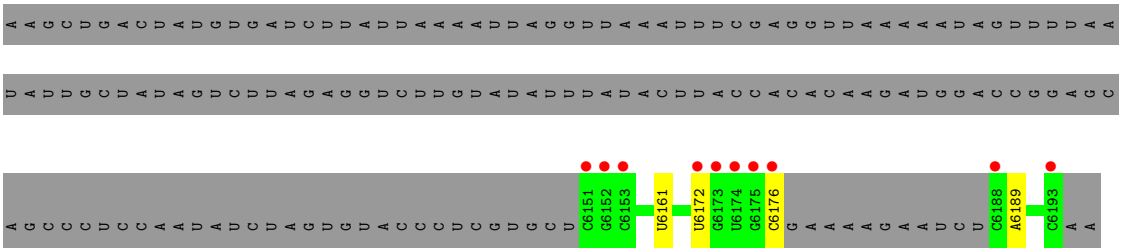
- Molecule 52: 5S ribosomal RNA

Chain B5S:



- Molecule 53: IRES RNA

Chain AIRE:



- Molecule 53: IRES RNA

Chain BIRE:

A
G
C
C
C
U
C
C
A
A
U
A
U
C
U
A
G
U
G
U
A
C
C
C
U
C
G
U
G
C
U
C6151
U6161
U6174
G6175
C6176
G
A
A
A
A
G
A
A
U
C
U
C6188
A6189
C6193
A
A

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.05Å 447.22Å 608.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 3.80 59.35 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.00-3.80) 99.9 (59.35-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.246 , 0.284 0.242 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (0.36%)	wwPDB-VP
Wilson B-factor (Å^2)	119.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 93.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	287293	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	AL02	0.33	0/2155	0.56	0/2905
1	BL02	0.40	0/2155	0.60	0/2905
2	AL03	0.31	0/1597	0.52	0/2153
2	BL03	0.33	0/1597	0.56	0/2153
3	AL04	0.31	0/1622	0.53	0/2194
3	BL04	0.32	0/1622	0.54	0/2194
4	AL05	0.22	0/1500	0.43	0/2017
4	BL05	0.23	0/1500	0.44	0/2017
5	AL06	0.25	0/1246	0.46	0/1682
5	BL06	0.33	0/1246	0.51	0/1682
6	AL09	0.29	0/1148	0.51	0/1552
6	BL09	0.30	0/1148	0.53	0/1552
7	AL11	0.22	0/1108	0.41	0/1500
7	BL11	0.25	0/1108	0.43	0/1500
8	AL13	0.37	0/1124	0.56	0/1515
8	BL13	0.32	0/1124	0.51	0/1515
9	AL14	0.29	0/942	0.51	0/1268
9	BL14	0.31	0/942	0.51	0/1268
10	AL15	0.31	0/1131	0.59	0/1504
10	BL15	0.37	0/1131	0.65	0/1504
11	AL16	0.31	0/1085	0.52	0/1449
11	BL16	0.32	0/1085	0.52	0/1449
12	AL17	0.37	0/974	0.57	0/1302
12	BL17	0.32	0/974	0.53	0/1302
13	AL18	0.25	0/779	0.43	0/1036
13	BL18	0.26	0/779	0.44	0/1036
14	AL19	0.27	0/1158	0.49	0/1544
14	BL19	0.27	0/1158	0.48	0/1544
15	AL20	0.32	0/982	0.47	0/1306
15	BL20	0.31	0/982	0.51	0/1306
16	AL21	0.31	0/790	0.52	0/1057
16	BL21	0.35	0/790	0.56	0/1057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AL22	0.31	0/902	0.53	0/1209
17	BL22	0.32	0/902	0.51	0/1209
18	AL23	0.28	0/740	0.49	0/993
18	BL23	0.33	0/740	0.49	0/993
19	AL24	0.50	2/789 (0.3%)	1.34	4/1051 (0.4%)
19	BL24	0.34	0/789	0.58	0/1051
20	AL25	0.28	0/1515	0.46	0/2056
20	BL25	0.28	0/1515	0.48	0/2056
21	AL27	0.27	0/613	0.50	0/816
21	BL27	0.27	0/613	0.49	0/816
22	AL28	0.32	0/702	0.59	1/932 (0.1%)
22	BL28	0.34	0/702	0.60	0/932
23	AL29	0.27	0/523	0.49	0/690
23	BL29	0.32	0/523	0.55	0/690
24	AL30	0.24	0/473	0.44	0/634
24	BL30	0.27	0/473	0.47	0/634
25	AL32	0.38	0/419	0.59	0/567
25	BL32	0.41	0/419	0.63	0/567
26	AL33	0.28	0/388	0.52	0/518
26	BL33	0.24	0/388	0.47	0/518
27	AL34	0.35	0/427	0.49	0/561
27	BL34	0.39	0/427	0.54	0/561
28	AL35	0.36	0/516	0.56	0/679
28	BL35	0.43	0/516	0.70	1/679 (0.1%)
29	AS02	0.27	0/1936	0.46	1/2609 (0.0%)
29	BS02	0.26	0/1936	0.45	0/2609
30	AS03	0.89	8/1637 (0.5%)	0.95	13/2205 (0.6%)
30	BS03	0.26	0/1637	0.42	0/2205
31	AS04	0.30	0/1733	0.49	0/2318
31	BS04	0.25	0/1733	0.42	0/2318
32	AS05	0.24	0/1172	0.45	0/1576
32	BS05	0.25	0/1172	0.44	0/1576
33	AS06	0.23	0/856	0.44	0/1154
33	BS06	0.25	0/856	0.45	0/1154
34	AS07	0.25	0/1276	0.42	0/1709
34	BS07	0.26	0/1276	0.42	0/1709
35	AS08	0.23	0/1136	0.45	0/1527
35	BS08	0.24	0/1136	0.44	0/1527
36	AS09	0.25	0/1029	0.41	0/1378
36	BS09	0.21	0/1029	0.40	0/1378
37	AS10	0.28	0/808	0.47	0/1085
37	BS10	0.25	0/808	0.46	0/1085
38	AS11	0.27	0/857	0.48	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	BS11	0.28	0/857	0.47	0/1157
39	AS12	0.29	0/973	0.50	0/1301
39	BS12	0.28	0/973	0.48	0/1301
40	AS13	0.27	0/944	0.43	0/1265
40	BS13	0.21	0/944	0.43	0/1265
41	AS14	0.30	0/501	0.45	0/664
41	BS14	0.22	0/501	0.39	0/664
42	AS15	0.39	0/745	0.54	0/992
42	BS15	0.38	0/745	0.52	0/992
43	AS16	0.31	0/717	0.48	0/963
43	BS16	0.25	0/717	0.46	0/963
44	AS17	0.31	0/837	0.48	0/1117
44	BS17	0.30	0/837	0.49	0/1117
45	AS18	0.24	0/579	0.43	0/768
45	BS18	0.25	0/579	0.45	0/768
46	AS19	0.30	0/643	0.46	0/865
46	BS19	0.27	0/643	0.46	0/865
47	AS20	0.26	0/764	0.47	0/1006
47	BS20	0.27	0/764	0.47	0/1006
48	ATHX	0.19	0/213	0.37	0/277
48	BTHX	0.20	0/213	0.40	0/277
49	AL31	0.20	0/229	0.45	0/309
49	BL31	0.20	0/229	0.41	0/309
50	A16S	0.27	0/36194	0.59	0/56493
50	B16S	0.25	0/36193	0.57	0/56490
51	A23S	0.39	2/69356 (0.0%)	0.71	11/108266 (0.0%)
51	B23S	0.39	0/69359	0.74	23/108270 (0.0%)
52	A5S	0.24	0/2853	0.55	0/4451
52	B5S	0.24	0/2853	0.56	0/4451
53	AIRE	0.25	0/748	0.50	0/1160
53	BIRE	0.27	0/748	0.57	0/1160
All	All	0.34	12/312170 (0.0%)	0.64	54/466611 (0.0%)

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
10	AL15	0	1
10	BL15	0	1
19	AL24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	AS03	0	2
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A23S	253	C	C4-N4	40.77	1.70	1.33
51	A23S	253	C	N3-C4	19.94	1.48	1.33
30	AS03	69	HIS	C-O	13.83	1.49	1.23
30	AS03	70	VAL	CB-CG1	13.29	1.80	1.52
30	AS03	69	HIS	N-CA	12.82	1.72	1.46
30	AS03	69	HIS	CA-CB	11.94	1.80	1.53
30	AS03	68	VAL	CB-CG2	-11.80	1.28	1.52
19	AL24	6	HIS	CG-ND1	-7.05	1.23	1.38
30	AS03	70	VAL	CB-CG2	-7.03	1.38	1.52
30	AS03	69	HIS	CA-C	6.49	1.69	1.52
30	AS03	68	VAL	C-O	-5.25	1.13	1.23
19	AL24	6	HIS	CG-CD2	-5.17	1.26	1.35

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	A23S	1444(A)	A	P-O3'-C3'	37.85	165.12	119.70
19	AL24	6	HIS	CG-ND1-CE1	-32.52	62.67	108.20
30	AS03	69	HIS	CB-CG-ND1	-19.53	74.38	123.20
19	AL24	6	HIS	CG-CD2-NE2	-17.32	76.28	109.20
30	AS03	69	HIS	N-CA-CB	17.00	141.21	110.60
51	A23S	253	C	N3-C4-N4	-16.70	106.31	118.00
51	A23S	253	C	C5-C4-N4	16.02	131.41	120.20
51	A23S	1444	G	OP1-P-O3'	15.52	139.34	105.20
51	A23S	1444	G	OP2-P-O3'	-13.24	76.08	105.20
19	AL24	6	HIS	CB-CG-ND1	-12.21	92.67	123.20
30	AS03	68	VAL	CA-C-N	11.90	143.39	117.20
30	AS03	68	VAL	CA-C-O	-8.60	102.04	120.10
51	A23S	253	C	C2-N3-C4	-7.75	116.03	119.90
28	BL35	31	HIS	CB-CA-C	7.30	125.00	110.40
51	B23S	2081	C	C4-C5-C6	7.27	121.03	117.40
30	AS03	68	VAL	O-C-N	-7.19	111.20	122.70
30	AS03	68	VAL	C-N-CA	-6.84	104.59	121.70
30	AS03	71	ALA	N-CA-CB	6.75	119.55	110.10
30	AS03	69	HIS	CB-CA-C	-6.74	96.92	110.40
30	AS03	69	HIS	ND1-CG-CD2	-6.72	96.59	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AS03	69	HIS	C-N-CA	-6.68	105.00	121.70
19	AL24	6	HIS	CB-CG-CD2	-6.62	110.29	130.80
51	B23S	733	G	N1-C6-O6	6.61	123.87	119.90
51	B23S	2081	C	C5-C6-N1	6.30	124.15	121.00
30	AS03	70	VAL	CA-CB-CG1	6.27	120.31	110.90
51	B23S	1332	G	N3-C4-C5	6.22	131.71	128.60
51	B23S	1332	G	N3-C4-N9	-6.15	122.31	126.00
51	A23S	1776	G	C4-N9-C1'	6.08	134.40	126.50
51	B23S	733	G	C4-C5-N7	6.03	113.21	110.80
51	B23S	2447	G	N1-C6-O6	6.01	123.50	119.90
51	B23S	450	G	C5-C6-N1	-5.95	108.53	111.50
51	B23S	733	G	C6-C5-N7	-5.94	126.84	130.40
29	AS02	140	HIS	CB-CA-C	5.92	122.23	110.40
51	B23S	2616	C	C6-N1-C2	5.60	122.54	120.30
51	B23S	528	A	N1-C2-N3	5.57	132.08	129.30
51	B23S	774	A	N1-C6-N6	5.57	121.94	118.60
51	B23S	450	G	C4-C5-C6	5.54	122.12	118.80
51	A23S	1776	G	C8-N9-C1'	-5.51	119.83	127.00
22	AL28	35	THR	N-CA-C	5.42	125.62	111.00
51	B23S	733	G	C5-N7-C8	-5.36	101.62	104.30
30	AS03	70	VAL	N-CA-CB	-5.32	99.81	111.50
51	B23S	2501	C	C2-N1-C1'	-5.31	112.96	118.80
51	B23S	2593	U	N3-C4-C5	-5.29	111.43	114.60
51	A23S	2447	G	C4-N9-C1'	5.25	133.33	126.50
51	B23S	2061	G	C6-C5-N7	-5.21	127.27	130.40
30	AS03	69	HIS	O-C-N	-5.18	114.41	122.70
51	B23S	1493	C	C2-N1-C1'	5.17	124.49	118.80
51	B23S	769	G	C4-N9-C1'	-5.17	119.78	126.50
51	B23S	748	G	N1-C6-O6	-5.13	116.82	119.90
51	B23S	528	A	C2-N3-C4	-5.12	108.04	110.60
51	A23S	650	C	C3'-C2'-C1'	5.08	105.57	101.50
51	B23S	788	A	C8-N9-C4	5.05	107.82	105.80
51	B23S	450	G	C4-N9-C1'	5.03	133.04	126.50
51	A23S	2585	U	C2-N1-C1'	5.01	123.72	117.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AL15	51	PHE	Peptide
19	AL24	6	HIS	Sidechain
30	AS03	68	VAL	Mainchain

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Mol	Chain	Res	Type	Group
30	AS03	69	HIS	Sidechain
10	BL15	51	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AL02	2105	0	0	0	0
1	BL02	2105	0	0	0	0
2	AL03	1564	0	0	0	0
2	BL03	1564	0	0	0	0
3	AL04	1587	0	0	0	0
3	BL04	1587	0	0	0	0
4	AL05	1475	0	0	0	0
4	BL05	1475	0	0	0	0
5	AL06	1223	0	0	0	0
5	BL06	1223	0	0	0	0
6	AL09	1133	0	0	0	0
6	BL09	1133	0	0	0	0
7	AL11	1088	0	0	0	0
7	BL11	1088	0	0	0	0
8	AL13	1097	0	0	0	0
8	BL13	1097	0	0	0	0
9	AL14	932	0	0	0	0
9	BL14	932	0	0	0	0
10	AL15	1114	0	0	0	0
10	BL15	1114	0	0	0	0
11	AL16	1065	0	0	0	0
11	BL16	1065	0	0	0	0
12	AL17	960	0	0	0	0
12	BL17	960	0	0	0	0
13	AL18	771	0	0	0	0
13	BL18	771	0	0	0	0
14	AL19	1144	0	0	0	0
14	BL19	1144	0	0	0	0
15	AL20	964	0	0	0	0
15	BL20	964	0	0	0	0
16	AL21	779	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	BL21	779	0	0	0	0
17	AL22	891	0	0	0	0
17	BL22	891	0	0	0	0
18	AL23	726	0	0	0	0
18	BL23	726	0	0	0	0
19	AL24	776	0	0	0	0
19	BL24	776	0	0	0	0
20	AL25	1483	0	0	0	0
20	BL25	1483	0	0	0	0
21	AL27	605	0	0	0	0
21	BL27	605	0	0	0	0
22	AL28	695	0	0	0	0
22	BL28	695	0	0	0	0
23	AL29	521	0	0	0	0
23	BL29	521	0	0	0	0
24	AL30	468	0	0	0	0
24	BL30	468	0	0	0	0
25	AL32	405	0	0	0	0
25	BL32	405	0	0	0	0
26	AL33	381	0	0	0	0
26	BL33	381	0	0	0	0
27	AL34	419	0	0	0	0
27	BL34	419	0	0	0	0
28	AL35	508	0	0	0	0
28	BL35	508	0	0	0	0
29	AS02	1901	0	0	0	0
29	BS02	1901	0	0	0	0
30	AS03	1613	0	0	0	0
30	BS03	1613	0	0	0	0
31	AS04	1703	0	0	0	0
31	BS04	1703	0	0	0	0
32	AS05	1156	0	0	0	0
32	BS05	1156	0	0	0	0
33	AS06	843	0	0	0	0
33	BS06	843	0	0	0	0
34	AS07	1257	0	0	0	0
34	BS07	1257	0	0	0	0
35	AS08	1116	0	0	0	0
35	BS08	1116	0	0	0	0
36	AS09	1011	0	0	0	0
36	BS09	1011	0	0	0	0
37	AS10	795	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BS10	795	0	0	0	0
38	AS11	843	0	0	0	0
38	BS11	843	0	0	0	0
39	AS12	957	0	0	0	0
39	BS12	957	0	0	0	0
40	AS13	934	0	0	0	0
40	BS13	934	0	0	0	0
41	AS14	492	0	0	0	0
41	BS14	492	0	0	0	0
42	AS15	734	0	0	0	0
42	BS15	734	0	0	0	0
43	AS16	701	0	0	0	0
43	BS16	701	0	0	0	0
44	AS17	824	0	0	0	0
44	BS17	824	0	0	0	0
45	AS18	574	0	0	0	0
45	BS18	574	0	0	0	0
46	AS19	630	0	0	0	0
46	BS19	630	0	0	0	0
47	AS20	762	0	0	0	0
47	BS20	762	0	0	0	0
48	ATHX	209	0	0	0	0
48	BTHX	209	0	0	0	0
49	AL31	226	0	0	0	0
49	BL31	226	0	0	0	0
50	A16S	32332	0	0	0	0
50	B16S	32331	0	0	0	0
51	A23S	61929	0	0	0	0
51	B23S	61931	0	0	0	0
52	A5S	2551	0	1295	97	0
52	B5S	2551	0	1295	104	0
53	AIRE	672	0	0	0	0
53	BIRE	672	0	0	0	0
54	AS04	1	0	0	0	0
54	AS14	1	0	0	0	0
54	BS04	1	0	0	0	0
54	BS14	1	0	0	0	0
All	All	287293	0	2590	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A5S:51:G:H21	52:A5S:52:A:H62	1.05	0.95
52:B5S:40:U:H3'	52:B5S:41:U:H5"	1.50	0.89
52:A5S:40:U:H3'	52:A5S:41:U:H5"	1.55	0.89
52:B5S:10:C:C2	52:B5S:11:C:H5	1.90	0.88
52:A5S:56:G:H21	52:A5S:59:A:H61	1.21	0.86
52:B5S:49:C:H2'	52:B5S:50:G:H8	1.43	0.83
52:A5S:95:U:H2'	52:A5S:96:G:C8	2.12	0.83
52:A5S:51:G:H21	52:A5S:52:A:N6	1.76	0.83
52:B5S:89(A):G:H2'	52:B5S:89(B):A:C8	2.13	0.83
52:B5S:49:C:H2'	52:B5S:50:G:C8	2.15	0.80
52:A5S:89(A):G:H2'	52:A5S:89(B):A:H8	1.47	0.79
52:A5S:84:C:H2'	52:A5S:85:G:H8	1.47	0.78
52:A5S:89(A):G:H2'	52:A5S:89(B):A:C8	2.18	0.78
52:A5S:51:G:N2	52:A5S:52:A:H62	1.81	0.75
52:B5S:80:U:H2'	52:B5S:81:G:H21	1.53	0.74
52:A5S:21:G:H2'	52:A5S:22:U:C6	2.23	0.73
52:B5S:112:G:O2'	52:B5S:113:C:H5'	1.88	0.73
52:B5S:68:C:H2'	52:B5S:69:G:O4'	1.92	0.69
52:B5S:78:A:H2'	52:B5S:79:C:O4'	1.92	0.69
52:A5S:84:C:H2'	52:A5S:85:G:C8	2.25	0.69
52:B5S:13:A:N7	52:B5S:70:C:H4'	2.09	0.67
52:A5S:28:C:H2'	52:A5S:29:A:C8	2.29	0.67
52:B5S:13:A:H2'	52:B5S:14:U:H5"	1.76	0.67
52:B5S:40:U:C3'	52:B5S:41:U:H5"	2.24	0.67
52:B5S:81:G:C2	52:B5S:82:G:N7	2.63	0.67
52:B5S:40:U:H3'	52:B5S:41:U:C5'	2.24	0.66
52:A5S:81:G:C2	52:A5S:82:G:N7	2.64	0.65
52:B5S:78:A:H61	52:B5S:98:G:H1'	1.61	0.65
52:B5S:75:G:N1	52:B5S:102:G:N2	2.44	0.64
52:A5S:29:A:H1'	52:A5S:59:A:C2	2.33	0.64
52:B5S:7:G:H2'	52:B5S:8:U:O4'	1.98	0.64
52:A5S:95:U:H2'	52:A5S:96:G:H8	1.63	0.63
52:B5S:55:U:H2'	52:B5S:56:G:C8	2.34	0.63
52:A5S:104:A:H2'	52:A5S:105:G:O4'	1.98	0.62
52:B5S:41:U:O2'	52:B5S:42:C:OP1	2.16	0.62
52:B5S:47:C:H2'	52:B5S:48:A:H5'	1.81	0.62
52:A5S:113:C:H2'	52:A5S:114:G:H8	1.65	0.61
52:B5S:5:C:H2'	52:B5S:6:C:H6	1.64	0.61
52:A5S:52:A:H2'	52:A5S:53:A:H8	1.66	0.60
52:A5S:40:U:H3'	52:A5S:41:U:C5'	2.30	0.60
52:B5S:95:U:H2'	52:B5S:96:G:H8	1.65	0.60
52:A5S:93:C:H2'	52:A5S:94:C:H6	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A5S:93:C:O2'	52:A5S:94:C:H5'	2.01	0.60
52:B5S:18:G:H1	52:B5S:65:C:H42	1.50	0.60
52:A5S:4:C:H2'	52:A5S:5:C:C6	2.37	0.59
52:A5S:56:G:H4'	52:A5S:57:A:H8	1.67	0.59
52:B5S:89(A):G:C6	52:B5S:89(B):A:N6	2.71	0.59
52:A5S:55:U:H2'	52:A5S:56:G:C8	2.38	0.59
52:B5S:14:U:H2'	52:B5S:15:A:H2	1.65	0.59
52:B5S:39:A:O2'	52:B5S:40:U:H5'	2.03	0.59
52:B5S:13:A:N6	52:B5S:70:C:H5'	2.16	0.58
52:B5S:5:C:H2'	52:B5S:6:C:C6	2.37	0.58
52:A5S:55:U:H2'	52:A5S:56:G:H8	1.69	0.58
52:B5S:86:G:H2'	52:B5S:87:G:H8	1.68	0.58
52:B5S:21:G:O2'	52:B5S:22:U:H5'	2.04	0.57
52:A5S:7:G:H2'	52:A5S:8:U:O4'	2.05	0.57
52:A5S:11:C:O2'	52:A5S:12:C:O4'	2.23	0.57
52:A5S:111:U:H2'	52:A5S:112:G:H8	1.70	0.57
52:B5S:47:C:C2'	52:B5S:48:A:H5'	2.34	0.57
52:A5S:15:A:H5'	52:A5S:16:G:C8	2.40	0.56
52:A5S:56:G:H4'	52:A5S:57:A:C8	2.41	0.56
52:A5S:86:G:H2'	52:A5S:87:G:H8	1.70	0.55
52:B5S:17:C:N4	52:B5S:18:G:C6	2.73	0.55
52:A5S:57:A:H2'	52:A5S:58:A:H8	1.71	0.55
52:B5S:10:C:C2	52:B5S:11:C:C5	2.82	0.55
52:A5S:66:A:H61	52:A5S:107:U:H2'	1.71	0.55
52:B5S:4:C:H2'	52:B5S:5:C:C6	2.42	0.55
52:B5S:86:G:H2'	52:B5S:87:G:C8	2.42	0.54
52:A5S:46:A:C6	52:A5S:47:C:N3	2.76	0.54
52:B5S:70:C:H2'	52:B5S:71:C:C6	2.43	0.54
52:B5S:82:G:O2'	52:B5S:83:G:H5'	2.07	0.54
52:A5S:73:A:C8	52:A5S:74:U:C5	2.96	0.54
52:A5S:56:G:H21	52:A5S:59:A:N6	2.00	0.54
52:A5S:22:U:H3	52:A5S:61:G:H1	1.55	0.54
52:B5S:52:A:H2'	52:B5S:53:A:H5'	1.90	0.54
52:A5S:78:A:C2	52:A5S:99:A:C4	2.97	0.53
52:A5S:11:C:H2'	52:A5S:12:C:C6	2.44	0.53
52:A5S:48:A:C2	52:A5S:49:C:C2	2.96	0.53
52:A5S:83:G:C2	52:A5S:84:C:C2	2.97	0.53
52:A5S:86:G:H2'	52:A5S:87:G:C8	2.44	0.53
52:A5S:24:G:C6	52:A5S:56:G:C2	2.96	0.52
52:B5S:18:G:H2'	52:B5S:19:G:H8	1.73	0.52
52:B5S:11:C:N4	52:B5S:110:G:N1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:A5S:21:G:H2'	52:A5S:22:U:H6	1.74	0.52
52:A5S:7:G:O2'	52:A5S:8:U:H5'	2.10	0.52
52:A5S:82:G:C2	52:A5S:83:G:C8	2.98	0.52
52:B5S:75:G:H1	52:B5S:102:G:N2	2.07	0.51
52:A5S:108:C:H5'	52:A5S:109:G:O5'	2.09	0.51
52:B5S:66:A:C2	52:B5S:68:C:N4	2.78	0.51
52:B5S:104:A:H2'	52:B5S:105:G:O4'	2.10	0.51
52:A5S:72:G:N2	52:A5S:105:G:C6	2.78	0.51
52:B5S:46:A:C6	52:B5S:47:C:C4	2.99	0.51
52:B5S:55:U:O2'	52:B5S:57:A:C8	2.64	0.50
52:A5S:17:C:C5	52:A5S:18:G:N7	2.80	0.50
52:A5S:33:G:N2	52:A5S:50:G:C4	2.79	0.50
52:B5S:51:G:H2'	52:B5S:51:G:N3	2.26	0.50
52:B5S:95:U:H2'	52:B5S:96:G:C8	2.45	0.50
52:A5S:113:C:H2'	52:A5S:114:G:C8	2.44	0.50
52:B5S:10:C:H2'	52:B5S:11:C:H6	1.75	0.50
52:A5S:20:C:H2'	52:A5S:21:G:O4'	2.12	0.50
52:B5S:108:C:H5'	52:B5S:109:G:O5'	2.12	0.50
52:B5S:9:G:C6	52:B5S:112:G:C6	2.99	0.49
52:A5S:76:G:H2'	52:A5S:77:U:O4'	2.12	0.49
52:B5S:35:U:C5	52:B5S:36:C:C5	3.00	0.49
52:A5S:43:C:N4	52:A5S:45:A:C6	2.81	0.49
52:A5S:49:C:H2'	52:A5S:50:G:H8	1.76	0.49
52:A5S:66:A:N6	52:A5S:107:U:H2'	2.28	0.49
52:A5S:76:G:H8	52:A5S:76:G:O5'	1.96	0.49
52:A5S:28:C:H2'	52:A5S:29:A:H8	1.78	0.49
52:A5S:81:G:H2'	52:A5S:82:G:H5'	1.94	0.49
52:B5S:66:A:H61	52:B5S:107:U:H2'	1.78	0.49
52:A5S:4:C:H2'	52:A5S:5:C:H6	1.76	0.48
52:B5S:13:A:C2'	52:B5S:14:U:H5"	2.43	0.48
52:B5S:18:G:H2'	52:B5S:19:G:C8	2.48	0.48
52:B5S:28:C:H2'	52:B5S:29:A:O4'	2.13	0.48
52:B5S:52:A:C2'	52:B5S:53:A:H5'	2.43	0.48
52:B5S:86:G:C2	52:B5S:91:C:C2	3.01	0.48
52:B5S:80:U:H2'	52:B5S:81:G:N2	2.25	0.48
52:B5S:13:A:O2'	52:B5S:14:U:H3'	2.13	0.48
52:A5S:56:G:O4'	52:A5S:57:A:N7	2.47	0.47
52:B5S:112:G:C2'	52:B5S:113:C:H5'	2.44	0.47
52:A5S:13:A:O2'	52:A5S:14:U:H3'	2.14	0.47
52:B5S:13:A:H62	52:B5S:70:C:H5'	1.78	0.47
52:A5S:57:A:H2'	52:A5S:58:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B5S:14:U:C2'	52:B5S:15:A:H2	2.26	0.47
52:B5S:33:G:C6	52:B5S:34:U:C4	3.03	0.47
52:B5S:70:C:H2'	52:B5S:71:C:H6	1.79	0.47
52:B5S:9:G:H2'	52:B5S:10:C:O4'	2.15	0.47
52:A5S:52:A:C5	52:A5S:53:A:N7	2.82	0.47
52:B5S:74:U:C4	52:B5S:75:G:C5	3.02	0.47
52:B5S:11:C:O2'	52:B5S:12:C:O4'	2.32	0.47
52:A5S:11:C:C2'	52:A5S:12:C:C6	2.98	0.46
52:A5S:66:A:C2	52:A5S:68:C:N4	2.84	0.46
52:B5S:40:U:H1'	52:B5S:43:C:H5	1.81	0.46
52:A5S:44:G:N3	52:A5S:47:C:N4	2.64	0.45
52:B5S:39:A:C2	52:B5S:40:U:C4	3.03	0.45
52:A5S:59:A:H2'	52:A5S:60:C:O4'	2.16	0.45
52:A5S:73:A:C4	52:A5S:104:A:C2	3.04	0.45
52:B5S:11:C:HO2'	52:B5S:12:C:C4'	2.29	0.45
52:A5S:11:C:N4	52:A5S:110:G:C2	2.85	0.45
52:A5S:56:G:N2	52:A5S:59:A:H61	2.01	0.45
52:A5S:77:U:O2'	52:A5S:78:A:H5'	2.15	0.45
52:A5S:74:U:O4	52:A5S:75:G:C6	2.70	0.45
52:B5S:74:U:C2'	52:B5S:75:G:H5'	2.47	0.45
52:A5S:79:C:C2'	52:A5S:80:U:H5'	2.46	0.45
52:B5S:20:C:H2'	52:B5S:21:G:H8	1.80	0.45
52:B5S:47:C:H2'	52:B5S:48:A:C5'	2.47	0.45
52:B5S:99:A:C4	52:B5S:100:G:C8	3.05	0.45
52:A5S:41:U:O2'	52:A5S:42:C:C5'	2.66	0.44
52:A5S:57:A:H2'	52:A5S:58:A:O4'	2.17	0.44
52:B5S:36:C:H2'	52:B5S:37:C:C6	2.52	0.44
52:B5S:74:U:H2'	52:B5S:75:G:C5'	2.48	0.44
52:A5S:72:G:O2'	52:A5S:104:A:N6	2.43	0.44
52:B5S:11:C:N4	52:B5S:110:G:H1	2.16	0.44
52:A5S:11:C:H2'	52:A5S:12:C:C5	2.53	0.44
52:B5S:12:C:H4'	52:B5S:13:A:OP1	2.17	0.44
52:B5S:18:G:N2	52:B5S:65:C:N3	2.63	0.44
52:B5S:43:C:C5	52:B5S:45:A:N6	2.86	0.44
52:B5S:93:C:H6	52:B5S:93:C:O5'	2.01	0.44
52:B5S:81:G:N1	52:B5S:82:G:N7	2.66	0.44
52:B5S:82:G:H2'	52:B5S:83:G:H8	1.82	0.44
52:A5S:97:G:C2'	52:A5S:98:G:H5'	2.48	0.43
52:B5S:10:C:N3	52:B5S:11:C:H5	2.12	0.43
52:B5S:24:G:N3	52:B5S:27:C:N4	2.64	0.43
52:B5S:74:U:H2'	52:B5S:75:G:H5'	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:B5S:79:C:C2'	52:B5S:80:U:H5'	2.47	0.43
52:B5S:85:G:N1	52:B5S:92:G:C6	2.87	0.43
52:A5S:33:G:N1	52:A5S:50:G:C6	2.87	0.43
52:A5S:97:G:O2'	52:A5S:98:G:H5'	2.18	0.43
52:B5S:11:C:H2'	52:B5S:12:C:H6	1.82	0.43
52:B5S:21:G:N3	52:B5S:63:G:N2	2.67	0.43
52:A5S:37:C:C4	52:A5S:38:C:C2	3.07	0.43
52:B5S:66:A:H2	52:B5S:68:C:N4	2.16	0.43
52:B5S:50:G:C6	52:B5S:51:G:C8	3.06	0.42
52:A5S:42:C:C5	52:A5S:43:C:C5	3.07	0.42
52:A5S:110:G:C2	52:A5S:111:U:C2	3.07	0.42
52:B5S:5:C:O2	52:B5S:116:G:C2	2.72	0.42
52:B5S:78:A:N6	52:B5S:98:G:H1'	2.30	0.42
52:A5S:66:A:H2	52:A5S:68:C:N4	2.17	0.42
52:B5S:10:C:H2'	52:B5S:11:C:C6	2.54	0.42
52:B5S:5:C:O2'	52:B5S:27:C:H1'	2.20	0.42
52:B5S:115:G:C2	52:B5S:116:G:C4	3.08	0.42
52:A5S:71:C:H2'	52:A5S:72:G:H5'	2.02	0.41
52:A5S:49:C:H2'	52:A5S:50:G:C8	2.54	0.41
52:B5S:33:G:C5	52:B5S:34:U:C4	3.08	0.41
52:B5S:86:G:C2	52:B5S:87:G:C5	3.08	0.41
52:B5S:115:G:C2	52:B5S:116:G:C5	3.09	0.41
52:A5S:28:C:H2'	52:A5S:29:A:O4'	2.21	0.41
52:A5S:56:G:C4'	52:A5S:57:A:C8	3.04	0.41
52:A5S:45:A:N3	52:A5S:45:A:H2'	2.36	0.41
52:A5S:110:G:C6	52:A5S:111:U:C4	3.09	0.41
52:B5S:18:G:H1	52:B5S:65:C:N4	2.15	0.41
52:B5S:21:G:C2	52:B5S:63:G:C2	3.08	0.41
52:A5S:71:C:C2'	52:A5S:72:G:H5'	2.51	0.41
52:A5S:81:G:N1	52:A5S:96:G:C2	2.89	0.41
52:A5S:106:G:C6	52:A5S:107:U:C4	3.09	0.41
52:A5S:9:G:C2	52:A5S:112:G:C4	3.09	0.40
52:A5S:35:U:O2'	52:A5S:36:C:H5'	2.21	0.40
52:A5S:94:C:N3	52:A5S:95:U:C4	2.90	0.40
52:B5S:16:G:N2	52:B5S:69:G:H1'	2.37	0.40
52:B5S:29:A:H2'	52:B5S:30:C:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AL02	269/271 (99%)	197 (73%)	49 (18%)	23 (9%)	1 12
1	BL02	269/271 (99%)	184 (68%)	56 (21%)	29 (11%)	0 8
2	AL03	202/204 (99%)	145 (72%)	41 (20%)	16 (8%)	1 14
2	BL03	202/204 (99%)	140 (69%)	46 (23%)	16 (8%)	1 14
3	AL04	200/202 (99%)	154 (77%)	31 (16%)	15 (8%)	1 15
3	BL04	200/202 (99%)	142 (71%)	41 (20%)	17 (8%)	1 12
4	AL05	179/181 (99%)	134 (75%)	35 (20%)	10 (6%)	2 21
4	BL05	179/181 (99%)	128 (72%)	35 (20%)	16 (9%)	1 12
5	AL06	157/159 (99%)	117 (74%)	35 (22%)	5 (3%)	4 32
5	BL06	157/159 (99%)	119 (76%)	27 (17%)	11 (7%)	1 17
6	AL09	143/145 (99%)	112 (78%)	26 (18%)	5 (4%)	3 31
6	BL09	143/145 (99%)	97 (68%)	37 (26%)	9 (6%)	1 20
7	AL11	145/147 (99%)	100 (69%)	36 (25%)	9 (6%)	1 20
7	BL11	145/147 (99%)	108 (74%)	28 (19%)	9 (6%)	1 20
8	AL13	135/137 (98%)	95 (70%)	23 (17%)	17 (13%)	0 5
8	BL13	135/137 (98%)	90 (67%)	30 (22%)	15 (11%)	0 7
9	AL14	120/122 (98%)	95 (79%)	16 (13%)	9 (8%)	1 15
9	BL14	120/122 (98%)	94 (78%)	15 (12%)	11 (9%)	1 12
10	AL15	144/146 (99%)	76 (53%)	36 (25%)	32 (22%)	0 1
10	BL15	144/146 (99%)	83 (58%)	41 (28%)	20 (14%)	0 4
11	AL16	132/134 (98%)	93 (70%)	28 (21%)	11 (8%)	1 13
11	BL16	132/134 (98%)	99 (75%)	20 (15%)	13 (10%)	0 10
12	AL17	115/117 (98%)	89 (77%)	17 (15%)	9 (8%)	1 15
12	BL17	115/117 (98%)	82 (71%)	27 (24%)	6 (5%)	2 23
13	AL18	96/98 (98%)	66 (69%)	17 (18%)	13 (14%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BL18	96/98 (98%)	61 (64%)	24 (25%)	11 (12%)	0	7
14	AL19	135/137 (98%)	85 (63%)	32 (24%)	18 (13%)	0	4
14	BL19	135/137 (98%)	88 (65%)	31 (23%)	16 (12%)	0	6
15	AL20	115/117 (98%)	88 (76%)	21 (18%)	6 (5%)	2	23
15	BL20	115/117 (98%)	88 (76%)	22 (19%)	5 (4%)	2	26
16	AL21	99/101 (98%)	70 (71%)	23 (23%)	6 (6%)	1	20
16	BL21	99/101 (98%)	75 (76%)	14 (14%)	10 (10%)	0	9
17	AL22	110/112 (98%)	86 (78%)	19 (17%)	5 (4%)	2	25
17	BL22	110/112 (98%)	81 (74%)	24 (22%)	5 (4%)	2	25
18	AL23	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	6	39
18	BL23	90/92 (98%)	78 (87%)	10 (11%)	2 (2%)	6	39
19	AL24	98/100 (98%)	62 (63%)	23 (24%)	13 (13%)	0	4
19	BL24	98/100 (98%)	53 (54%)	28 (29%)	17 (17%)	0	3
20	AL25	185/187 (99%)	144 (78%)	34 (18%)	7 (4%)	3	29
20	BL25	185/187 (99%)	142 (77%)	37 (20%)	6 (3%)	4	32
21	AL27	74/76 (97%)	56 (76%)	12 (16%)	6 (8%)	1	14
21	BL27	74/76 (97%)	58 (78%)	12 (16%)	4 (5%)	2	22
22	AL28	86/88 (98%)	60 (70%)	12 (14%)	14 (16%)	0	3
22	BL28	86/88 (98%)	58 (67%)	14 (16%)	14 (16%)	0	3
23	AL29	60/62 (97%)	45 (75%)	12 (20%)	3 (5%)	2	23
23	BL29	60/62 (97%)	44 (73%)	9 (15%)	7 (12%)	0	6
24	AL30	57/59 (97%)	49 (86%)	6 (10%)	2 (4%)	3	31
24	BL30	57/59 (97%)	41 (72%)	13 (23%)	3 (5%)	2	23
25	AL32	50/52 (96%)	36 (72%)	10 (20%)	4 (8%)	1	14
25	BL32	50/52 (96%)	40 (80%)	7 (14%)	3 (6%)	1	20
26	AL33	42/44 (96%)	27 (64%)	12 (29%)	3 (7%)	1	17
26	BL33	42/44 (96%)	26 (62%)	12 (29%)	4 (10%)	0	11
27	AL34	46/48 (96%)	40 (87%)	4 (9%)	2 (4%)	2	26
27	BL34	46/48 (96%)	36 (78%)	7 (15%)	3 (6%)	1	19
28	AL35	61/63 (97%)	36 (59%)	20 (33%)	5 (8%)	1	13
28	BL35	61/63 (97%)	39 (64%)	14 (23%)	8 (13%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AS02	232/234 (99%)	184 (79%)	34 (15%)	14 (6%)	1	20
29	BS02	232/234 (99%)	183 (79%)	44 (19%)	5 (2%)	6	39
30	AS03	204/206 (99%)	159 (78%)	32 (16%)	13 (6%)	1	20
30	BS03	204/206 (99%)	146 (72%)	47 (23%)	11 (5%)	2	22
31	AS04	206/208 (99%)	154 (75%)	40 (19%)	12 (6%)	1	21
31	BS04	206/208 (99%)	153 (74%)	40 (19%)	13 (6%)	1	20
32	AS05	149/151 (99%)	114 (76%)	30 (20%)	5 (3%)	3	31
32	BS05	149/151 (99%)	120 (80%)	23 (15%)	6 (4%)	3	28
33	AS06	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	23
33	BS06	99/101 (98%)	79 (80%)	14 (14%)	6 (6%)	1	20
34	AS07	153/155 (99%)	132 (86%)	19 (12%)	2 (1%)	12	48
34	BS07	153/155 (99%)	128 (84%)	22 (14%)	3 (2%)	7	41
35	AS08	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	1	21
35	BS08	136/138 (99%)	106 (78%)	24 (18%)	6 (4%)	2	25
36	AS09	125/127 (98%)	94 (75%)	23 (18%)	8 (6%)	1	20
36	BS09	125/127 (98%)	98 (78%)	23 (18%)	4 (3%)	4	32
37	AS10	96/98 (98%)	76 (79%)	16 (17%)	4 (4%)	3	26
37	BS10	96/98 (98%)	73 (76%)	21 (22%)	2 (2%)	7	40
38	AS11	112/114 (98%)	85 (76%)	19 (17%)	8 (7%)	1	17
38	BS11	112/114 (98%)	91 (81%)	18 (16%)	3 (3%)	5	35
39	AS12	120/122 (98%)	90 (75%)	26 (22%)	4 (3%)	4	32
39	BS12	120/122 (98%)	91 (76%)	25 (21%)	4 (3%)	4	32
40	AS13	115/117 (98%)	96 (84%)	17 (15%)	2 (2%)	9	43
40	BS13	115/117 (98%)	93 (81%)	17 (15%)	5 (4%)	2	26
41	AS14	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	9	43
41	BS14	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	31
42	AS15	86/88 (98%)	69 (80%)	15 (17%)	2 (2%)	6	38
42	BS15	86/88 (98%)	69 (80%)	16 (19%)	1 (1%)	13	50
43	AS16	81/83 (98%)	61 (75%)	15 (18%)	5 (6%)	1	20
43	BS16	81/83 (98%)	63 (78%)	16 (20%)	2 (2%)	5	36
44	AS17	97/99 (98%)	74 (76%)	18 (19%)	5 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BS17	97/99 (98%)	81 (84%)	11 (11%)	5 (5%)	2	23
45	AS18	68/70 (97%)	48 (71%)	16 (24%)	4 (6%)	1	21
45	BS18	68/70 (97%)	45 (66%)	20 (29%)	3 (4%)	2	25
46	AS19	76/78 (97%)	53 (70%)	18 (24%)	5 (7%)	1	19
46	BS19	76/78 (97%)	50 (66%)	20 (26%)	6 (8%)	1	14
47	AS20	97/99 (98%)	73 (75%)	14 (14%)	10 (10%)	0	9
47	BS20	97/99 (98%)	72 (74%)	21 (22%)	4 (4%)	3	27
48	ATHX	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
48	BTHX	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	12
49	AL31	28/30 (93%)	15 (54%)	11 (39%)	2 (7%)	1	17
49	BL31	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	0	8
All	All	11410/11606 (98%)	8465 (74%)	2170 (19%)	775 (7%)	1	18

All (775) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AL02	26	LYS
1	AL02	33	LEU
1	AL02	34	VAL
1	AL02	154	LYS
1	AL02	239	ARG
2	AL03	17	ASP
2	AL03	86	PRO
2	AL03	132	HIS
2	AL03	134	ILE
2	AL03	144	ARG
3	AL04	66	PRO
3	AL04	73	ALA
3	AL04	74	ARG
3	AL04	128	ALA
3	AL04	133	ASN
3	AL04	134	GLY
3	AL04	166	ALA
4	AL05	75	LYS
4	AL05	84	LYS
6	AL09	10	GLU
6	AL09	135	GLU
7	AL11	99	ILE

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Mol	Chain	Res	Type
7	AL11	118	THR
8	AL13	41	ALA
8	AL13	46	LEU
8	AL13	86	THR
8	AL13	149	PRO
8	AL13	157	ARG
9	AL14	5	GLN
9	AL14	26	LYS
9	AL14	29	ASN
10	AL15	11	GLY
10	AL15	14	LYS
10	AL15	15	ARG
10	AL15	16	ARG
10	AL15	19	VAL
10	AL15	35	HIS
10	AL15	47	ASP
10	AL15	49	ARG
10	AL15	52	GLU
10	AL15	59	LEU
10	AL15	65	ARG
10	AL15	74	GLU
10	AL15	106	LEU
11	AL16	21	THR
12	AL17	12	ARG
12	AL17	83	ILE
12	AL17	107	ASP
13	AL18	21	THR
13	AL18	59	LYS
13	AL18	86	ALA
14	AL19	3	ARG
14	AL19	86	ILE
14	AL19	90	GLN
14	AL19	107	ASP
14	AL19	116	ALA
15	AL20	91	ASP
15	AL20	114	LYS
16	AL21	50	PRO
16	AL21	66	ARG
16	AL21	80	GLN
17	AL22	63	ASP
19	AL24	17	SER
19	AL24	49	VAL

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Mol	Chain	Res	Type
19	AL24	56	PRO
19	AL24	77	PRO
19	AL24	78	ALA
21	AL27	73	GLY
22	AL28	32	LYS
23	AL29	48	HIS
25	AL32	4	HIS
25	AL32	21	SER
28	AL35	30	ARG
28	AL35	51	ALA
28	AL35	62	LEU
29	AS02	123	ALA
29	AS02	169	LYS
31	AS04	5	ILE
31	AS04	166	LYS
33	AS06	15	ASP
36	AS09	23	ASN
37	AS10	92	THR
38	AS11	91	ARG
42	AS15	49	ASP
44	AS17	12	SER
44	AS17	79	SER
45	AS18	86	VAL
46	AS19	11	VAL
46	AS19	29	ARG
46	AS19	80	TYR
47	AS20	71	THR
47	AS20	99	LEU
1	BL02	26	LYS
1	BL02	33	LEU
1	BL02	34	VAL
1	BL02	52	ARG
2	BL03	129	HIS
3	BL04	68	LYS
3	BL04	72	ARG
3	BL04	73	ALA
4	BL05	75	LYS
5	BL06	47	GLU
5	BL06	65	HIS
5	BL06	143	GLN
5	BL06	144	VAL
5	BL06	167	GLU

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Mol	Chain	Res	Type
6	BL09	121	LYS
6	BL09	135	GLU
8	BL13	89	LYS
8	BL13	147	ALA
9	BL14	26	LYS
9	BL14	29	ASN
9	BL14	91	LEU
10	BL15	9	ASN
10	BL15	16	ARG
10	BL15	31	ALA
10	BL15	49	ARG
10	BL15	52	GLU
10	BL15	59	LEU
10	BL15	149	GLU
11	BL16	136	ALA
12	BL17	6	SER
12	BL17	8	ARG
13	BL18	107	GLU
14	BL19	3	ARG
14	BL19	42	ILE
14	BL19	58	ASN
14	BL19	98	LYS
14	BL19	105	LEU
14	BL19	115	ARG
15	BL20	9	VAL
15	BL20	90	VAL
15	BL20	93	LYS
16	BL21	50	PRO
16	BL21	64	HIS
16	BL21	78	LYS
17	BL22	63	ASP
19	BL24	3	VAL
19	BL24	7	VAL
19	BL24	8	LYS
19	BL24	23	ARG
19	BL24	49	VAL
19	BL24	63	LYS
19	BL24	77	PRO
19	BL24	96	ILE
21	BL27	47	PRO
22	BL28	11	ARG
22	BL28	16	ASN

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Mol	Chain	Res	Type
22	BL28	21	ARG
22	BL28	83	GLU
22	BL28	87	PRO
23	BL29	3	LEU
23	BL29	17	SER
23	BL29	43	GLN
23	BL29	44	LEU
23	BL29	48	HIS
24	BL30	29	ARG
25	BL32	4	HIS
26	BL33	31	PRO
28	BL35	31	HIS
28	BL35	62	LEU
30	BS03	45	LYS
30	BS03	206	GLU
31	BS04	5	ILE
31	BS04	30	LYS
32	BS05	11	ILE
35	BS08	99	GLU
36	BS09	127	LYS
38	BS11	106	LYS
39	BS12	50	ALA
46	BS19	11	VAL
46	BS19	80	TYR
47	BS20	84	LEU
1	AL02	32	SER
1	AL02	57	GLY
1	AL02	59	LYS
1	AL02	144	ALA
1	AL02	198	ASN
2	AL03	89	ASP
2	AL03	121	ASN
2	AL03	127	ASP
3	AL04	69	HIS
4	AL05	35	GLU
4	AL05	116	ASP
6	AL09	89	TYR
7	AL11	51	ALA
8	AL13	40	ASP
8	AL13	60	LYS
8	AL13	87	GLY
8	AL13	154	GLN

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Mol	Chain	Res	Type
10	AL15	13	ASN
10	AL15	70	GLN
10	AL15	90	ARG
10	AL15	110	TYR
10	AL15	146	VAL
10	AL15	149	GLU
11	AL16	81	VAL
11	AL16	136	ALA
11	AL16	137	TYR
12	AL17	6	SER
12	AL17	10	LEU
12	AL17	45	ARG
12	AL17	59	ASP
12	AL17	82	GLU
13	AL18	62	LYS
13	AL18	90	GLY
13	AL18	103	GLU
14	AL19	2	ASN
14	AL19	12	SER
14	AL19	55	ASN
14	AL19	118	ARG
14	AL19	124	ASP
15	AL20	88	ILE
15	AL20	90	VAL
15	AL20	117	GLN
17	AL22	89	ALA
17	AL22	110	LYS
19	AL24	3	VAL
19	AL24	96	ILE
19	AL24	98	VAL
20	AL25	93	ASP
20	AL25	163	LEU
21	AL27	11	LYS
22	AL28	53	VAL
22	AL28	85	LEU
23	AL29	17	SER
23	AL29	44	LEU
26	AL33	31	PRO
27	AL34	12	ARG
27	AL34	44	PRO
28	AL35	34	TRP
28	AL35	37	SER

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Mol	Chain	Res	Type
29	AS02	14	GLY
29	AS02	88	ALA
29	AS02	126	GLU
29	AS02	141	GLU
30	AS03	4	LYS
30	AS03	47	LEU
30	AS03	60	ALA
30	AS03	145	GLY
31	AS04	23	GLY
31	AS04	44	GLY
31	AS04	55	ALA
33	AS06	39	LYS
33	AS06	44	GLY
33	AS06	47	ARG
35	AS08	83	ILE
35	AS08	99	GLU
36	AS09	31	GLN
36	AS09	127	LYS
37	AS10	91	PRO
39	AS12	86	GLY
43	AS16	78	GLY
44	AS17	31	LEU
44	AS17	80	GLY
44	AS17	99	SER
45	AS18	41	LYS
45	AS18	60	ALA
47	AS20	82	SER
1	BL02	18	VAL
1	BL02	31	LYS
1	BL02	41	GLY
1	BL02	44	ASN
1	BL02	56	GLY
1	BL02	57	GLY
1	BL02	69	ARG
1	BL02	146	GLU
1	BL02	159	ALA
1	BL02	201	HIS
1	BL02	202	LYS
1	BL02	236	GLY
1	BL02	239	ARG
2	BL03	40	GLU
2	BL03	108	SER

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Mol	Chain	Res	Type
2	BL03	144	ARG
2	BL03	169	ASN
2	BL03	189	PRO
3	BL04	66	PRO
3	BL04	127	GLU
3	BL04	128	ALA
3	BL04	160	ASN
4	BL05	22	ARG
4	BL05	35	GLU
4	BL05	48	GLU
4	BL05	90	LEU
4	BL05	116	ASP
4	BL05	128	ARG
6	BL09	84	GLY
6	BL09	120	ILE
6	BL09	140	LEU
7	BL11	34	ILE
8	BL13	59	GLY
8	BL13	70	ALA
8	BL13	150	ASP
9	BL14	49	ARG
10	BL15	11	GLY
10	BL15	17	LYS
10	BL15	46	LYS
10	BL15	76	LYS
10	BL15	106	LEU
11	BL16	10	ARG
11	BL16	18	LYS
11	BL16	23	GLY
11	BL16	82	ARG
12	BL17	107	ASP
13	BL18	24	LEU
13	BL18	35	ILE
13	BL18	90	GLY
14	BL19	2	ASN
14	BL19	55	ASN
14	BL19	86	ILE
14	BL19	118	ARG
16	BL21	40	LEU
16	BL21	80	GLN
17	BL22	99	ARG
19	BL24	5	MET

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Mol	Chain	Res	Type
19	BL24	29	GLU
19	BL24	78	ALA
19	BL24	88	LYS
20	BL25	31	ARG
22	BL28	32	LYS
22	BL28	54	ALA
23	BL29	47	ASN
24	BL30	32	GLN
26	BL33	51	GLU
27	BL34	2	LYS
28	BL35	7	HIS
28	BL35	37	SER
28	BL35	40	GLU
28	BL35	51	ALA
29	BS02	14	GLY
29	BS02	66	GLY
29	BS02	169	LYS
30	BS03	60	ALA
30	BS03	163	ALA
30	BS03	180	ALA
30	BS03	181	ASN
30	BS03	189	ALA
31	BS04	3	ARG
31	BS04	6	GLY
31	BS04	88	VAL
31	BS04	171	GLY
31	BS04	186	LEU
32	BS05	77	PRO
33	BS06	45	LEU
34	BS07	7	ALA
35	BS08	20	TYR
35	BS08	91	ARG
37	BS10	30	SER
38	BS11	99	GLN
39	BS12	18	ARG
39	BS12	44	PRO
40	BS13	85	GLY
41	BS14	40	CYS
44	BS17	80	GLY
47	BS20	101	GLY
48	BTHX	7	ARG
48	BTHX	24	ARG

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Mol	Chain	Res	Type
49	BL31	54	LYS
1	AL02	35	LYS
1	AL02	127	VAL
2	AL03	52	LEU
3	AL04	89	VAL
3	AL04	132	VAL
4	AL05	24	GLY
4	AL05	36	LYS
4	AL05	96	ARG
7	AL11	86	LYS
7	AL11	141	ALA
7	AL11	142	PRO
8	AL13	74	PHE
8	AL13	99	SER
8	AL13	150	ASP
9	AL14	11	ALA
10	AL15	18	ARG
10	AL15	31	ALA
10	AL15	33	ARG
10	AL15	57	THR
10	AL15	72	PRO
10	AL15	104	GLY
10	AL15	141	ALA
11	AL16	19	GLY
11	AL16	133	ARG
11	AL16	135	ASP
12	AL17	5	LYS
13	AL18	31	SER
13	AL18	35	ILE
13	AL18	44	LYS
13	AL18	95	HIS
14	AL19	58	ASN
14	AL19	115	ARG
15	AL20	56	ASP
17	AL22	5	ALA
18	AL23	32	PRO
19	AL24	41	GLY
20	AL25	79	ARG
21	AL27	12	ASN
22	AL28	10	LYS
22	AL28	52	ARG
22	AL28	87	PRO

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Mol	Chain	Res	Type
25	AL32	51	TYR
26	AL33	44	ARG
29	AS02	100	GLY
29	AS02	129	GLU
29	AS02	130	ARG
29	AS02	228	GLY
29	AS02	235	SER
30	AS03	27	LYS
30	AS03	49	SER
30	AS03	81	GLY
30	AS03	96	GLY
31	AS04	45	GLN
32	AS05	64	ARG
32	AS05	140	ARG
35	AS08	98	LYS
36	AS09	10	ARG
37	AS10	58	ASP
38	AS11	106	LYS
38	AS11	116	HIS
38	AS11	122	LYS
47	AS20	84	LEU
47	AS20	97	ALA
47	AS20	98	PRO
1	BL02	35	LYS
1	BL02	40	THR
1	BL02	192	THR
1	BL02	266	SER
2	BL03	17	ASP
2	BL03	52	LEU
2	BL03	89	ASP
2	BL03	126	PRO
2	BL03	132	HIS
2	BL03	201	THR
3	BL04	113	ALA
3	BL04	133	ASN
4	BL05	36	LYS
4	BL05	83	ARG
4	BL05	85	GLY
5	BL06	22	GLY
6	BL09	25	TYR
7	BL11	51	ALA
7	BL11	95	LYS

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Mol	Chain	Res	Type
7	BL11	141	ALA
9	BL14	25	LEU
9	BL14	27	GLY
9	BL14	120	GLU
10	BL15	12	ALA
10	BL15	57	THR
10	BL15	146	VAL
11	BL16	13	GLN
11	BL16	118	LEU
11	BL16	133	ARG
11	BL16	135	ASP
12	BL17	10	LEU
12	BL17	12	ARG
13	BL18	42	ASP
13	BL18	103	GLU
14	BL19	45	PHE
15	BL20	66	ASN
16	BL21	17	GLY
16	BL21	48	GLY
17	BL22	5	ALA
17	BL22	110	LYS
18	BL23	32	PRO
18	BL23	93	GLU
19	BL24	17	SER
21	BL27	11	LYS
22	BL28	10	LYS
22	BL28	31	GLY
22	BL28	33	LYS
26	BL33	41	PRO
27	BL34	12	ARG
28	BL35	3	LYS
29	BS02	130	ARG
29	BS02	235	SER
30	BS03	81	GLY
32	BS05	21	ALA
34	BS07	99	LEU
35	BS08	2	LEU
35	BS08	23	SER
36	BS09	31	GLN
38	BS11	118	GLY
40	BS13	101	GLN
40	BS13	117	VAL

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Mol	Chain	Res	Type
42	BS15	18	PHE
43	BS16	49	LEU
44	BS17	4	LYS
44	BS17	74	LEU
45	BS18	45	SER
1	AL02	31	LYS
2	AL03	30	PRO
2	AL03	189	PRO
3	AL04	53	THR
4	AL05	14	GLU
5	AL06	56	SER
7	AL11	34	ILE
7	AL11	145	LYS
10	AL15	12	ALA
10	AL15	17	LYS
10	AL15	56	SER
11	AL16	126	PRO
13	AL18	27	SER
14	AL19	43	GLN
14	AL19	56	GLY
17	AL22	72	LYS
18	AL23	85	PRO
19	AL24	39	VAL
21	AL27	33	ALA
21	AL27	49	LYS
22	AL28	11	ARG
24	AL30	50	VAL
25	AL32	47	PRO
29	AS02	16	HIS
29	AS02	78	GLN
30	AS03	22	TRP
30	AS03	69	HIS
30	AS03	195	VAL
30	AS03	196	LEU
31	AS04	7	PRO
31	AS04	168	ARG
32	AS05	38	GLN
32	AS05	67	VAL
33	AS06	64	GLN
34	AS07	149	ARG
35	AS08	104	ARG
36	AS09	33	PHE

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Mol	Chain	Res	Type
38	AS11	35	PRO
38	AS11	123	LYS
39	AS12	50	ALA
40	AS13	101	GLN
41	AS14	26	ARG
43	AS16	48	TRP
43	AS16	50	LYS
47	AS20	102	GLY
1	BL02	188	GLU
1	BL02	191	ALA
3	BL04	172	TRP
3	BL04	178	PRO
4	BL05	177	GLY
5	BL06	29	PRO
5	BL06	164	TYR
6	BL09	42	SER
7	BL11	136	VAL
7	BL11	145	LYS
8	BL13	60	LYS
8	BL13	68	ASN
8	BL13	110	LEU
8	BL13	149	PRO
8	BL13	155	ALA
9	BL14	2	ILE
9	BL14	48	PRO
9	BL14	75	SER
10	BL15	18	ARG
10	BL15	102	ARG
11	BL16	21	THR
11	BL16	117	ALA
13	BL18	19	LYS
13	BL18	57	LYS
13	BL18	59	LYS
14	BL19	57	PHE
14	BL19	68	TYR
14	BL19	107	ASP
20	BL25	146	ILE
21	BL27	18	ALA
21	BL27	64	ASP
22	BL28	52	ARG
25	BL32	24	ALA
26	BL33	35	GLU

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Mol	Chain	Res	Type
30	BS03	164	ARG
31	BS04	9	CYS
31	BS04	47	ARG
31	BS04	48	ALA
31	BS04	69	GLY
33	BS06	37	VAL
33	BS06	49	ALA
33	BS06	96	PRO
39	BS12	26	LEU
40	BS13	67	GLU
44	BS17	79	SER
46	BS19	9	VAL
47	BS20	11	SER
49	AL31	61	VAL
49	BL31	61	VAL
1	AL02	13	ARG
1	AL02	28	GLU
1	AL02	69	ARG
1	AL02	236	GLY
2	AL03	169	ASN
3	AL04	30	PRO
3	AL04	181	LEU
5	AL06	46	GLU
5	AL06	167	GLU
5	AL06	168	PRO
8	AL13	51	THR
9	AL14	49	ARG
9	AL14	77	ILE
10	AL15	10	PRO
13	AL18	24	LEU
13	AL18	42	ASP
14	AL19	81	PRO
14	AL19	84	GLN
14	AL19	128	GLU
16	AL21	78	LYS
19	AL24	59	GLY
22	AL28	16	ASN
22	AL28	33	LYS
22	AL28	83	GLU
24	AL30	16	PRO
26	AL33	28	ARG
29	AS02	216	SER

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Mol	Chain	Res	Type
30	AS03	15	THR
31	AS04	28	SER
31	AS04	32	ALA
35	AS08	29	SER
36	AS09	44	VAL
36	AS09	61	ALA
38	AS11	68	ALA
43	AS16	49	LEU
45	AS18	61	LYS
47	AS20	11	SER
47	AS20	95	ALA
47	AS20	96	GLY
1	BL02	59	LYS
1	BL02	214	TRP
1	BL02	246	PRO
2	BL03	14	ILE
2	BL03	56	PRO
3	BL04	67	GLN
3	BL04	104	LYS
3	BL04	171	PRO
3	BL04	181	LEU
4	BL05	14	GLU
4	BL05	87	PRO
5	BL06	15	VAL
7	BL11	91	PRO
7	BL11	142	PRO
8	BL13	54	ALA
8	BL13	152	PRO
10	BL15	47	ASP
11	BL16	8	LYS
11	BL16	99	PRO
14	BL19	78	LEU
19	BL24	39	VAL
19	BL24	56	PRO
20	BL25	92	SER
22	BL28	53	VAL
23	BL29	4	SER
24	BL30	30	ARG
27	BL34	11	LYS
30	BS03	47	LEU
31	BS04	84	LYS
31	BS04	130	GLY

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Mol	Chain	Res	Type
32	BS05	67	VAL
33	BS06	15	ASP
34	BS07	19	GLY
35	BS08	3	THR
36	BS09	105	ASP
37	BS10	88	LEU
40	BS13	13	LYS
45	BS18	86	VAL
46	BS19	29	ARG
49	AL31	54	LYS
1	AL02	125	ILE
1	AL02	249	PRO
2	AL03	56	PRO
2	AL03	184	VAL
6	AL09	86	THR
7	AL11	25	PRO
9	AL14	4	PRO
9	AL14	96	THR
9	AL14	119	PRO
10	AL15	34	GLY
11	AL16	8	LYS
14	AL19	68	TYR
19	AL24	60	PHE
20	AL25	81	ARG
22	AL28	45	ASN
22	AL28	58	ILE
22	AL28	84	GLY
31	AS04	30	LYS
31	AS04	195	ALA
32	AS05	62	ALA
35	AS08	2	LEU
35	AS08	120	THR
37	AS10	59	SER
38	AS11	118	GLY
40	AS13	117	VAL
42	AS15	18	PHE
3	BL04	76	GLY
4	BL05	77	ILE
4	BL05	81	LYS
5	BL06	117	PRO
6	BL09	127	VAL
9	BL14	5	GLN

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Mol	Chain	Res	Type
10	BL15	39	LYS
12	BL17	117	VAL
13	BL18	97	ARG
20	BL25	62	PRO
20	BL25	101	PRO
22	BL28	56	GLN
22	BL28	85	LEU
25	BL32	28	PRO
28	BL35	34	TRP
32	BS05	128	PRO
41	BS14	56	VAL
44	BS17	56	VAL
45	BS18	33	ASP
2	AL03	75	VAL
2	AL03	88	GLY
3	AL04	183	VAL
8	AL13	134	PRO
8	AL13	148	GLY
8	AL13	152	PRO
11	AL16	23	GLY
20	AL25	114	GLY
35	AS08	73	ASP
43	AS16	63	GLY
1	BL02	74	GLY
1	BL02	244	ARG
5	BL06	107	VAL
7	BL11	92	GLY
8	BL13	53	ILE
10	BL15	104	GLY
19	BL24	42	VAL
46	BS19	8	GLY
4	AL05	157	ILE
5	AL06	126	PRO
8	AL13	158	PRO
11	AL16	127	ILE
16	AL21	48	GLY
19	AL24	61	ILE
20	AL25	62	PRO
39	AS12	124	PRO
46	AS19	8	GLY
2	BL03	59	VAL
8	BL13	100	GLY

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Mol	Chain	Res	Type
16	BL21	16	PRO
16	BL21	54	GLY
1	AL02	244	ARG
3	AL04	78	ILE
6	AL09	15	VAL
10	AL15	71	VAL
20	AL25	106	GLY
34	AS07	69	VAL
36	AS09	109	VAL
39	AS12	38	VAL
46	AS19	26	GLY
4	BL05	140	ILE
6	BL09	18	VAL
8	BL13	85	VAL
13	BL18	22	GLY
14	BL19	81	PRO
16	BL21	28	GLU
19	BL24	41	GLY
30	BS03	80	GLY
32	BS05	109	ILE
33	BS06	11	ASN
1	AL02	47	GLY
1	AL02	178	PRO
4	AL05	140	ILE
16	AL21	16	PRO
3	BL04	89	VAL
15	BL20	65	ILE
20	BL25	106	GLY
36	BS09	24	GLY
43	BS16	79	VAL
46	BS19	26	GLY
47	BS20	97	ALA
49	BL31	55	PRO
1	AL02	36	PRO
21	AL27	28	GLY
22	AL28	12	PRO
1	BL02	86	PRO
2	BL03	191	PRO
17	BL22	87	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AL02	213/213 (100%)	185 (87%)	28 (13%)	4 23
1	BL02	213/213 (100%)	177 (83%)	36 (17%)	2 14
2	AL03	165/165 (100%)	137 (83%)	28 (17%)	2 14
2	BL03	165/165 (100%)	131 (79%)	34 (21%)	1 8
3	AL04	161/161 (100%)	150 (93%)	11 (7%)	16 47
3	BL04	161/161 (100%)	141 (88%)	20 (12%)	4 24
4	AL05	155/155 (100%)	133 (86%)	22 (14%)	3 21
4	BL05	155/155 (100%)	136 (88%)	19 (12%)	4 24
5	AL06	132/132 (100%)	123 (93%)	9 (7%)	16 47
5	BL06	132/132 (100%)	116 (88%)	16 (12%)	5 25
6	AL09	122/122 (100%)	97 (80%)	25 (20%)	1 8
6	BL09	122/122 (100%)	102 (84%)	20 (16%)	2 15
7	AL11	111/111 (100%)	105 (95%)	6 (5%)	22 53
7	BL11	111/111 (100%)	106 (96%)	5 (4%)	27 57
8	AL13	116/116 (100%)	100 (86%)	16 (14%)	3 22
8	BL13	116/116 (100%)	98 (84%)	18 (16%)	2 17
9	AL14	100/100 (100%)	87 (87%)	13 (13%)	4 23
9	BL14	100/100 (100%)	89 (89%)	11 (11%)	6 29
10	AL15	112/112 (100%)	82 (73%)	30 (27%)	0 3
10	BL15	112/112 (100%)	80 (71%)	32 (29%)	0 2
11	AL16	105/105 (100%)	96 (91%)	9 (9%)	10 40
11	BL16	105/105 (100%)	88 (84%)	17 (16%)	2 15
12	AL17	100/100 (100%)	87 (87%)	13 (13%)	4 23
12	BL17	100/100 (100%)	86 (86%)	14 (14%)	3 21
13	AL18	77/77 (100%)	70 (91%)	7 (9%)	9 36
13	BL18	77/77 (100%)	68 (88%)	9 (12%)	5 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AL19	121/121 (100%)	105 (87%)	16 (13%)	4	22
14	BL19	121/121 (100%)	106 (88%)	15 (12%)	4	24
15	AL20	93/93 (100%)	79 (85%)	14 (15%)	3	18
15	BL20	93/93 (100%)	83 (89%)	10 (11%)	6	30
16	AL21	82/82 (100%)	68 (83%)	14 (17%)	2	14
16	BL21	82/82 (100%)	67 (82%)	15 (18%)	1	11
17	AL22	91/91 (100%)	83 (91%)	8 (9%)	10	38
17	BL22	91/91 (100%)	83 (91%)	8 (9%)	10	38
18	AL23	74/74 (100%)	67 (90%)	7 (10%)	8	34
18	BL23	74/74 (100%)	67 (90%)	7 (10%)	8	34
19	AL24	84/84 (100%)	69 (82%)	15 (18%)	2	12
19	BL24	84/84 (100%)	71 (84%)	13 (16%)	2	17
20	AL25	162/162 (100%)	150 (93%)	12 (7%)	13	44
20	BL25	162/162 (100%)	151 (93%)	11 (7%)	16	47
21	AL27	61/61 (100%)	56 (92%)	5 (8%)	11	40
21	BL27	61/61 (100%)	52 (85%)	9 (15%)	3	19
22	AL28	73/73 (100%)	60 (82%)	13 (18%)	2	12
22	BL28	73/73 (100%)	60 (82%)	13 (18%)	2	12
23	AL29	58/58 (100%)	52 (90%)	6 (10%)	7	31
23	BL29	58/58 (100%)	47 (81%)	11 (19%)	1	10
24	AL30	51/51 (100%)	47 (92%)	4 (8%)	12	42
24	BL30	51/51 (100%)	42 (82%)	9 (18%)	2	13
25	AL32	45/45 (100%)	38 (84%)	7 (16%)	2	17
25	BL32	45/45 (100%)	40 (89%)	5 (11%)	6	29
26	AL33	43/43 (100%)	36 (84%)	7 (16%)	2	15
26	BL33	43/43 (100%)	34 (79%)	9 (21%)	1	8
27	AL34	41/41 (100%)	37 (90%)	4 (10%)	8	33
27	BL34	41/41 (100%)	33 (80%)	8 (20%)	1	9
28	AL35	53/53 (100%)	45 (85%)	8 (15%)	3	18
28	BL35	53/53 (100%)	49 (92%)	4 (8%)	13	44
29	AS02	202/202 (100%)	186 (92%)	16 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BS02	202/202 (100%)	186 (92%)	16 (8%)	12	42
30	AS03	160/160 (100%)	140 (88%)	20 (12%)	4	24
30	BS03	160/160 (100%)	147 (92%)	13 (8%)	11	41
31	AS04	180/180 (100%)	163 (91%)	17 (9%)	8	35
31	BS04	180/180 (100%)	162 (90%)	18 (10%)	7	32
32	AS05	116/116 (100%)	101 (87%)	15 (13%)	4	23
32	BS05	116/116 (100%)	106 (91%)	10 (9%)	10	40
33	AS06	90/90 (100%)	82 (91%)	8 (9%)	9	38
33	BS06	90/90 (100%)	83 (92%)	7 (8%)	12	42
34	AS07	126/126 (100%)	121 (96%)	5 (4%)	31	59
34	BS07	126/126 (100%)	121 (96%)	5 (4%)	31	59
35	AS08	119/119 (100%)	108 (91%)	11 (9%)	9	35
35	BS08	119/119 (100%)	112 (94%)	7 (6%)	19	51
36	AS09	98/98 (100%)	91 (93%)	7 (7%)	14	45
36	BS09	98/98 (100%)	91 (93%)	7 (7%)	14	45
37	AS10	88/88 (100%)	79 (90%)	9 (10%)	7	31
37	BS10	88/88 (100%)	80 (91%)	8 (9%)	9	36
38	AS11	86/86 (100%)	79 (92%)	7 (8%)	11	41
38	BS11	86/86 (100%)	77 (90%)	9 (10%)	7	30
39	AS12	103/103 (100%)	92 (89%)	11 (11%)	6	30
39	BS12	103/103 (100%)	93 (90%)	10 (10%)	8	33
40	AS13	94/94 (100%)	92 (98%)	2 (2%)	53	74
40	BS13	94/94 (100%)	90 (96%)	4 (4%)	29	58
41	AS14	49/49 (100%)	45 (92%)	4 (8%)	11	40
41	BS14	49/49 (100%)	46 (94%)	3 (6%)	18	50
42	AS15	79/79 (100%)	71 (90%)	8 (10%)	7	32
42	BS15	79/79 (100%)	68 (86%)	11 (14%)	3	21
43	AS16	72/72 (100%)	63 (88%)	9 (12%)	4	24
43	BS16	72/72 (100%)	68 (94%)	4 (6%)	21	52
44	AS17	94/94 (100%)	85 (90%)	9 (10%)	8	34
44	BS17	94/94 (100%)	87 (93%)	7 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	AS18	61/61 (100%)	58 (95%)	3 (5%)	25	55
45	BS18	61/61 (100%)	53 (87%)	8 (13%)	4	23
46	AS19	69/69 (100%)	63 (91%)	6 (9%)	10	38
46	BS19	69/69 (100%)	62 (90%)	7 (10%)	7	32
47	AS20	76/76 (100%)	72 (95%)	4 (5%)	22	54
47	BS20	76/76 (100%)	72 (95%)	4 (5%)	22	54
48	ATHX	19/19 (100%)	18 (95%)	1 (5%)	22	54
48	BTHX	19/19 (100%)	19 (100%)	0	100	100
49	AL31	27/27 (100%)	26 (96%)	1 (4%)	34	62
49	BL31	27/27 (100%)	25 (93%)	2 (7%)	13	44
All	All	9618/9618 (100%)	8530 (89%)	1088 (11%)	6	28

All (1088) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AL02	5	LYS
1	AL02	10	THR
1	AL02	18	VAL
1	AL02	33	LEU
1	AL02	35	LYS
1	AL02	46	GLN
1	AL02	63	ARG
1	AL02	88	ARG
1	AL02	94	LEU
1	AL02	95	LEU
1	AL02	104	TYR
1	AL02	106	ILE
1	AL02	111	LEU
1	AL02	117	VAL
1	AL02	126	GLN
1	AL02	131	LEU
1	AL02	141	VAL
1	AL02	150	LYS
1	AL02	157	ARG
1	AL02	166	GLN
1	AL02	183	ARG
1	AL02	192	THR
1	AL02	198	ASN

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Mol	Chain	Res	Type
1	AL02	201	HIS
1	AL02	212	SER
1	AL02	242	ARG
1	AL02	255	LYS
1	AL02	268	ARG
2	AL03	5	LEU
2	AL03	14	ILE
2	AL03	17	ASP
2	AL03	27	LEU
2	AL03	31	CYS
2	AL03	33	VAL
2	AL03	51	PHE
2	AL03	54	GLN
2	AL03	57	LYS
2	AL03	78	LEU
2	AL03	87	GLU
2	AL03	90	THR
2	AL03	92	THR
2	AL03	102	VAL
2	AL03	107	THR
2	AL03	117	MET
2	AL03	119	ARG
2	AL03	122	PHE
2	AL03	128	SER
2	AL03	129	HIS
2	AL03	144	ARG
2	AL03	154	LYS
2	AL03	168	MET
2	AL03	174	ASP
2	AL03	183	LEU
2	AL03	184	VAL
2	AL03	196	VAL
2	AL03	197	ILE
3	AL04	8	GLN
3	AL04	9	ILE
3	AL04	24	LEU
3	AL04	45	ARG
3	AL04	67	GLN
3	AL04	70	THR
3	AL04	106	ARG
3	AL04	129	PHE
3	AL04	151	SER

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Mol	Chain	Res	Type
3	AL04	164	ARG
3	AL04	175	THR
4	AL05	5	LEU
4	AL05	11	TYR
4	AL05	18	GLU
4	AL05	34	LEU
4	AL05	35	GLU
4	AL05	47	LYS
4	AL05	80	PHE
4	AL05	83	ARG
4	AL05	86	MET
4	AL05	90	LEU
4	AL05	94	LEU
4	AL05	97	ASP
4	AL05	102	PHE
4	AL05	113	ARG
4	AL05	115	ARG
4	AL05	118	ARG
4	AL05	121	ASN
4	AL05	128	ARG
4	AL05	143	GLU
4	AL05	155	MET
4	AL05	156	ASP
4	AL05	157	ILE
5	AL06	13	LYS
5	AL06	23	ARG
5	AL06	47	GLU
5	AL06	86	GLU
5	AL06	101	ARG
5	AL06	111	HIS
5	AL06	123	PHE
5	AL06	124	GLU
5	AL06	136	ILE
6	AL09	1	MET
6	AL09	3	VAL
6	AL09	4	ILE
6	AL09	5	LEU
6	AL09	6	LEU
6	AL09	12	LEU
6	AL09	19	VAL
6	AL09	25	TYR
6	AL09	56	LYS

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Mol	Chain	Res	Type
6	AL09	62	LYS
6	AL09	66	GLU
6	AL09	67	ARG
6	AL09	92	VAL
6	AL09	95	LYS
6	AL09	97	ILE
6	AL09	107	ILE
6	AL09	109	ILE
6	AL09	110	ASP
6	AL09	114	LEU
6	AL09	128	LEU
6	AL09	131	LYS
6	AL09	135	GLU
6	AL09	140	LEU
6	AL09	141	LYS
6	AL09	144	VAL
7	AL11	27	LEU
7	AL11	65	PHE
7	AL11	76	TYR
7	AL11	93	ARG
7	AL11	101	TRP
7	AL11	115	LEU
8	AL13	57	LEU
8	AL13	58	ARG
8	AL13	61	HIS
8	AL13	68	ASN
8	AL13	71	MET
8	AL13	86	THR
8	AL13	94	ILE
8	AL13	114	LEU
8	AL13	117	HIS
8	AL13	119	GLU
8	AL13	132	LYS
8	AL13	135	LEU
8	AL13	143	LEU
8	AL13	144	LYS
8	AL13	154	GLN
8	AL13	160	LYS
9	AL14	8	LEU
9	AL14	9	GLU
9	AL14	14	THR
9	AL14	24	VAL

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Mol	Chain	Res	Type
9	AL14	31	LYS
9	AL14	32	TYR
9	AL14	38	VAL
9	AL14	40	VAL
9	AL14	47	ILE
9	AL14	77	ILE
9	AL14	96	THR
9	AL14	114	ILE
9	AL14	115	VAL
10	AL15	6	LEU
10	AL15	13	ASN
10	AL15	15	ARG
10	AL15	16	ARG
10	AL15	18	ARG
10	AL15	19	VAL
10	AL15	32	THR
10	AL15	40	SER
10	AL15	45	LEU
10	AL15	49	ARG
10	AL15	50	ARG
10	AL15	51	PHE
10	AL15	56	SER
10	AL15	58	THR
10	AL15	59	LEU
10	AL15	61	ARG
10	AL15	62	LEU
10	AL15	64	LYS
10	AL15	67	MET
10	AL15	70	GLN
10	AL15	75	ILE
10	AL15	81	GLN
10	AL15	83	VAL
10	AL15	105	LEU
10	AL15	106	LEU
10	AL15	115	LEU
10	AL15	117	GLU
10	AL15	135	LEU
10	AL15	144	GLU
10	AL15	148	LEU
11	AL16	9	TYR
11	AL16	10	ARG
11	AL16	14	ARG

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Mol	Chain	Res	Type
11	AL16	17	LEU
11	AL16	35	VAL
11	AL16	45	GLN
11	AL16	82	ARG
11	AL16	109	VAL
11	AL16	133	ARG
12	AL17	2	ARG
12	AL17	17	ARG
12	AL17	28	LEU
12	AL17	44	LEU
12	AL17	67	LEU
12	AL17	70	LEU
12	AL17	71	GLN
12	AL17	76	VAL
12	AL17	79	LEU
12	AL17	81	ASP
12	AL17	97	VAL
12	AL17	99	LYS
12	AL17	104	ARG
13	AL18	12	PHE
13	AL18	14	VAL
13	AL18	26	LEU
13	AL18	44	LYS
13	AL18	57	LYS
13	AL18	61	ASN
13	AL18	101	LEU
14	AL19	22	PHE
14	AL19	26	ASP
14	AL19	30	VAL
14	AL19	36	GLU
14	AL19	41	ARG
14	AL19	42	ILE
14	AL19	59	THR
14	AL19	60	THR
14	AL19	74	ARG
14	AL19	78	LEU
14	AL19	80	SER
14	AL19	89	VAL
14	AL19	93	ARG
14	AL19	99	LEU
14	AL19	112	ARG
14	AL19	115	ARG

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Mol	Chain	Res	Type
15	AL20	8	VAL
15	AL20	27	LEU
15	AL20	28	ARG
15	AL20	30	LYS
15	AL20	31	SER
15	AL20	38	THR
15	AL20	52	ARG
15	AL20	60	LEU
15	AL20	75	ASN
15	AL20	79	PHE
15	AL20	88	ILE
15	AL20	92	ARG
15	AL20	104	GLN
15	AL20	112	ARG
16	AL21	5	VAL
16	AL21	7	THR
16	AL21	10	LYS
16	AL21	13	ARG
16	AL21	18	LEU
16	AL21	33	VAL
16	AL21	46	VAL
16	AL21	47	VAL
16	AL21	64	HIS
16	AL21	72	VAL
16	AL21	80	GLN
16	AL21	82	ARG
16	AL21	88	ARG
16	AL21	99	ILE
17	AL22	2	GLU
17	AL22	11	ARG
17	AL22	69	LEU
17	AL22	70	TYR
17	AL22	76	VAL
17	AL22	85	VAL
17	AL22	105	VAL
17	AL22	107	LEU
18	AL23	8	ILE
18	AL23	28	PHE
18	AL23	52	VAL
18	AL23	65	ARG
18	AL23	68	ARG
18	AL23	80	ILE

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Mol	Chain	Res	Type
18	AL23	83	VAL
19	AL24	4	LYS
19	AL24	6	HIS
19	AL24	8	LYS
19	AL24	9	LYS
19	AL24	12	THR
19	AL24	21	LYS
19	AL24	27	VAL
19	AL24	29	GLU
19	AL24	35	TYR
19	AL24	39	VAL
19	AL24	46	LYS
19	AL24	75	ILE
19	AL24	76	CYS
19	AL24	85	VAL
19	AL24	90	LEU
20	AL25	24	LEU
20	AL25	31	ARG
20	AL25	42	VAL
20	AL25	71	VAL
20	AL25	72	ARG
20	AL25	78	LYS
20	AL25	118	GLN
20	AL25	125	LEU
20	AL25	132	ASN
20	AL25	133	ILE
20	AL25	146	ILE
20	AL25	154	ASP
21	AL27	11	LYS
21	AL27	21	LEU
21	AL27	25	ARG
21	AL27	32	ARG
21	AL27	80	HIS
22	AL28	16	ASN
22	AL28	21	ARG
22	AL28	26	ARG
22	AL28	27	GLU
22	AL28	37	ILE
22	AL28	41	ARG
22	AL28	45	ASN
22	AL28	58	ILE
22	AL28	80	LEU

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Mol	Chain	Res	Type
22	AL28	82	LEU
22	AL28	88	LYS
22	AL28	92	LYS
22	AL28	95	LEU
23	AL29	1	MET
23	AL29	5	GLU
23	AL29	21	LEU
23	AL29	25	VAL
23	AL29	44	LEU
23	AL29	60	LEU
24	AL30	8	LEU
24	AL30	17	LYS
24	AL30	37	LEU
24	AL30	52	HIS
25	AL32	21	SER
25	AL32	22	HIS
25	AL32	25	LEU
25	AL32	29	ILE
25	AL32	44	THR
25	AL32	51	TYR
25	AL32	52	TYR
26	AL33	11	LEU
26	AL33	12	GLU
26	AL33	24	GLU
26	AL33	34	LEU
26	AL33	36	LEU
26	AL33	42	TRP
26	AL33	43	CYS
27	AL34	4	THR
27	AL34	8	ASN
27	AL34	31	LEU
27	AL34	34	ARG
28	AL35	19	SER
28	AL35	27	THR
28	AL35	30	ARG
28	AL35	34	TRP
28	AL35	49	VAL
28	AL35	52	LYS
28	AL35	57	ARG
28	AL35	64	TYR
29	AS02	15	VAL
29	AS02	17	PHE

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Mol	Chain	Res	Type
29	AS02	69	LEU
29	AS02	71	VAL
29	AS02	74	LYS
29	AS02	75	LYS
29	AS02	96	ARG
29	AS02	97	TRP
29	AS02	119	GLU
29	AS02	126	GLU
29	AS02	142	LEU
29	AS02	153	ARG
29	AS02	154	LEU
29	AS02	158	LEU
29	AS02	169	LYS
29	AS02	198	ASP
30	AS03	5	ILE
30	AS03	10	PHE
30	AS03	16	ARG
30	AS03	21	ARG
30	AS03	29	TYR
30	AS03	31	HIS
30	AS03	56	ASP
30	AS03	62	ASP
30	AS03	67	THR
30	AS03	70	VAL
30	AS03	79	ARG
30	AS03	104	GLN
30	AS03	124	ILE
30	AS03	131	ARG
30	AS03	135	LYS
30	AS03	172	ARG
30	AS03	175	LEU
30	AS03	191	THR
30	AS03	195	VAL
30	AS03	196	LEU
31	AS04	4	TYR
31	AS04	12	CYS
31	AS04	21	LEU
31	AS04	26	CYS
31	AS04	30	LYS
31	AS04	59	ARG
31	AS04	66	ARG
31	AS04	72	GLU

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Mol	Chain	Res	Type
31	AS04	73	ARG
31	AS04	114	ARG
31	AS04	119	GLN
31	AS04	122	ARG
31	AS04	135	LEU
31	AS04	150	GLU
31	AS04	166	LYS
31	AS04	179	GLU
31	AS04	194	LEU
32	AS05	7	GLU
32	AS05	10	MET
32	AS05	11	ILE
32	AS05	12	LEU
32	AS05	20	GLN
32	AS05	25	ARG
32	AS05	26	PHE
32	AS05	43	LEU
32	AS05	47	LYS
32	AS05	64	ARG
32	AS05	68	GLU
32	AS05	76	ILE
32	AS05	79	GLU
32	AS05	101	ILE
32	AS05	121	LYS
33	AS06	6	VAL
33	AS06	14	LEU
33	AS06	21	LEU
33	AS06	33	TYR
33	AS06	46	ARG
33	AS06	47	ARG
33	AS06	75	LEU
33	AS06	100	ASN
34	AS07	5	ARG
34	AS07	28	ASN
34	AS07	75	VAL
34	AS07	113	GLU
34	AS07	155	ARG
35	AS08	1	MET
35	AS08	26	VAL
35	AS08	37	ARG
35	AS08	41	ARG
35	AS08	50	ARG

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Mol	Chain	Res	Type
35	AS08	73	ASP
35	AS08	98	LYS
35	AS08	102	ARG
35	AS08	111	ILE
35	AS08	135	CYS
35	AS08	138	TRP
36	AS09	10	ARG
36	AS09	32	ASP
36	AS09	95	LYS
36	AS09	96	LEU
36	AS09	104	ARG
36	AS09	112	LYS
36	AS09	121	ARG
37	AS10	16	LEU
37	AS10	22	LYS
37	AS10	54	PHE
37	AS10	55	LYS
37	AS10	57	LYS
37	AS10	74	ILE
37	AS10	86	MET
37	AS10	92	THR
37	AS10	96	ILE
38	AS11	18	ARG
38	AS11	26	ASN
38	AS11	31	THR
38	AS11	80	VAL
38	AS11	84	VAL
38	AS11	92	GLU
38	AS11	104	GLN
39	AS12	5	THR
39	AS12	12	LYS
39	AS12	19	LYS
39	AS12	26	LEU
39	AS12	41	THR
39	AS12	51	LEU
39	AS12	52	ARG
39	AS12	63	TYR
39	AS12	76	LEU
39	AS12	81	VAL
39	AS12	91	ASP
40	AS13	93	ARG
40	AS13	115	LYS

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Mol	Chain	Res	Type
41	AS14	6	LEU
41	AS14	26	ARG
41	AS14	40	CYS
41	AS14	44	LEU
42	AS15	3	ILE
42	AS15	5	LYS
42	AS15	17	ARG
42	AS15	41	GLU
42	AS15	44	LYS
42	AS15	45	VAL
42	AS15	65	ARG
42	AS15	82	ILE
43	AS16	5	ARG
43	AS16	8	ARG
43	AS16	11	SER
43	AS16	36	ILE
43	AS16	39	TYR
43	AS16	45	THR
43	AS16	55	ARG
43	AS16	76	GLN
43	AS16	82	GLN
44	AS17	7	THR
44	AS17	25	ARG
44	AS17	38	ARG
44	AS17	52	LYS
44	AS17	60	ILE
44	AS17	70	ARG
44	AS17	74	LEU
44	AS17	81	ARG
44	AS17	100	LYS
45	AS18	65	ILE
45	AS18	87	ARG
45	AS18	88	LYS
46	AS19	6	LYS
46	AS19	7	LYS
46	AS19	29	ARG
46	AS19	30	LEU
46	AS19	37	ARG
46	AS19	44	MET
47	AS20	24	LEU
47	AS20	62	LEU
47	AS20	72	LEU

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Mol	Chain	Res	Type
47	AS20	75	ASN
48	ATHX	5	ASP
1	BL02	10	THR
1	BL02	14	ARG
1	BL02	23	GLU
1	BL02	24	ILE
1	BL02	33	LEU
1	BL02	35	LYS
1	BL02	40	THR
1	BL02	44	ASN
1	BL02	46	GLN
1	BL02	54	ARG
1	BL02	61	LEU
1	BL02	94	LEU
1	BL02	95	LEU
1	BL02	105	ILE
1	BL02	106	ILE
1	BL02	117	VAL
1	BL02	118	VAL
1	BL02	125	ILE
1	BL02	134	ARG
1	BL02	140	THR
1	BL02	142	VAL
1	BL02	145	VAL
1	BL02	147	LEU
1	BL02	150	LYS
1	BL02	166	GLN
1	BL02	182	LEU
1	BL02	200	ASP
1	BL02	212	SER
1	BL02	217	ARG
1	BL02	237	GLU
1	BL02	242	ARG
1	BL02	250	TRP
1	BL02	254	THR
1	BL02	255	LYS
1	BL02	257	LEU
1	BL02	270	ILE
2	BL03	5	LEU
2	BL03	12	THR
2	BL03	13	ARG
2	BL03	17	ASP

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Mol	Chain	Res	Type
2	BL03	19	ARG
2	BL03	25	VAL
2	BL03	41	LYS
2	BL03	45	THR
2	BL03	54	GLN
2	BL03	57	LYS
2	BL03	59	VAL
2	BL03	77	ILE
2	BL03	78	LEU
2	BL03	79	ARG
2	BL03	82	ARG
2	BL03	87	GLU
2	BL03	92	THR
2	BL03	111	ARG
2	BL03	113	PHE
2	BL03	118	LYS
2	BL03	119	ARG
2	BL03	122	PHE
2	BL03	132	HIS
2	BL03	140	SER
2	BL03	145	LYS
2	BL03	150	VAL
2	BL03	151	TYR
2	BL03	159	HIS
2	BL03	163	GLU
2	BL03	169	ASN
2	BL03	184	VAL
2	BL03	188	VAL
2	BL03	192	ASN
2	BL03	196	VAL
3	BL04	8	GLN
3	BL04	9	ILE
3	BL04	24	LEU
3	BL04	30	PRO
3	BL04	33	LEU
3	BL04	50	SER
3	BL04	54	ARG
3	BL04	57	VAL
3	BL04	72	ARG
3	BL04	74	ARG
3	BL04	95	ARG
3	BL04	99	TYR

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Mol	Chain	Res	Type
3	BL04	101	LEU
3	BL04	106	ARG
3	BL04	132	VAL
3	BL04	161	GLU
3	BL04	174	VAL
3	BL04	189	THR
3	BL04	192	LEU
3	BL04	195	ASP
4	BL05	11	TYR
4	BL05	33	ARG
4	BL05	34	LEU
4	BL05	35	GLU
4	BL05	45	GLU
4	BL05	47	LYS
4	BL05	52	ILE
4	BL05	62	LEU
4	BL05	74	LYS
4	BL05	80	PHE
4	BL05	86	MET
4	BL05	90	LEU
4	BL05	91	ARG
4	BL05	115	ARG
4	BL05	121	ASN
4	BL05	128	ARG
4	BL05	148	MET
4	BL05	155	MET
4	BL05	157	ILE
5	BL06	13	LYS
5	BL06	23	ARG
5	BL06	43	VAL
5	BL06	46	GLU
5	BL06	47	GLU
5	BL06	79	VAL
5	BL06	86	GLU
5	BL06	87	LEU
5	BL06	101	ARG
5	BL06	103	LEU
5	BL06	104	GLU
5	BL06	106	THR
5	BL06	111	HIS
5	BL06	116	GLU
5	BL06	123	PHE

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Mol	Chain	Res	Type
5	BL06	124	GLU
6	BL09	1	MET
6	BL09	2	LYS
6	BL09	6	LEU
6	BL09	10	GLU
6	BL09	22	LYS
6	BL09	31	LEU
6	BL09	33	ARG
6	BL09	44	LEU
6	BL09	67	ARG
6	BL09	71	ILE
6	BL09	74	ASN
6	BL09	77	LEU
6	BL09	89	TYR
6	BL09	92	VAL
6	BL09	109	ILE
6	BL09	112	LYS
6	BL09	118	LYS
6	BL09	121	LYS
6	BL09	140	LEU
6	BL09	141	LYS
7	BL11	65	PHE
7	BL11	93	ARG
7	BL11	101	TRP
7	BL11	110	GLN
7	BL11	125	ARG
8	BL13	38	LEU
8	BL13	56	LEU
8	BL13	58	ARG
8	BL13	61	HIS
8	BL13	68	ASN
8	BL13	69	VAL
8	BL13	71	MET
8	BL13	90	LEU
8	BL13	94	ILE
8	BL13	110	LEU
8	BL13	117	HIS
8	BL13	122	LEU
8	BL13	132	LYS
8	BL13	135	LEU
8	BL13	138	ARG
8	BL13	143	LEU

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Mol	Chain	Res	Type
8	BL13	154	GLN
8	BL13	161	LEU
9	BL14	5	GLN
9	BL14	32	TYR
9	BL14	35	VAL
9	BL14	38	VAL
9	BL14	66	LYS
9	BL14	90	GLN
9	BL14	91	LEU
9	BL14	98	VAL
9	BL14	99	PHE
9	BL14	108	GLU
9	BL14	112	MET
10	BL15	13	ASN
10	BL15	16	ARG
10	BL15	21	ARG
10	BL15	32	THR
10	BL15	35	HIS
10	BL15	39	LYS
10	BL15	40	SER
10	BL15	42	SER
10	BL15	45	LEU
10	BL15	49	ARG
10	BL15	50	ARG
10	BL15	51	PHE
10	BL15	52	GLU
10	BL15	59	LEU
10	BL15	61	ARG
10	BL15	62	LEU
10	BL15	67	MET
10	BL15	68	GLN
10	BL15	75	ILE
10	BL15	83	VAL
10	BL15	84	ASN
10	BL15	86	LYS
10	BL15	101	VAL
10	BL15	105	LEU
10	BL15	106	LEU
10	BL15	114	ILE
10	BL15	115	LEU
10	BL15	117	GLU
10	BL15	138	LEU

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Mol	Chain	Res	Type
10	BL15	144	GLU
10	BL15	147	LEU
10	BL15	148	LEU
11	BL16	9	TYR
11	BL16	22	LYS
11	BL16	32	PHE
11	BL16	35	VAL
11	BL16	45	GLN
11	BL16	47	ILE
11	BL16	54	MET
11	BL16	56	ARG
11	BL16	68	ILE
11	BL16	75	THR
11	BL16	81	VAL
11	BL16	82	ARG
11	BL16	96	VAL
11	BL16	106	VAL
11	BL16	133	ARG
11	BL16	134	ARG
11	BL16	135	ASP
12	BL17	2	ARG
12	BL17	4	LEU
12	BL17	9	LYS
12	BL17	36	THR
12	BL17	37	THR
12	BL17	43	GLU
12	BL17	65	LEU
12	BL17	67	LEU
12	BL17	75	LEU
12	BL17	76	VAL
12	BL17	99	LYS
12	BL17	104	ARG
12	BL17	107	ASP
12	BL17	113	LEU
13	BL18	12	PHE
13	BL18	14	VAL
13	BL18	30	ARG
13	BL18	38	GLN
13	BL18	42	ASP
13	BL18	44	LYS
13	BL18	57	LYS
13	BL18	61	ASN

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Mol	Chain	Res	Type
13	BL18	92	TYR
14	BL19	1	MET
14	BL19	27	THR
14	BL19	48	ILE
14	BL19	53	ARG
14	BL19	59	THR
14	BL19	78	LEU
14	BL19	85	LYS
14	BL19	87	ASP
14	BL19	98	LYS
14	BL19	99	LEU
14	BL19	105	LEU
14	BL19	107	ASP
14	BL19	112	ARG
14	BL19	115	ARG
14	BL19	121	ILE
15	BL20	8	VAL
15	BL20	27	LEU
15	BL20	31	SER
15	BL20	34	LYS
15	BL20	44	ASN
15	BL20	49	HIS
15	BL20	60	LEU
15	BL20	92	ARG
15	BL20	97	ASP
15	BL20	104	GLN
16	BL21	2	PHE
16	BL21	7	THR
16	BL21	10	LYS
16	BL21	13	ARG
16	BL21	18	LEU
16	BL21	35	LEU
16	BL21	47	VAL
16	BL21	57	VAL
16	BL21	61	VAL
16	BL21	80	GLN
16	BL21	82	ARG
16	BL21	88	ARG
16	BL21	91	TYR
16	BL21	95	LEU
16	BL21	99	ILE
17	BL22	8	ARG

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Mol	Chain	Res	Type
17	BL22	11	ARG
17	BL22	17	VAL
17	BL22	51	LEU
17	BL22	85	VAL
17	BL22	88	ARG
17	BL22	92	ARG
17	BL22	100	THR
18	BL23	27	THR
18	BL23	28	PHE
18	BL23	55	ASN
18	BL23	65	ARG
18	BL23	70	LEU
18	BL23	80	ILE
18	BL23	83	VAL
19	BL24	4	LYS
19	BL24	6	HIS
19	BL24	8	LYS
19	BL24	9	LYS
19	BL24	14	LEU
19	BL24	23	ARG
19	BL24	27	VAL
19	BL24	49	VAL
19	BL24	60	PHE
19	BL24	75	ILE
19	BL24	76	CYS
19	BL24	83	THR
19	BL24	88	LYS
20	BL25	24	LEU
20	BL25	37	VAL
20	BL25	71	VAL
20	BL25	87	ASP
20	BL25	118	GLN
20	BL25	123	ASP
20	BL25	131	ARG
20	BL25	151	HIS
20	BL25	157	LEU
20	BL25	168	GLU
20	BL25	180	VAL
21	BL27	11	LYS
21	BL27	20	ARG
21	BL27	21	LEU
21	BL27	32	ARG

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Mol	Chain	Res	Type
21	BL27	53	MET
21	BL27	55	ARG
21	BL27	60	PHE
21	BL27	64	ASP
21	BL27	80	HIS
22	BL28	18	ILE
22	BL28	21	ARG
22	BL28	27	GLU
22	BL28	35	THR
22	BL28	37	ILE
22	BL28	41	ARG
22	BL28	45	ASN
22	BL28	58	ILE
22	BL28	59	THR
22	BL28	61	ARG
22	BL28	82	LEU
22	BL28	88	LYS
22	BL28	95	LEU
23	BL29	2	LYS
23	BL29	5	GLU
23	BL29	7	ARG
23	BL29	9	GLN
23	BL29	16	LEU
23	BL29	24	LEU
23	BL29	48	HIS
23	BL29	50	ILE
23	BL29	51	ARG
23	BL29	59	ARG
23	BL29	60	LEU
24	BL30	6	VAL
24	BL30	29	ARG
24	BL30	30	ARG
24	BL30	31	LEU
24	BL30	40	THR
24	BL30	44	ARG
24	BL30	48	GLU
24	BL30	56	VAL
24	BL30	58	VAL
25	BL32	3	LYS
25	BL32	6	VAL
25	BL32	31	VAL
25	BL32	51	TYR

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Mol	Chain	Res	Type
25	BL32	52	TYR
26	BL33	11	LEU
26	BL33	12	GLU
26	BL33	14	THR
26	BL33	20	ASN
26	BL33	24	GLU
26	BL33	34	LEU
26	BL33	36	LEU
26	BL33	44	ARG
26	BL33	46	HIS
27	BL34	2	LYS
27	BL34	4	THR
27	BL34	8	ASN
27	BL34	19	ARG
27	BL34	21	ARG
27	BL34	24	THR
27	BL34	37	LYS
27	BL34	46	VAL
28	BL35	4	MET
28	BL35	52	LYS
28	BL35	57	ARG
28	BL35	64	TYR
29	BS02	9	GLU
29	BS02	17	PHE
29	BS02	44	LEU
29	BS02	48	MET
29	BS02	96	ARG
29	BS02	97	TRP
29	BS02	101	MET
29	BS02	119	GLU
29	BS02	128	GLU
29	BS02	153	ARG
29	BS02	154	LEU
29	BS02	163	PHE
29	BS02	169	LYS
29	BS02	172	ILE
29	BS02	198	ASP
29	BS02	221	LEU
30	BS03	5	ILE
30	BS03	10	PHE
30	BS03	11	ARG
30	BS03	12	LEU

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Mol	Chain	Res	Type
30	BS03	14	ILE
30	BS03	21	ARG
30	BS03	28	GLN
30	BS03	29	TYR
30	BS03	56	ASP
30	BS03	79	ARG
30	BS03	167	TRP
30	BS03	175	LEU
30	BS03	196	LEU
31	BS04	12	CYS
31	BS04	15	GLU
31	BS04	21	LEU
31	BS04	26	CYS
31	BS04	33	MET
31	BS04	66	ARG
31	BS04	73	ARG
31	BS04	76	ARG
31	BS04	103	ASN
31	BS04	114	ARG
31	BS04	122	ARG
31	BS04	131	ARG
31	BS04	135	LEU
31	BS04	144	ASP
31	BS04	150	GLU
31	BS04	159	ARG
31	BS04	166	LYS
31	BS04	194	LEU
32	BS05	10	MET
32	BS05	12	LEU
32	BS05	20	GLN
32	BS05	47	LYS
32	BS05	60	TYR
32	BS05	80	ILE
32	BS05	107	ARG
32	BS05	120	THR
32	BS05	123	LEU
32	BS05	135	THR
33	BS06	14	LEU
33	BS06	30	LEU
33	BS06	46	ARG
33	BS06	69	GLU
33	BS06	75	LEU

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Mol	Chain	Res	Type
33	BS06	86	ARG
33	BS06	100	ASN
34	BS07	5	ARG
34	BS07	12	LEU
34	BS07	28	ASN
34	BS07	148	ASN
34	BS07	153	HIS
35	BS08	1	MET
35	BS08	56	LYS
35	BS08	73	ASP
35	BS08	75	ARG
35	BS08	83	ILE
35	BS08	102	ARG
35	BS08	137	VAL
36	BS09	10	ARG
36	BS09	62	TYR
36	BS09	95	LYS
36	BS09	104	ARG
36	BS09	109	VAL
36	BS09	121	ARG
36	BS09	124	GLN
37	BS10	22	LYS
37	BS10	54	PHE
37	BS10	55	LYS
37	BS10	61	GLU
37	BS10	62	HIS
37	BS10	86	MET
37	BS10	92	THR
37	BS10	96	ILE
38	BS11	29	ILE
38	BS11	31	THR
38	BS11	33	THR
38	BS11	80	VAL
38	BS11	87	THR
38	BS11	92	GLU
38	BS11	93	GLN
38	BS11	96	ARG
38	BS11	123	LYS
39	BS12	19	LYS
39	BS12	26	LEU
39	BS12	39	VAL
39	BS12	40	ARG

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Mol	Chain	Res	Type
39	BS12	51	LEU
39	BS12	52	ARG
39	BS12	61	SER
39	BS12	78	GLU
39	BS12	84	ILE
39	BS12	119	TYR
40	BS13	19	LEU
40	BS13	64	TRP
40	BS13	93	ARG
40	BS13	115	LYS
41	BS14	6	LEU
41	BS14	8	GLU
41	BS14	31	ARG
42	BS15	4	THR
42	BS15	5	LYS
42	BS15	15	PHE
42	BS15	17	ARG
42	BS15	25	THR
42	BS15	26	GLU
42	BS15	44	LYS
42	BS15	52	SER
42	BS15	54	ARG
42	BS15	62	GLN
42	BS15	82	ILE
43	BS16	8	ARG
43	BS16	55	ARG
43	BS16	82	GLN
43	BS16	83	GLU
44	BS17	38	ARG
44	BS17	52	LYS
44	BS17	55	ASP
44	BS17	74	LEU
44	BS17	93	GLN
44	BS17	96	GLN
44	BS17	100	LYS
45	BS18	19	LYS
45	BS18	31	LEU
45	BS18	38	GLU
45	BS18	76	LEU
45	BS18	78	LEU
45	BS18	84	LYS
45	BS18	87	ARG

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Mol	Chain	Res	Type
45	BS18	88	LYS
46	BS19	6	LYS
46	BS19	7	LYS
46	BS19	14	HIS
46	BS19	29	ARG
46	BS19	37	ARG
46	BS19	44	MET
46	BS19	53	ASN
47	BS20	13	LEU
47	BS20	62	LEU
47	BS20	73	HIS
47	BS20	86	ARG
49	AL31	62	CYS
49	BL31	39	ARG
49	BL31	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A16S	1503/1506 (99%)	247 (16%)	21 (1%)
50	B16S	1503/1506 (99%)	249 (16%)	21 (1%)
51	A23S	2872/2879 (99%)	541 (18%)	29 (1%)
51	B23S	2872/2879 (99%)	552 (19%)	26 (0%)
52	A5S	118/119 (99%)	18 (15%)	0
52	B5S	118/119 (99%)	15 (12%)	0
53	AIRE	30/196 (15%)	4 (13%)	0
53	BIRE	30/196 (15%)	4 (13%)	0
All	All	9046/9400 (96%)	1630 (18%)	97 (1%)

All (1630) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A16S	6	G
50	A16S	7	G
50	A16S	9	G
50	A16S	16	A
50	A16S	17	U
50	A16S	31	G

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Mol	Chain	Res	Type
50	A16S	32	A
50	A16S	39	G
50	A16S	47	C
50	A16S	48	C
50	A16S	50	A
50	A16S	51	A
50	A16S	59	A
50	A16S	61	G
50	A16S	68(I)	G
50	A16S	68(N)	U
50	A16S	68(P)	C
50	A16S	101	A
50	A16S	108	G
50	A16S	116	A
50	A16S	121	C
50	A16S	131	C
50	A16S	144	G
50	A16S	163	C
50	A16S	169	C
50	A16S	174	C
50	A16S	181	G
50	A16S	182	U
50	A16S	186(H)	U
50	A16S	186(I)	U
50	A16S	195	A
50	A16S	197	A
50	A16S	198	G
50	A16S	201(C)	U
50	A16S	216	G
50	A16S	220	G
50	A16S	244	U
50	A16S	245	C
50	A16S	247	G
50	A16S	251	G
50	A16S	267	C
50	A16S	289	G
50	A16S	296	U
50	A16S	321	A
50	A16S	328	C
50	A16S	329	A
50	A16S	330	C
50	A16S	332	G

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Mol	Chain	Res	Type
50	A16S	341	C
50	A16S	345	C
50	A16S	346	G
50	A16S	351	G
50	A16S	352	C
50	A16S	353	A
50	A16S	354	G
50	A16S	356	A
50	A16S	367	U
50	A16S	372	C
50	A16S	373	A
50	A16S	384	G
50	A16S	390	C
50	A16S	392	G
50	A16S	397	A
50	A16S	398	C
50	A16S	406	G
50	A16S	412	A
50	A16S	414	A
50	A16S	422	C
50	A16S	423	G
50	A16S	429	U
50	A16S	440	A
50	A16S	452	A
50	A16S	453	A
50	A16S	455	C
50	A16S	458(B)	A
50	A16S	458(D)	G
50	A16S	497	A
50	A16S	498	U
50	A16S	500	G
50	A16S	509	A
50	A16S	510	A
50	A16S	511	C
50	A16S	518	C
50	A16S	527	G
50	A16S	531	U
50	A16S	532	A
50	A16S	533	A
50	A16S	547	A
50	A16S	561	U
50	A16S	562	C

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Mol	Chain	Res	Type
50	A16S	563	A
50	A16S	564	C
50	A16S	572	A
50	A16S	573	A
50	A16S	576	G
50	A16S	577	G
50	A16S	596	C
50	A16S	632	A
50	A16S	653	A
50	A16S	660	G
50	A16S	665	A
50	A16S	670	G
50	A16S	671	G
50	A16S	688	G
50	A16S	695	A
50	A16S	701	C
50	A16S	702	A
50	A16S	703	G
50	A16S	721	G
50	A16S	722	A
50	A16S	724	G
50	A16S	748	C
50	A16S	749	C
50	A16S	777	A
50	A16S	791	G
50	A16S	793	U
50	A16S	794	A
50	A16S	799	G
50	A16S	802	A
50	A16S	816	A
50	A16S	817	C
50	A16S	818	G
50	A16S	819	A
50	A16S	821	G
50	A16S	828	A
50	A16S	838(A)	U
50	A16S	838(B)	C
50	A16S	838(C)	U
50	A16S	848	C
50	A16S	851	G
50	A16S	859	A
50	A16S	871	U

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Mol	Chain	Res	Type
50	A16S	872	A
50	A16S	873	A
50	A16S	902	G
50	A16S	914	A
50	A16S	926	G
50	A16S	927	G
50	A16S	934	C
50	A16S	935	A
50	A16S	943	U
50	A16S	960	U
50	A16S	961	U
50	A16S	969	A
50	A16S	971	G
50	A16S	974	A
50	A16S	976	G
50	A16S	977	A
50	A16S	978	A
50	A16S	980	C
50	A16S	991	U
50	A16S	992	U
50	A16S	993	G
50	A16S	1004	A
50	A16S	1025	U
50	A16S	1050	G
50	A16S	1053	G
50	A16S	1054	C
50	A16S	1055	A
50	A16S	1065	U
50	A16S	1067	A
50	A16S	1068	G
50	A16S	1094	G
50	A16S	1095	U
50	A16S	1101	A
50	A16S	1102	A
50	A16S	1104	G
50	A16S	1118	C
50	A16S	1126	U
50	A16S	1129	C
50	A16S	1130	A
50	A16S	1131	G
50	A16S	1137	C
50	A16S	1138	G

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Mol	Chain	Res	Type
50	A16S	1139	G
50	A16S	1140	C
50	A16S	1145	C
50	A16S	1146	A
50	A16S	1152	A
50	A16S	1154	G
50	A16S	1158	C
50	A16S	1159	U
50	A16S	1171	G
50	A16S	1181	G
50	A16S	1184	G
50	A16S	1193	G
50	A16S	1196	U
50	A16S	1200	C
50	A16S	1201	A
50	A16S	1202	G
50	A16S	1212	U
50	A16S	1213	A
50	A16S	1225	A
50	A16S	1226	C
50	A16S	1227	A
50	A16S	1238	A
50	A16S	1241	G
50	A16S	1257	U
50	A16S	1258	G
50	A16S	1260	C
50	A16S	1278	U
50	A16S	1280	A
50	A16S	1281	U
50	A16S	1286	A
50	A16S	1287	A
50	A16S	1290	G
50	A16S	1298	C
50	A16S	1300	G
50	A16S	1301	U
50	A16S	1302	U
50	A16S	1317	C
50	A16S	1319	A
50	A16S	1320	C
50	A16S	1322	C
50	A16S	1323	G
50	A16S	1331	G

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Mol	Chain	Res	Type
50	A16S	1338	G
50	A16S	1340	A
50	A16S	1346	A
50	A16S	1347	G
50	A16S	1353	G
50	A16S	1362(A)	C
50	A16S	1364	U
50	A16S	1365	G
50	A16S	1377	A
50	A16S	1378	C
50	A16S	1398	A
50	A16S	1419	G
50	A16S	1434	A
50	A16S	1440(C)	G
50	A16S	1440(D)	A
50	A16S	1440(E)	G
50	A16S	1440(I)	A
50	A16S	1440(J)	C
50	A16S	1440(K)	G
50	A16S	1440(L)	G
50	A16S	1487	G
50	A16S	1492	A
50	A16S	1502	A
50	A16S	1504	G
50	A16S	1505	G
50	A16S	1506	U
50	A16S	1507	A
50	A16S	1517	G
50	A16S	1520	G
50	A16S	1529	G
50	A16S	1530	G
51	A23S	10	G
51	A23S	17	G
51	A23S	23	G
51	A23S	35	G
51	A23S	46	C
51	A23S	55	G
51	A23S	57	C
51	A23S	63	U
51	A23S	72	U
51	A23S	74	A
51	A23S	75	G

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Mol	Chain	Res	Type
51	A23S	84	A
51	A23S	99	U
51	A23S	101	G
51	A23S	102	G
51	A23S	118	A
51	A23S	120	U
51	A23S	137(B)	G
51	A23S	137(D)	A
51	A23S	155(B)	U
51	A23S	178	G
51	A23S	181	A
51	A23S	188	G
51	A23S	195	A
51	A23S	196	A
51	A23S	197	A
51	A23S	199	A
51	A23S	204	A
51	A23S	205	G
51	A23S	215	G
51	A23S	216	A
51	A23S	221	A
51	A23S	222	A
51	A23S	228	A
51	A23S	229	A
51	A23S	230	U
51	A23S	231	C
51	A23S	245	G
51	A23S	248	G
51	A23S	252	G
51	A23S	266	G
51	A23S	270(L)	U
51	A23S	270(M)	U
51	A23S	270(O)	U
51	A23S	270(P)	C
51	A23S	270(Q)	C
51	A23S	270(S)	G
51	A23S	271(C)	U
51	A23S	271(D)	G
51	A23S	271(M)	G
51	A23S	271(N)	G
51	A23S	271(P)	C
51	A23S	271(Q)	A

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Mol	Chain	Res	Type
51	A23S	271(R)	C
51	A23S	295	G
51	A23S	296	C
51	A23S	302	C
51	A23S	317	G
51	A23S	327	G
51	A23S	329	G
51	A23S	330	A
51	A23S	335	C
51	A23S	336	C
51	A23S	353	G
51	A23S	357(M)	C
51	A23S	372	G
51	A23S	376	C
51	A23S	385	C
51	A23S	386	G
51	A23S	396	G
51	A23S	404	C
51	A23S	405	U
51	A23S	407	G
51	A23S	411	G
51	A23S	428	A
51	A23S	435	C
51	A23S	444	C
51	A23S	455	C
51	A23S	457	A
51	A23S	470	A
51	A23S	475	U
51	A23S	480	A
51	A23S	481	G
51	A23S	494	G
51	A23S	505	A
51	A23S	508	G
51	A23S	509	C
51	A23S	512	G
51	A23S	513	A
51	A23S	518	G
51	A23S	530	G
51	A23S	531	C
51	A23S	532	A
51	A23S	533	G
51	A23S	534	U

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Mol	Chain	Res	Type
51	A23S	543(B)	C
51	A23S	550	G
51	A23S	563	G
51	A23S	572	A
51	A23S	573	G
51	A23S	574	C
51	A23S	575	A
51	A23S	595	C
51	A23S	603	A
51	A23S	610	G
51	A23S	611(D)	U
51	A23S	611(E)	G
51	A23S	611(G)	G
51	A23S	620	G
51	A23S	621	A
51	A23S	627	A
51	A23S	629	G
51	A23S	637	A
51	A23S	643	A
51	A23S	645	C
51	A23S	646	A
51	A23S	647	G
51	A23S	649	G
51	A23S	650	C
51	A23S	651	G
51	A23S	653	C
51	A23S	654	U
51	A23S	668	G
51	A23S	671	C
51	A23S	676	A
51	A23S	682	G
51	A23S	685	A
51	A23S	686	G
51	A23S	695	G
51	A23S	717	G
51	A23S	730	C
51	A23S	738	G
51	A23S	748	G
51	A23S	764	A
51	A23S	765	G
51	A23S	776	G
51	A23S	781	A

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Mol	Chain	Res	Type
51	A23S	782	A
51	A23S	784	A
51	A23S	785	G
51	A23S	789	A
51	A23S	792	G
51	A23S	800	A
51	A23S	805	G
51	A23S	811	U
51	A23S	812	C
51	A23S	819	A
51	A23S	827	U
51	A23S	828	U
51	A23S	832	G
51	A23S	839	U
51	A23S	846	C
51	A23S	847	U
51	A23S	848	G
51	A23S	859	G
51	A23S	879	G
51	A23S	886	C
51	A23S	887	A
51	A23S	890	A
51	A23S	896	A
51	A23S	897	C
51	A23S	910	A
51	A23S	917	A
51	A23S	932	G
51	A23S	933	A
51	A23S	941	A
51	A23S	944	G
51	A23S	945	A
51	A23S	946	G
51	A23S	959	A
51	A23S	961	C
51	A23S	973	A
51	A23S	974	G
51	A23S	974(A)	C
51	A23S	975	G
51	A23S	980	A
51	A23S	983	A
51	A23S	996	A
51	A23S	999	U

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Mol	Chain	Res	Type
51	A23S	1003	G
51	A23S	1009	A
51	A23S	1010	A
51	A23S	1011	G
51	A23S	1012	U
51	A23S	1013	C
51	A23S	1017	G
51	A23S	1022	G
51	A23S	1023	U
51	A23S	1025	G
51	A23S	1026	U
51	A23S	1027	A
51	A23S	1033	U
51	A23S	1047	G
51	A23S	1048	A
51	A23S	1061	U
51	A23S	1070	A
51	A23S	1072	C
51	A23S	1078	U
51	A23S	1079	C
51	A23S	1088	A
51	A23S	1089	G
51	A23S	1112	G
51	A23S	1129	A
51	A23S	1130	U
51	A23S	1135	C
51	A23S	1136	G
51	A23S	1139	G
51	A23S	1141(A)	U
51	A23S	1142	A
51	A23S	1143	A
51	A23S	1155	A
51	A23S	1174	U
51	A23S	1205	U
51	A23S	1210	A
51	A23S	1211	U
51	A23S	1226	A
51	A23S	1227	G
51	A23S	1236	G
51	A23S	1244	G
51	A23S	1248	G
51	A23S	1250	G

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Mol	Chain	Res	Type
51	A23S	1253	A
51	A23S	1256	G
51	A23S	1265	A
51	A23S	1271	G
51	A23S	1272	A
51	A23S	1273	U
51	A23S	1300	U
51	A23S	1301	A
51	A23S	1302	A
51	A23S	1310	G
51	A23S	1313	U
51	A23S	1314	C
51	A23S	1321	A
51	A23S	1325	G
51	A23S	1329	U
51	A23S	1332	G
51	A23S	1341	U
51	A23S	1342	A
51	A23S	1349	A
51	A23S	1352	U
51	A23S	1359	A
51	A23S	1365	A
51	A23S	1378	A
51	A23S	1380	G
51	A23S	1384	A
51	A23S	1385	G
51	A23S	1392	A
51	A23S	1394	U
51	A23S	1395	A
51	A23S	1396	U
51	A23S	1398	C
51	A23S	1416	G
51	A23S	1420	U
51	A23S	1421	G
51	A23S	1427	A
51	A23S	1428	C
51	A23S	1444(A)	A
51	A23S	1445	C
51	A23S	1446	C
51	A23S	1448	G
51	A23S	1453	A
51	A23S	1454	U

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Mol	Chain	Res	Type
51	A23S	1455	G
51	A23S	1459	G
51	A23S	1460	A
51	A23S	1467	C
51	A23S	1483	G
51	A23S	1490	A
51	A23S	1493	C
51	A23S	1494	A
51	A23S	1495	A
51	A23S	1497	U
51	A23S	1506(A)	A
51	A23S	1506(C)	A
51	A23S	1535	U
51	A23S	1536	A
51	A23S	1538	G
51	A23S	1542	G
51	A23S	1543	A
51	A23S	1543(A)	C
51	A23S	1554	A
51	A23S	1558	A
51	A23S	1559	G
51	A23S	1560	G
51	A23S	1566	A
51	A23S	1569	A
51	A23S	1579	A
51	A23S	1582	C
51	A23S	1584	C
51	A23S	1603	A
51	A23S	1608	A
51	A23S	1609	A
51	A23S	1610	A
51	A23S	1616	A
51	A23S	1617	C
51	A23S	1618	A
51	A23S	1632	A
51	A23S	1635	G
51	A23S	1646	C
51	A23S	1647	G
51	A23S	1648	C
51	A23S	1649	G
51	A23S	1651	G
51	A23S	1653	G

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Mol	Chain	Res	Type
51	A23S	1654	A
51	A23S	1658	C
51	A23S	1665	A
51	A23S	1667	G
51	A23S	1674	G
51	A23S	1683	C
51	A23S	1693	U
51	A23S	1696	G
51	A23S	1707	G
51	A23S	1712(H)	A
51	A23S	1712(K)	A
51	A23S	1756	G
51	A23S	1763	G
51	A23S	1764	G
51	A23S	1773	A
51	A23S	1779	U
51	A23S	1780	A
51	A23S	1784	A
51	A23S	1785	A
51	A23S	1786	A
51	A23S	1787	A
51	A23S	1791	A
51	A23S	1800	C
51	A23S	1811	G
51	A23S	1816	G
51	A23S	1829	A
51	A23S	1833	U
51	A23S	1847	A
51	A23S	1888	G
51	A23S	1889	A
51	A23S	1902	C
51	A23S	1903	G
51	A23S	1905	C
51	A23S	1906	G
51	A23S	1912	A
51	A23S	1913	A
51	A23S	1915	U
51	A23S	1919	A
51	A23S	1929	G
51	A23S	1930	G
51	A23S	1936	A
51	A23S	1937	A

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Mol	Chain	Res	Type
51	A23S	1938	A
51	A23S	1939	U
51	A23S	1945	G
51	A23S	1955	U
51	A23S	1963	U
51	A23S	1964	G
51	A23S	1967	C
51	A23S	1970	A
51	A23S	1971	A
51	A23S	1972	A
51	A23S	1982	C
51	A23S	1991	U
51	A23S	1992	G
51	A23S	1993	U
51	A23S	1997	G
51	A23S	2017	U
51	A23S	2020	A
51	A23S	2021	C
51	A23S	2023	G
51	A23S	2027	G
51	A23S	2030	A
51	A23S	2031	A
51	A23S	2032	G
51	A23S	2033	A
51	A23S	2036	C
51	A23S	2052	G
51	A23S	2055	C
51	A23S	2056	G
51	A23S	2060	A
51	A23S	2061	G
51	A23S	2069	G
51	A23S	2098	U
51	A23S	2108	C
51	A23S	2111	C
51	A23S	2116	G
51	A23S	2117	A
51	A23S	2118	U
51	A23S	2119	A
51	A23S	2120	G
51	A23S	2126	A
51	A23S	2131	G
51	A23S	2133	G

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Mol	Chain	Res	Type
51	A23S	2146	C
51	A23S	2147	G
51	A23S	2159	G
51	A23S	2171	A
51	A23S	2172	U
51	A23S	2173	A
51	A23S	2198	A
51	A23S	2202(C)	G
51	A23S	2202(D)	G
51	A23S	2202(E)	A
51	A23S	2202(F)	U
51	A23S	2202(G)	G
51	A23S	2225	A
51	A23S	2226	C
51	A23S	2227	A
51	A23S	2238	G
51	A23S	2239	G
51	A23S	2263	C
51	A23S	2273	A
51	A23S	2275	C
51	A23S	2278	A
51	A23S	2283	C
51	A23S	2287	A
51	A23S	2288	A
51	A23S	2297	C
51	A23S	2304	G
51	A23S	2305	A
51	A23S	2306	C
51	A23S	2307	G
51	A23S	2311	A
51	A23S	2319	G
51	A23S	2320	A
51	A23S	2321	G
51	A23S	2325	G
51	A23S	2334	G
51	A23S	2336	A
51	A23S	2345	G
51	A23S	2346	A
51	A23S	2347	C
51	A23S	2354	G
51	A23S	2358	G
51	A23S	2372	G

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Mol	Chain	Res	Type
51	A23S	2379	G
51	A23S	2383	G
51	A23S	2385	C
51	A23S	2392	A
51	A23S	2402	C
51	A23S	2403	C
51	A23S	2406	U
51	A23S	2407	G
51	A23S	2410	G
51	A23S	2416	C
51	A23S	2419	U
51	A23S	2422	A
51	A23S	2423	U
51	A23S	2424	C
51	A23S	2425	A
51	A23S	2427	C
51	A23S	2429	G
51	A23S	2430	A
51	A23S	2431	U
51	A23S	2434	A
51	A23S	2435	A
51	A23S	2439	A
51	A23S	2441	C
51	A23S	2445	G
51	A23S	2448	A
51	A23S	2470	G
51	A23S	2476	A
51	A23S	2477	C
51	A23S	2478	A
51	A23S	2487	G
51	A23S	2494	G
51	A23S	2500	U
51	A23S	2501	C
51	A23S	2502	G
51	A23S	2504	U
51	A23S	2505	G
51	A23S	2506	U
51	A23S	2513	G
51	A23S	2518	A
51	A23S	2520	C
51	A23S	2529	G
51	A23S	2542	A

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Mol	Chain	Res	Type
51	A23S	2543	G
51	A23S	2553	G
51	A23S	2554	U
51	A23S	2566	A
51	A23S	2567	G
51	A23S	2572	A
51	A23S	2573	C
51	A23S	2574	G
51	A23S	2578	G
51	A23S	2585	U
51	A23S	2586	C
51	A23S	2596	U
51	A23S	2602	A
51	A23S	2609	U
51	A23S	2610	C
51	A23S	2611	U
51	A23S	2612	C
51	A23S	2614	A
51	A23S	2615	U
51	A23S	2630	G
51	A23S	2636	U
51	A23S	2646	C
51	A23S	2655	G
51	A23S	2665	A
51	A23S	2672	G
51	A23S	2679	A
51	A23S	2682	U
51	A23S	2683	C
51	A23S	2686	G
51	A23S	2689	U
51	A23S	2690	C
51	A23S	2703	C
51	A23S	2707	G
51	A23S	2712(A)	A
51	A23S	2713	A
51	A23S	2714	G
51	A23S	2720	U
51	A23S	2726	U
51	A23S	2731	G
51	A23S	2733	A
51	A23S	2748	A
51	A23S	2764	A

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Mol	Chain	Res	Type
51	A23S	2765	A
51	A23S	2766	G
51	A23S	2769	C
51	A23S	2776	A
51	A23S	2778	A
51	A23S	2779	U
51	A23S	2790	A
51	A23S	2791	C
51	A23S	2792	G
51	A23S	2794(B)	U
51	A23S	2794(D)	A
51	A23S	2805	G
51	A23S	2808	U
51	A23S	2818	G
51	A23S	2820	A
51	A23S	2821	A
51	A23S	2833	G
51	A23S	2834	G
51	A23S	2835	A
51	A23S	2849	U
51	A23S	2872	G
51	A23S	2873	A
51	A23S	2874	C
51	A23S	2875	C
51	A23S	2886	G
51	A23S	2894	G
52	A5S	15	A
52	A5S	16	G
52	A5S	24	G
52	A5S	28	C
52	A5S	41	U
52	A5S	42	C
52	A5S	44	G
52	A5S	51	G
52	A5S	52	A
52	A5S	63	G
52	A5S	66	A
52	A5S	67	G
52	A5S	73	A
52	A5S	81	G
52	A5S	87	G
52	A5S	90	C

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Mol	Chain	Res	Type
52	A5S	99	A
52	A5S	109	G
50	B16S	6	G
50	B16S	7	G
50	B16S	9	G
50	B16S	32	A
50	B16S	39	G
50	B16S	47	C
50	B16S	48	C
50	B16S	51	A
50	B16S	61	G
50	B16S	68(D)	C
50	B16S	68(N)	U
50	B16S	68(O)	A
50	B16S	101	A
50	B16S	108	G
50	B16S	116	A
50	B16S	120	A
50	B16S	121	C
50	B16S	129(A)	G
50	B16S	131	C
50	B16S	134	A
50	B16S	151	A
50	B16S	163	C
50	B16S	169	C
50	B16S	174	C
50	B16S	179	A
50	B16S	181	G
50	B16S	182	U
50	B16S	186(J)	G
50	B16S	195	A
50	B16S	197	A
50	B16S	201(C)	U
50	B16S	216	G
50	B16S	244	U
50	B16S	247	G
50	B16S	251	G
50	B16S	266	G
50	B16S	267	C
50	B16S	268	C
50	B16S	279	A
50	B16S	280	C

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Mol	Chain	Res	Type
50	B16S	283	C
50	B16S	289	G
50	B16S	314	C
50	B16S	320	C
50	B16S	321	A
50	B16S	328	C
50	B16S	329	A
50	B16S	332	G
50	B16S	345	C
50	B16S	346	G
50	B16S	352	C
50	B16S	353	A
50	B16S	354	G
50	B16S	356	A
50	B16S	367	U
50	B16S	372	C
50	B16S	373	A
50	B16S	382	A
50	B16S	387	U
50	B16S	389	A
50	B16S	390	C
50	B16S	392	G
50	B16S	397	A
50	B16S	398	C
50	B16S	406	G
50	B16S	412	A
50	B16S	413	G
50	B16S	414	A
50	B16S	422	C
50	B16S	429	U
50	B16S	430	A
50	B16S	440	A
50	B16S	450	G
50	B16S	452	A
50	B16S	453	A
50	B16S	458(B)	A
50	B16S	485	G
50	B16S	497	A
50	B16S	498	U
50	B16S	499	A
50	B16S	500	G
50	B16S	503	C

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Mol	Chain	Res	Type
50	B16S	505	G
50	B16S	509	A
50	B16S	510	A
50	B16S	511	C
50	B16S	512	U
50	B16S	518	C
50	B16S	527	G
50	B16S	531	U
50	B16S	533	A
50	B16S	536	C
50	B16S	547	A
50	B16S	558	G
50	B16S	559	A
50	B16S	560	U
50	B16S	561	U
50	B16S	562	C
50	B16S	572	A
50	B16S	573	A
50	B16S	575	G
50	B16S	576	G
50	B16S	577	G
50	B16S	579	G
50	B16S	632	A
50	B16S	653	A
50	B16S	665	A
50	B16S	672	U
50	B16S	688	G
50	B16S	690	G
50	B16S	702	A
50	B16S	703	G
50	B16S	717	C
50	B16S	722	A
50	B16S	723	U
50	B16S	748	C
50	B16S	749	C
50	B16S	755	G
50	B16S	774	G
50	B16S	777	A
50	B16S	793	U
50	B16S	794	A
50	B16S	816	A
50	B16S	817	C

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Mol	Chain	Res	Type
50	B16S	818	G
50	B16S	819	A
50	B16S	827	U
50	B16S	828	A
50	B16S	838(A)	U
50	B16S	838(B)	C
50	B16S	838(C)	U
50	B16S	859	A
50	B16S	861	G
50	B16S	867	G
50	B16S	872	A
50	B16S	873	A
50	B16S	874	G
50	B16S	890	G
50	B16S	891	U
50	B16S	902	G
50	B16S	914	A
50	B16S	922	G
50	B16S	926	G
50	B16S	927	G
50	B16S	934	C
50	B16S	935	A
50	B16S	951	G
50	B16S	960	U
50	B16S	961	U
50	B16S	969	A
50	B16S	971	G
50	B16S	974	A
50	B16S	975	A
50	B16S	976	G
50	B16S	977	A
50	B16S	978	A
50	B16S	980	C
50	B16S	992	U
50	B16S	993	G
50	B16S	1004	A
50	B16S	1027	C
50	B16S	1045	C
50	B16S	1054	C
50	B16S	1055	A
50	B16S	1065	U
50	B16S	1067	A

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Mol	Chain	Res	Type
50	B16S	1081	G
50	B16S	1094	G
50	B16S	1095	U
50	B16S	1101	A
50	B16S	1118	C
50	B16S	1125	U
50	B16S	1126	U
50	B16S	1129	C
50	B16S	1130	A
50	B16S	1131	G
50	B16S	1132	C
50	B16S	1137	C
50	B16S	1138	G
50	B16S	1139	G
50	B16S	1140	C
50	B16S	1146	A
50	B16S	1152	A
50	B16S	1158	C
50	B16S	1159	U
50	B16S	1160	G
50	B16S	1171	G
50	B16S	1181	G
50	B16S	1182	G
50	B16S	1184	G
50	B16S	1193	G
50	B16S	1196	U
50	B16S	1200	C
50	B16S	1201	A
50	B16S	1202	G
50	B16S	1212	U
50	B16S	1213	A
50	B16S	1226	C
50	B16S	1227	A
50	B16S	1238	A
50	B16S	1241	G
50	B16S	1257	U
50	B16S	1258	G
50	B16S	1260	C
50	B16S	1278	U
50	B16S	1280	A
50	B16S	1281	U
50	B16S	1286	A

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Mol	Chain	Res	Type
50	B16S	1287	A
50	B16S	1288	A
50	B16S	1300	G
50	B16S	1301	U
50	B16S	1302	U
50	B16S	1317	C
50	B16S	1322	C
50	B16S	1323	G
50	B16S	1331	G
50	B16S	1336	C
50	B16S	1338	G
50	B16S	1346	A
50	B16S	1347	G
50	B16S	1362(A)	C
50	B16S	1364	U
50	B16S	1378	C
50	B16S	1398	A
50	B16S	1406	U
50	B16S	1408	A
50	B16S	1419	G
50	B16S	1440(B)	G
50	B16S	1440(C)	G
50	B16S	1440(D)	A
50	B16S	1440(E)	G
50	B16S	1440(I)	A
50	B16S	1440(J)	C
50	B16S	1440(K)	G
50	B16S	1440(L)	G
50	B16S	1492	A
50	B16S	1497	G
50	B16S	1502	A
50	B16S	1504	G
50	B16S	1505	G
50	B16S	1506	U
50	B16S	1507	A
50	B16S	1508	G
50	B16S	1517	G
50	B16S	1519	A
50	B16S	1520	G
50	B16S	1529	G
50	B16S	1530	G
51	B23S	34	C

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Mol	Chain	Res	Type
51	B23S	35	G
51	B23S	46	C
51	B23S	55	G
51	B23S	58	G
51	B23S	61	G
51	B23S	71	A
51	B23S	72	U
51	B23S	74	A
51	B23S	75	G
51	B23S	84	A
51	B23S	91	A
51	B23S	99	U
51	B23S	101	G
51	B23S	102	G
51	B23S	118	A
51	B23S	119	A
51	B23S	120	U
51	B23S	131	G
51	B23S	137(B)	G
51	B23S	155	C
51	B23S	155(B)	U
51	B23S	181	A
51	B23S	186	G
51	B23S	196	A
51	B23S	197	A
51	B23S	204	A
51	B23S	205	G
51	B23S	215	G
51	B23S	216	A
51	B23S	222	A
51	B23S	227	A
51	B23S	229	A
51	B23S	230	U
51	B23S	240	G
51	B23S	245	G
51	B23S	248	G
51	B23S	252	G
51	B23S	267	C
51	B23S	269	U
51	B23S	270(L)	U
51	B23S	270(M)	U
51	B23S	270(Q)	C

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Mol	Chain	Res	Type
51	B23S	270(Y)	G
51	B23S	271(C)	U
51	B23S	271(D)	G
51	B23S	271(M)	G
51	B23S	271(N)	G
51	B23S	271(P)	C
51	B23S	271(R)	C
51	B23S	271(S)	C
51	B23S	271(V)	A
51	B23S	301	G
51	B23S	302	C
51	B23S	312	G
51	B23S	316	C
51	B23S	324	A
51	B23S	329	G
51	B23S	335	C
51	B23S	336	C
51	B23S	338	G
51	B23S	352	G
51	B23S	353	G
51	B23S	354	G
51	B23S	356	G
51	B23S	357(L)	A
51	B23S	357(M)	C
51	B23S	372	G
51	B23S	383	U
51	B23S	385	C
51	B23S	386	G
51	B23S	396	G
51	B23S	405	U
51	B23S	406	G
51	B23S	411	G
51	B23S	412	A
51	B23S	444	C
51	B23S	446	G
51	B23S	454	A
51	B23S	455	C
51	B23S	457	A
51	B23S	470	A
51	B23S	471	A
51	B23S	473	G
51	B23S	475	U

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Mol	Chain	Res	Type
51	B23S	480	A
51	B23S	481	G
51	B23S	492	A
51	B23S	505	A
51	B23S	508	G
51	B23S	509	C
51	B23S	510	C
51	B23S	512	G
51	B23S	513	A
51	B23S	527	C
51	B23S	530	G
51	B23S	531	C
51	B23S	532	A
51	B23S	533	G
51	B23S	543	C
51	B23S	551	G
51	B23S	563	G
51	B23S	573	G
51	B23S	575	A
51	B23S	587	C
51	B23S	599	G
51	B23S	603	A
51	B23S	611(D)	U
51	B23S	611(F)	A
51	B23S	611(G)	G
51	B23S	620	G
51	B23S	621	A
51	B23S	622	G
51	B23S	627	A
51	B23S	637	A
51	B23S	645	C
51	B23S	646	A
51	B23S	647	G
51	B23S	650	C
51	B23S	651	G
51	B23S	653	C
51	B23S	654	U
51	B23S	655	A
51	B23S	668	G
51	B23S	669	G
51	B23S	670	A
51	B23S	671	C

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Mol	Chain	Res	Type
51	B23S	685	A
51	B23S	686	G
51	B23S	688	U
51	B23S	717	G
51	B23S	722	A
51	B23S	730	C
51	B23S	746	A
51	B23S	762	U
51	B23S	764	A
51	B23S	765	G
51	B23S	775	G
51	B23S	776	G
51	B23S	782	A
51	B23S	784	A
51	B23S	785	G
51	B23S	786	C
51	B23S	787	U
51	B23S	789	A
51	B23S	792	G
51	B23S	805	G
51	B23S	812	C
51	B23S	819	A
51	B23S	820	A
51	B23S	827	U
51	B23S	828	U
51	B23S	830	G
51	B23S	831	G
51	B23S	832	G
51	B23S	846	C
51	B23S	847	U
51	B23S	848	G
51	B23S	859	G
51	B23S	879	G
51	B23S	886	C
51	B23S	890	A
51	B23S	896	A
51	B23S	897	C
51	B23S	898	C
51	B23S	907	U
51	B23S	910	A
51	B23S	914	C
51	B23S	915	C

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Mol	Chain	Res	Type
51	B23S	917	A
51	B23S	919	G
51	B23S	926	A
51	B23S	932	G
51	B23S	938	G
51	B23S	941	A
51	B23S	945	A
51	B23S	946	G
51	B23S	953	A
51	B23S	959	A
51	B23S	961	C
51	B23S	962	G
51	B23S	974	G
51	B23S	974(A)	C
51	B23S	975	G
51	B23S	979	G
51	B23S	980	A
51	B23S	983	A
51	B23S	990	A
51	B23S	996	A
51	B23S	999	U
51	B23S	1003	G
51	B23S	1005	C
51	B23S	1009	A
51	B23S	1010	A
51	B23S	1011	G
51	B23S	1012	U
51	B23S	1013	C
51	B23S	1020	A
51	B23S	1023	U
51	B23S	1025	G
51	B23S	1026	U
51	B23S	1033	U
51	B23S	1047	G
51	B23S	1048	A
51	B23S	1061	U
51	B23S	1062	G
51	B23S	1065	U
51	B23S	1070	A
51	B23S	1072	C
51	B23S	1074	G
51	B23S	1079	C

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Mol	Chain	Res	Type
51	B23S	1088	A
51	B23S	1112	G
51	B23S	1129	A
51	B23S	1130	U
51	B23S	1135	C
51	B23S	1136	G
51	B23S	1141(A)	U
51	B23S	1142	A
51	B23S	1151	G
51	B23S	1155	A
51	B23S	1174	U
51	B23S	1177	A
51	B23S	1186	G
51	B23S	1205	U
51	B23S	1210	A
51	B23S	1211	U
51	B23S	1219(A)	A
51	B23S	1220	C
51	B23S	1227	G
51	B23S	1236	G
51	B23S	1240	U
51	B23S	1244	G
51	B23S	1248	G
51	B23S	1250	G
51	B23S	1252	G
51	B23S	1253	A
51	B23S	1256	G
51	B23S	1271	G
51	B23S	1272	A
51	B23S	1300	U
51	B23S	1301	A
51	B23S	1302	A
51	B23S	1309	G
51	B23S	1313	U
51	B23S	1314	C
51	B23S	1321	A
51	B23S	1329	U
51	B23S	1330	C
51	B23S	1344	G
51	B23S	1345	C
51	B23S	1349	A
51	B23S	1359	A

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Mol	Chain	Res	Type
51	B23S	1365	A
51	B23S	1366	A
51	B23S	1380	G
51	B23S	1384	A
51	B23S	1385	G
51	B23S	1386	C
51	B23S	1395	A
51	B23S	1396	U
51	B23S	1416	G
51	B23S	1428	C
51	B23S	1444(A)	A
51	B23S	1453	A
51	B23S	1454	U
51	B23S	1455	G
51	B23S	1458	C
51	B23S	1460	A
51	B23S	1467	C
51	B23S	1483	G
51	B23S	1490	A
51	B23S	1493	C
51	B23S	1494	A
51	B23S	1495	A
51	B23S	1497	U
51	B23S	1506(C)	A
51	B23S	1535	U
51	B23S	1538	G
51	B23S	1542	G
51	B23S	1543	A
51	B23S	1543(A)	C
51	B23S	1558	A
51	B23S	1559	G
51	B23S	1566	A
51	B23S	1569	A
51	B23S	1578	U
51	B23S	1579	A
51	B23S	1584	C
51	B23S	1586	A
51	B23S	1603	A
51	B23S	1608	A
51	B23S	1609	A
51	B23S	1610	A
51	B23S	1617	C

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Mol	Chain	Res	Type
51	B23S	1639	U
51	B23S	1644	C
51	B23S	1646	C
51	B23S	1648	C
51	B23S	1651	G
51	B23S	1653	G
51	B23S	1674	G
51	B23S	1681	G
51	B23S	1685	C
51	B23S	1689	A
51	B23S	1694	C
51	B23S	1695	G
51	B23S	1698	A
51	B23S	1712(H)	A
51	B23S	1712(I)	U
51	B23S	1712(K)	A
51	B23S	1712(Q)	G
51	B23S	1750	G
51	B23S	1754	C
51	B23S	1756	G
51	B23S	1763	G
51	B23S	1764	G
51	B23S	1773	A
51	B23S	1785	A
51	B23S	1787	A
51	B23S	1788	C
51	B23S	1791	A
51	B23S	1800	C
51	B23S	1801	G
51	B23S	1811	G
51	B23S	1816	G
51	B23S	1833	U
51	B23S	1838	C
51	B23S	1839	G
51	B23S	1840	G
51	B23S	1847	A
51	B23S	1859	A
51	B23S	1860	G
51	B23S	1878	G
51	B23S	1889	A
51	B23S	1903	G
51	B23S	1904	G

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Mol	Chain	Res	Type
51	B23S	1906	G
51	B23S	1913	A
51	B23S	1914	C
51	B23S	1919	A
51	B23S	1929	G
51	B23S	1934	C
51	B23S	1936	A
51	B23S	1937	A
51	B23S	1938	A
51	B23S	1939	U
51	B23S	1945	G
51	B23S	1955	U
51	B23S	1963	U
51	B23S	1964	G
51	B23S	1966	A
51	B23S	1967	C
51	B23S	1970	A
51	B23S	1971	A
51	B23S	1972	A
51	B23S	1974	C
51	B23S	1981	A
51	B23S	1982	C
51	B23S	1984	G
51	B23S	1991	U
51	B23S	1992	G
51	B23S	1993	U
51	B23S	1997	G
51	B23S	2004	G
51	B23S	2006	C
51	B23S	2021	C
51	B23S	2023	G
51	B23S	2031	A
51	B23S	2032	G
51	B23S	2033	A
51	B23S	2036	C
51	B23S	2043	C
51	B23S	2052	G
51	B23S	2055	C
51	B23S	2056	G
51	B23S	2058	A
51	B23S	2060	A
51	B23S	2061	G

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Mol	Chain	Res	Type
51	B23S	2069	G
51	B23S	2080	G
51	B23S	2086	U
51	B23S	2108	C
51	B23S	2111	C
51	B23S	2112	G
51	B23S	2118	U
51	B23S	2119	A
51	B23S	2120	G
51	B23S	2131	G
51	B23S	2133	G
51	B23S	2147	G
51	B23S	2148	G
51	B23S	2159	G
51	B23S	2171	A
51	B23S	2172	U
51	B23S	2173	A
51	B23S	2190	G
51	B23S	2198	A
51	B23S	2202(C)	G
51	B23S	2202(D)	G
51	B23S	2202(E)	A
51	B23S	2202(F)	U
51	B23S	2202(G)	G
51	B23S	2225	A
51	B23S	2226	C
51	B23S	2238	G
51	B23S	2239	G
51	B23S	2243	U
51	B23S	2251	G
51	B23S	2266	A
51	B23S	2269	A
51	B23S	2273	A
51	B23S	2275	C
51	B23S	2278	A
51	B23S	2283	C
51	B23S	2287	A
51	B23S	2296	U
51	B23S	2304	G
51	B23S	2305	A
51	B23S	2306	C
51	B23S	2307	G

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Mol	Chain	Res	Type
51	B23S	2310	A
51	B23S	2319	G
51	B23S	2320	A
51	B23S	2321	G
51	B23S	2325	G
51	B23S	2334	G
51	B23S	2336	A
51	B23S	2344	U
51	B23S	2345	G
51	B23S	2346	A
51	B23S	2347	C
51	B23S	2350	C
51	B23S	2361	A
51	B23S	2379	G
51	B23S	2383	G
51	B23S	2385	C
51	B23S	2388	A
51	B23S	2392	A
51	B23S	2402	C
51	B23S	2403	C
51	B23S	2406	U
51	B23S	2410	G
51	B23S	2422	A
51	B23S	2424	C
51	B23S	2425	A
51	B23S	2429	G
51	B23S	2430	A
51	B23S	2431	U
51	B23S	2433	A
51	B23S	2434	A
51	B23S	2435	A
51	B23S	2436	G
51	B23S	2439	A
51	B23S	2440	C
51	B23S	2441	C
51	B23S	2446	G
51	B23S	2448	A
51	B23S	2464	C
51	B23S	2468	G
51	B23S	2469	A
51	B23S	2470	G
51	B23S	2476	A

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Mol	Chain	Res	Type
51	B23S	2477	C
51	B23S	2478	A
51	B23S	2484	G
51	B23S	2489	G
51	B23S	2491	U
51	B23S	2494	G
51	B23S	2500	U
51	B23S	2501	C
51	B23S	2502	G
51	B23S	2503	A
51	B23S	2504	U
51	B23S	2505	G
51	B23S	2506	U
51	B23S	2513	G
51	B23S	2518	A
51	B23S	2520	C
51	B23S	2529	G
51	B23S	2542	A
51	B23S	2543	G
51	B23S	2554	U
51	B23S	2566	A
51	B23S	2567	G
51	B23S	2569	G
51	B23S	2572	A
51	B23S	2573	C
51	B23S	2578	G
51	B23S	2585	U
51	B23S	2586	C
51	B23S	2593	U
51	B23S	2602	A
51	B23S	2603	G
51	B23S	2604	U
51	B23S	2605	U
51	B23S	2609	U
51	B23S	2610	C
51	B23S	2611	U
51	B23S	2612	C
51	B23S	2614	A
51	B23S	2615	U
51	B23S	2630	G
51	B23S	2634	G
51	B23S	2636	U

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Mol	Chain	Res	Type
51	B23S	2641	G
51	B23S	2654	A
51	B23S	2655	G
51	B23S	2658	C
51	B23S	2663	G
51	B23S	2665	A
51	B23S	2686	G
51	B23S	2689	U
51	B23S	2690	C
51	B23S	2691	C
51	B23S	2693	A
51	B23S	2694	G
51	B23S	2712(A)	A
51	B23S	2713	A
51	B23S	2714	G
51	B23S	2726	U
51	B23S	2733	A
51	B23S	2734	A
51	B23S	2751	G
51	B23S	2758	A
51	B23S	2765	A
51	B23S	2766	G
51	B23S	2769	C
51	B23S	2778	A
51	B23S	2779	U
51	B23S	2781	A
51	B23S	2782	G
51	B23S	2789	C
51	B23S	2790	A
51	B23S	2791	C
51	B23S	2792	G
51	B23S	2794(D)	A
51	B23S	2805	G
51	B23S	2808	U
51	B23S	2818	G
51	B23S	2820	A
51	B23S	2821	A
51	B23S	2823	A
51	B23S	2831	G
51	B23S	2835	A
51	B23S	2849	U
51	B23S	2872	G

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Mol	Chain	Res	Type
51	B23S	2873	A
51	B23S	2875	C
51	B23S	2883	A
51	B23S	2886	G
51	B23S	2894	G
52	B5S	12	C
52	B5S	13	A
52	B5S	41	U
52	B5S	42	C
52	B5S	45	A
52	B5S	52	A
52	B5S	56	G
52	B5S	57	A
52	B5S	63	G
52	B5S	67	G
52	B5S	73	A
52	B5S	81	G
52	B5S	84	C
52	B5S	90	C
52	B5S	109	G
53	AIRE	6161	U
53	AIRE	6172	U
53	AIRE	6176	C
53	AIRE	6189	A
53	BIRE	6161	U
53	BIRE	6174	U
53	BIRE	6176	C
53	BIRE	6189	A

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	A16S	60	A
50	A16S	115	G
50	A16S	197	A
50	A16S	243	A
50	A16S	328	C
50	A16S	428	G
50	A16S	499	A
50	A16S	509	A
50	A16S	560	U
50	A16S	687	A

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Mol	Chain	Res	Type
50	A16S	748	C
50	A16S	913	A
50	A16S	991	U
50	A16S	1049	U
50	A16S	1064	G
50	A16S	1067	A
50	A16S	1101	A
50	A16S	1145	C
50	A16S	1201	A
50	A16S	1285	A
50	A16S	1504	G
51	A23S	196	A
51	A23S	221	A
51	A23S	265	A
51	A23S	271(B)	G
51	A23S	357(L)	A
51	A23S	474	G
51	A23S	479	A
51	A23S	650	C
51	A23S	775	G
51	A23S	846	C
51	A23S	960	A
51	A23S	1022	G
51	A23S	1060	U
51	A23S	1210	A
51	A23S	1300	U
51	A23S	1379	A
51	A23S	1444(A)	A
51	A23S	1542	G
51	A23S	1558	A
51	A23S	1786	A
51	A23S	1935	G
51	A23S	1937	A
51	A23S	2097	C
51	A23S	2225	A
51	A23S	2428	G
51	A23S	2447	G
51	A23S	2609	U
51	A23S	2689	U
51	A23S	2719	G
50	B16S	60	A
50	B16S	68(N)	U

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Mol	Chain	Res	Type
50	B16S	115	G
50	B16S	328	C
50	B16S	428	G
50	B16S	429	U
50	B16S	484	G
50	B16S	499	A
50	B16S	509	A
50	B16S	560	U
50	B16S	687	A
50	B16S	748	C
50	B16S	913	A
50	B16S	991	U
50	B16S	992	U
50	B16S	1064	G
50	B16S	1145	C
50	B16S	1201	A
50	B16S	1285	A
50	B16S	1491	G
50	B16S	1504	G
51	B23S	196	A
51	B23S	214	G
51	B23S	271(B)	G
51	B23S	271(Q)	A
51	B23S	474	G
51	B23S	479	A
51	B23S	611(E)	G
51	B23S	611(F)	A
51	B23S	775	G
51	B23S	791	C
51	B23S	846	C
51	B23S	1009	A
51	B23S	1022	G
51	B23S	1060	U
51	B23S	1210	A
51	B23S	1300	U
51	B23S	1379	A
51	B23S	1427	A
51	B23S	1558	A
51	B23S	1786	A
51	B23S	1858	G
51	B23S	2225	A
51	B23S	2433	A

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Mol	Chain	Res	Type
51	B23S	2503	A
51	B23S	2609	U
51	B23S	2750	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AL02	271/271 (100%)	0.09	4 (1%)	73	66	54, 99, 150, 228	0
1	BL02	271/271 (100%)	-0.01	1 (0%)	92	89	42, 88, 128, 197	0
2	AL03	204/204 (100%)	0.39	7 (3%)	45	37	63, 120, 179, 294	0
2	BL03	204/204 (100%)	0.16	6 (2%)	51	42	52, 114, 168, 253	0
3	AL04	202/202 (100%)	0.04	4 (1%)	65	58	60, 113, 184, 265	0
3	BL04	202/202 (100%)	0.03	3 (1%)	73	66	52, 109, 174, 242	0
4	AL05	181/181 (100%)	1.30	54 (29%)	0	0	134, 212, 272, 318	0
4	BL05	181/181 (100%)	1.42	51 (28%)	0	0	149, 227, 281, 309	0
5	AL06	159/159 (100%)	1.68	60 (37%)	0	0	124, 217, 285, 314	0
5	BL06	159/159 (100%)	0.40	9 (5%)	23	19	91, 142, 199, 240	0
6	AL09	145/145 (100%)	1.17	44 (30%)	0	0	82, 185, 244, 324	0
6	BL09	145/145 (100%)	0.75	21 (14%)	2	2	76, 156, 202, 244	0
7	AL11	147/147 (100%)	3.85	118 (80%)	0	0	256, 322, 358, 387	0
7	BL11	147/147 (100%)	4.54	113 (76%)	0	0	225, 321, 363, 388	0
8	AL13	137/137 (100%)	0.32	8 (5%)	23	18	82, 133, 194, 207	0
8	BL13	137/137 (100%)	0.34	6 (4%)	34	29	69, 120, 186, 258	0
9	AL14	122/122 (100%)	0.08	0	100	100	63, 111, 148, 180	0
9	BL14	122/122 (100%)	0.34	3 (2%)	57	49	65, 101, 142, 171	0
10	AL15	146/146 (100%)	0.45	8 (5%)	25	21	63, 138, 225, 281	0
10	BL15	146/146 (100%)	0.55	13 (8%)	9	8	46, 134, 208, 283	0
11	AL16	134/134 (100%)	0.46	10 (7%)	14	11	85, 136, 201, 289	0
11	BL16	134/134 (100%)	0.55	11 (8%)	11	9	77, 126, 219, 300	0
12	AL17	117/117 (100%)	0.52	8 (6%)	17	13	64, 113, 171, 197	0
12	BL17	117/117 (100%)	0.49	2 (1%)	70	62	67, 105, 162, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AL18	98/98 (100%)	1.15	26 (26%)	0	0	125, 187, 243, 293	0
13	BL18	98/98 (100%)	0.72	17 (17%)	1	1	140, 201, 253, 275	0
14	AL19	137/137 (100%)	0.27	7 (5%)	28	24	78, 132, 216, 266	0
14	BL19	137/137 (100%)	0.15	4 (2%)	51	42	74, 124, 226, 284	0
15	AL20	117/117 (100%)	0.04	2 (1%)	70	62	66, 113, 181, 243	0
15	BL20	117/117 (100%)	-0.17	0	100	100	62, 112, 172, 232	0
16	AL21	101/101 (100%)	0.27	2 (1%)	65	58	86, 140, 206, 307	0
16	BL21	101/101 (100%)	0.18	5 (4%)	28	25	75, 130, 202, 283	0
17	AL22	112/112 (100%)	0.60	4 (3%)	42	35	71, 104, 172, 250	0
17	BL22	112/112 (100%)	0.30	3 (2%)	54	45	57, 95, 152, 210	0
18	AL23	92/92 (100%)	0.13	0	100	100	77, 117, 171, 217	0
18	BL23	92/92 (100%)	0.37	2 (2%)	62	54	62, 97, 139, 182	0
19	AL24	100/100 (100%)	1.14	20 (20%)	1	1	103, 144, 262, 296	0
19	BL24	100/100 (100%)	0.82	10 (10%)	7	6	83, 129, 234, 266	0
20	AL25	187/187 (100%)	0.96	41 (21%)	0	1	119, 190, 253, 309	0
20	BL25	187/187 (100%)	0.35	14 (7%)	14	11	111, 179, 225, 276	0
21	AL27	76/76 (100%)	0.34	5 (6%)	18	14	91, 135, 187, 233	0
21	BL27	76/76 (100%)	0.42	5 (6%)	18	14	88, 132, 198, 248	0
22	AL28	88/88 (100%)	0.35	3 (3%)	45	37	61, 109, 186, 283	0
22	BL28	88/88 (100%)	0.37	4 (4%)	33	28	61, 105, 182, 248	0
23	AL29	62/62 (100%)	0.33	4 (6%)	18	14	99, 137, 237, 255	0
23	BL29	62/62 (100%)	0.28	6 (9%)	7	7	59, 108, 218, 253	0
24	AL30	59/59 (100%)	1.40	15 (25%)	0	0	101, 132, 214, 248	0
24	BL30	59/59 (100%)	0.92	5 (8%)	10	9	78, 131, 207, 286	0
25	AL32	52/52 (100%)	0.51	7 (13%)	3	3	66, 117, 205, 239	0
25	BL32	52/52 (100%)	0.06	2 (3%)	40	33	54, 105, 215, 269	0
26	AL33	44/44 (100%)	9.55	44 (100%)	0	0	140, 241, 282, 301	0
26	BL33	44/44 (100%)	5.13	39 (88%)	0	0	193, 248, 287, 304	0
27	AL34	48/48 (100%)	-0.04	0	100	100	59, 89, 129, 203	0
27	BL34	48/48 (100%)	0.14	0	100	100	41, 71, 113, 175	0
28	AL35	63/63 (100%)	0.21	1 (1%)	72	64	69, 119, 192, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	BL35	63/63 (100%)	0.16	1 (1%)	72	64	71, 114, 188, 225	0
29	AS02	234/234 (100%)	0.56	22 (9%)	8	7	128, 202, 274, 300	0
29	BS02	234/234 (100%)	0.64	26 (11%)	5	5	113, 213, 279, 309	0
30	AS03	206/206 (100%)	0.44	15 (7%)	15	12	124, 200, 264, 308	0
30	BS03	206/206 (100%)	0.34	12 (5%)	23	18	119, 196, 253, 298	0
31	AS04	208/208 (100%)	0.23	5 (2%)	59	50	99, 152, 216, 239	0
31	BS04	208/208 (100%)	0.73	31 (14%)	2	2	128, 204, 275, 307	0
32	AS05	151/151 (100%)	0.11	4 (2%)	56	47	94, 144, 199, 262	0
32	BS05	151/151 (100%)	0.04	5 (3%)	46	38	105, 164, 216, 261	0
33	AS06	101/101 (100%)	0.17	5 (4%)	28	25	122, 172, 234, 258	0
33	BS06	101/101 (100%)	-0.10	2 (1%)	65	58	96, 149, 203, 230	0
34	AS07	155/155 (100%)	0.91	32 (20%)	1	1	154, 214, 272, 300	0
34	BS07	155/155 (100%)	0.95	30 (19%)	1	1	151, 222, 282, 309	0
35	AS08	138/138 (100%)	0.47	12 (8%)	10	8	92, 142, 195, 229	0
35	BS08	138/138 (100%)	0.58	14 (10%)	7	6	95, 168, 215, 256	0
36	AS09	127/127 (100%)	1.61	38 (29%)	0	0	139, 274, 335, 355	0
36	BS09	127/127 (100%)	1.31	31 (24%)	0	0	150, 262, 310, 343	0
37	AS10	98/98 (100%)	2.25	49 (50%)	0	0	138, 260, 344, 356	0
37	BS10	98/98 (100%)	1.61	33 (33%)	0	0	142, 246, 308, 339	0
38	AS11	114/114 (100%)	0.43	13 (11%)	5	5	95, 150, 210, 267	0
38	BS11	114/114 (100%)	0.11	3 (2%)	56	47	85, 138, 193, 251	0
39	AS12	122/122 (100%)	0.72	12 (9%)	7	7	74, 121, 166, 201	0
39	BS12	122/122 (100%)	0.53	8 (6%)	18	14	105, 147, 192, 230	0
40	AS13	117/117 (100%)	1.65	41 (35%)	0	0	152, 259, 315, 352	0
40	BS13	117/117 (100%)	1.11	30 (25%)	0	0	159, 253, 318, 340	0
41	AS14	60/60 (100%)	1.05	11 (18%)	1	1	148, 194, 241, 329	0
41	BS14	60/60 (100%)	1.02	9 (15%)	2	2	144, 196, 242, 301	0
42	AS15	88/88 (100%)	0.32	5 (5%)	23	19	100, 139, 183, 229	0
42	BS15	88/88 (100%)	0.48	5 (5%)	23	19	92, 146, 201, 215	0
43	AS16	83/83 (100%)	0.84	12 (14%)	2	2	104, 137, 187, 233	0
43	BS16	83/83 (100%)	1.44	27 (32%)	0	0	148, 199, 260, 310	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AS17	99/99 (100%)	0.15	3 (3%) 50 40	92, 125, 166, 223	0
44	BS17	99/99 (100%)	0.36	3 (3%) 50 40	105, 149, 191, 235	0
45	AS18	70/70 (100%)	0.85	9 (12%) 3 4	110, 174, 234, 253	0
45	BS18	70/70 (100%)	0.49	1 (1%) 75 68	100, 150, 195, 247	0
46	AS19	78/78 (100%)	2.27	38 (48%) 0 0	170, 255, 301, 353	0
46	BS19	78/78 (100%)	1.70	28 (35%) 0 0	172, 257, 302, 314	0
47	AS20	99/99 (100%)	0.69	9 (9%) 9 7	106, 149, 228, 256	0
47	BS20	99/99 (100%)	1.18	22 (22%) 0 0	120, 178, 249, 291	0
48	ATHX	24/24 (100%)	0.68	1 (4%) 36 30	153, 263, 279, 301	0
48	BTHX	24/24 (100%)	1.20	8 (33%) 0 0	209, 276, 325, 350	0
49	AL31	30/30 (100%)	1.85	13 (43%) 0 0	206, 272, 323, 351	0
49	BL31	30/30 (100%)	1.81	11 (36%) 0 0	216, 303, 332, 352	0
50	A16S	1504/1506 (99%)	0.19	50 (3%) 46 38	76, 144, 270, 413	0
50	B16S	1504/1506 (99%)	0.23	56 (3%) 41 34	79, 171, 296, 397	0
51	A23S	2876/2879 (99%)	0.23	126 (4%) 34 29	58, 115, 252, 440	0
51	B23S	2876/2879 (99%)	0.14	117 (4%) 37 31	52, 103, 243, 414	0
52	A5S	119/119 (100%)	-0.03	1 (0%) 86 81	122, 178, 230, 282	0
52	B5S	119/119 (100%)	-0.19	1 (0%) 86 81	124, 178, 236, 309	0
53	AIRE	32/196 (16%)	1.84	10 (31%) 0 0	131, 266, 505, 516	0
53	BIRE	32/196 (16%)	0.48	2 (6%) 20 15	145, 222, 413, 466	0
All	All	20668/21006 (98%)	0.49	1913 (9%) 8 7	41, 141, 282, 516	0

All (1913) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BL11	1	MET	31.2
26	AL33	49	HIS	20.9
26	AL33	13	CYS	20.3
26	AL33	47	THR	17.4
26	AL33	22	ALA	16.8
26	AL33	24	GLU	16.1
26	AL33	50	ARG	15.4
26	AL33	26	ASN	15.0
26	BL33	9	LEU	14.8
26	AL33	40	CYS	14.8

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Mol	Chain	Res	Type	RSRZ
51	A23S	1078	U	14.7
50	B16S	1028(D)	C	14.4
7	BL11	31	GLY	14.3
26	AL33	41	PRO	13.9
26	AL33	51	GLU	13.3
26	BL33	24	GLU	13.2
7	BL11	4	VAL	13.2
51	A23S	1087	G	13.1
26	AL33	46	HIS	12.5
26	BL33	11	LEU	12.5
51	A23S	1089	G	12.4
7	BL11	124	ALA	12.1
7	BL11	2	LYS	12.0
7	BL11	125	ARG	11.9
26	AL33	14	THR	11.8
26	BL33	22	ALA	11.7
7	BL11	66	THR	11.7
36	BS09	8	GLY	11.6
26	AL33	37	ARG	11.3
46	AS19	74	PHE	11.3
24	BL30	1	MET	11.1
51	A23S	2146	C	11.0
7	AL11	136	VAL	11.0
34	BS07	80	VAL	10.8
26	AL33	39	TYR	10.7
26	AL33	20	ASN	10.7
51	B23S	2116	G	10.7
50	B16S	68(L)	U	10.6
51	A23S	1080	C	10.4
26	BL33	23	THR	10.3
7	AL11	95	LYS	10.2
26	AL33	35	GLU	10.2
51	A23S	1083	U	10.0
7	BL11	65	PHE	10.0
17	AL22	112	GLY	9.9
26	AL33	21	TYR	9.9
7	AL11	47	ASN	9.8
26	AL33	36	LEU	9.7
7	AL11	32	ALA	9.5
26	AL33	12	GLU	9.5
26	AL33	25	LYS	9.5
7	AL11	137	GLU	9.4

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Mol	Chain	Res	Type	RSRZ
7	BL11	5	VAL	9.4
37	AS10	10	GLY	9.3
19	AL24	52	SER	9.2
26	AL33	23	THR	9.1
7	BL11	91	PRO	9.1
7	AL11	19	PRO	9.1
7	BL11	60	TYR	9.1
7	AL11	57	ILE	9.0
40	AS13	112	GLY	8.9
5	AL06	161	GLY	8.9
7	BL11	92	GLY	8.9
40	AS13	6	GLY	8.9
7	BL11	69	THR	8.9
7	BL11	18	THR	8.8
40	AS13	7	VAL	8.8
50	A16S	68(L)	U	8.8
26	AL33	27	LYS	8.7
51	A23S	1084	A	8.6
26	BL33	10	LEU	8.6
26	AL33	38	LYS	8.6
26	BL33	12	GLU	8.5
19	BL24	51	VAL	8.5
51	B23S	1075	C	8.5
7	BL11	132	ARG	8.4
51	A23S	1077	A	8.2
34	BS07	82	GLY	8.2
7	BL11	145	LYS	8.1
26	AL33	45	LYS	8.0
24	AL30	1	MET	8.0
26	AL33	11	LEU	8.0
26	AL33	16	CYS	8.0
46	AS19	75	ALA	8.0
7	BL11	128	ALA	8.0
26	BL33	26	ASN	8.0
51	B23S	1087	G	7.9
26	AL33	32	ASN	7.9
7	BL11	17	ALA	7.9
51	A23S	2139	C	7.9
51	B23S	2125	G	7.8
26	BL33	51	GLU	7.8
7	AL11	20	ALA	7.8
7	BL11	59	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
7	BL11	133	SER	7.8
7	AL11	72	PRO	7.7
7	BL11	34	ILE	7.7
36	AS09	15	ALA	7.7
50	A16S	1028(D)	C	7.6
26	AL33	52	VAL	7.6
7	AL11	27	LEU	7.6
7	BL11	140	GLY	7.5
7	AL11	76	TYR	7.5
19	BL24	52	SER	7.5
7	AL11	62	ASP	7.5
26	BL33	21	TYR	7.4
26	AL33	29	ASN	7.4
7	AL11	58	THR	7.4
51	A23S	888	C	7.4
7	BL11	94	GLU	7.4
51	A23S	1090	U	7.4
7	AL11	94	GLU	7.3
51	A23S	1081	U	7.3
51	A23S	2125	G	7.3
51	B23S	1076	C	7.3
51	B23S	1078	U	7.2
7	BL11	3	LYS	7.2
36	BS09	7	THR	7.2
34	BS07	81	GLY	7.1
4	BL05	48	GLU	7.1
26	AL33	30	THR	7.1
36	AS09	47	LEU	7.1
7	AL11	30	HIS	7.1
7	AL11	71	THR	7.1
51	A23S	1075	C	7.1
46	BS19	81	ARG	7.1
7	AL11	131	ALA	7.1
7	BL11	64	SER	7.0
46	AS19	81	ARG	7.0
37	AS10	67	THR	7.0
51	A23S	2165	G	7.0
51	B23S	1093	G	6.9
26	BL33	31	PRO	6.9
36	AS09	32	ASP	6.9
7	AL11	18	THR	6.9
51	B23S	2147	G	6.9

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Mol	Chain	Res	Type	RSRZ
53	AIRE	6153	C	6.8
51	A23S	1079	C	6.8
26	BL33	52	VAL	6.8
7	BL11	97	GLY	6.8
7	BL11	82	ALA	6.8
51	B23S	2794(C)	C	6.8
7	AL11	70	LYS	6.7
7	BL11	146	ASP	6.7
40	AS13	116	THR	6.7
51	B23S	1089	G	6.7
7	BL11	30	HIS	6.7
34	AS07	20	ASP	6.7
37	AS10	72	VAL	6.7
49	BL31	45	GLY	6.7
51	A23S	2116	G	6.7
19	AL24	50	ARG	6.7
4	BL05	108	ASN	6.7
7	AL11	88	ALA	6.7
51	A23S	1076	C	6.6
5	AL06	159	GLU	6.6
7	BL11	129	GLY	6.6
7	AL11	23	VAL	6.6
51	B23S	1079	C	6.6
7	AL11	33	ASN	6.6
26	AL33	28	ARG	6.6
53	AIRE	6176	C	6.5
51	A23S	2121	G	6.5
51	A23S	2123	G	6.5
53	AIRE	6152	G	6.5
50	B16S	201(C)	U	6.5
36	AS09	14	VAL	6.5
19	AL24	51	VAL	6.5
19	AL24	53	PRO	6.5
49	BL31	44	CYS	6.4
51	A23S	2145	C	6.4
46	BS19	59	PRO	6.4
37	BS10	73	ASP	6.4
7	BL11	139	VAL	6.4
26	BL33	14	THR	6.3
19	BL24	50	ARG	6.3
7	AL11	135	GLY	6.3
4	BL05	177	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
51	B23S	1083	U	6.3
4	AL05	88	ILE	6.3
13	AL18	58	LEU	6.3
19	BL24	53	PRO	6.3
46	AS19	52	TYR	6.3
7	BL11	85	GLU	6.3
50	A16S	1028(E)	G	6.2
36	AS09	81	ILE	6.2
26	AL33	43	CYS	6.2
7	BL11	98	ARG	6.2
36	AS09	8	GLY	6.2
7	AL11	75	SER	6.2
51	B23S	1077	A	6.2
4	BL05	176	LEU	6.1
46	AS19	78	ARG	6.1
7	BL11	114	ASP	6.1
4	BL05	137	GLU	6.1
40	AS13	113	PRO	6.1
37	BS10	72	VAL	6.0
32	AS05	29	GLY	6.0
34	AS07	12	LEU	6.0
50	B16S	1028(E)	G	6.0
46	AS19	35	SER	6.0
7	BL11	12	LEU	6.0
7	BL11	96	VAL	5.9
26	AL33	48	VAL	5.9
51	A23S	1046	A	5.9
26	AL33	34	LEU	5.9
51	A23S	1074	G	5.9
37	BS10	71	LEU	5.9
51	A23S	2147	G	5.9
7	AL11	51	ALA	5.9
26	AL33	31	PRO	5.9
51	A23S	2152	G	5.9
51	A23S	2155	G	5.9
7	BL11	67	PHE	5.8
26	BL33	20	ASN	5.8
37	AS10	6	ILE	5.8
4	BL05	73	ALA	5.8
7	AL11	34	ILE	5.8
46	AS19	69	HIS	5.8
51	A23S	2110	G	5.8

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Mol	Chain	Res	Type	RSRZ
51	A23S	2174	C	5.8
51	A23S	2794(C)	C	5.8
51	B23S	1092	C	5.8
7	BL11	93	ARG	5.8
47	BS20	85	MET	5.7
26	AL33	19	ARG	5.7
49	BL31	46	ASN	5.7
31	BS04	108	LEU	5.6
50	A16S	68(K)	U	5.6
7	AL11	130	SER	5.6
34	BS07	79	ARG	5.6
6	AL09	80	PRO	5.6
7	AL11	78	ILE	5.6
7	AL11	102	GLU	5.6
51	B23S	2117	A	5.6
51	A23S	2124	G	5.6
36	AS09	64	THR	5.6
7	BL11	16	LYS	5.6
46	AS19	53	ASN	5.6
29	BS02	132	LYS	5.6
7	AL11	127	ILE	5.5
37	AS10	71	LEU	5.5
7	BL11	32	ALA	5.5
51	B23S	2124	G	5.5
51	A23S	2138	C	5.5
7	BL11	71	THR	5.5
46	AS19	71	LEU	5.5
7	BL11	58	THR	5.5
26	BL33	29	ASN	5.5
7	AL11	8	VAL	5.5
37	AS10	68	HIS	5.5
7	AL11	69	THR	5.5
2	AL03	204	ALA	5.5
29	BS02	96	ARG	5.4
37	AS10	69	ASN	5.4
10	BL15	122	PRO	5.4
4	BL05	157	ILE	5.4
50	B16S	1257	U	5.4
7	BL11	113	PRO	5.4
26	BL33	25	LYS	5.4
43	BS16	22	THR	5.4
4	AL05	2	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
5	AL06	155	SER	5.4
34	BS07	83	ALA	5.4
37	AS10	99	LYS	5.4
51	B23S	2115	G	5.4
38	AS11	109	VAL	5.4
7	AL11	66	THR	5.4
51	B23S	2167	U	5.4
6	BL09	100	ALA	5.3
34	BS07	16	LEU	5.3
46	AS19	77	THR	5.3
50	A16S	1492	A	5.3
37	AS10	65	LEU	5.3
46	AS19	70	LYS	5.3
36	BS09	105	ASP	5.3
51	A23S	2127	G	5.3
51	A23S	2166	G	5.3
26	AL33	9	LEU	5.3
5	AL06	168	PRO	5.3
40	AS13	98	VAL	5.3
13	AL18	52	SER	5.3
43	BS16	34	GLU	5.3
7	BL11	57	ILE	5.3
53	AIRE	6188	C	5.3
7	BL11	127	ILE	5.3
40	BS13	40	ASN	5.2
7	BL11	77	LEU	5.2
7	AL11	63	ARG	5.2
11	AL16	135	ASP	5.2
7	AL11	74	ALA	5.2
23	BL29	16	LEU	5.2
5	AL06	100	GLY	5.2
50	A16S	68(J)	G	5.2
51	A23S	2151	G	5.2
51	A23S	2154	G	5.2
7	BL11	83	GLY	5.2
29	BS02	101	MET	5.2
34	AS07	104	LEU	5.2
40	AS13	117	VAL	5.2
37	AS10	100	THR	5.2
37	AS10	64	GLU	5.1
10	AL15	150	ALA	5.1
7	BL11	88	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
46	AS19	76	PRO	5.1
4	AL05	43	LEU	5.1
7	BL11	81	ALA	5.1
36	AS09	9	ARG	5.1
10	BL15	119	GLU	5.1
23	BL29	15	LYS	5.1
51	A23S	1088	A	5.1
51	A23S	2794(B)	U	5.1
40	AS13	3	ARG	5.1
50	A16S	68(M)	U	5.1
51	A23S	2132	U	5.1
51	B23S	2122	U	5.1
7	BL11	14	ALA	5.1
7	BL11	121	GLU	5.0
40	AS13	103	THR	5.0
51	B23S	2148	G	5.0
40	AS13	30	ALA	5.0
7	AL11	44	ALA	5.0
51	B23S	2114	A	5.0
4	BL05	87	PRO	5.0
53	AIRE	6193	C	5.0
7	BL11	100	THR	5.0
7	AL11	7	VAL	5.0
7	AL11	109	LYS	5.0
26	BL33	36	LEU	4.9
7	BL11	47	ASN	4.9
4	AL05	90	LEU	4.9
46	BS19	71	LEU	4.9
51	B23S	2402	C	4.9
7	AL11	79	ARG	4.9
7	AL11	132	ARG	4.9
51	A23S	2140	C	4.9
7	BL11	111	LYS	4.9
7	BL11	6	ALA	4.9
6	AL09	116	LEU	4.9
24	AL30	28	LEU	4.9
29	BS02	128	GLU	4.9
43	BS16	36	ILE	4.9
40	BS13	98	VAL	4.9
19	BL24	59	GLY	4.9
4	BL05	72	ARG	4.9
5	AL06	101	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
36	AS09	65	VAL	4.8
39	AS12	72	GLU	4.8
5	AL06	89	ILE	4.8
50	B16S	1028(C)	G	4.8
50	B16S	68(M)	U	4.8
26	BL33	28	ARG	4.8
34	AS07	15	ASP	4.8
10	AL15	110	TYR	4.8
7	AL11	61	ALA	4.8
26	AL33	15	GLU	4.8
41	BS14	2	ALA	4.8
51	A23S	2163	C	4.8
4	AL05	41	GLN	4.8
7	AL11	138	VAL	4.8
37	BS10	35	SER	4.8
50	A16S	1257	U	4.8
13	AL18	41	ASP	4.8
7	BL11	72	PRO	4.8
36	BS09	65	VAL	4.8
49	AL31	54	LYS	4.8
29	AS02	19	HIS	4.7
51	A23S	1100	C	4.7
19	AL24	86	ARG	4.7
26	BL33	32	ASN	4.7
13	AL18	35	ILE	4.7
5	AL06	104	GLU	4.7
7	BL11	70	LYS	4.7
26	BL33	42	TRP	4.7
26	BL33	13	CYS	4.7
46	BS19	48	THR	4.7
46	AS19	40	ILE	4.7
7	AL11	104	VAL	4.7
5	AL06	162	ILE	4.7
7	BL11	90	LYS	4.7
26	BL33	34	LEU	4.7
51	A23S	2173	A	4.7
24	AL30	2	PRO	4.7
6	AL09	91	SER	4.7
51	B23S	1090	U	4.7
46	AS19	36	ARG	4.7
7	AL11	134	MET	4.7
5	AL06	90	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
50	B16S	380	G	4.7
51	A23S	1091	G	4.6
7	BL11	35	MET	4.6
36	AS09	29	ASN	4.6
26	BL33	30	THR	4.6
37	AS10	28	ARG	4.6
53	AIRE	6151	C	4.6
6	AL09	36	ALA	4.6
51	B23S	2121	G	4.6
38	BS11	11	LYS	4.6
51	B23S	1173	A	4.6
51	B23S	2107	C	4.6
7	AL11	105	LEU	4.6
7	AL11	144	VAL	4.6
13	AL18	57	LYS	4.6
34	AS07	11	GLN	4.6
41	AS14	56	VAL	4.6
7	BL11	141	ALA	4.6
37	BS10	70	ARG	4.6
53	BIRE	6188	C	4.6
48	BTHX	5	ASP	4.6
51	A23S	2159	G	4.6
7	BL11	56	GLU	4.6
4	AL05	155	MET	4.6
47	BS20	9	ASN	4.6
37	AS10	5	ARG	4.5
7	BL11	63	ARG	4.5
4	BL05	46	ALA	4.5
23	BL29	12	GLU	4.5
51	A23S	2141	G	4.5
34	BS07	78	ARG	4.5
7	AL11	31	GLY	4.5
51	A23S	2158	A	4.5
20	AL25	159	PRO	4.5
50	A16S	68(N)	U	4.5
38	BS11	12	ARG	4.5
43	BS16	21	VAL	4.5
51	A23S	2144	U	4.5
37	BS10	6	ILE	4.5
7	AL11	10	LEU	4.5
20	BL25	163	LEU	4.5
34	AS07	88	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
38	BS11	13	GLN	4.5
51	A23S	2153	G	4.5
51	A23S	2122	U	4.5
13	AL18	37	ALA	4.5
51	B23S	2168	G	4.5
7	BL11	87	GLY	4.4
14	BL19	136	GLN	4.4
7	BL11	123	ALA	4.4
26	AL33	44	ARG	4.4
4	BL05	51	ARG	4.4
46	AS19	49	ILE	4.4
36	AS09	77	ILE	4.4
46	AS19	79	THR	4.4
40	AS13	100	GLY	4.4
31	BS04	70	ILE	4.4
46	BS19	5	LEU	4.4
40	AS13	115	LYS	4.4
7	BL11	131	ALA	4.4
34	AS07	18	TYR	4.4
7	AL11	77	LEU	4.4
5	AL06	112	PRO	4.4
51	B23S	1072	C	4.4
7	AL11	73	PRO	4.4
37	BS10	5	ARG	4.4
51	B23S	888	C	4.4
5	AL06	160	LYS	4.4
26	AL33	18	ARG	4.4
36	BS09	47	LEU	4.4
11	BL16	91	GLU	4.3
36	AS09	13	ALA	4.3
7	AL11	59	ILE	4.3
7	BL11	99	ILE	4.3
40	AS13	29	ARG	4.3
51	B23S	2166	G	4.3
14	AL19	2	ASN	4.3
51	B23S	2165	G	4.3
41	BS14	54	PRO	4.3
4	BL05	131	TYR	4.3
7	BL11	137	GLU	4.3
37	AS10	27	ALA	4.3
51	B23S	2794(B)	U	4.3
29	AS02	36	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
7	BL11	138	VAL	4.3
7	AL11	11	GLN	4.3
46	BS19	41	VAL	4.3
41	AS14	57	ARG	4.3
46	AS19	33	THR	4.3
13	AL18	87	PHE	4.3
41	BS14	14	PRO	4.3
5	AL06	98	LEU	4.3
26	AL33	33	LYS	4.3
46	AS19	80	TYR	4.3
29	BS02	125	PRO	4.3
46	AS19	67	VAL	4.3
26	BL33	17	LYS	4.3
36	AS09	44	VAL	4.3
51	A23S	2161	C	4.3
6	AL09	111	PRO	4.3
40	BS13	25	ILE	4.3
51	B23S	1091	G	4.2
51	A23S	1173	A	4.2
11	AL16	91	GLU	4.2
13	AL18	39	ILE	4.2
4	AL05	109	VAL	4.2
34	AS07	80	VAL	4.2
5	AL06	154	PRO	4.2
51	A23S	1082	U	4.2
51	A23S	2135	A	4.2
7	BL11	95	LYS	4.2
46	BS19	61	TYR	4.2
29	BS02	227	GLY	4.2
7	AL11	6	ALA	4.2
40	AS13	101	GLN	4.2
50	A16S	994	A	4.2
51	A23S	2128	C	4.2
51	A23S	2168	G	4.2
51	B23S	2141	G	4.2
7	AL11	14	ALA	4.2
37	AS10	61	GLU	4.2
7	BL11	48	MET	4.2
4	BL05	41	GLN	4.2
23	AL29	15	LYS	4.2
47	BS20	50	GLU	4.2
5	AL06	24	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
41	AS14	14	PRO	4.2
37	AS10	70	ARG	4.2
34	BS07	84	ASN	4.2
39	BS12	94	GLY	4.2
7	AL11	103	GLN	4.1
34	AS07	125	MET	4.1
51	A23S	2136	C	4.1
4	AL05	152	LEU	4.1
51	A23S	2176	A	4.1
7	AL11	106	GLU	4.1
51	A23S	2167	U	4.1
21	BL27	85	ALA	4.1
23	AL29	12	GLU	4.1
51	A23S	2794(D)	A	4.1
36	AS09	51	ARG	4.1
7	AL11	1	MET	4.1
43	BS16	35	LYS	4.1
7	AL11	128	ALA	4.1
13	AL18	51	ALA	4.1
37	AS10	20	ALA	4.1
19	AL24	2	ARG	4.1
5	AL06	80	SER	4.1
38	AS11	119	CYS	4.1
4	AL05	34	LEU	4.1
5	AL06	103	LEU	4.1
7	AL11	91	PRO	4.1
50	A16S	1226	C	4.1
5	AL06	29	PRO	4.1
10	AL15	149	GLU	4.1
19	BL24	2	ARG	4.1
29	BS02	228	GLY	4.1
40	AS13	92	HIS	4.1
7	BL11	84	LEU	4.1
7	BL11	62	ASP	4.1
46	BS19	40	ILE	4.1
51	A23S	2162	G	4.1
49	AL31	51	TYR	4.1
6	AL09	143	SER	4.1
23	BL29	9	GLN	4.1
7	BL11	147	ALA	4.0
51	A23S	2160	G	4.0
51	B23S	2123	G	4.0

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Mol	Chain	Res	Type	RSRZ
40	AS13	93	ARG	4.0
7	BL11	19	PRO	4.0
45	AS18	88	LYS	4.0
43	BS16	23	ASP	4.0
51	B23S	2793	G	4.0
36	BS09	9	ARG	4.0
36	BS09	36	TYR	4.0
30	BS03	151	VAL	4.0
35	BS08	132	GLU	4.0
51	A23S	2120	G	4.0
7	AL11	81	ALA	4.0
25	AL32	48	GLU	4.0
13	AL18	36	TYR	4.0
40	AS13	114	ARG	4.0
7	AL11	100	THR	4.0
5	AL06	51	ARG	4.0
51	A23S	2175	C	4.0
5	AL06	48	GLY	4.0
20	AL25	165	VAL	4.0
51	A23S	2119	A	4.0
24	AL30	29	ARG	4.0
49	BL31	41	ILE	4.0
7	AL11	21	PRO	3.9
13	AL18	28	VAL	3.9
51	A23S	2126	A	3.9
5	BL06	170	ARG	3.9
6	AL09	85	GLU	3.9
42	BS15	31	LEU	3.9
51	A23S	1066	U	3.9
20	AL25	95	PRO	3.9
51	B23S	1084	A	3.9
51	B23S	2805	G	3.9
32	BS05	155	GLU	3.9
40	BS13	116	THR	3.9
50	B16S	1362(A)	C	3.9
13	BL18	59	LYS	3.9
5	AL06	53	GLU	3.9
7	BL11	68	VAL	3.9
7	BL11	144	VAL	3.9
19	BL24	17	SER	3.9
34	AS07	16	LEU	3.9
4	AL05	131	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
51	B23S	2146	C	3.9
5	BL06	61	HIS	3.9
40	AS13	94	ARG	3.9
7	AL11	28	GLY	3.9
37	BS10	33	GLN	3.9
51	B23S	1080	C	3.9
7	AL11	54	PRO	3.9
40	BS13	15	VAL	3.9
20	AL25	98	MET	3.9
20	BL25	162	GLU	3.8
7	AL11	24	GLY	3.8
29	BS02	97	TRP	3.8
51	B23S	2139	C	3.8
51	B23S	2177	C	3.8
51	A23S	2171	A	3.8
51	B23S	2119	A	3.8
36	BS09	81	ILE	3.8
37	AS10	8	LEU	3.8
43	AS16	83	GLU	3.8
45	AS18	76	LEU	3.8
6	AL09	78	THR	3.8
48	BTHX	2	GLY	3.8
26	BL33	16	CYS	3.8
4	BL05	34	LEU	3.8
50	A16S	999	U	3.8
51	A23S	2164	C	3.8
7	BL11	142	PRO	3.8
34	AS07	2	ALA	3.8
34	BS07	20	ASP	3.8
6	AL09	123	LEU	3.8
26	AL33	17	LYS	3.8
37	BS10	99	LYS	3.8
47	AS20	81	LYS	3.8
4	AL05	89	GLY	3.8
25	BL32	2	ALA	3.8
17	BL22	108	GLY	3.8
7	AL11	13	PRO	3.8
4	BL05	2	PRO	3.8
37	AS10	33	GLN	3.8
47	BS20	51	GLU	3.8
7	BL11	15	GLY	3.7
51	A23S	508	G	3.7

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Mol	Chain	Res	Type	RSRZ
36	AS09	33	PHE	3.7
51	B23S	1067	A	3.7
51	B23S	2169	A	3.7
4	AL05	101	ILE	3.7
51	A23S	2156	G	3.7
7	BL11	61	ALA	3.7
47	BS20	104	LEU	3.7
51	A23S	2108	C	3.7
7	AL11	17	ALA	3.7
34	AS07	17	VAL	3.7
30	AS03	10	PHE	3.7
50	B16S	68(J)	G	3.7
4	AL05	62	LEU	3.7
5	AL06	170	ARG	3.7
20	AL25	126	VAL	3.7
35	BS08	61	VAL	3.7
10	AL15	148	LEU	3.7
51	B23S	2118	U	3.7
7	AL11	108	ALA	3.7
7	BL11	86	LYS	3.7
7	AL11	68	VAL	3.7
37	BS10	98	ILE	3.7
51	A23S	1099	G	3.7
51	A23S	2157	G	3.7
29	AS02	48	MET	3.7
34	AS07	79	ARG	3.7
50	B16S	1248	A	3.7
26	BL33	39	TYR	3.6
47	BS20	100	ILE	3.6
46	BS19	76	PRO	3.6
19	AL24	87	LYS	3.6
36	AS09	34	ASN	3.6
46	BS19	39	THR	3.6
13	BL18	52	SER	3.6
20	BL25	88	PHE	3.6
4	BL05	107	LEU	3.6
16	AL21	36	PRO	3.6
37	AS10	98	ILE	3.6
51	A23S	2112	G	3.6
40	AS13	108	ARG	3.6
33	AS06	90	VAL	3.6
34	BS07	101	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
40	BS13	42	ALA	3.6
4	AL05	97	ASP	3.6
7	AL11	50	ASP	3.6
51	A23S	2115	G	3.6
30	BS03	168	ALA	3.6
2	AL03	186	GLY	3.6
7	AL11	64	SER	3.6
7	BL11	55	VAL	3.6
50	B16S	201(A)	U	3.6
50	B16S	838(C)	U	3.6
37	AS10	29	ARG	3.6
40	AS13	4	ILE	3.6
26	BL33	46	HIS	3.6
51	B23S	2803	C	3.6
4	BL05	134	GLY	3.6
20	AL25	186	GLU	3.6
7	BL11	52	ILE	3.6
31	BS04	134	ASP	3.6
43	AS16	68	ASP	3.6
6	BL09	123	LEU	3.6
6	AL09	100	ALA	3.6
6	AL09	20	ASP	3.6
4	AL05	17	PRO	3.5
26	BL33	38	LYS	3.5
51	B23S	1074	G	3.5
34	BS07	17	VAL	3.5
7	AL11	16	LYS	3.5
7	BL11	20	ALA	3.5
20	AL25	189	ALA	3.5
43	AS16	51	VAL	3.5
51	A23S	1058	G	3.5
33	BS06	101	ALA	3.5
43	BS16	19	ILE	3.5
24	AL30	34	GLU	3.5
4	AL05	70	VAL	3.5
4	AL05	142	PRO	3.5
19	BL24	22	GLY	3.5
50	A16S	1287	A	3.5
50	B16S	958	A	3.5
51	A23S	271(M)	G	3.5
41	AS14	2	ALA	3.5
46	BS19	38	SER	3.5

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Mol	Chain	Res	Type	RSRZ
5	AL06	106	THR	3.5
21	BL27	75	LEU	3.5
10	BL15	94	GLU	3.5
5	AL06	141	VAL	3.5
7	BL11	76	TYR	3.5
37	BS10	95	GLU	3.5
43	BS16	39	TYR	3.5
50	B16S	1252	A	3.5
6	AL09	92	VAL	3.5
42	AS15	2	PRO	3.5
43	BS16	2	VAL	3.5
4	AL05	122	PRO	3.5
4	BL05	49	ASP	3.5
36	AS09	63	ILE	3.5
43	BS16	37	GLY	3.5
50	B16S	1249	C	3.5
46	AS19	39	THR	3.5
4	AL05	157	ILE	3.5
51	A23S	2100	G	3.5
4	BL05	39	ILE	3.5
33	AS06	89	MET	3.5
5	AL06	81	GLU	3.5
11	BL16	90	VAL	3.5
36	BS09	37	PHE	3.5
46	AS19	9	VAL	3.5
7	AL11	99	ILE	3.5
20	AL25	99	TYR	3.5
30	AS03	201	TYR	3.5
36	AS09	71	SER	3.5
26	AL33	42	TRP	3.4
7	BL11	110	GLN	3.4
46	AS19	51	VAL	3.4
13	AL18	97	ARG	3.4
36	AS09	66	ARG	3.4
51	B23S	2152	G	3.4
4	BL05	161	THR	3.4
5	AL06	145	ALA	3.4
43	BS16	3	LYS	3.4
36	AS09	17	VAL	3.4
6	AL09	84	GLY	3.4
40	BS13	100	GLY	3.4
6	BL09	4	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
51	A23S	2793	G	3.4
37	AS10	21	GLN	3.4
37	BS10	30	SER	3.4
4	BL05	21	ARG	3.4
41	AS14	55	GLY	3.4
13	AL18	72	ALA	3.4
43	AS16	48	TRP	3.4
7	BL11	13	PRO	3.4
7	BL11	89	HIS	3.4
47	AS20	64	ASP	3.4
37	BS10	69	ASN	3.4
34	AS07	101	LEU	3.4
50	A16S	1531	A	3.4
51	B23S	1088	A	3.4
6	AL09	120	ILE	3.4
21	BL27	78	TYR	3.4
40	BS13	4	ILE	3.4
50	A16S	744	C	3.4
53	AIRE	6175	G	3.4
36	AS09	101	PHE	3.4
51	B23S	2794(D)	A	3.4
7	BL11	79	ARG	3.4
4	BL05	142	PRO	3.4
34	AS07	34	GLY	3.4
46	BS19	32	LYS	3.4
46	AS19	50	ALA	3.4
50	B16S	1286	A	3.4
37	AS10	66	ARG	3.4
7	AL11	147	ALA	3.3
4	BL05	136	ARG	3.3
29	BS02	165	VAL	3.3
37	AS10	40	LEU	3.3
21	BL27	76	GLY	3.3
26	BL33	27	LYS	3.3
5	AL06	43	VAL	3.3
7	BL11	102	GLU	3.3
49	BL31	43	GLY	3.3
40	AS13	19	LEU	3.3
4	BL05	86	MET	3.3
7	BL11	49	GLY	3.3
33	AS06	63	TYR	3.3
29	AS02	95	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
43	BS16	54	GLU	3.3
36	BS09	94	ALA	3.3
7	AL11	2	LYS	3.3
50	A16S	958	A	3.3
5	AL06	97	ARG	3.3
12	BL17	112	ALA	3.3
49	BL31	47	VAL	3.3
7	AL11	101	TRP	3.3
40	AS13	64	TRP	3.3
7	AL11	146	ASP	3.3
36	AS09	62	TYR	3.3
36	BS09	15	ALA	3.3
4	BL05	174	GLU	3.3
7	BL11	54	PRO	3.3
7	AL11	82	ALA	3.3
34	BS07	85	TYR	3.3
26	AL33	10	LEU	3.3
2	BL03	88	GLY	3.3
4	BL05	146	TYR	3.3
24	AL30	39	ASP	3.3
7	AL11	46	ALA	3.3
7	AL11	53	VAL	3.3
37	AS10	63	PHE	3.3
31	BS04	169	LYS	3.3
31	BS04	184	LYS	3.3
40	AS13	102	ARG	3.3
50	B16S	1253	G	3.3
36	BS09	43	ALA	3.3
41	AS14	60	SER	3.3
11	BL16	105	GLU	3.3
4	AL05	68	PRO	3.3
40	BS13	58	GLU	3.3
40	BS13	103	THR	3.3
50	B16S	1254	C	3.3
7	BL11	50	ASP	3.3
37	AS10	38	ILE	3.3
5	AL06	47	GLU	3.3
35	AS08	1	MET	3.3
46	BS19	4	SER	3.3
5	AL06	52	VAL	3.3
51	A23S	2794(E)	A	3.3
53	AIRE	6174	U	3.3

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Mol	Chain	Res	Type	RSRZ
3	AL04	167	ALA	3.3
6	AL09	128	LEU	3.3
49	AL31	43	GLY	3.3
51	A23S	2131	G	3.3
35	BS08	92	ARG	3.2
41	AS14	12	ARG	3.2
4	AL05	23	PHE	3.2
46	BS19	60	VAL	3.2
51	A23S	1102	C	3.2
51	B23S	2175	C	3.2
10	BL15	89	ALA	3.2
4	AL05	52	ILE	3.2
50	A16S	1000	A	3.2
29	AS02	101	MET	3.2
29	AS02	122	PHE	3.2
46	AS19	73	GLU	3.2
4	AL05	100	TRP	3.2
39	BS12	27	LYS	3.2
20	AL25	43	GLU	3.2
34	BS07	37	ASN	3.2
37	BS10	8	LEU	3.2
51	A23S	2169	A	3.2
16	BL21	53	GLU	3.2
11	BL16	89	ASN	3.2
37	BS10	76	ASN	3.2
12	BL17	118	GLU	3.2
37	BS10	94	VAL	3.2
46	AS19	59	PRO	3.2
30	BS03	59	ARG	3.2
20	BL25	27	VAL	3.2
5	AL06	148	ILE	3.2
37	BS10	4	ILE	3.2
36	AS09	82	ALA	3.2
4	AL05	58	GLN	3.2
29	BS02	98	LEU	3.2
36	AS09	21	PRO	3.2
10	BL15	118	GLY	3.2
4	AL05	143	GLU	3.2
40	BS13	111	LYS	3.2
4	BL05	135	LEU	3.2
7	AL11	56	GLU	3.2
4	AL05	179	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
43	BS16	53	VAL	3.2
31	BS04	5	ILE	3.2
7	AL11	42	ASN	3.2
4	BL05	37	VAL	3.2
5	AL06	88	LEU	3.2
6	AL09	71	ILE	3.2
37	AS10	62	HIS	3.2
47	BS20	84	LEU	3.2
51	B23S	271(M)	G	3.2
40	BS13	16	ASP	3.2
20	AL25	28	MET	3.2
29	BS02	102	LEU	3.2
34	AS07	19	GLY	3.2
38	AS11	108	ILE	3.2
7	AL11	125	ARG	3.1
20	AL25	166	SER	3.1
50	A16S	1225	A	3.1
51	A23S	2792	G	3.1
51	B23S	2156	G	3.1
4	AL05	113	ARG	3.1
31	BS04	101	LEU	3.1
46	BS19	49	ILE	3.1
50	B16S	201(B)	U	3.1
5	AL06	129	THR	3.1
6	AL09	82	ARG	3.1
7	AL11	118	THR	3.1
7	AL11	22	PRO	3.1
50	B16S	1243	C	3.1
5	AL06	114	VAL	3.1
6	AL09	145	VAL	3.1
47	BS20	88	VAL	3.1
7	AL11	141	ALA	3.1
34	AS07	85	TYR	3.1
37	BS10	67	THR	3.1
7	AL11	140	GLY	3.1
3	BL04	156	LEU	3.1
46	BS19	75	ALA	3.1
6	AL09	10	GLU	3.1
7	AL11	133	SER	3.1
19	AL24	79	CYS	3.1
48	BTHX	24	ARG	3.1
14	BL19	2	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
40	AS13	106	ASN	3.1
29	BS02	142	LEU	3.1
30	AS03	170	GLN	3.1
32	BS05	5	ASP	3.1
23	AL29	4	SER	3.1
51	B23S	508	G	3.1
30	AS03	151	VAL	3.1
20	AL25	167	PRO	3.1
45	BS18	31	LEU	3.1
47	BS20	48	LYS	3.1
49	AL31	37	PRO	3.1
5	AL06	169	VAL	3.1
37	AS10	17	ASP	3.1
51	A23S	2107	C	3.1
40	AS13	67	GLU	3.1
4	BL05	178	PHE	3.1
6	AL09	4	ILE	3.1
7	BL11	108	ALA	3.1
41	AS14	30	ALA	3.1
4	AL05	92	VAL	3.1
12	AL17	82	GLU	3.1
51	A23S	2113	U	3.1
51	B23S	1065	U	3.1
51	B23S	2132	U	3.1
7	BL11	136	VAL	3.1
5	AL06	124	GLU	3.1
51	A23S	1085	A	3.1
37	AS10	34	VAL	3.1
8	BL13	31	GLN	3.1
34	AS07	61	VAL	3.1
36	BS09	5	TYR	3.1
11	AL16	139	GLU	3.1
36	BS09	64	THR	3.1
6	AL09	96	ASP	3.0
13	BL18	37	ALA	3.0
29	BS02	135	GLN	3.0
41	AS14	10	ALA	3.0
36	AS09	18	PHE	3.0
17	BL22	112	GLY	3.0
20	AL25	171	ILE	3.0
40	BS13	22	ILE	3.0
46	AS19	32	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
51	A23S	2137	C	3.0
7	BL11	27	LEU	3.0
37	AS10	41	PRO	3.0
40	BS13	69	GLU	3.0
50	A16S	1363	A	3.0
50	B16S	1492	A	3.0
4	BL05	133	LEU	3.0
51	A23S	2894	G	3.0
51	B23S	2149	G	3.0
7	AL11	92	GLY	3.0
40	AS13	61	GLU	3.0
40	BS13	117	VAL	3.0
41	BS14	12	ARG	3.0
5	BL06	100	GLY	3.0
7	BL11	51	ALA	3.0
13	AL18	53	SER	3.0
13	AL18	60	GLY	3.0
19	AL24	43	ASN	3.0
40	AS13	69	GLU	3.0
50	B16S	1226	C	3.0
10	BL15	148	LEU	3.0
13	BL18	61	ASN	3.0
8	AL13	118	PRO	3.0
43	AS16	7	ALA	3.0
4	AL05	13	GLU	3.0
40	BS13	65	LYS	3.0
45	AS18	87	ARG	3.0
43	AS16	53	VAL	3.0
19	BL24	14	LEU	3.0
51	A23S	1067	A	3.0
30	AS03	57	ILE	3.0
6	BL09	82	ARG	3.0
9	BL14	15	GLY	3.0
4	AL05	77	ILE	3.0
20	AL25	96	VAL	3.0
51	A23S	2109	U	3.0
51	B23S	1066	U	3.0
41	BS14	8	GLU	3.0
14	AL19	106	SER	3.0
7	AL11	129	GLY	3.0
37	BS10	96	ILE	3.0
14	AL19	39	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
7	AL11	96	VAL	3.0
26	BL33	35	GLU	3.0
35	AS08	132	GLU	3.0
51	A23S	2402	C	3.0
51	B23S	2108	C	3.0
39	BS12	31	PHE	3.0
7	AL11	5	VAL	3.0
40	BS13	5	ALA	3.0
46	BS19	46	GLY	3.0
29	AS02	119	GLU	3.0
46	BS19	78	ARG	3.0
41	BS14	56	VAL	2.9
35	BS08	46	LYS	2.9
50	B16S	68(A)	G	2.9
42	BS15	50	HIS	2.9
6	BL09	25	TYR	2.9
51	B23S	2137	C	2.9
46	BS19	50	ALA	2.9
36	BS09	98	PRO	2.9
34	BS07	9	VAL	2.9
1	BL02	167	GLY	2.9
50	A16S	723	U	2.9
13	AL18	68	GLN	2.9
7	AL11	90	LYS	2.9
6	BL09	103	ARG	2.9
7	BL11	126	MET	2.9
8	BL13	157	ARG	2.9
50	B16S	63	C	2.9
6	AL09	76	THR	2.9
35	BS08	62	TYR	2.9
8	AL13	95	TYR	2.9
4	BL05	69	ALA	2.9
20	AL25	91	LEU	2.9
14	AL19	1	MET	2.9
16	AL21	16	PRO	2.9
7	BL11	43	ALA	2.9
50	B16S	1028(F)	A	2.9
11	BL16	92	GLY	2.9
46	AS19	4	SER	2.9
51	B23S	2157	G	2.9
7	AL11	4	VAL	2.9
38	AS11	12	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
40	BS13	19	LEU	2.9
40	BS13	51	ALA	2.9
16	BL21	36	PRO	2.9
6	BL09	85	GLU	2.9
30	BS03	35	GLU	2.9
5	AL06	68	THR	2.9
47	BS20	8	ARG	2.9
37	AS10	39	PRO	2.9
45	AS18	62	GLU	2.9
35	AS08	94	TYR	2.9
36	BS09	93	ARG	2.9
41	BS14	52	GLN	2.9
6	AL09	83	ALA	2.9
35	AS08	111	ILE	2.9
51	B23S	2176	A	2.9
40	BS13	43	THR	2.9
49	AL31	53	THR	2.9
37	AS10	7	LYS	2.9
36	AS09	35	GLU	2.9
36	AS09	10	ARG	2.9
37	AS10	19	SER	2.9
14	BL19	6	LEU	2.9
21	AL27	12	ASN	2.9
7	AL11	15	GLY	2.8
7	AL11	45	THR	2.8
7	AL11	124	ALA	2.9
11	AL16	105	GLU	2.8
29	BS02	194	PRO	2.8
4	BL05	88	ILE	2.8
37	BS10	65	LEU	2.8
47	BS20	77	ALA	2.8
51	A23S	271(C)	U	2.8
37	BS10	97	GLU	2.8
47	BS20	57	ARG	2.8
4	AL05	133	LEU	2.8
51	A23S	2148	G	2.8
51	B23S	2142	C	2.8
53	AIRE	6173	G	2.8
4	AL05	69	ALA	2.8
7	AL11	26	ALA	2.8
7	AL11	49	GLY	2.8
13	BL18	51	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
24	AL30	56	VAL	2.8
50	A16S	1346	A	2.8
19	AL24	88	LYS	2.8
20	AL25	150	LEU	2.8
11	BL16	24	GLY	2.8
11	AL16	31	ASP	2.8
5	BL06	116	GLU	2.8
6	AL09	35	LEU	2.8
10	BL15	88	LEU	2.8
40	BS13	99	ARG	2.8
48	BTHX	7	ARG	2.8
7	BL11	36	GLU	2.8
51	A23S	2180	U	2.8
50	B16S	1355	G	2.8
7	BL11	33	ASN	2.8
46	AS19	42	PRO	2.8
4	AL05	145	THR	2.8
30	AS03	149	ALA	2.8
49	BL31	61	VAL	2.8
49	AL31	56	GLU	2.8
7	AL11	139	VAL	2.8
38	AS11	35	PRO	2.8
51	A23S	2129	C	2.8
44	AS17	8	GLY	2.8
13	BL18	53	SER	2.8
50	B16S	1002	G	2.8
12	AL17	81	ASP	2.8
34	AS07	14	PRO	2.8
36	BS09	101	PHE	2.8
31	BS04	105	VAL	2.8
51	A23S	405	U	2.8
30	BS03	3	ASN	2.8
47	BS20	99	LEU	2.8
51	B23S	2106	G	2.8
4	AL05	39	ILE	2.8
40	BS13	112	GLY	2.8
38	AS11	13	GLN	2.8
29	BS02	95	GLN	2.8
45	AS18	72	ARG	2.8
46	AS19	41	VAL	2.8
52	A5S	88	C	2.8
31	AS04	104	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
51	B23S	1913	A	2.8
20	BL25	69	THR	2.8
13	AL18	86	ALA	2.8
30	BS03	2	GLY	2.8
50	A16S	993	G	2.8
50	A16S	1028(C)	G	2.8
35	AS08	129	VAL	2.8
42	BS15	30	ALA	2.8
50	A16S	68(O)	A	2.8
32	AS05	14	ARG	2.7
39	AS12	70	PRO	2.7
46	BS19	31	ILE	2.7
4	BL05	85	GLY	2.7
7	BL11	104	VAL	2.7
13	BL18	58	LEU	2.7
30	BS03	149	ALA	2.7
47	BS20	96	GLY	2.7
5	AL06	152	ARG	2.7
12	AL17	63	ARG	2.7
1	AL02	30	GLU	2.7
36	BS09	19	LEU	2.7
51	A23S	645	C	2.7
51	A23S	2143	C	2.7
42	BS15	19	PRO	2.7
50	A16S	1028(F)	A	2.7
4	AL05	146	TYR	2.7
20	AL25	27	VAL	2.7
36	BS09	17	VAL	2.7
46	AS19	44	MET	2.7
4	AL05	137	GLU	2.7
51	B23S	2113	U	2.7
36	BS09	18	PHE	2.7
51	B23S	2794(A)	G	2.7
23	AL29	16	LEU	2.7
7	AL11	87	GLY	2.7
9	BL14	16	ALA	2.7
50	A16S	977	A	2.7
6	AL09	21	VAL	2.7
13	BL18	38	GLN	2.7
37	BS10	80	LYS	2.7
44	AS17	58	GLU	2.7
47	BS20	54	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
6	AL09	132	PRO	2.7
47	BS20	70	SER	2.7
34	BS07	8	GLU	2.7
51	A23S	2794(A)	G	2.7
34	BS07	155	ARG	2.7
29	AS02	165	VAL	2.7
4	AL05	46	ALA	2.7
4	AL05	171	ALA	2.7
5	AL06	96	ALA	2.7
10	BL15	92	GLU	2.7
40	BS13	21	TYR	2.7
7	BL11	42	ASN	2.7
30	AS03	204	LEU	2.7
4	BL05	159	VAL	2.7
20	AL25	47	VAL	2.7
11	AL16	33	GLY	2.7
47	BS20	81	LYS	2.7
31	BS04	11	LEU	2.7
12	AL17	49	ASP	2.7
31	BS04	138	TYR	2.7
43	BS16	68	ASP	2.7
51	B23S	2804	C	2.7
51	B23S	1073	A	2.7
36	AS09	61	ALA	2.7
5	AL06	69	ARG	2.6
10	BL15	130	PHE	2.7
30	AS03	11	ARG	2.6
19	AL24	64	GLU	2.6
50	B16S	68(Y)	C	2.6
5	AL06	17	VAL	2.6
6	BL09	11	ASN	2.6
51	B23S	2170	A	2.6
18	BL23	26	TYR	2.6
37	AS10	59	SER	2.6
37	BS10	100	THR	2.6
39	AS12	71	GLY	2.6
51	A23S	1063	G	2.6
51	A23S	2133	G	2.6
29	AS02	118	LEU	2.6
30	AS03	47	LEU	2.6
5	AL06	19	VAL	2.6
36	AS09	11	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
50	B16S	1025	U	2.6
50	B16S	754	C	2.6
29	BS02	193	ASP	2.6
35	AS08	24	THR	2.6
51	A23S	357(B)	A	2.6
51	B23S	2158	A	2.6
4	BL05	35	GLU	2.6
4	BL05	155	MET	2.6
35	AS08	133	LEU	2.6
37	AS10	45	ARG	2.6
43	BS16	24	ALA	2.6
50	A16S	1042	G	2.6
13	AL18	88	ASP	2.6
23	BL29	10	LEU	2.6
53	AIRE	6172	U	2.6
3	AL04	104	LYS	2.6
51	A23S	2790	A	2.6
33	AS06	59	TYR	2.6
37	BS10	87	THR	2.6
50	B16S	723	U	2.6
51	A23S	1535	U	2.6
6	BL09	128	LEU	2.6
7	AL11	29	GLN	2.6
37	AS10	44	VAL	2.6
50	A16S	1028	C	2.6
51	B23S	2896	C	2.6
29	BS02	170	GLU	2.6
37	AS10	73	ASP	2.6
11	AL16	32	PHE	2.6
31	AS04	5	ILE	2.6
51	A23S	6	A	2.6
4	BL05	109	VAL	2.6
13	BL18	68	GLN	2.6
16	BL21	49	THR	2.6
50	A16S	1359	C	2.6
47	BS20	58	LYS	2.6
5	AL06	57	ASP	2.6
14	BL19	1	MET	2.6
34	BS07	4	ARG	2.6
31	BS04	133	VAL	2.6
35	BS08	79	VAL	2.6
31	BS04	10	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
34	BS07	11	GLN	2.6
50	A16S	1224	G	2.6
51	B23S	2159	G	2.6
21	AL27	75	LEU	2.6
36	AS09	46	ALA	2.6
12	AL17	85	PRO	2.6
26	BL33	18	ARG	2.6
31	AS04	116	GLN	2.6
50	A16S	1150	U	2.6
51	B23S	1081	U	2.6
39	BS12	67	ALA	2.6
7	AL11	120	LEU	2.6
20	AL25	125	LEU	2.6
20	AL25	168	GLU	2.6
30	AS03	152	ILE	2.6
51	A23S	2805	G	2.6
47	AS20	68	LYS	2.6
20	AL25	132	ASN	2.6
3	BL04	155	LEU	2.6
43	AS16	54	GLU	2.6
6	BL09	3	VAL	2.6
12	AL17	66	VAL	2.6
4	AL05	72	ARG	2.6
4	AL05	172	LEU	2.6
30	AS03	56	ASP	2.6
6	AL09	86	THR	2.6
7	BL11	53	VAL	2.6
37	BS10	10	GLY	2.6
29	AS02	96	ARG	2.6
31	BS04	3	ARG	2.6
13	AL18	24	LEU	2.5
49	AL31	44	CYS	2.5
50	B16S	68(O)	A	2.5
51	A23S	2170	A	2.5
13	AL18	59	LYS	2.5
25	AL32	37	LYS	2.5
2	AL03	184	VAL	2.5
20	BL25	39	VAL	2.5
26	BL33	41	PRO	2.5
46	BS19	57	HIS	2.5
16	BL21	7	THR	2.5
34	AS07	108	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	AL05	182	LYS	2.5
14	AL19	36	GLU	2.5
51	A23S	2111	C	2.5
51	A23S	2896	C	2.5
5	BL06	48	GLY	2.5
6	BL09	35	LEU	2.5
5	AL06	144	VAL	2.5
20	AL25	169	GLU	2.5
19	AL24	59	GLY	2.5
34	BS07	156	TRP	2.5
46	BS19	42	PRO	2.5
19	AL24	47	LYS	2.5
7	BL11	143	GLU	2.5
13	BL18	49	VAL	2.5
51	B23S	2179	C	2.5
20	AL25	81	ARG	2.5
37	AS10	9	ARG	2.5
24	BL30	2	PRO	2.5
7	AL11	3	LYS	2.5
30	AS03	53	ALA	2.5
33	BS06	94	GLN	2.5
19	AL24	39	VAL	2.5
22	BL28	34	THR	2.5
34	BS07	61	VAL	2.5
2	AL03	182	LEU	2.5
6	BL09	104	GLN	2.5
46	BS19	47	HIS	2.5
13	AL18	71	ARG	2.5
7	AL11	145	LYS	2.5
15	AL20	73	GLY	2.5
34	BS07	48	LYS	2.5
50	A16S	1331	G	2.5
51	B23S	2318	G	2.5
37	BS10	39	PRO	2.5
13	BL18	28	VAL	2.5
4	AL05	156	ASP	2.5
46	AS19	55	LYS	2.5
50	A16S	1250	A	2.5
8	AL13	108	ILE	2.5
32	AS05	13	ILE	2.5
36	AS09	85	LEU	2.5
49	AL31	41	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
4	AL05	21	ARG	2.5
5	AL06	149	ARG	2.5
26	BL33	40	CYS	2.5
39	AS12	53	LYS	2.5
50	B16S	1026	G	2.5
5	AL06	151	ILE	2.5
24	AL30	6	VAL	2.5
5	BL06	47	GLU	2.5
7	AL11	48	MET	2.5
6	AL09	114	LEU	2.5
21	AL27	42	GLY	2.5
34	AS07	100	ALA	2.5
35	BS08	60	ARG	2.5
38	AS11	47	VAL	2.5
30	BS03	150	LYS	2.5
42	AS15	89	GLY	2.5
34	AS07	23	VAL	2.5
4	AL05	105	LYS	2.5
51	B23S	1064	C	2.5
20	AL25	66	SER	2.5
37	AS10	35	SER	2.5
43	BS16	17	TYR	2.5
46	AS19	10	PHE	2.5
44	BS17	22	LEU	2.5
4	BL05	55	LYS	2.5
13	BL18	19	LYS	2.5
30	AS03	67	THR	2.5
4	AL05	35	GLU	2.5
7	BL11	37	PHE	2.5
34	AS07	26	PHE	2.5
49	BL31	49	GLU	2.5
51	B23S	1068	G	2.5
46	AS19	68	GLY	2.5
51	B23S	2602	A	2.5
39	AS12	111	ASP	2.5
4	AL05	3	LEU	2.5
13	AL18	38	GLN	2.5
46	BS19	80	TYR	2.5
20	AL25	163	LEU	2.5
10	BL15	121	LYS	2.5
39	AS12	69	ILE	2.5
7	AL11	142	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
11	AL16	39	PRO	2.4
29	AS02	102	LEU	2.4
35	AS08	3	THR	2.4
48	BTHX	8	THR	2.4
19	AL24	3	VAL	2.4
22	AL28	30	VAL	2.4
24	BL30	10	LYS	2.4
29	BS02	139	LYS	2.4
34	BS07	23	VAL	2.4
24	BL30	30	ARG	2.4
29	AS02	111	ARG	2.4
36	BS09	73	GLN	2.4
40	BS13	115	LYS	2.4
43	BS16	1	MET	2.4
30	BS03	169	ALA	2.4
51	A23S	229	A	2.4
51	B23S	884	C	2.4
29	AS02	112	VAL	2.4
25	AL32	53	ALA	2.4
26	BL33	47	THR	2.4
7	AL11	143	GLU	2.4
31	BS04	182	LYS	2.4
36	BS09	102	LEU	2.4
20	AL25	140	ASP	2.4
30	AS03	183	ASP	2.4
37	AS10	23	ILE	2.4
47	BS20	64	ASP	2.4
50	B16S	110	C	2.4
51	B23S	229	A	2.4
51	B23S	2317	C	2.4
29	AS02	116	GLU	2.4
49	BL31	60	GLU	2.4
2	BL03	10	GLY	2.4
40	BS13	95	GLY	2.4
49	BL31	57	ILE	2.4
31	BS04	42	GLN	2.4
5	BL06	115	VAL	2.4
6	AL09	3	VAL	2.4
17	BL22	47	VAL	2.4
21	AL27	78	TYR	2.4
49	AL31	46	ASN	2.4
4	BL05	52	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
31	BS04	181	MET	2.4
45	AS18	77	GLY	2.4
53	BIRE	6193	C	2.4
31	AS04	110	PHE	2.4
4	BL05	97	ASP	2.4
5	AL06	164	TYR	2.4
37	BS10	78	ASN	2.4
38	AS11	14	VAL	2.4
2	BL03	56	PRO	2.4
7	BL11	26	ALA	2.4
50	B16S	1393	U	2.4
51	A23S	2172	U	2.4
24	AL30	40	THR	2.4
37	AS10	24	VAL	2.4
39	BS12	92	LEU	2.4
50	A16S	1260	C	2.4
50	B16S	1363	A	2.4
51	B23S	2140	C	2.4
36	AS09	80	GLY	2.4
50	B16S	1117	G	2.4
34	BS07	86	GLN	2.4
36	BS09	104	ARG	2.4
40	AS13	96	LEU	2.4
31	BS04	137	SER	2.4
35	BS08	109	ILE	2.4
44	BS17	17	LYS	2.4
39	AS12	98	HIS	2.4
40	AS13	97	PRO	2.4
50	B16S	1362	C	2.4
51	A23S	1073	A	2.4
51	B23S	2138	C	2.4
2	AL03	24	THR	2.4
11	AL16	103	MET	2.4
29	AS02	150	SER	2.4
36	BS09	69	GLY	2.4
42	BS15	49	ASP	2.4
5	AL06	25	LYS	2.4
5	AL06	95	ARG	2.4
36	AS09	84	ALA	2.4
17	AL22	20	VAL	2.4
31	BS04	140	VAL	2.4
51	B23S	1082	U	2.4

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Mol	Chain	Res	Type	RSRZ
51	B23S	2897	U	2.4
6	BL09	107	ILE	2.4
36	AS09	74	ILE	2.4
3	AL04	175	THR	2.4
7	BL11	44	ALA	2.4
36	BS09	106	ALA	2.4
40	AS13	12	ASN	2.4
4	BL05	80	PHE	2.4
7	AL11	98	ARG	2.4
31	BS04	109	GLY	2.4
47	AS20	65	LYS	2.4
25	BL32	53	ALA	2.4
46	AS19	38	SER	2.4
39	AS12	121	THR	2.4
41	AS14	13	THR	2.4
4	AL05	80	PHE	2.4
49	AL31	55	PRO	2.4
19	AL24	58	GLY	2.4
48	BTHX	4	GLY	2.4
24	AL30	42	ALA	2.4
33	AS06	40	VAL	2.4
34	AS07	103	TRP	2.4
37	AS10	83	GLU	2.4
39	AS12	124	PRO	2.4
2	BL03	186	GLY	2.4
7	AL11	12	LEU	2.4
18	BL23	86	GLY	2.4
36	AS09	50	LEU	2.4
10	BL15	137	LYS	2.4
15	AL20	91	ASP	2.4
50	B16S	1288	A	2.4
40	AS13	111	LYS	2.4
4	AL05	66	GLN	2.3
42	AS15	38	ARG	2.3
6	AL09	140	LEU	2.3
50	A16S	1235	U	2.3
37	BS10	26	ALA	2.3
19	BL24	47	LYS	2.3
51	B23S	1099	G	2.3
5	AL06	55	PRO	2.3
2	BL03	187	ALA	2.3
7	BL11	112	MET	2.3

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Mol	Chain	Res	Type	RSRZ
51	A23S	2602	A	2.3
51	B23S	2794	C	2.3
13	AL18	92	TYR	2.3
7	AL11	113	PRO	2.3
7	BL11	101	TRP	2.3
45	AS18	46	GLU	2.3
34	BS07	22	LEU	2.3
29	BS02	94	ASN	2.3
50	A16S	971	G	2.3
51	A23S	2117	A	2.3
7	AL11	38	VAL	2.3
8	AL13	87	GLY	2.3
20	AL25	93	ASP	2.3
6	AL09	115	ALA	2.3
51	A23S	1072	C	2.3
13	BL18	23	ARG	2.3
22	BL28	11	ARG	2.3
4	AL05	45	GLU	2.3
7	BL11	38	VAL	2.3
31	BS04	104	VAL	2.3
16	BL21	16	PRO	2.3
47	BS20	18	GLN	2.3
20	AL25	4	ARG	2.3
21	BL27	72	ARG	2.3
29	AS02	33	TYR	2.3
40	AS13	80	ARG	2.3
51	A23S	2319	G	2.3
51	A23S	1101	U	2.3
8	AL13	122	LEU	2.3
5	AL06	27	LYS	2.3
29	AS02	109	SER	2.3
37	AS10	30	SER	2.3
49	AL31	45	GLY	2.3
5	AL06	102	ALA	2.3
47	AS20	46	GLU	2.3
43	BS16	65	GLN	2.3
51	B23S	849	A	2.3
4	BL05	147	ASP	2.3
43	AS16	19	ILE	2.3
51	B23S	2155	G	2.3
4	AL05	82	LEU	2.3
8	AL13	75	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
8	BL13	33	GLU	2.3
28	AL35	35	GLN	2.3
22	AL28	85	LEU	2.3
34	AS07	45	ASP	2.3
34	AS07	129	GLU	2.3
43	BS16	73	LEU	2.3
34	BS07	62	PHE	2.3
51	B23S	2134	A	2.3
20	BL25	81	ARG	2.3
50	A16S	1241	G	2.3
29	BS02	163	PHE	2.3
29	AS02	194	PRO	2.3
32	BS05	153	LYS	2.3
47	BS20	14	LYS	2.3
51	B23S	2794(E)	A	2.3
2	AL03	174	ASP	2.3
25	AL32	39	MET	2.3
29	AS02	163	PHE	2.3
51	B23S	2174	C	2.3
47	AS20	77	ALA	2.3
34	AS07	75	VAL	2.3
40	AS13	65	LYS	2.3
46	AS19	31	ILE	2.3
49	AL31	52	SER	2.3
40	AS13	73	GLU	2.3
46	BS19	43	GLU	2.3
31	AS04	147	ALA	2.3
1	AL02	35	LYS	2.3
10	AL15	132	LYS	2.3
51	A23S	1086	A	2.3
7	AL11	41	PHE	2.3
20	AL25	185	GLU	2.3
7	AL11	35	MET	2.3
20	AL25	160	GLY	2.3
6	BL09	86	THR	2.3
13	BL18	54	LEU	2.3
35	AS08	112	LEU	2.3
50	A16S	1125	U	2.3
24	BL30	19	GLN	2.3
20	BL25	160	GLY	2.3
51	B23S	887	A	2.3
50	B16S	1297	C	2.3

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Mol	Chain	Res	Type	RSRZ
50	B16S	1354	C	2.3
37	BS10	61	GLU	2.2
50	B16S	68(K)	U	2.2
51	A23S	1093	G	2.2
3	BL04	167	ALA	2.2
5	AL06	105	LEU	2.2
20	AL25	164	ALA	2.2
29	BS02	177	ALA	2.2
42	AS15	49	ASP	2.2
28	BL35	54	GLU	2.2
32	BS05	125	SER	2.2
35	BS08	87	SER	2.2
39	AS12	125	LYS	2.2
43	BS16	41	PRO	2.2
50	A16S	972	C	2.2
43	BS16	9	PHE	2.2
43	BS16	32	TYR	2.2
4	BL05	13	GLU	2.2
6	BL09	20	ASP	2.2
6	AL09	104	GLN	2.2
6	AL09	125	GLU	2.2
50	B16S	66	G	2.2
5	AL06	87	LEU	2.2
6	BL09	109	ILE	2.2
20	BL25	159	PRO	2.2
47	BS20	55	ILE	2.2
31	BS04	141	ARG	2.2
31	BS04	145	GLU	2.2
35	BS08	52	ASP	2.2
37	AS10	25	GLU	2.2
7	BL11	28	GLY	2.2
6	BL09	21	VAL	2.2
10	AL15	146	VAL	2.2
20	AL25	54	HIS	2.2
36	AS09	73	GLN	2.2
30	BS03	200	ALA	2.2
31	BS04	37	PRO	2.2
34	AS07	9	VAL	2.2
40	BS13	96	LEU	2.2
12	AL17	33	ARG	2.2
37	AS10	79	ARG	2.2
46	BS19	53	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
20	BL25	70	LEU	2.2
36	BS09	77	ILE	2.2
5	AL06	117	PRO	2.2
51	B23S	2145	C	2.2
13	BL18	39	ILE	2.2
34	BS07	5	ARG	2.2
36	AS09	20	ARG	2.2
6	AL09	2	LYS	2.2
30	AS03	150	LYS	2.2
43	AS16	17	TYR	2.2
50	A16S	1365	G	2.2
51	B23S	2184	G	2.2
51	B23S	2135	A	2.2
20	AL25	127	LYS	2.2
35	BS08	44	PHE	2.2
37	BS10	9	ARG	2.2
40	BS13	3	ARG	2.2
51	B23S	2178	C	2.2
43	AS16	66	PRO	2.2
4	AL05	14	GLU	2.2
7	AL11	83	GLY	2.2
34	BS07	64	GLN	2.2
35	BS08	89	PRO	2.2
50	B16S	1493	A	2.2
26	BL33	43	CYS	2.2
8	AL13	106	LYS	2.2
24	AL30	35	ARG	2.2
38	AS11	83	ILE	2.2
6	AL09	130	TYR	2.2
43	BS16	59	TRP	2.2
7	AL11	85	GLU	2.2
2	BL03	204	ALA	2.2
5	BL06	141	VAL	2.2
6	AL09	105	HIS	2.2
6	BL09	38	LEU	2.2
50	B16S	68(C)	C	2.2
11	BL16	21	THR	2.2
47	AS20	71	THR	2.2
48	BTHX	18	TYR	2.2
43	BS16	72	ARG	2.2
49	AL31	47	VAL	2.2
4	AL05	147	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	BL05	158	ALA	2.2
7	AL11	43	ALA	2.2
38	AS11	94	ALA	2.2
50	A16S	1184	G	2.2
50	B16S	1356	G	2.2
51	B23S	2153	G	2.2
39	AS12	99	ILE	2.2
29	BS02	140	HIS	2.2
24	AL30	19	GLN	2.2
25	AL32	35	GLU	2.2
29	AS02	153	ARG	2.2
34	AS07	22	LEU	2.2
50	A16S	1288	A	2.2
45	AS18	48	GLY	2.2
39	AS12	50	ALA	2.2
51	A23S	271(L)	C	2.2
21	AL27	71	ASP	2.2
8	BL13	95	TYR	2.2
11	BL16	93	TYR	2.2
36	BS09	14	VAL	2.2
31	BS04	146	ILE	2.2
40	AS13	110	ARG	2.2
20	AL25	162	GLU	2.2
37	AS10	77	PRO	2.1
41	BS14	30	ALA	2.1
40	AS13	58	GLU	2.1
48	ATHX	2	GLY	2.1
50	B16S	972	C	2.1
50	B16S	988	G	2.1
51	A23S	2804	C	2.1
51	B23S	2112	G	2.1
20	BL25	182	LYS	2.1
26	BL33	50	ARG	2.1
29	BS02	136	VAL	2.1
5	AL06	72	ILE	2.1
6	BL09	96	ASP	2.1
13	BL18	40	ILE	2.1
11	BL16	12	GLN	2.1
19	AL24	99	CYS	2.1
24	AL30	33	GLN	2.1
10	AL15	122	PRO	2.1
40	AS13	87	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
12	AL17	80	PHE	2.1
11	BL16	25	ASP	2.1
37	AS10	87	THR	2.1
50	B16S	1003	G	2.1
51	B23S	2449	U	2.1
8	BL13	52	LYS	2.1
29	BS02	7	VAL	2.1
44	BS17	21	VAL	2.1
10	BL15	114	ILE	2.1
20	AL25	135	GLU	2.1
22	BL28	27	GLU	2.1
38	AS11	42	TRP	2.1
37	BS10	7	LYS	2.1
31	BS04	142	PRO	2.1
40	AS13	51	ALA	2.1
47	AS20	48	LYS	2.1
4	BL05	175	LEU	2.1
6	AL09	37	VAL	2.1
20	AL25	161	VAL	2.1
31	BS04	107	ARG	2.1
50	A16S	174	C	2.1
50	A16S	934	C	2.1
51	B23S	2099	U	2.1
7	BL11	78	ILE	2.1
7	AL11	121	GLU	2.1
51	A23S	271(T)	G	2.1
4	BL05	173	LEU	2.1
10	BL15	85	LEU	2.1
29	AS02	237	ALA	2.1
32	BS05	120	THR	2.1
31	BS04	136	PRO	2.1
20	AL25	124	ILE	2.1
51	B23S	2126	A	2.1
1	AL02	83	GLU	2.1
8	AL13	89	LYS	2.1
13	AL18	107	GLU	2.1
31	BS04	69	GLY	2.1
50	B16S	186(A)	C	2.1
5	AL06	99	VAL	2.1
6	BL09	12	LEU	2.1
5	AL06	30	LYS	2.1
40	AS13	85	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
6	AL09	26	ALA	2.1
8	BL13	122	LEU	2.1
9	BL14	46	ALA	2.1
19	AL24	5	MET	2.1
36	BS09	46	ALA	2.1
37	AS10	49	VAL	2.1
50	A16S	1440(I)	A	2.1
39	BS12	97	TYR	2.1
35	AS08	98	LYS	2.1
51	B23S	2164	C	2.1
30	BS03	190	ARG	2.1
25	AL32	38	ALA	2.1
35	AS08	95	VAL	2.1
36	BS09	85	LEU	2.1
34	BS07	13	GLN	2.1
13	BL18	82	ILE	2.1
50	B16S	1353	G	2.1
6	AL09	19	VAL	2.1
29	AS02	203	GLY	2.1
34	AS07	8	GLU	2.1
39	BS12	14	ARG	2.1
43	BS16	71	ARG	2.1
40	AS13	5	ALA	2.1
45	AS18	78	LEU	2.1
6	AL09	109	ILE	2.1
51	A23S	2177	C	2.1
51	B23S	2111	C	2.1
39	BS12	93	PRO	2.1
40	AS13	91	ARG	2.1
23	BL29	43	GLN	2.1
4	BL05	94	LEU	2.1
5	AL06	18	GLU	2.1
26	BL33	19	ARG	2.1
51	A23S	2099	U	2.1
51	B23S	2506	U	2.1
6	AL09	101	LEU	2.1
19	AL24	27	VAL	2.1
11	AL16	28	ALA	2.1
43	BS16	7	ALA	2.1
50	A16S	1027	C	2.1
51	B23S	1297	C	2.1
51	B23S	2477	C	2.1

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Mol	Chain	Res	Type	RSRZ
36	BS09	62	TYR	2.1
46	AS19	45	VAL	2.1
11	BL16	36	ALA	2.1
24	AL30	18	ASP	2.1
14	AL19	65	LYS	2.1
46	AS19	34	TRP	2.1
50	B16S	1028(H)	G	2.1
51	B23S	2109	U	2.1
31	BS04	65	ARG	2.1
4	BL05	59	GLU	2.1
10	AL15	85	LEU	2.1
34	BS07	104	LEU	2.1
40	BS13	6	GLY	2.1
41	BS14	55	GLY	2.1
50	B16S	1129	C	2.1
51	A23S	2789	C	2.1
6	AL09	110	ASP	2.1
2	AL03	59	VAL	2.1
35	AS08	2	LEU	2.1
5	BL06	168	PRO	2.0
25	AL32	34	PRO	2.0
26	BL33	33	LYS	2.0
37	BS10	36	GLY	2.1
42	AS15	52	SER	2.0
49	BL31	37	PRO	2.0
52	B5S	52	A	2.0
4	BL05	25	TYR	2.0
5	AL06	94	TYR	2.0
34	AS07	10	ARG	2.0
36	BS09	89	ASN	2.0
50	A16S	998(A)	C	2.0
17	AL22	30	GLU	2.0
20	BL25	185	GLU	2.0
22	AL28	93	GLU	2.0
40	BS13	67	GLU	2.0
32	AS05	10	MET	2.0
43	AS16	59	TRP	2.0
4	AL05	25	TYR	2.0
6	AL09	25	TYR	2.0
3	AL04	156	LEU	2.0
47	AS20	88	VAL	2.0
20	AL25	26	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
46	BS19	17	GLU	2.0
46	BS19	56	GLN	2.0
51	B23S	2151	G	2.0
51	B23S	2160	G	2.0
38	AS11	50	TYR	2.0
6	AL09	30	LEU	2.0
20	AL25	67	LEU	2.0
30	BS03	207	VAL	2.0
38	AS11	110	ASP	2.0
44	AS17	55	ASP	2.0
4	BL05	14	GLU	2.0
29	BS02	129	GLU	2.0
4	AL05	63	ILE	2.0
14	AL19	64	ARG	2.0
29	BS02	31	TYR	2.0
35	BS08	129	VAL	2.0
37	BS10	40	LEU	2.0
50	A16S	1228	C	2.0
50	B16S	186(B)	C	2.0
50	B16S	979	C	2.0
51	B23S	543(B)	C	2.0
51	B23S	2131	G	2.0
26	BL33	37	ARG	2.0
34	BS07	121	ALA	2.0
13	AL18	26	LEU	2.0
20	AL25	92	SER	2.0
22	BL28	12	PRO	2.0
1	AL02	233	HIS	2.0
20	BL25	179	ASP	2.0
40	BS13	50	GLU	2.0
43	BS16	4	ILE	2.0
51	B23S	1098	A	2.0
34	AS07	84	ASN	2.0
17	AL22	102	HIS	2.0
19	AL24	91	GLU	2.0
41	AS14	51	GLY	2.0
51	B23S	2150	U	2.0
6	BL09	139	GLN	2.0
7	BL11	45	THR	2.0
20	AL25	87	ASP	2.0
31	BS04	67	ILE	2.0
35	BS08	25	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
36	AS09	76	ALA	2.0
48	BTHX	17	THR	2.0
4	BL05	81	LYS	2.0
13	AL18	33	LYS	2.0
20	BL25	161	VAL	2.0
37	AS10	37	PRO	2.0
43	AS16	49	LEU	2.0
24	AL30	48	GLU	2.0
31	BS04	6	GLY	2.0
46	AS19	43	GLU	2.0
50	A16S	1123	A	2.0
50	A16S	1280	A	2.0
51	B23S	1494	A	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	ZN	BS04	301	1/1	0.90	0.23	100,100,100,100	0
54	ZN	AS14	101	1/1	0.95	0.13	120,120,120,120	0
54	ZN	BS14	101	1/1	0.96	0.10	137,137,137,137	0
54	ZN	AS04	301	1/1	0.99	0.24	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.