



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 06:45 AM EDT

PDB ID : 4V7J
Title : Structure of RelE nuclease bound to the 70S ribosome (precleavage state)
Authors : Neubauer, C.; Gao, Y.-G.; Andersen, K.R.; Dunham, C.M.; Kelley, A.C.;
Hentschel, J.; Gerdes, K.; Ramakrishnan, V.; Brodersen, D.E.
Deposited on : 2009-11-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

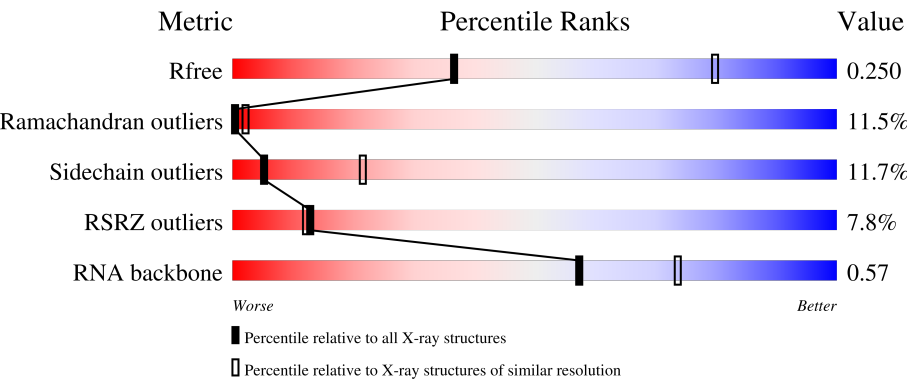
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

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 3.30 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	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	Ab	256	<div><div>8%</div><div>77%</div><div>14%</div><div>9%</div></div>
1	Bb	256	<div><div>7%</div><div>77%</div><div>14%</div><div>9%</div></div>
2	Ac	239	<div><div>7%</div><div>69%</div><div>17%</div><div>14%</div></div>
2	Bc	239	<div><div>9%</div><div>69%</div><div>16%</div><div>14%</div></div>
3	Ad	209	<div><div>%</div><div>82%</div><div>15%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Bd	209	
4	Ae	162	
4	Be	162	
5	Af	101	
5	Bf	101	
6	Ag	156	
6	Bg	156	
7	Ah	138	
7	Bh	138	
8	Ai	128	
8	Bi	128	
9	Aj	105	
9	Bj	105	
10	Ak	129	
10	Bk	129	
11	Al	132	
11	Bl	132	
12	Am	126	
12	Bm	126	
13	An	61	
13	Bn	61	
14	Ao	89	
14	Bo	89	
15	Ap	88	
15	Bp	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	Aq	105	
16	Bq	105	
17	Ar	88	
17	Br	88	
18	As	93	
18	Bs	93	
19	At	106	
19	Bt	106	
20	Au	27	
20	Bu	27	
21	Ay	95	
21	By	95	
22	Aa	1504	
22	Ba	1504	
23	Ax	25	
23	Bx	25	
24	Av	77	
24	Bv	77	
25	Aw	77	
25	Bw	77	
26	AC	229	
26	BC	229	
27	AD	276	
27	BD	276	
28	AE	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BE	206	
29	AF	210	
29	BF	210	
30	AG	182	
30	BG	182	
31	AH	180	
31	BH	180	
32	AI	148	
32	BI	148	
33	AJ	173	
33	BJ	173	
34	AN	140	
34	BN	140	
35	AO	122	
35	BO	122	
36	AP	150	
36	BP	150	
37	AQ	141	
37	BQ	141	
38	AR	118	
38	BR	118	
39	AS	112	
39	BS	112	
40	AT	146	
40	BT	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	AU	118	
41	BU	118	
42	AV	101	
42	BV	101	
43	AW	113	
43	BW	113	
44	AX	96	
44	BX	96	
45	AY	110	
45	BY	110	
46	AZ	206	
46	BZ	206	
47	A0	85	
47	B0	85	
48	A1	98	
48	B1	98	
49	A2	72	
49	B2	72	
50	A3	60	
50	B3	60	
51	A4	71	
51	B4	71	
52	A5	60	
52	B5	60	
53	A6	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B6	54	
54	A7	49	
54	B7	49	
55	A8	65	
55	B8	65	
56	A9	37	
56	B9	37	
57	AA	2848	
57	BA	2848	
58	AB	119	
58	BB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	A7	101	-	-	-	X
60	MG	AA	2917	-	-	-	X
60	MG	AA	2925	-	-	-	X
60	MG	AA	2946	-	-	-	X
60	MG	AA	2968	-	-	-	X
60	MG	AA	2975	-	-	-	X
60	MG	AA	3002	-	-	-	X
60	MG	AA	3016	-	-	-	X
60	MG	AA	3030	-	-	-	X
60	MG	AA	3040	-	-	-	X
60	MG	AA	3067	-	-	-	X
60	MG	AA	3069	-	-	-	X
60	MG	AA	3084	-	-	-	X
60	MG	AA	3087	-	-	-	X
60	MG	AA	3102	-	-	-	X
60	MG	AA	3103	-	-	-	X
60	MG	AA	3106	-	-	-	X
60	MG	AA	3112	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3138	-	-	-	X
60	MG	AA	3139	-	-	-	X
60	MG	AA	3143	-	-	-	X
60	MG	AA	3146	-	-	-	X
60	MG	AA	3149	-	-	-	X
60	MG	AA	3152	-	-	-	X
60	MG	AA	3165	-	-	-	X
60	MG	AA	3168	-	-	-	X
60	MG	AA	3176	-	-	-	X
60	MG	AA	3185	-	-	-	X
60	MG	AA	3194	-	-	-	X
60	MG	AA	3206	-	-	-	X
60	MG	AA	3207	-	-	-	X
60	MG	AA	3209	-	-	-	X
60	MG	AA	3219	-	-	-	X
60	MG	AA	3222	-	-	-	X
60	MG	AA	3224	-	-	-	X
60	MG	AA	3225	-	-	-	X
60	MG	AA	3230	-	-	-	X
60	MG	AA	3236	-	-	-	X
60	MG	AA	3237	-	-	-	X
60	MG	AA	3239	-	-	-	X
60	MG	AA	3241	-	-	-	X
60	MG	AA	3242	-	-	-	X
60	MG	AA	3248	-	-	-	X
60	MG	AA	3249	-	-	-	X
60	MG	AA	3253	-	-	-	X
60	MG	AA	3257	-	-	-	X
60	MG	AA	3260	-	-	-	X
60	MG	AA	3261	-	-	-	X
60	MG	AA	3262	-	-	-	X
60	MG	AA	3264	-	-	-	X
60	MG	AA	3266	-	-	-	X
60	MG	AB	202	-	-	-	X
60	MG	AQ	201	-	-	-	X
60	MG	AX	101	-	-	-	X
60	MG	Aa	1610	-	-	-	X
60	MG	Aa	1611	-	-	-	X
60	MG	Aa	1616	-	-	-	X
60	MG	Aa	1618	-	-	-	X
60	MG	Aa	1623	-	-	-	X
60	MG	Aa	1630	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Aa	1633	-	-	-	X
60	MG	Aa	1637	-	-	-	X
60	MG	Aa	1641	-	-	-	X
60	MG	Aa	1651	-	-	-	X
60	MG	Aa	1652	-	-	-	X
60	MG	Aa	1658	-	-	-	X
60	MG	Aa	1665	-	-	-	X
60	MG	Aa	1677	-	-	-	X
60	MG	Aa	1681	-	-	-	X
60	MG	Aa	1700	-	-	-	X
60	MG	Aa	1706	-	-	-	X
60	MG	Aa	1713	-	-	-	X
60	MG	Aa	1714	-	-	-	X
60	MG	Aa	1723	-	-	-	X
60	MG	Aa	1727	-	-	-	X
60	MG	Aa	1730	-	-	-	X
60	MG	Am	201	-	-	-	X
60	MG	Aw	101	-	-	-	X
60	MG	B0	101	-	-	-	X
60	MG	BA	2921	-	-	-	X
60	MG	BA	2938	-	-	-	X
60	MG	BA	2945	-	-	-	X
60	MG	BA	2958	-	-	-	X
60	MG	BA	2965	-	-	-	X
60	MG	BA	2976	-	-	-	X
60	MG	BA	2984	-	-	-	X
60	MG	BA	2998	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3036	-	-	-	X
60	MG	BA	3049	-	-	-	X
60	MG	BA	3065	-	-	-	X
60	MG	BA	3071	-	-	-	X
60	MG	BA	3074	-	-	-	X
60	MG	BA	3086	-	-	-	X
60	MG	BA	3088	-	-	-	X
60	MG	BA	3109	-	-	-	X
60	MG	BA	3126	-	-	-	X
60	MG	BA	3129	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	BA	3136	-	-	-	X
60	MG	BA	3148	-	-	-	X
60	MG	BA	3149	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3150	-	-	-	X
60	MG	BA	3154	-	-	-	X
60	MG	BA	3157	-	-	-	X
60	MG	BA	3162	-	-	-	X
60	MG	BA	3173	-	-	-	X
60	MG	BA	3175	-	-	-	X
60	MG	BA	3180	-	-	-	X
60	MG	BA	3182	-	-	-	X
60	MG	BA	3191	-	-	-	X
60	MG	BA	3204	-	-	-	X
60	MG	BA	3206	-	-	-	X
60	MG	BA	3219	-	-	-	X
60	MG	BA	3229	-	-	-	X
60	MG	BA	3231	-	-	-	X
60	MG	BA	3235	-	-	-	X
60	MG	BA	3237	-	-	-	X
60	MG	BA	3244	-	-	-	X
60	MG	BA	3246	-	-	-	X
60	MG	BA	3253	-	-	-	X
60	MG	BA	3255	-	-	-	X
60	MG	BA	3258	-	-	-	X
60	MG	BA	3261	-	-	-	X
60	MG	BA	3265	-	-	-	X
60	MG	BB	203	-	-	-	X
60	MG	Ba	1610	-	-	-	X
60	MG	Ba	1631	-	-	-	X
60	MG	Ba	1640	-	-	-	X
60	MG	Ba	1643	-	-	-	X
60	MG	Ba	1645	-	-	-	X
60	MG	Ba	1646	-	-	-	X
60	MG	Ba	1647	-	-	-	X
60	MG	Ba	1648	-	-	-	X
60	MG	Ba	1660	-	-	-	X
60	MG	Ba	1664	-	-	-	X
60	MG	Ba	1665	-	-	-	X
60	MG	Ba	1670	-	-	-	X
60	MG	Ba	1676	-	-	-	X
60	MG	Ba	1680	-	-	-	X
60	MG	Ba	1682	-	-	-	X
60	MG	Ba	1695	-	-	-	X
60	MG	Ba	1698	-	-	-	X
60	MG	Ba	1699	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Ba	1706	-	-	-	X
60	MG	Ba	1712	-	-	-	X
60	MG	Ba	1716	-	-	-	X
60	MG	Ba	1717	-	-	-	X
60	MG	Ba	1728	-	-	-	X
60	MG	Ba	1732	-	-	-	X
60	MG	Ba	1739	-	-	-	X
60	MG	Bm	202	-	-	-	X
60	MG	Bv	104	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297206 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ab	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
1	Bb	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ac	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
2	Bc	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Ae	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
4	Be	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Aj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
9	Bj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Al	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
11	Bl	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Am	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
12	Bm	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Ap	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
15	Bp	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Aq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
16	Bq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	As	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
18	Bs	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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

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

- Molecule 20 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Au	24	Total	C	N	O	0	0	0
			208	128	50	30			
20	Bu	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 21 is a protein called Toxin relE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Ay	94	Total	C	N	O	S	0	0	0
			770	496	133	139	2			
21	By	94	Total	C	N	O	S	0	0	0
			766	495	130	139	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ay	45	ALA	ARG	engineered mutation	UNP P0C077
Ay	81	ALA	ARG	engineered mutation	UNP P0C077
By	45	ALA	ARG	engineered mutation	UNP P0C077
By	81	ALA	ARG	engineered mutation	UNP P0C077

- Molecule 22 is a RNA chain called RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Aa	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
22	Ba	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 23 is a RNA chain called RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Ax	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			
23	Bx	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			

- Molecule 24 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Av	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
24	Bv	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 25 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Aw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
25	Bw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
26	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
29	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

Continued on next page...

Continued from previous page...

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			
31	BH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
32	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	AJ	130	Total	C	N	O	0	0	0
			641	381	130	130			
33	BJ	130	Total	C	N	O	0	0	0
			641	381	130	130			

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
37	BQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AS	98	Total	C	N	O	0	0	0
			770	486	154	130			
39	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
40	BT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	AX	92	Total	C	N	O	0	0	0
			725	471	131	123			
44	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	A1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
48	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	A2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	A3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
50	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	A4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			
51	B4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	A5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			
52	B5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	A6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
53	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	A7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
54	B7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 57 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	AA	2848	Total 61341	C 27300	N 11478	O 19716	P 2847	0	0	0
57	BA	2848	Total 61341	C 27300	N 11478	O 19716	P 2847	0	0	0

- Molecule 58 is a RNA chain called RNA (119-MER).

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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Ad	1	Total 1	Zn 1	0	0
59	An	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0
59	Bd	1	Total 1	Zn 1	0	0
59	Bn	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Am	1	Total 1	Mg 1	0	0
60	Aq	1	Total 1	Mg 1	0	0
60	Aa	145	Total 145	Mg 145	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Av	4	Total 4	Mg 4	0	0
60	Aw	1	Total 1	Mg 1	0	0
60	AD	2	Total 2	Mg 2	0	0
60	AF	1	Total 1	Mg 1	0	0
60	AQ	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	A1	1	Total 1	Mg 1	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A7	2	Total 2	Mg 2	0	0
60	AA	368	Total 368	Mg 368	0	0
60	AB	3	Total 3	Mg 3	0	0
60	Bm	2	Total 2	Mg 2	0	0
60	Bq	1	Total 1	Mg 1	0	0
60	Ba	143	Total 143	Mg 143	0	0
60	Bx	1	Total 1	Mg 1	0	0
60	Bv	5	Total 5	Mg 5	0	0
60	Bw	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0

Continued on next page...

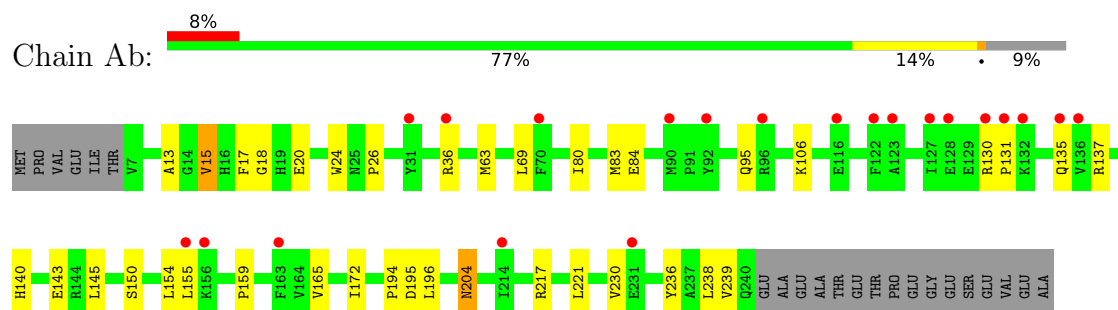
Continued from previous page...

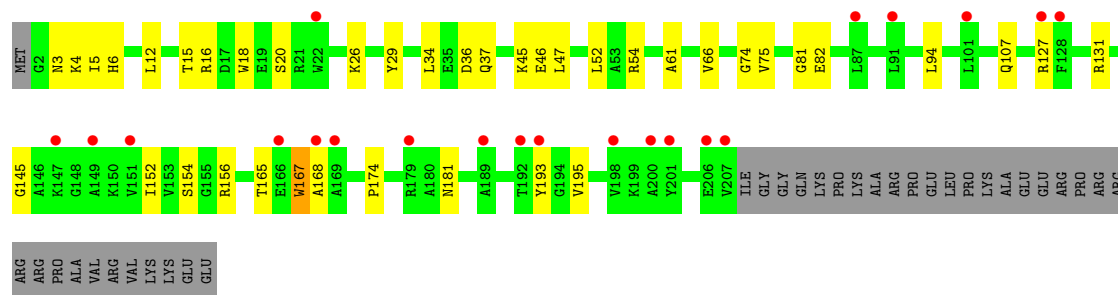
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B0	2	Total 2	Mg 2	0	0
60	B5	1	Total 1	Mg 1	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BA	366	Total 366	Mg 366	0	0
60	BB	3	Total 3	Mg 3	0	0

3 Residue-property plots [i](#)

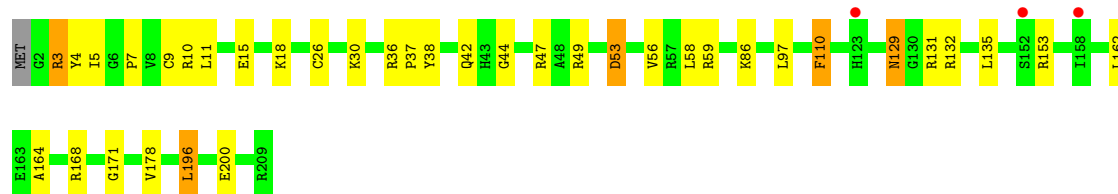
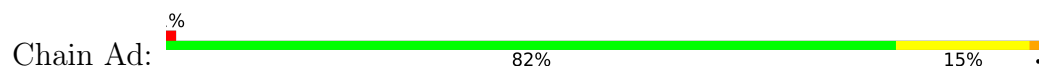
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 30S ribosomal protein S2

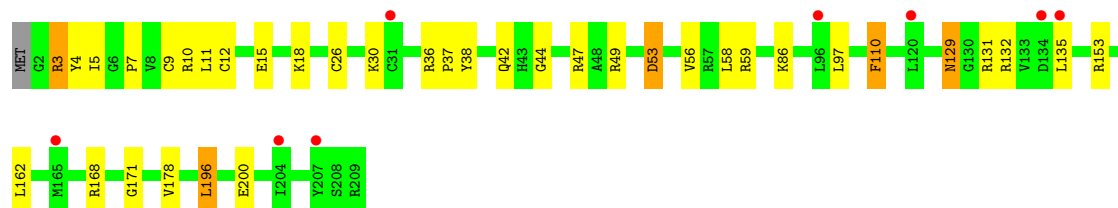
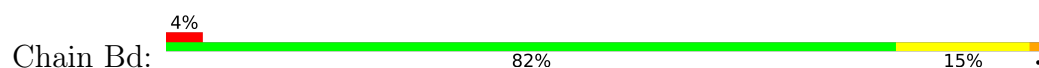




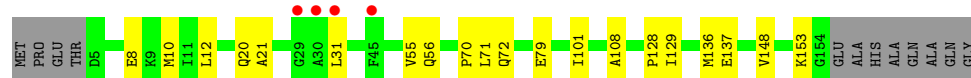
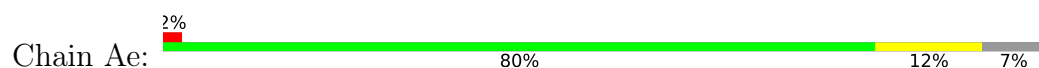
• Molecule 3: 30S ribosomal protein S4



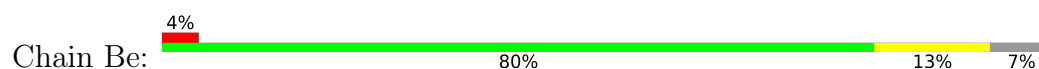
• Molecule 3: 30S ribosomal protein S4



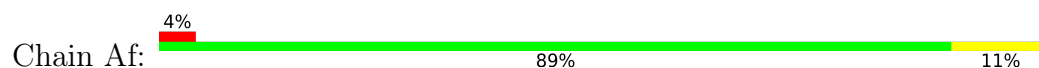
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

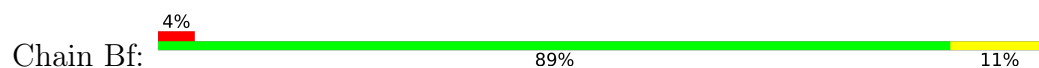


• Molecule 5: 30S ribosomal protein S6

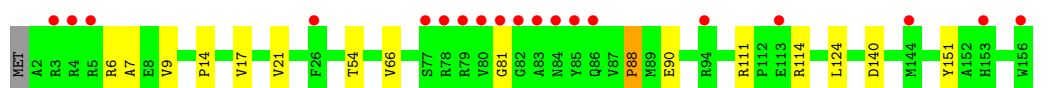
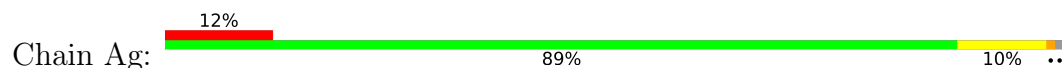




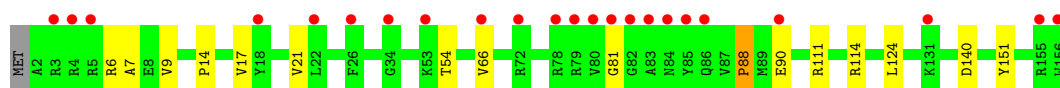
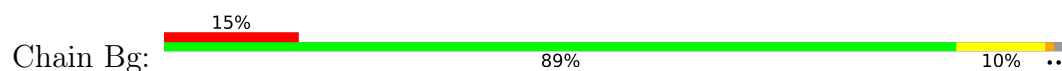
- Molecule 5: 30S ribosomal protein S6



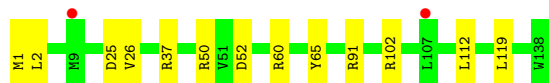
- Molecule 6: 30S ribosomal protein S7



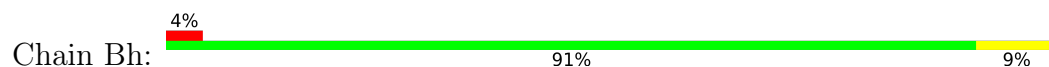
- Molecule 6: 30S ribosomal protein S7



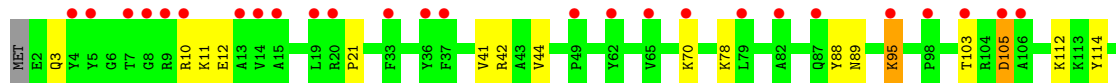
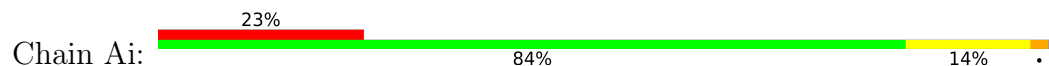
- Molecule 7: 30S ribosomal protein S8

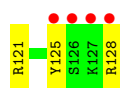


- Molecule 7: 30S ribosomal protein S8

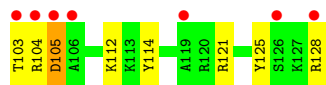
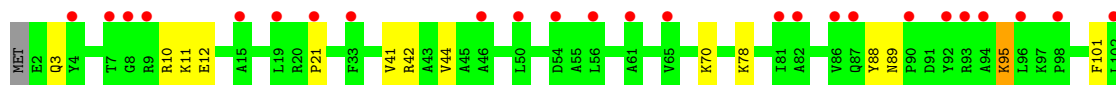
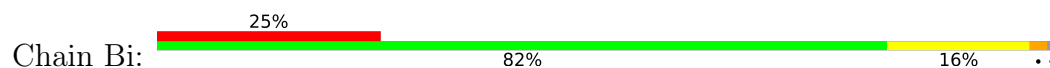


- Molecule 8: 30S ribosomal protein S9

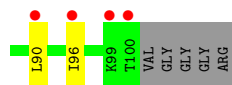
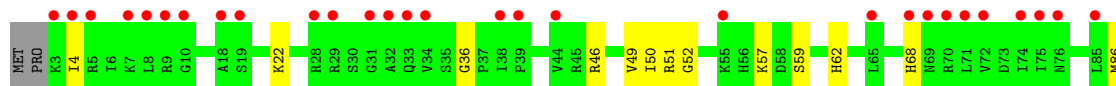
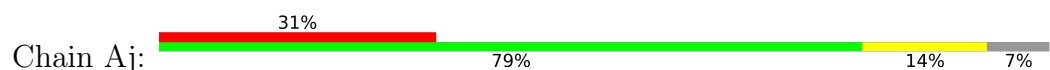




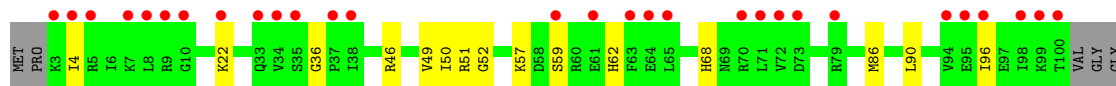
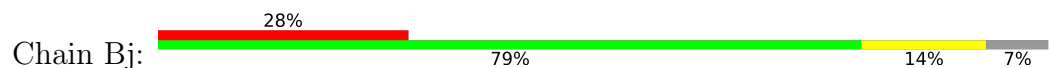
• Molecule 8: 30S ribosomal protein S9



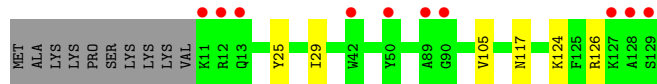
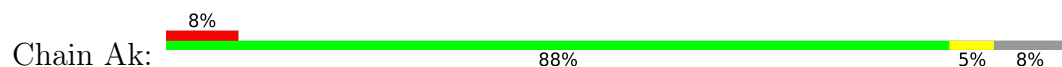
• Molecule 9: 30S ribosomal protein S10



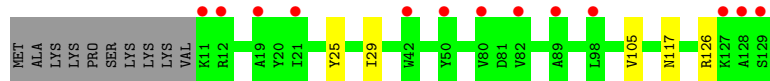
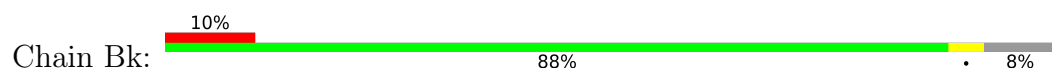
• Molecule 9: 30S ribosomal protein S10



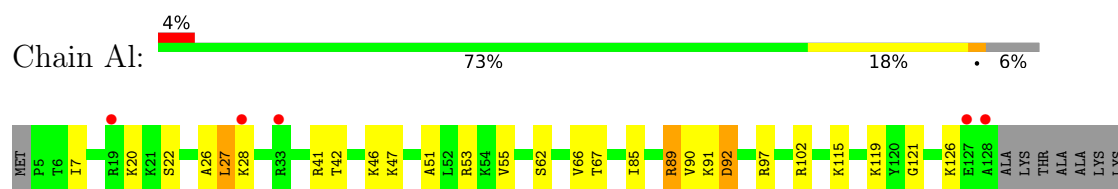
• Molecule 10: 30S ribosomal protein S11



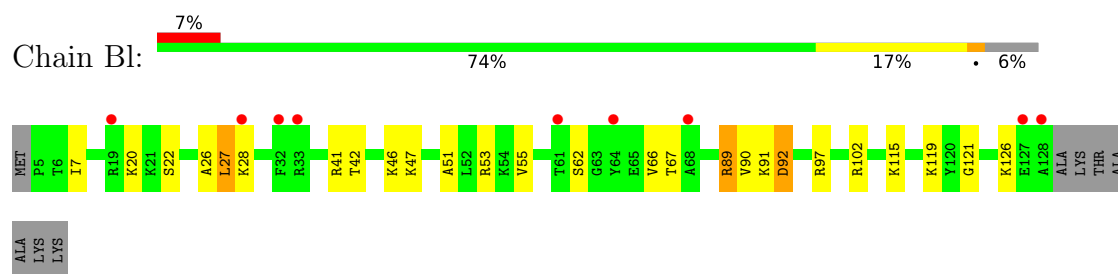
• Molecule 10: 30S ribosomal protein S11



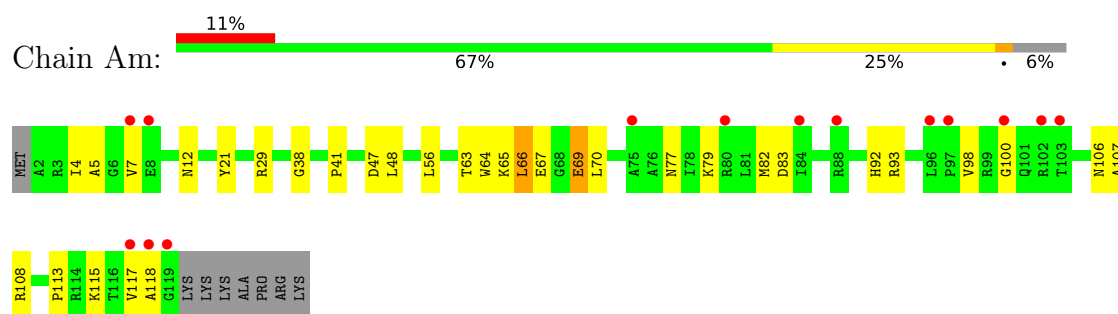
- Molecule 11: 30S ribosomal protein S12



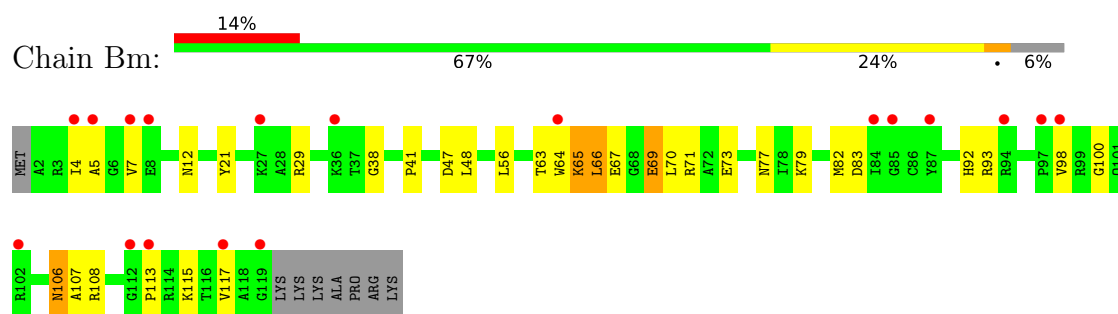
- Molecule 11: 30S ribosomal protein S12



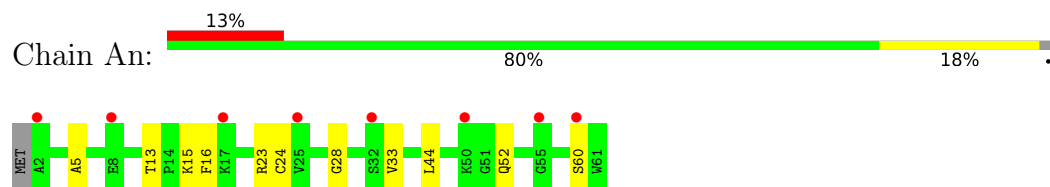
- Molecule 12: 30S ribosomal protein S13



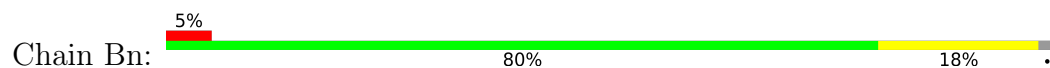
- Molecule 12: 30S ribosomal protein S13

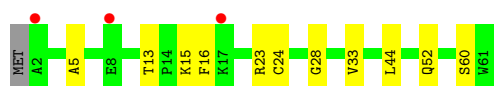


- Molecule 13: 30S ribosomal protein S14 type Z

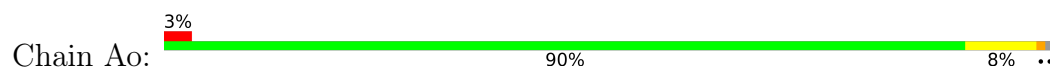


- Molecule 13: 30S ribosomal protein S14 type Z

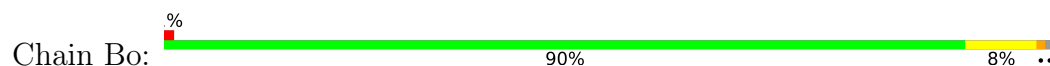




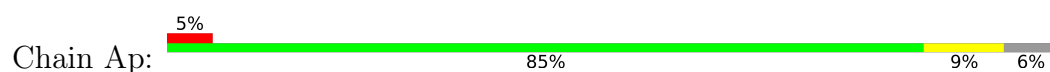
- Molecule 14: 30S ribosomal protein S15



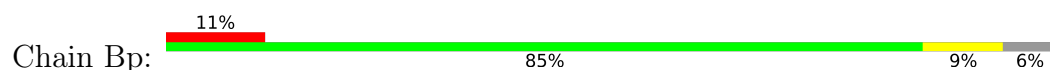
- Molecule 14: 30S ribosomal protein S15



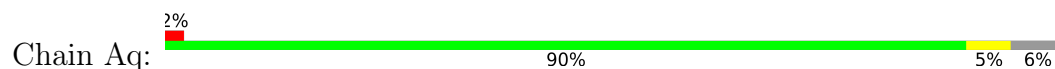
- Molecule 15: 30S ribosomal protein S16



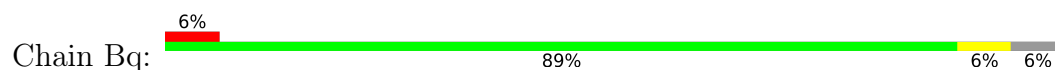
- Molecule 15: 30S ribosomal protein S16



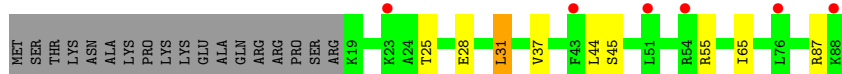
- Molecule 16: 30S ribosomal protein S17



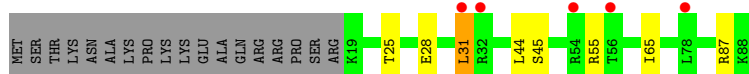
- Molecule 16: 30S ribosomal protein S17



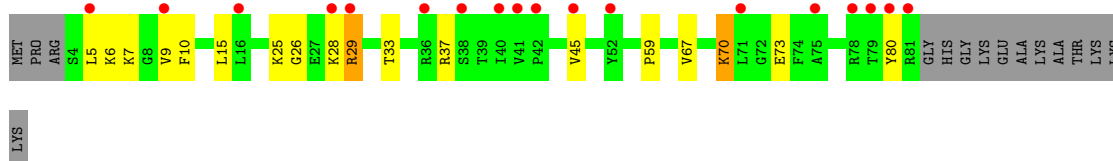
- Molecule 17: 30S ribosomal protein S18



- Molecule 17: 30S ribosomal protein S18



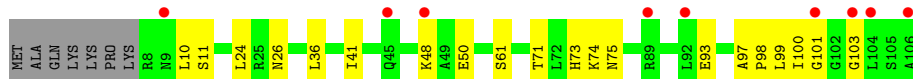
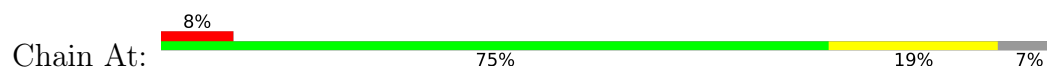
- Molecule 18: 30S ribosomal protein S19



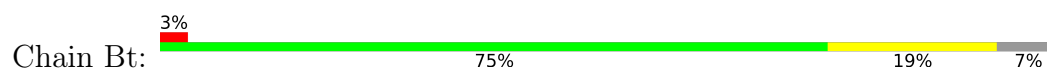
- Molecule 18: 30S ribosomal protein S19



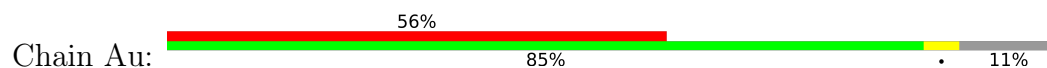
- Molecule 19: 30S ribosomal protein S20

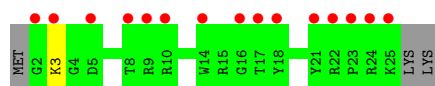


- Molecule 19: 30S ribosomal protein S20

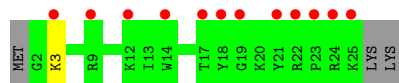
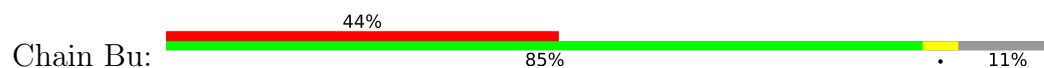


- Molecule 20: 30S ribosomal protein Thx

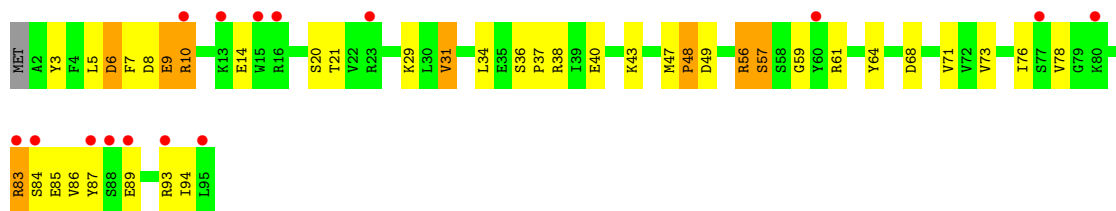




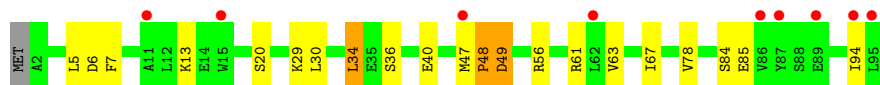
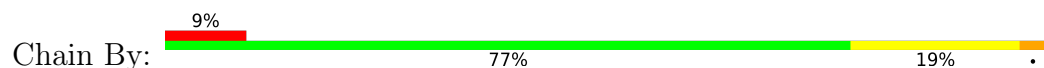
- Molecule 20: 30S ribosomal protein Thx



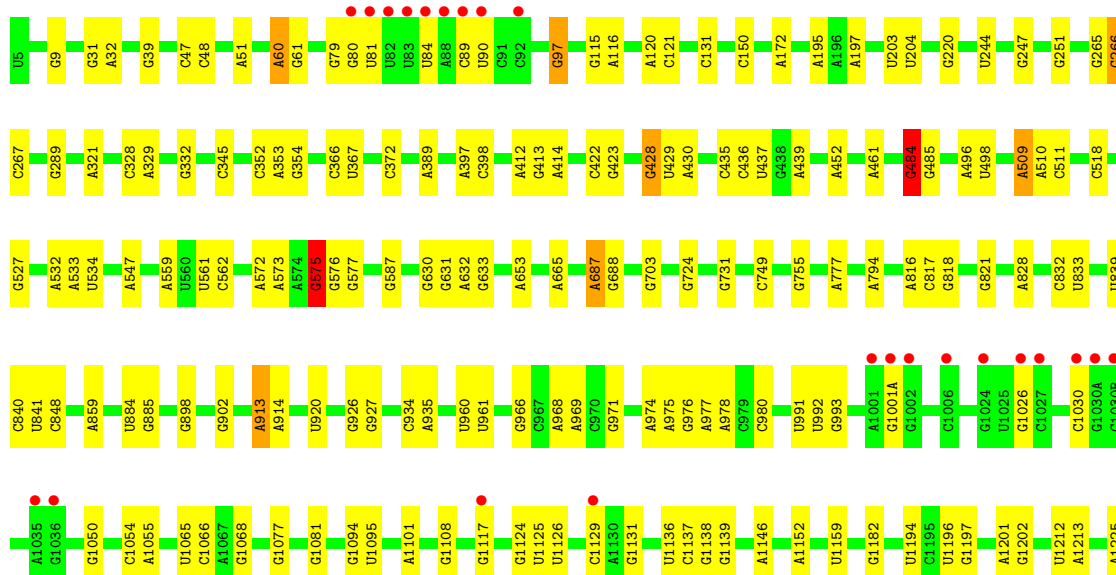
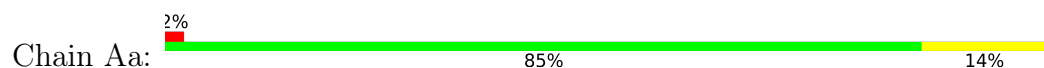
- Molecule 21: Toxin relE



- Molecule 21: Toxin relE

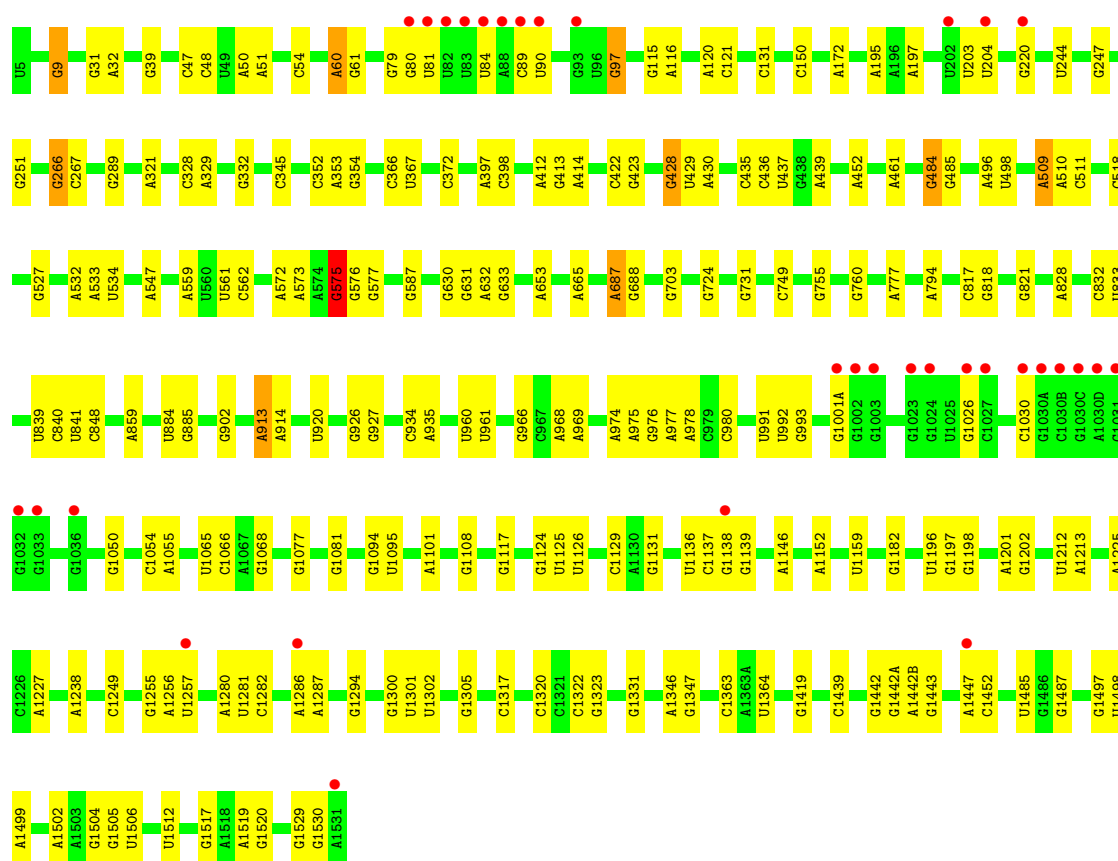
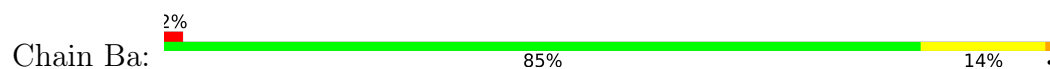


- Molecule 22: RNA (1504-MER)

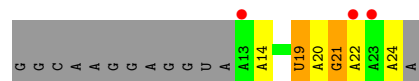
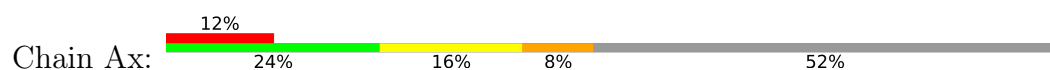




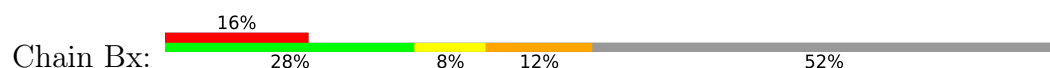
• Molecule 22: RNA (1504-MER)

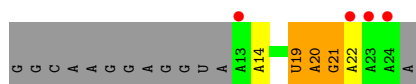


• Molecule 23: RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3')

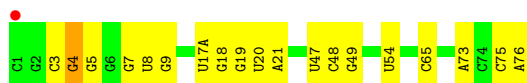
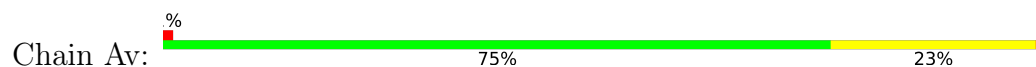


• Molecule 23: RNA (5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*A*AP*AP*AP*AP*UP*GP*(OMU)P*(A2M)P*(OMG)P*AP*AP*AP*A)-3')

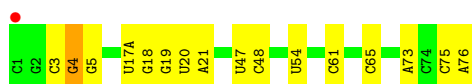
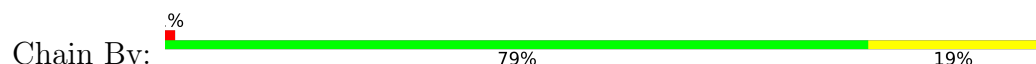




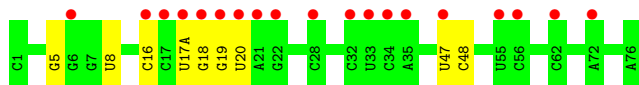
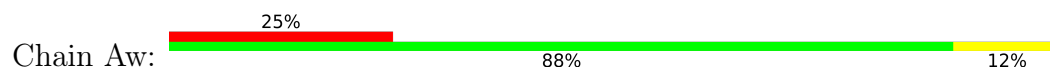
- Molecule 24: RNA (77-MER)



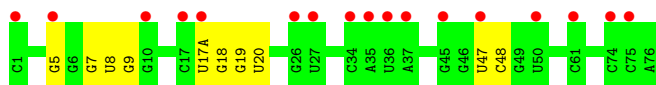
- Molecule 24: RNA (77-MER)



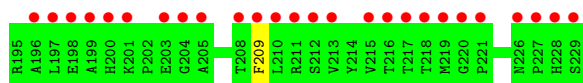
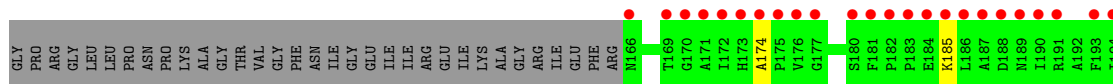
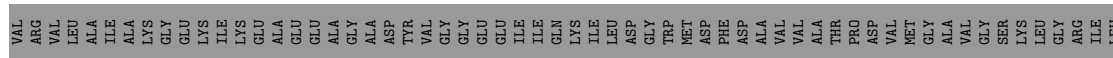
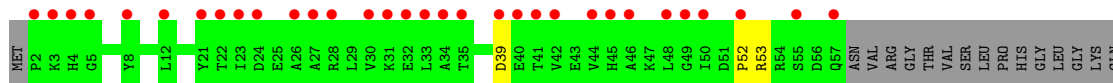
- Molecule 25: RNA (77-MER)



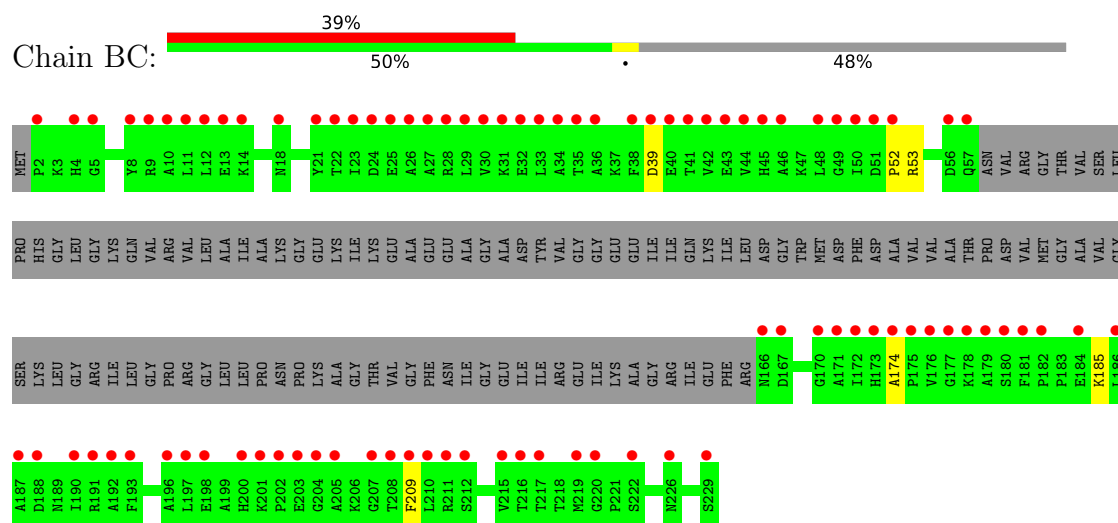
- Molecule 25: RNA (77-MER)



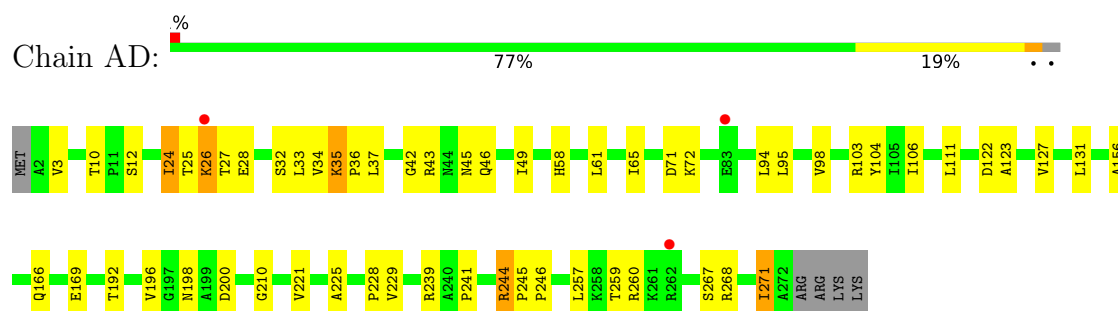
- Molecule 26: 50S ribosomal protein L1



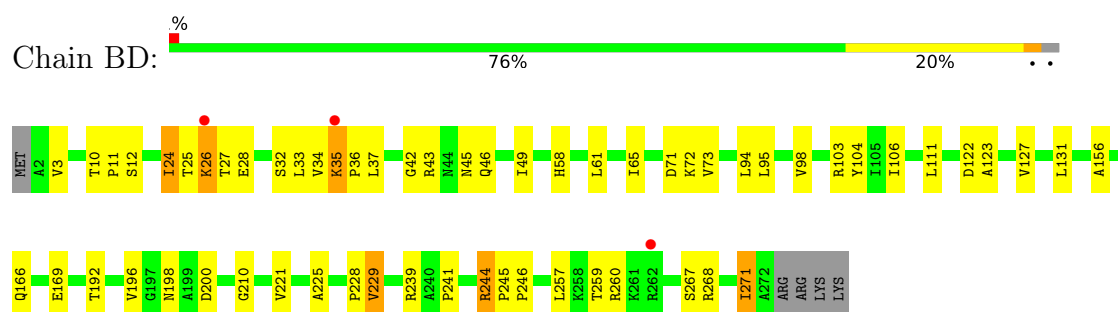
- Molecule 26: 50S ribosomal protein L1



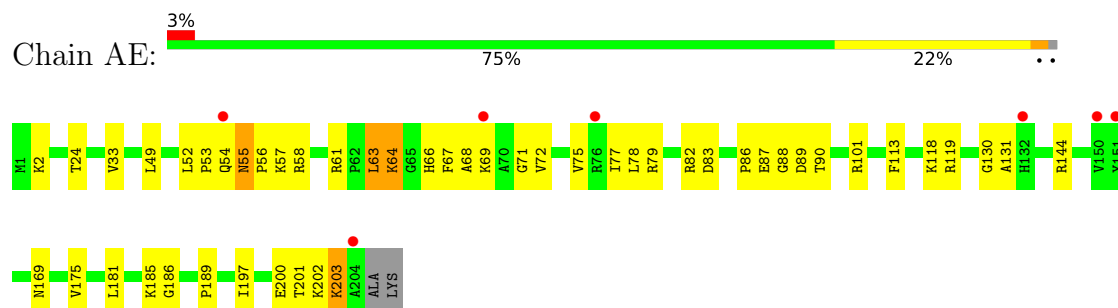
- Molecule 27: 50S ribosomal protein L2



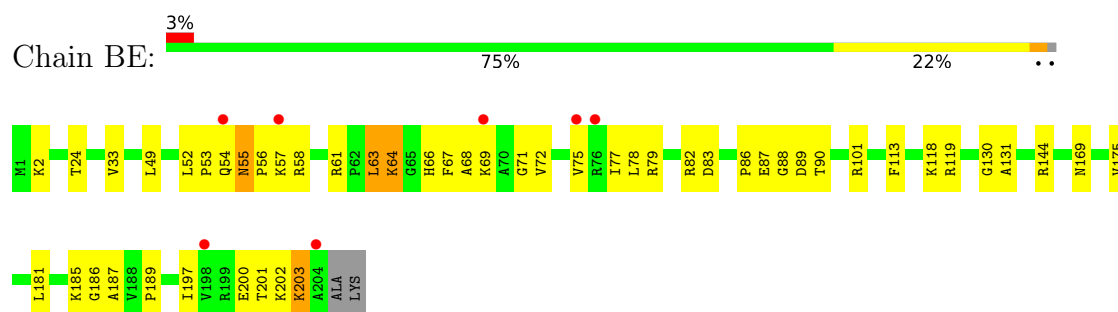
- Molecule 27: 50S ribosomal protein L2



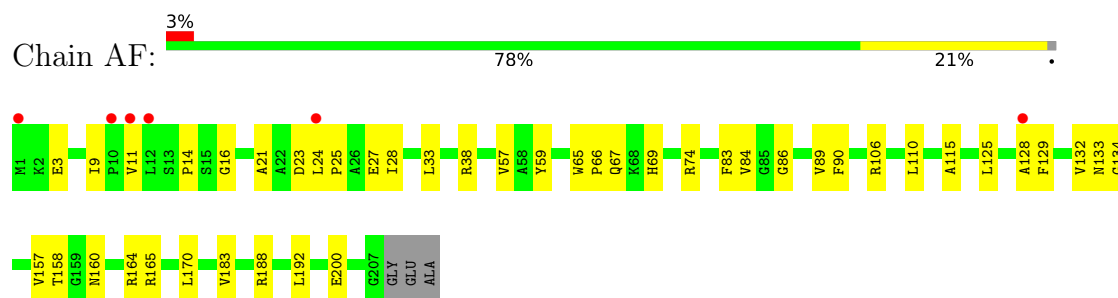
- Molecule 28: 50S ribosomal protein L3



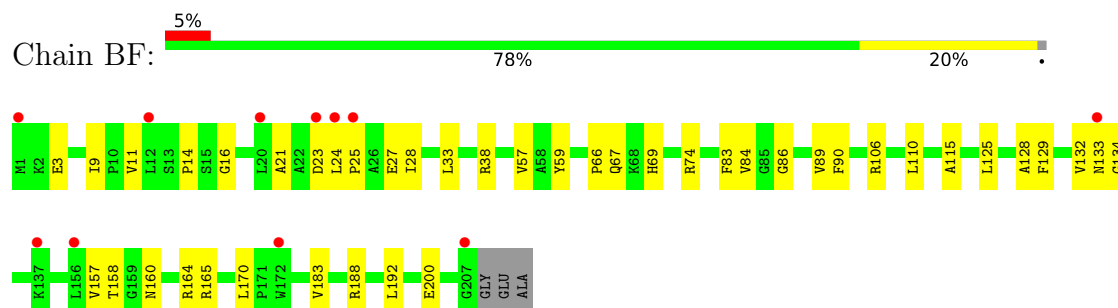
- Molecule 28: 50S ribosomal protein L3



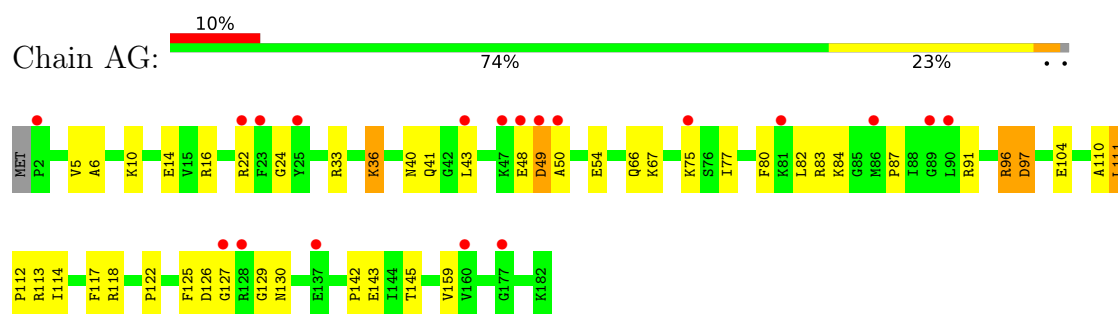
- Molecule 29: 50S ribosomal protein L4



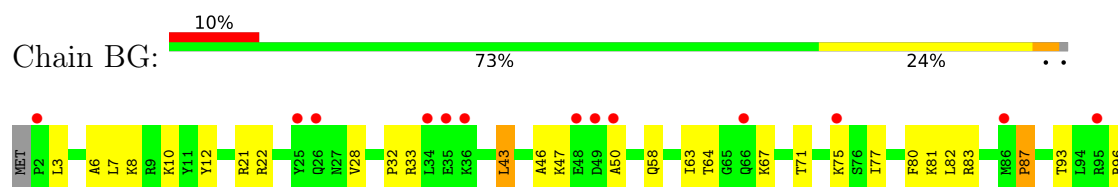
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

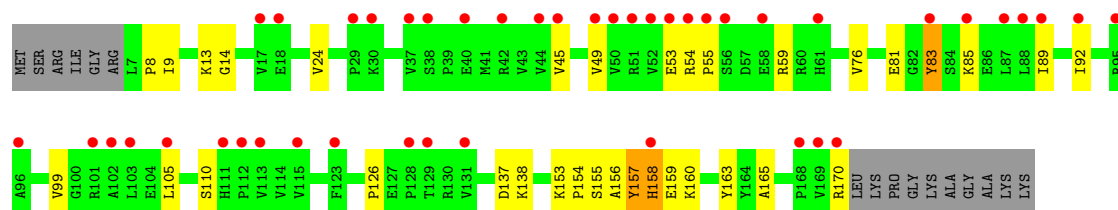
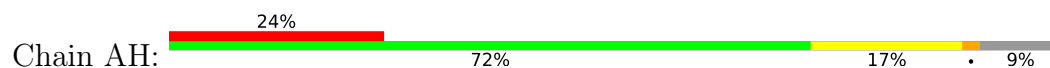


- Molecule 30: 50S ribosomal protein L5

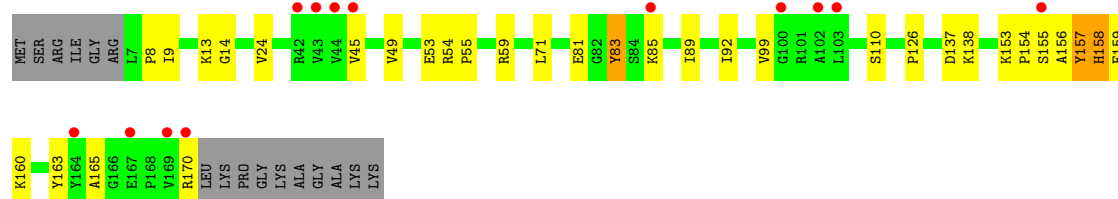
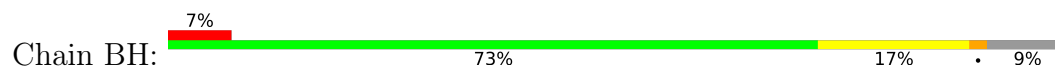




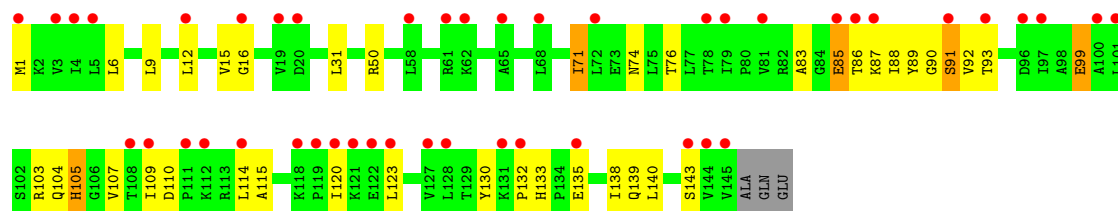
- Molecule 31: 50S ribosomal protein L6



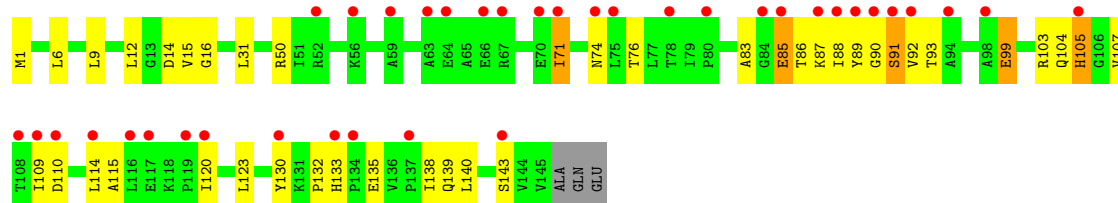
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

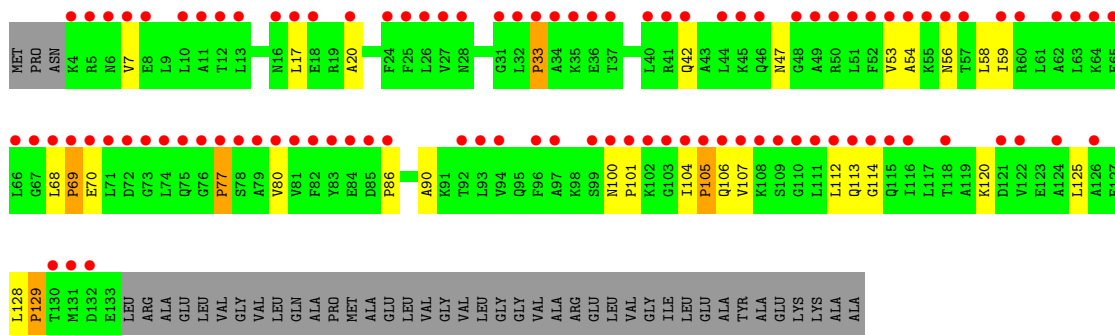


- Molecule 32: 50S ribosomal protein L9

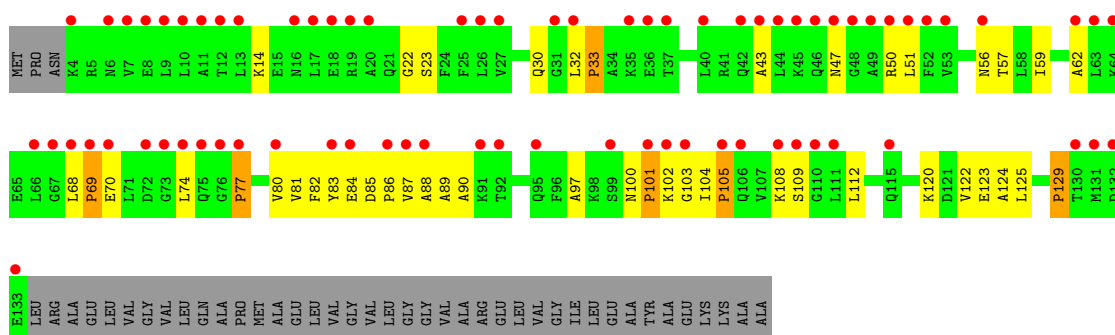
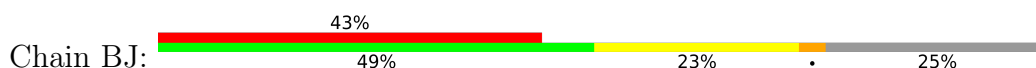


- Molecule 33: 50S ribosomal protein L10

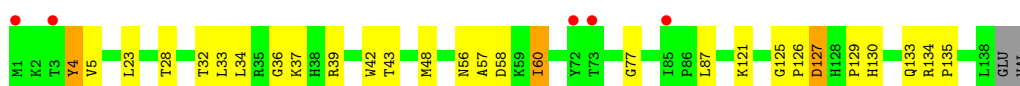
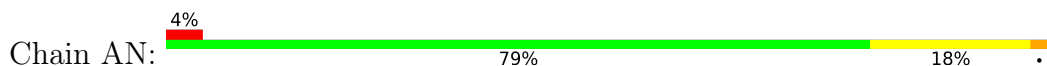




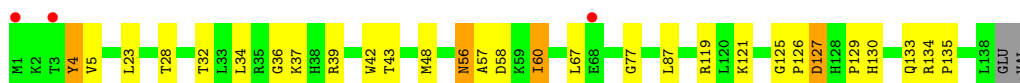
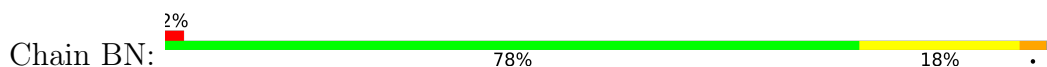
- Molecule 33: 50S ribosomal protein L10



- Molecule 34: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L13

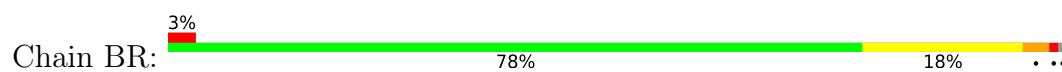


- Molecule 35: 50S ribosomal protein L14

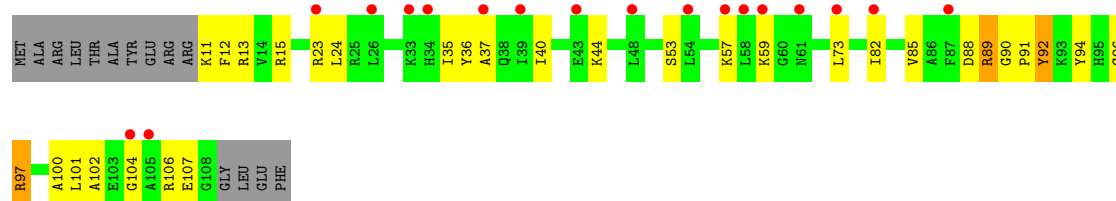


- Molecule 35: 50S ribosomal protein L14

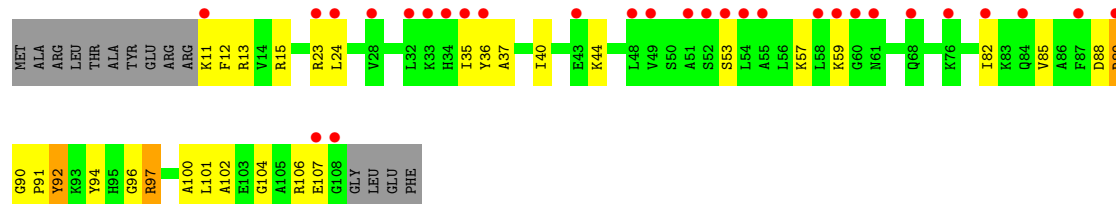




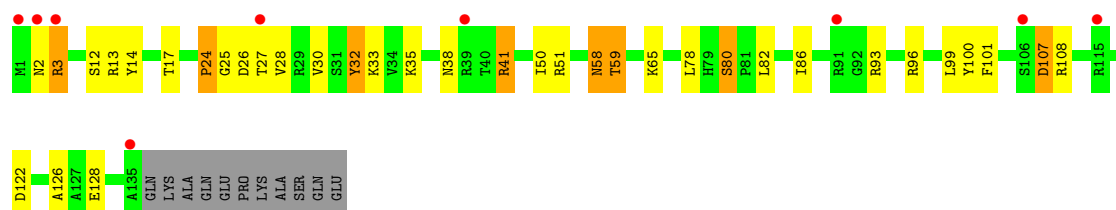
- Molecule 39: 50S ribosomal protein L18



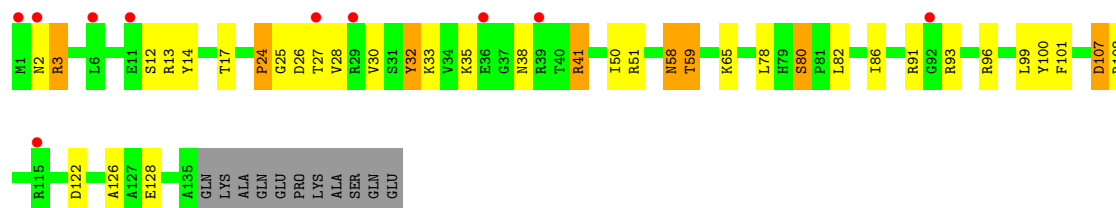
- Molecule 39: 50S ribosomal protein L18



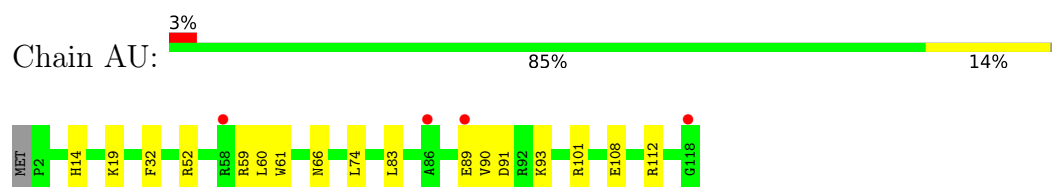
- Molecule 40: 50S ribosomal protein L19



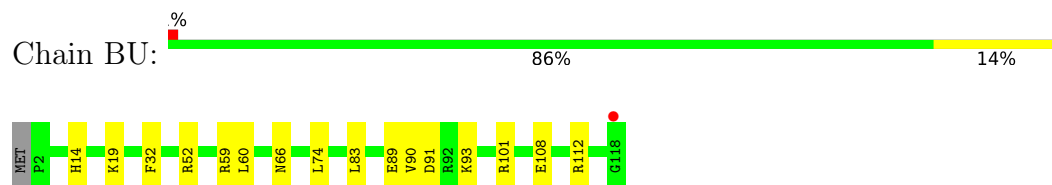
- Molecule 40: 50S ribosomal protein L19



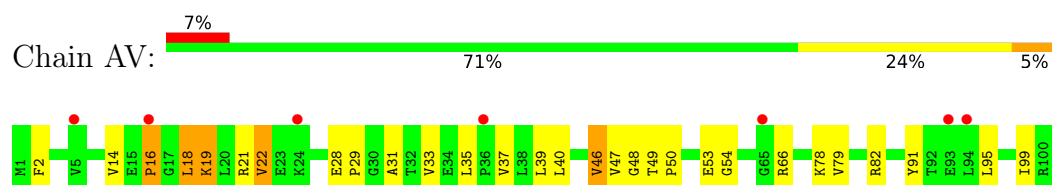
- Molecule 41: 50S ribosomal protein L20



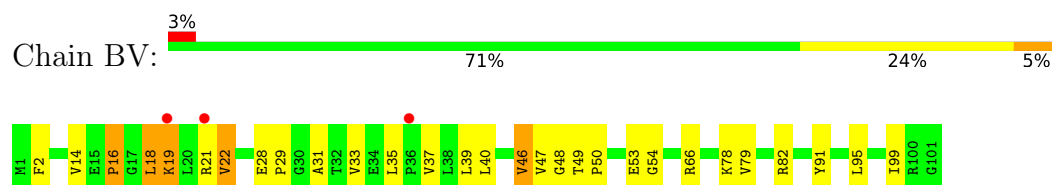
- Molecule 41: 50S ribosomal protein L20



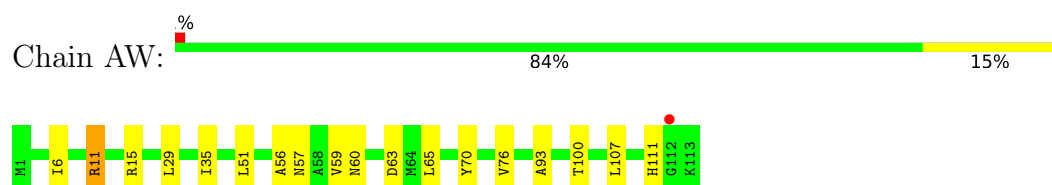
- Molecule 42: 50S ribosomal protein L21



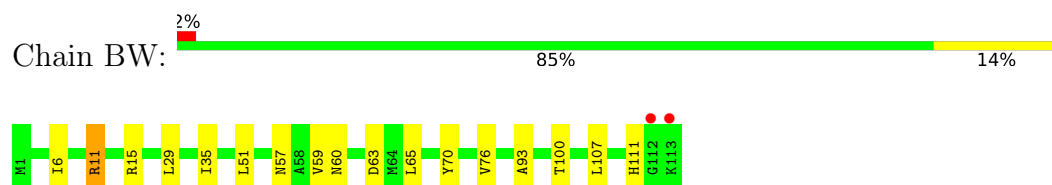
- Molecule 42: 50S ribosomal protein L21



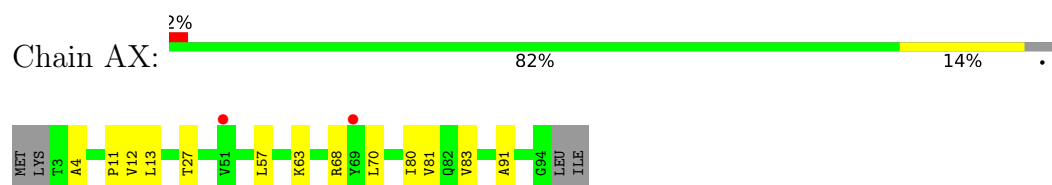
- Molecule 43: 50S ribosomal protein L22




- Molecule 43: 50S ribosomal protein L22

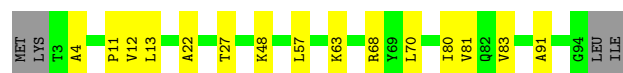


- Molecule 44: 50S ribosomal protein L23



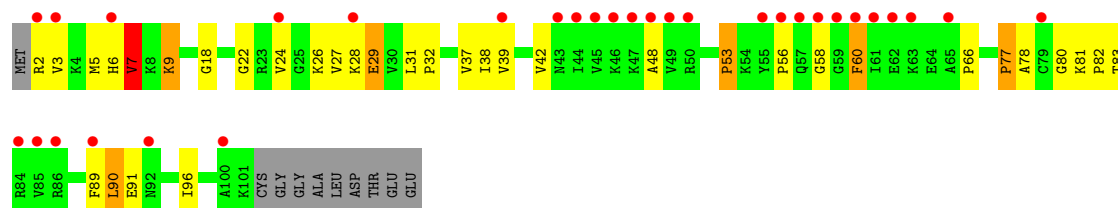
- Molecule 44: 50S ribosomal protein L23

Chain BX:  80% 16% 4%



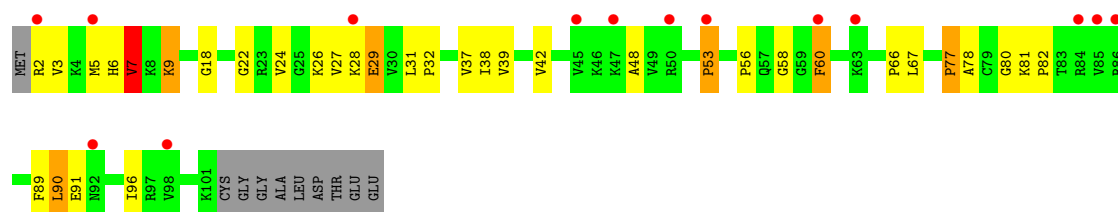
- Molecule 45: 50S ribosomal protein L24

Chain AY: 



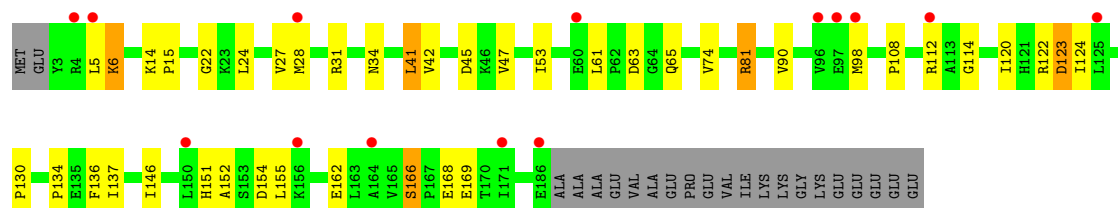
- Molecule 45: 50S ribosomal protein L24

Chain BY: 



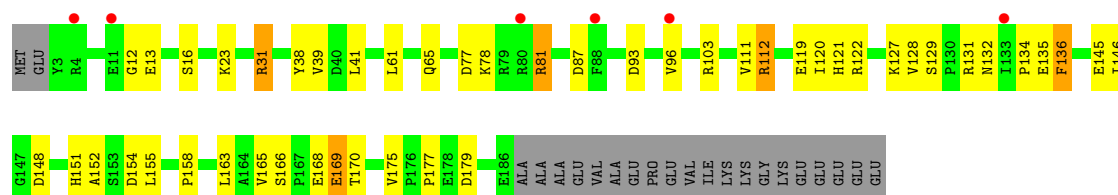
- Molecule 46: 50S ribosomal protein L25

Chain AZ: 

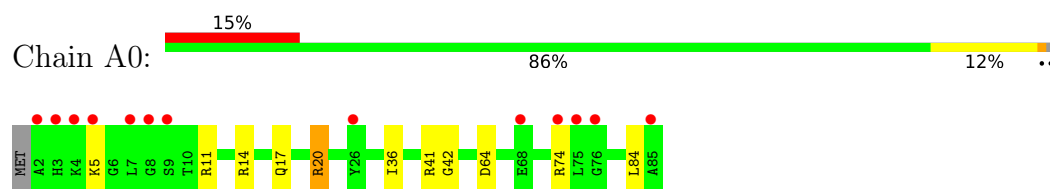


- Molecule 46: 50S ribosomal protein L25

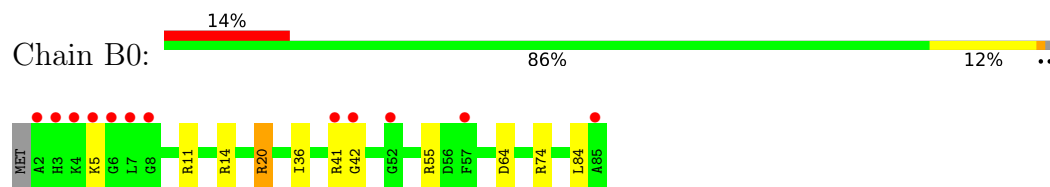
Chain BZ:



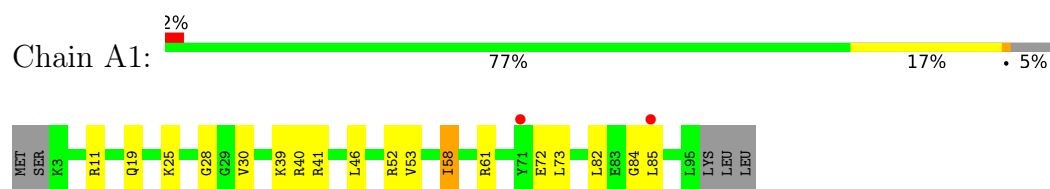
• Molecule 47: 50S ribosomal protein L27



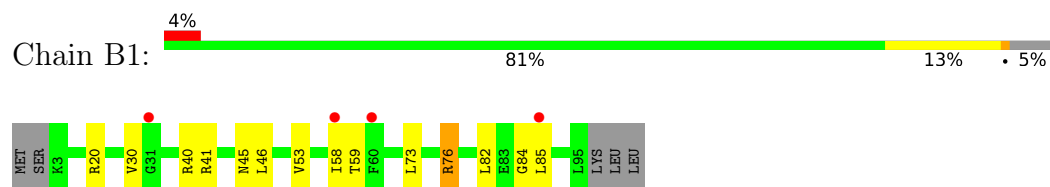
• Molecule 47: 50S ribosomal protein L27



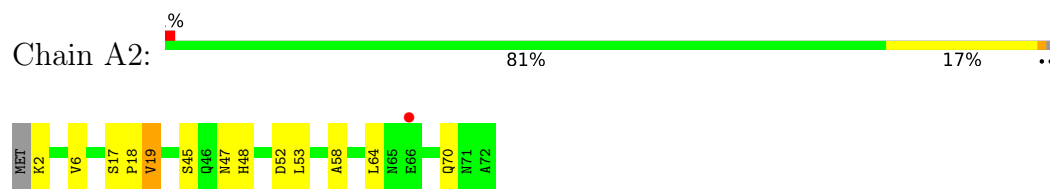
• Molecule 48: 50S ribosomal protein L28



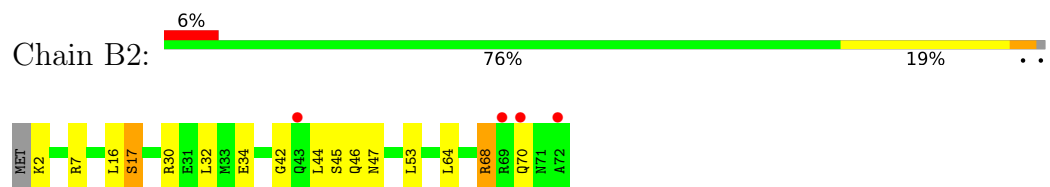
• Molecule 48: 50S ribosomal protein L28



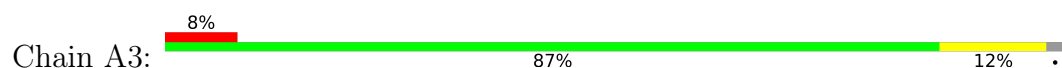
• Molecule 49: 50S ribosomal protein L29

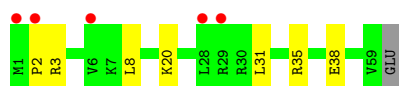


• Molecule 49: 50S ribosomal protein L29

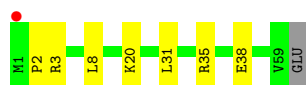
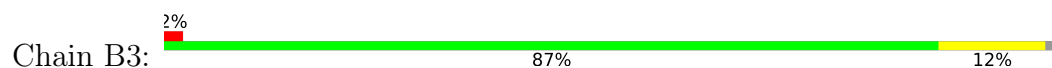


• Molecule 50: 50S ribosomal protein L30

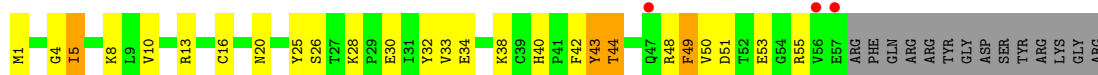
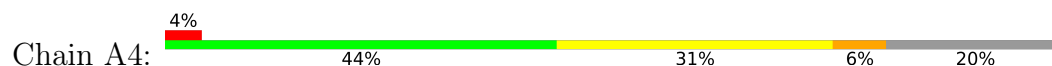




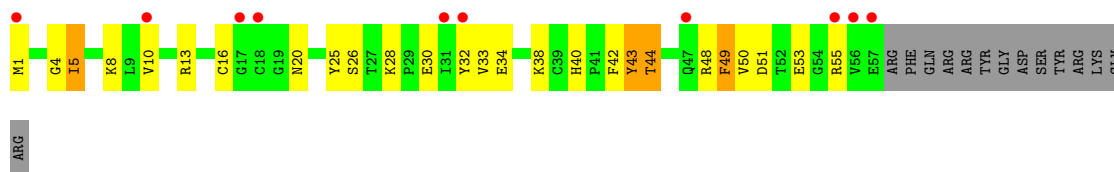
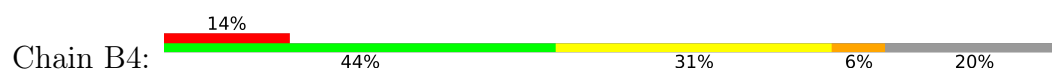
- Molecule 50: 50S ribosomal protein L30



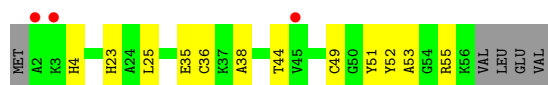
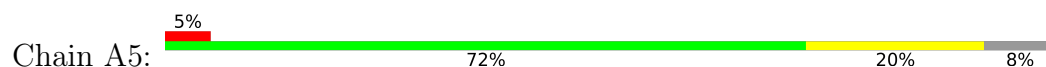
- Molecule 51: 50S ribosomal protein L31



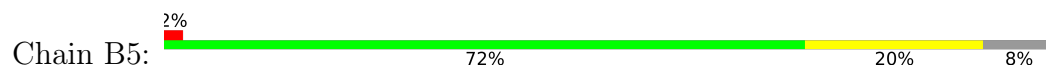
- Molecule 51: 50S ribosomal protein L31



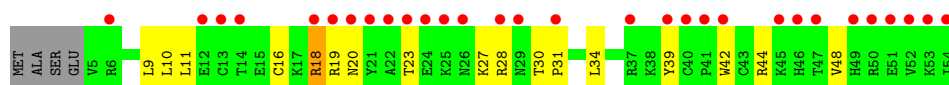
- Molecule 52: 50S ribosomal protein L32



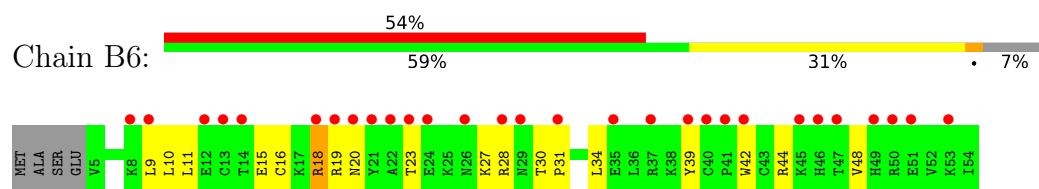
- Molecule 52: 50S ribosomal protein L32



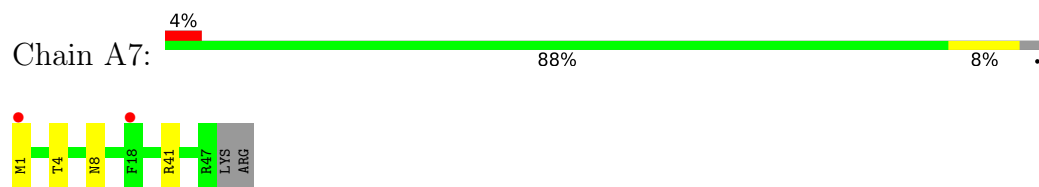
- Molecule 53: 50S ribosomal protein L33



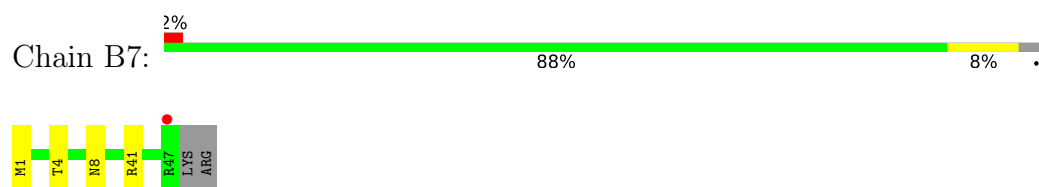
• Molecule 53: 50S ribosomal protein L33



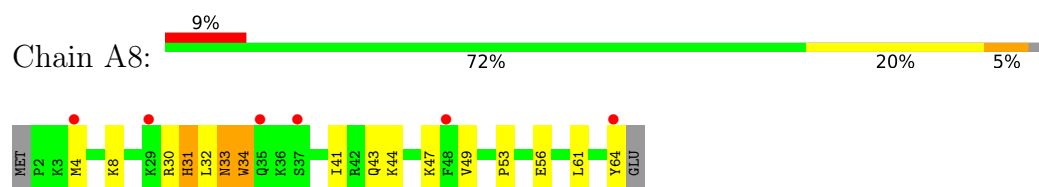
• Molecule 54: 50S ribosomal protein L34



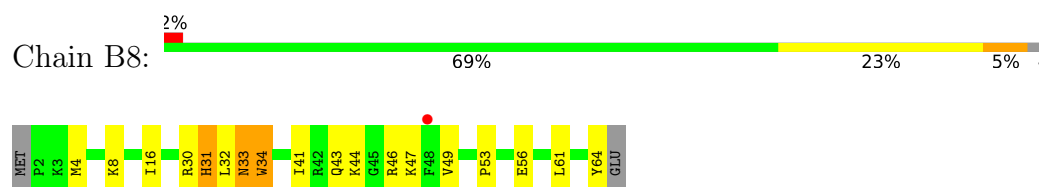
• Molecule 54: 50S ribosomal protein L34



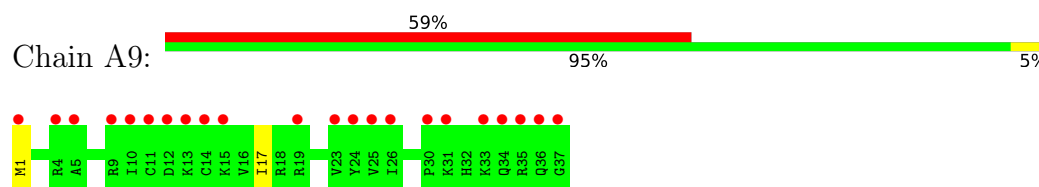
• Molecule 55: 50S ribosomal protein L35



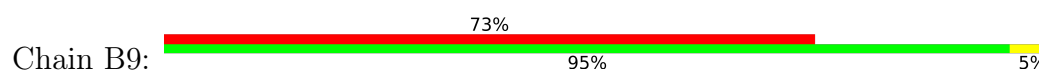
• Molecule 55: 50S ribosomal protein L35

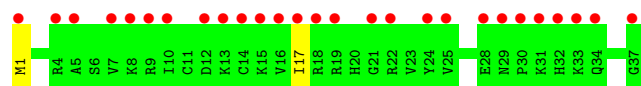


• Molecule 56: 50S ribosomal protein L36

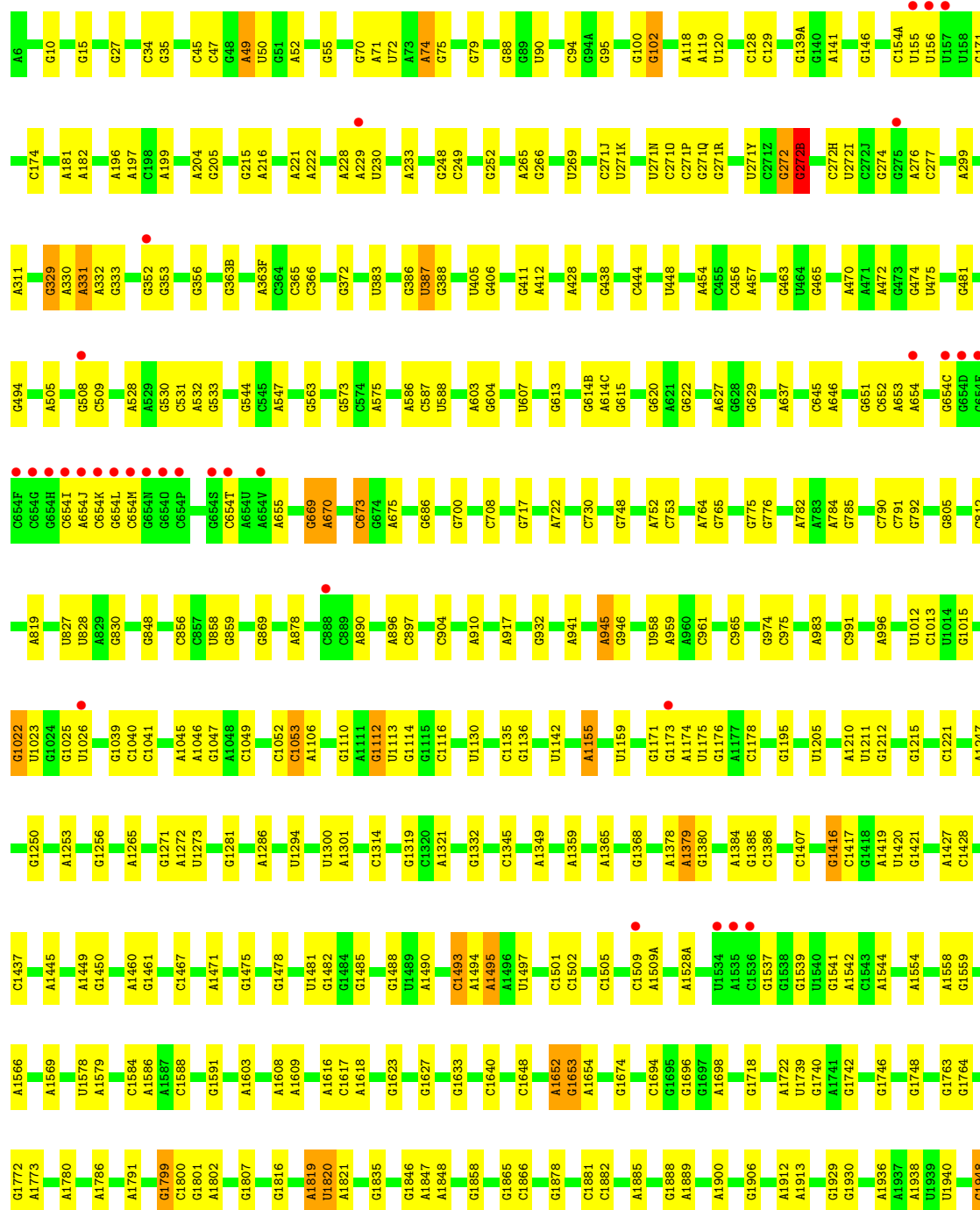
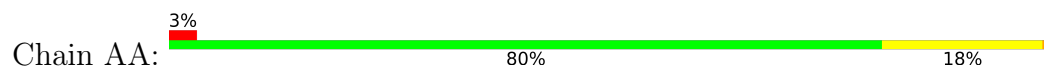


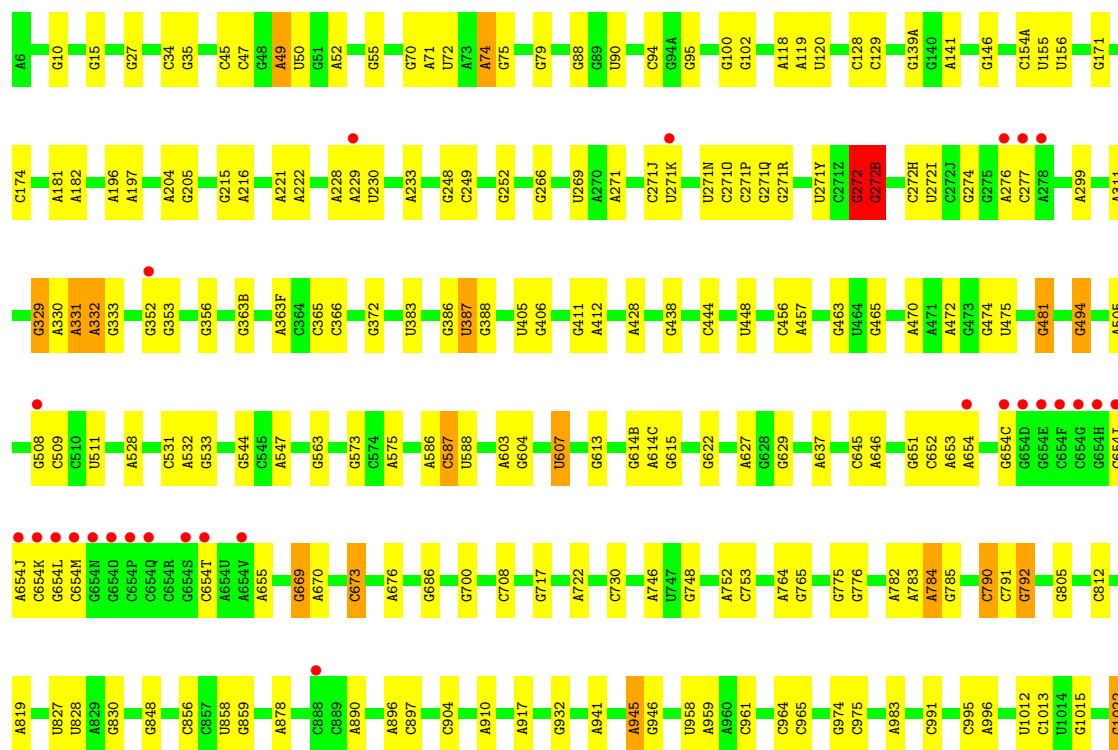
• Molecule 56: 50S ribosomal protein L36

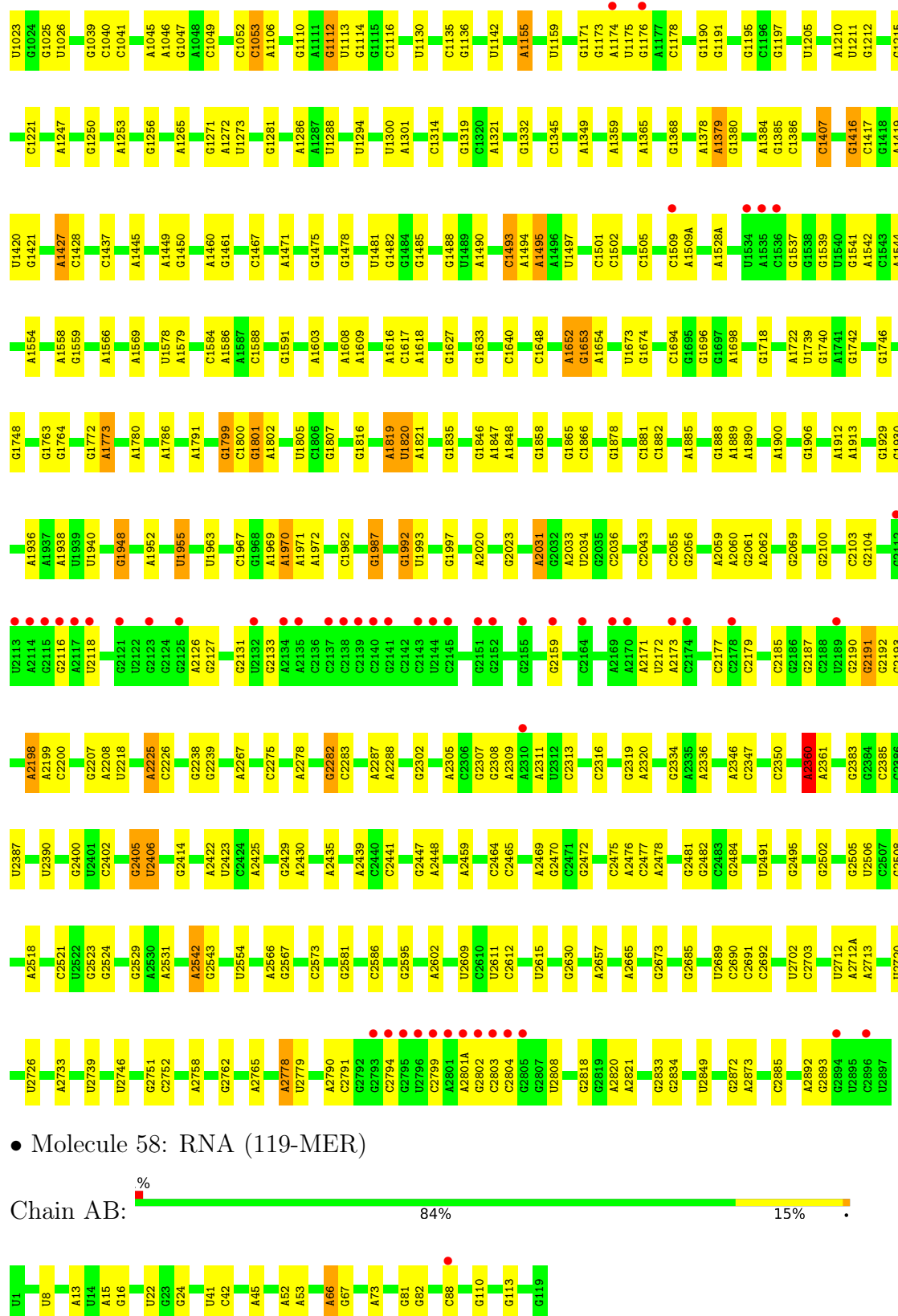


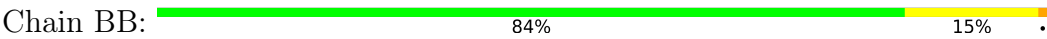


● Molecule 57: RNA (2848-MER)









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.57Å 451.96Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.9 (49.99-3.30)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.247 0.221 , 0.250	Depositor DCC
R_{free} test set	40918 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297206	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMG, ZN, A2M, MG, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	Ab	0.34	0/1935	0.61	0/2609
1	Bb	0.34	0/1935	0.61	0/2609
2	Ac	0.33	0/1636	0.57	0/2205
2	Bc	0.33	0/1636	0.57	0/2205
3	Ad	0.38	0/1733	0.64	0/2318
3	Bd	0.38	0/1733	0.64	0/2318
4	Ae	0.35	0/1162	0.63	0/1564
4	Be	0.36	0/1162	0.63	0/1564
5	Af	0.33	0/856	0.65	0/1154
5	Bf	0.35	0/856	0.65	0/1154
6	Ag	0.32	0/1276	0.54	0/1709
6	Bg	0.32	0/1276	0.54	0/1709
7	Ah	0.35	0/1136	0.65	0/1527
7	Bh	0.35	0/1136	0.65	0/1527
8	Ai	0.33	0/1029	0.53	0/1379
8	Bi	0.34	0/1029	0.55	0/1379
9	Aj	0.34	0/807	0.62	0/1085
9	Bj	0.35	0/807	0.62	0/1085
10	Ak	0.34	0/900	0.62	0/1213
10	Bk	0.36	0/900	0.62	0/1213
11	Al	0.41	0/986	0.74	1/1320 (0.1%)
11	Bl	0.41	0/986	0.74	1/1320 (0.1%)
12	Am	0.30	0/947	0.63	0/1270
12	Bm	0.31	0/947	0.61	0/1270
13	An	0.34	0/501	0.57	0/664
13	Bn	0.35	0/501	0.58	0/664
14	Ao	0.33	0/745	0.60	0/992
14	Bo	0.34	0/745	0.61	0/992
15	Ap	0.34	0/716	0.60	0/963
15	Bp	0.34	0/716	0.59	0/963
16	Aq	0.35	0/836	0.64	0/1117
16	Bq	0.36	0/836	0.64	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ar	0.35	0/579	0.65	0/768
17	Br	0.36	0/579	0.65	0/768
18	As	0.34	0/642	0.63	0/865
18	Bs	0.34	0/642	0.63	0/865
19	At	0.34	0/765	0.61	0/1007
19	Bt	0.32	0/765	0.60	0/1007
20	Au	0.40	0/212	0.56	0/277
20	Bu	0.37	0/212	0.56	0/277
21	Ay	0.31	0/781	0.67	1/1045 (0.1%)
21	By	0.38	0/777	0.69	0/1040
22	Aa	0.41	0/36190	0.69	14/56486 (0.0%)
22	Ba	0.41	0/36190	0.69	14/56486 (0.0%)
23	Ax	0.52	0/219	0.74	0/340
23	Bx	0.45	0/219	0.75	0/340
24	Av	0.43	0/1810	0.70	0/2821
24	Bv	0.46	0/1810	0.72	1/2821 (0.0%)
25	Aw	0.42	0/1832	0.70	0/2855
25	Bw	0.44	0/1832	0.69	0/2855
26	AC	0.33	0/956	0.53	0/1288
26	BC	0.34	0/956	0.53	0/1288
27	AD	0.45	0/2154	0.81	3/2905 (0.1%)
27	BD	0.48	0/2154	0.82	4/2905 (0.1%)
28	AE	0.45	0/1596	0.79	0/2153
28	BE	0.47	0/1596	0.80	0/2153
29	AF	0.42	0/1658	0.72	0/2244
29	BF	0.45	0/1658	0.74	0/2244
30	AG	0.37	0/1499	0.69	1/2016 (0.0%)
30	BG	0.39	0/1499	0.71	1/2016 (0.0%)
31	AH	0.38	0/1284	0.74	1/1739 (0.1%)
31	BH	0.42	0/1284	0.76	1/1739 (0.1%)
32	AI	0.42	0/1146	0.92	3/1551 (0.2%)
32	BI	0.41	0/1146	0.93	3/1551 (0.2%)
33	AJ	0.36	0/640	0.78	7/889 (0.8%)
33	BJ	0.39	0/640	0.78	6/889 (0.7%)
34	AN	0.38	0/1131	0.74	0/1525
34	BN	0.42	0/1131	0.75	1/1525 (0.1%)
35	AO	0.44	0/943	0.69	0/1269
35	BO	0.45	0/943	0.70	0/1269
36	AP	0.49	0/1131	1.03	5/1504 (0.3%)
36	BP	0.53	0/1131	1.05	5/1504 (0.3%)
37	AQ	0.39	0/1133	0.65	0/1515
37	BQ	0.42	0/1133	0.66	0/1515
38	AR	0.41	0/974	0.79	2/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BR	0.42	0/974	0.80	3/1302 (0.2%)
39	AS	0.41	0/778	0.72	0/1036
39	BS	0.44	0/778	0.73	0/1036
40	AT	0.44	0/1137	0.82	2/1519 (0.1%)
40	BT	0.45	0/1137	0.83	2/1519 (0.1%)
41	AU	0.45	0/975	0.70	0/1297
41	BU	0.50	0/975	0.74	0/1297
42	AV	0.40	0/790	0.74	0/1057
42	BV	0.44	0/790	0.76	0/1057
43	AW	0.43	0/907	0.73	0/1216
43	BW	0.44	0/907	0.73	0/1216
44	AX	0.44	0/739	0.71	0/993
44	BX	0.47	0/739	0.73	0/993
45	AY	0.47	0/788	0.75	1/1051 (0.1%)
45	BY	0.51	0/788	0.77	1/1051 (0.1%)
46	AZ	0.36	0/1499	0.66	0/2035
46	BZ	0.39	0/1499	0.71	0/2035
47	A0	0.39	0/671	0.69	0/892
47	B0	0.43	0/671	0.71	0/892
48	A1	0.41	0/738	0.77	0/981
48	B1	0.44	0/738	0.80	0/981
49	A2	0.34	0/600	0.60	0/793
49	B2	0.43	0/600	0.70	0/793
50	A3	0.35	0/472	0.68	0/634
50	B3	0.38	0/472	0.68	0/634
51	A4	0.40	0/460	0.71	1/621 (0.2%)
51	B4	0.42	0/460	0.72	1/621 (0.2%)
52	A5	0.45	0/441	0.76	0/596
52	B5	0.48	0/441	0.79	0/596
53	A6	0.45	0/440	0.77	0/586
53	B6	0.46	0/440	0.77	0/586
54	A7	0.41	0/417	0.67	0/550
54	B7	0.46	0/417	0.67	0/550
55	A8	0.53	0/515	0.87	0/679
55	B8	0.53	0/515	0.88	0/679
56	A9	0.35	0/310	0.59	0/407
56	B9	0.37	0/310	0.60	0/407
57	AA	0.49	0/68704	0.74	49/107260 (0.0%)
57	BA	0.54	2/68704 (0.0%)	0.74	59/107260 (0.1%)
58	AB	0.41	0/2853	0.70	0/4451
58	BB	0.45	0/2853	0.71	0/4451
All	All	0.45	2/321416 (0.0%)	0.72	194/480209 (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
21	Ay	0	1
22	Aa	0	11
22	Ba	1	11
24	Av	0	1
24	Bv	0	1
38	AR	0	1
38	BR	0	1
52	A5	0	1
52	B5	0	1
57	AA	2	50
57	BA	2	68
58	AB	0	1
58	BB	0	1
All	All	5	149

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2685	G	C6-O6	5.93	1.29	1.24
57	BA	2506	U	N1-C2	5.03	1.43	1.38

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BI	50	ARG	NE-CZ-NH2	-14.23	113.19	120.30
32	AI	50	ARG	NE-CZ-NH1	-14.08	113.26	120.30
32	BI	50	ARG	NE-CZ-NH1	13.66	127.13	120.30
32	AI	50	ARG	NE-CZ-NH2	13.15	126.88	120.30
57	AA	1992	G	C2'-C3'-O3'	10.34	132.24	109.50
57	BA	1992	G	C2'-C3'-O3'	10.27	132.09	109.50
22	Ba	1498	U	C2'-C3'-O3'	10.21	131.97	109.50
24	Bv	4	G	N9-C1'-C2'	-9.39	101.67	112.00
57	BA	1653	G	C2'-C3'-O3'	9.18	129.69	109.50
57	AA	1653	G	C2'-C3'-O3'	9.12	129.55	109.50
57	AA	1799	G	C2'-C3'-O3'	9.12	129.55	109.50
57	BA	1786	A	N9-C1'-C2'	9.01	125.72	114.00
22	Aa	115	G	C2'-C3'-O3'	9.00	129.30	109.50
57	AA	1786	A	N9-C1'-C2'	9.00	125.70	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1819	A	C2'-C3'-O3'	9.00	129.31	109.50
57	BA	1799	G	C2'-C3'-O3'	8.99	129.27	109.50
57	BA	49	A	C2'-C3'-O3'	8.83	128.93	109.50
57	BA	331	A	C2'-C3'-O3'	8.77	128.80	109.50
57	AA	331	A	C2'-C3'-O3'	8.76	128.76	109.50
22	Ba	115	G	C2'-C3'-O3'	8.73	128.71	109.50
57	BA	1022	G	C2'-C3'-O3'	8.72	128.68	109.50
22	Ba	575	G	C2'-C3'-O3'	8.65	128.54	109.50
57	AA	1819	A	C2'-C3'-O3'	8.54	128.28	109.50
57	AA	49	A	C2'-C3'-O3'	8.49	128.18	109.50
57	AA	1022	G	C2'-C3'-O3'	8.46	128.10	109.50
22	Aa	575	G	C2'-C3'-O3'	8.39	127.96	109.50
36	BP	52	GLU	N-CA-C	8.21	133.17	111.00
36	AP	52	GLU	N-CA-C	8.20	133.15	111.00
57	BA	1820	U	C2'-C3'-O3'	7.93	126.95	109.50
57	BA	1652	A	C2'-C3'-O3'	7.92	126.91	109.50
57	AA	1652	A	C2'-C3'-O3'	7.86	126.78	109.50
57	AA	1820	U	C2'-C3'-O3'	7.80	126.66	109.50
36	BP	53	GLY	N-CA-C	-7.79	93.63	113.10
22	Aa	1498	U	C2'-C3'-O3'	7.79	126.63	109.50
57	AA	2360	A	N9-C1'-C2'	-7.72	103.51	112.00
36	AP	53	GLY	N-CA-C	-7.64	93.99	113.10
57	BA	2360	A	N9-C1'-C2'	-7.58	103.66	112.00
57	BA	387	U	C2'-C3'-O3'	7.54	126.09	109.50
38	AR	4	LEU	CA-CB-CG	7.42	132.36	115.30
57	AA	387	U	C2'-C3'-O3'	7.39	125.75	109.50
22	Ba	366	C	C2'-C3'-O3'	7.30	125.56	109.50
57	BA	945	A	N9-C1'-C2'	7.30	123.49	114.00
38	BR	4	LEU	CA-CB-CG	7.20	131.85	115.30
22	Aa	366	C	C2'-C3'-O3'	7.09	125.10	109.50
27	AD	244	ARG	C-N-CD	-7.06	105.08	120.60
32	BI	50	ARG	CD-NE-CZ	7.05	133.47	123.60
22	Ba	509	A	C2'-C3'-O3'	7.00	124.90	113.70
32	AI	50	ARG	CD-NE-CZ	6.99	133.39	123.60
22	Aa	913	A	C2'-C3'-O3'	6.98	124.87	113.70
27	BD	244	ARG	C-N-CD	-6.95	105.32	120.60
22	Aa	509	A	C2'-C3'-O3'	6.94	124.81	113.70
57	AA	945	A	N9-C1'-C2'	6.86	122.91	114.00
22	Ba	913	A	C2'-C3'-O3'	6.81	124.60	113.70
57	BA	2346	A	O4'-C1'-N9	6.72	113.57	108.20
57	AA	2346	A	N9-C1'-C2'	6.68	122.68	114.00
57	AA	2225	A	C2'-C3'-O3'	6.62	124.28	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1495	A	N9-C1'-C2'	6.55	122.52	114.00
57	AA	2346	A	O4'-C1'-N9	6.51	113.41	108.20
33	BJ	33	PRO	N-CA-CB	6.49	111.08	103.30
57	AA	1495	A	N9-C1'-C2'	6.47	122.42	114.00
22	Aa	428	G	C2'-C3'-O3'	6.42	123.97	113.70
57	BA	2225	A	C2'-C3'-O3'	6.38	123.91	113.70
22	Aa	60	A	C2'-C3'-O3'	6.38	123.91	113.70
33	BJ	105	PRO	N-CA-CB	6.37	110.94	103.30
57	BA	2346	A	N9-C1'-C2'	6.29	122.18	114.00
57	AA	272	G	C2'-C3'-O3'	6.28	123.75	113.70
57	BA	1948	G	C5'-C4'-O4'	-6.24	101.61	109.10
36	BP	41	ARG	N-CA-C	-6.21	94.23	111.00
36	AP	41	ARG	N-CA-C	-6.21	94.23	111.00
57	BA	1365	A	C5'-C4'-C3'	6.20	125.93	116.00
22	Ba	428	G	C2'-C3'-O3'	6.19	123.61	113.70
57	AA	2405	G	N9-C1'-C2'	6.16	122.00	114.00
30	BG	125	PHE	N-CA-C	-6.12	94.47	111.00
22	Ba	60	A	C2'-C3'-O3'	6.12	123.49	113.70
57	BA	1970	A	C5'-C4'-O4'	6.11	116.43	109.10
57	BA	1493	C	N1-C1'-C2'	6.07	121.89	114.00
22	Ba	266	G	C2'-C3'-O3'	6.04	123.36	113.70
57	AA	1970	A	C5'-C4'-O4'	6.03	116.33	109.10
57	BA	272	G	C2'-C3'-O3'	6.02	123.33	113.70
36	AP	58	THR	N-CA-C	-6.00	94.79	111.00
57	AA	1365	A	C5'-C4'-C3'	5.99	125.59	116.00
57	AA	74	A	C2'-C3'-O3'	5.94	123.20	113.70
57	AA	2191	G	C2'-C3'-O3'	5.92	123.17	113.70
22	Aa	266	G	C2'-C3'-O3'	5.88	123.11	113.70
22	Aa	687	A	C2'-C3'-O3'	5.88	123.10	113.70
36	BP	58	THR	N-CA-C	-5.85	95.20	111.00
57	BA	1970	A	C5'-C4'-C3'	5.84	125.34	116.00
57	BA	2191	G	C2'-C3'-O3'	5.82	123.02	113.70
22	Ba	687	A	C2'-C3'-O3'	5.78	122.95	113.70
31	AH	158	HIS	N-CA-C	5.78	126.59	111.00
36	AP	54	GLY	N-CA-C	-5.75	98.72	113.10
40	BT	80	SER	N-CA-C	5.73	126.47	111.00
30	AG	54	GLU	N-CA-C	-5.72	95.55	111.00
57	AA	1493	C	N1-C1'-C2'	5.72	121.44	114.00
31	BH	158	HIS	N-CA-C	5.71	126.42	111.00
36	BP	54	GLY	N-CA-C	-5.71	98.83	113.10
57	BA	1698	A	N9-C1'-C2'	5.71	121.42	114.00
11	Bl	119	LYS	N-CA-C	-5.70	95.62	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1155	A	C5'-C4'-O4'	-5.68	102.29	109.10
40	AT	59	THR	N-CA-C	-5.68	95.68	111.00
57	BA	1987	G	C5'-C4'-C3'	-5.67	106.92	116.00
57	AA	1155	A	C5'-C4'-O4'	-5.67	102.30	109.10
57	AA	1819	A	C4'-C3'-O3'	5.67	124.34	113.00
11	Al	119	LYS	N-CA-C	-5.67	95.70	111.00
57	BA	1799	G	C4'-C3'-O3'	5.66	124.33	113.00
57	BA	2447	G	OP1-P-O3'	5.66	117.66	105.20
57	BA	673	C	C5'-C4'-O4'	-5.66	102.31	109.10
33	AJ	69	PRO	N-CA-CB	5.66	110.09	103.30
22	Aa	484	G	N9-C1'-C2'	5.65	121.34	114.00
33	AJ	77	PRO	N-CA-CB	5.64	110.06	103.30
57	BA	272(B)	G	C5'-C4'-C3'	5.63	125.01	116.00
40	BT	59	THR	N-CA-C	-5.62	95.81	111.00
57	AA	673	C	C5'-C4'-O4'	-5.61	102.37	109.10
57	AA	1948	G	C5'-C4'-O4'	-5.61	102.37	109.10
51	A4	43	TYR	N-CA-C	5.58	126.08	111.00
22	Ba	484	G	N9-C1'-C2'	5.58	121.25	114.00
57	AA	272(B)	G	C5'-C4'-C3'	5.58	124.92	116.00
57	BA	74	A	C2'-C3'-O3'	5.57	122.61	113.70
33	AJ	105	PRO	N-CA-CB	5.55	109.96	103.30
33	AJ	33	PRO	N-CA-CB	5.52	109.93	103.30
57	BA	2405	G	N9-C1'-C2'	5.51	121.16	114.00
33	AJ	101	PRO	N-CA-CB	5.49	109.89	103.30
57	BA	2278	A	C5'-C4'-C3'	5.48	124.77	116.00
57	BA	784	A	N9-C1'-C2'	5.48	121.13	114.00
51	B4	43	TYR	N-CA-C	5.47	125.76	111.00
33	AJ	129	PRO	N-CA-CB	5.45	109.83	103.30
57	BA	1970	A	C1'-O4'-C4'	-5.44	105.55	109.90
57	AA	1698	A	N9-C1'-C2'	5.42	121.04	114.00
27	BD	210	GLY	N-CA-C	-5.42	99.55	113.10
57	BA	1159	U	C5'-C4'-C3'	-5.42	107.33	116.00
40	AT	80	SER	N-CA-C	5.41	125.62	111.00
57	BA	587	C	OP2-P-O3'	5.41	117.11	105.20
57	BA	2778	A	C5'-C4'-C3'	-5.41	107.35	116.00
57	AA	1159	U	C5'-C4'-C3'	-5.40	107.36	116.00
45	BY	7	VAL	N-CA-C	5.39	125.57	111.00
57	BA	669	G	N9-C1'-C2'	5.39	121.01	114.00
57	AA	1970	A	C5'-C4'-C3'	5.38	124.61	116.00
57	BA	1773	A	N9-C1'-C2'	-5.37	106.09	112.00
57	AA	1053	C	N1-C1'-C2'	5.37	120.98	114.00
57	AA	1799	G	C4'-C3'-O3'	5.36	123.72	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BR	58	GLY	N-CA-C	5.36	126.50	113.10
57	BA	1053	C	N1-C1'-C2'	5.35	120.96	114.00
57	BA	964	C	C5'-C4'-C3'	-5.35	107.44	116.00
45	AY	7	VAL	N-CA-C	5.35	125.44	111.00
22	Ba	920	U	C5'-C4'-C3'	-5.34	107.45	116.00
57	AA	2521	C	C5'-C4'-C3'	-5.33	107.47	116.00
33	BJ	101	PRO	N-CA-CB	5.32	109.69	103.30
33	BJ	69	PRO	N-CA-CB	5.32	109.69	103.30
57	BA	629	G	C5'-C4'-C3'	-5.32	107.49	116.00
27	AD	210	GLY	N-CA-C	-5.31	99.81	113.10
57	BA	790	C	C2'-C3'-O3'	5.31	122.20	113.70
57	AA	272(B)	G	O4'-C1'-N9	5.31	112.45	108.20
38	AR	58	GLY	N-CA-C	5.30	126.36	113.10
33	AJ	86	PRO	N-CA-CB	5.29	109.65	103.30
57	AA	629	G	C5'-C4'-C3'	-5.29	107.54	116.00
57	BA	272(B)	G	O4'-C1'-N9	5.27	112.42	108.20
33	BJ	77	PRO	N-CA-CB	5.27	109.62	103.30
38	BR	5	LYS	N-CA-C	-5.26	96.79	111.00
57	AA	2278	A	C5'-C4'-C3'	5.26	124.42	116.00
57	AA	1987	G	C5'-C4'-C3'	-5.26	107.59	116.00
57	AA	2778	A	C5'-C4'-C3'	-5.25	107.60	116.00
57	BA	1819	A	C4'-C3'-O3'	5.24	123.48	113.00
57	BA	783	A	N9-C1'-C2'	-5.23	106.25	112.00
57	BA	2521	C	C5'-C4'-C3'	-5.20	107.67	116.00
57	AA	2094	G	C5'-C4'-C3'	-5.19	107.70	116.00
57	BA	1820	U	C4'-C3'-C2'	5.17	107.77	102.60
33	BJ	129	PRO	N-CA-CB	5.17	109.50	103.30
57	AA	669	G	N9-C1'-C2'	5.16	120.71	114.00
57	AA	1820	U	C4'-C3'-C2'	5.16	107.76	102.60
22	Aa	920	U	C5'-C4'-C3'	-5.16	107.75	116.00
22	Aa	115	G	C4'-C3'-C2'	5.14	107.74	102.60
27	BD	111	LEU	CA-CB-CG	5.14	127.12	115.30
57	BA	494	G	C5'-C4'-C3'	-5.14	107.78	116.00
57	AA	1294	U	C5'-C4'-C3'	-5.14	107.78	116.00
57	BA	2751	G	N9-C1'-C2'	5.12	120.66	114.00
57	BA	1407	C	C5'-C4'-C3'	-5.10	107.85	116.00
27	AD	111	LEU	CA-CB-CG	5.09	127.02	115.30
57	AA	2751	G	N9-C1'-C2'	5.08	120.61	114.00
57	BA	748	G	N9-C1'-C2'	5.08	120.60	114.00
57	AA	2031	A	N9-C1'-C2'	5.07	120.59	114.00
22	Ba	115	G	C4'-C3'-C2'	5.07	107.67	102.60
57	BA	1294	U	C5'-C4'-C3'	-5.06	107.90	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	676	A	O4'-C1'-N9	5.05	112.24	108.20
57	BA	481	G	N9-C1'-C2'	5.04	120.56	114.00
57	BA	332	A	N9-C1'-C2'	5.03	120.53	114.00
57	AA	265	A	N9-C1'-C2'	5.02	120.53	114.00
57	AA	748	G	N9-C1'-C2'	5.02	120.53	114.00
34	BN	67	LEU	N-CA-C	-5.02	97.44	111.00
57	BA	1190	G	C5'-C4'-C3'	-5.02	107.97	116.00
27	BD	229	VAL	CB-CA-C	-5.02	101.86	111.40
21	Ay	31	VAL	N-CA-C	-5.01	97.46	111.00
57	AA	49	A	C4'-C3'-C2'	5.01	107.61	102.60
22	Aa	389	A	C5'-C4'-C3'	5.00	124.00	116.00
22	Ba	575	G	O4'-C1'-N9	-5.00	104.20	108.20

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	AA	1799	G	C3'
57	AA	1819	A	C3'
22	Ba	1498	U	C3'
57	BA	1799	G	C3'
57	BA	1819	A	C3'

All (149) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	A5	51	TYR	Sidechain
57	AA	102	G	Sidechain
57	AA	1040	C	Sidechain
57	AA	1112	G	Sidechain
57	AA	1215	G	Sidechain
57	AA	1379	A	Sidechain
57	AA	1416	G	Sidechain
57	AA	15	G	Sidechain
57	AA	1623	G	Sidechain
57	AA	1627	G	Sidechain
57	AA	1633	G	Sidechain
57	AA	1772	G	Sidechain
57	AA	1802	A	Sidechain
57	AA	1807	G	Sidechain
57	AA	1940	U	Sidechain
57	AA	1952	A	Sidechain
57	AA	1955	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
57	AA	2020	A	Sidechain
57	AA	2031	A	Sidechain
57	AA	2059	A	Sidechain
57	AA	2086	U	Sidechain
57	AA	2198	A	Sidechain
57	AA	2282	G	Sidechain
57	AA	2360	A	Sidechain
57	AA	2390	U	Sidechain
57	AA	2406	U	Sidechain
57	AA	2414	G	Sidechain
57	AA	2464	C	Sidechain
57	AA	249	C	Sidechain
57	AA	2494	G	Sidechain
57	AA	2508	G	Sidechain
57	AA	2523	G	Sidechain
57	AA	2542	A	Sidechain
57	AA	2595	G	Sidechain
57	AA	2665	A	Sidechain
57	AA	27	G	Sidechain
57	AA	271(K)	U	Sidechain
57	AA	271(Q)	G	Sidechain
57	AA	272(B)	G	Sidechain
57	AA	329	G	Sidechain
57	AA	383	U	Sidechain
57	AA	463	G	Sidechain
57	AA	465	G	Sidechain
57	AA	47	C	Sidechain
57	AA	472	A	Sidechain
57	AA	52	A	Sidechain
57	AA	652	C	Sidechain
57	AA	670	A	Sidechain
57	AA	675	A	Sidechain
57	AA	70	G	Sidechain
57	AA	700	G	Sidechain
58	AB	66	A	Sidechain
38	AR	87	TYR	Sidechain
22	Aa	1077	G	Sidechain
22	Aa	1487	G	Sidechain
22	Aa	265	G	Sidechain
22	Aa	436	C	Sidechain
22	Aa	484	G	Sidechain
22	Aa	575	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	Aa	587	G	Sidechain
22	Aa	832	C	Sidechain
22	Aa	884	U	Sidechain
22	Aa	898	G	Sidechain
22	Aa	97	G	Sidechain
24	Av	4	G	Sidechain
21	Ay	83	ARG	Sidechain
52	B5	51	TYR	Sidechain
57	BA	1040	C	Sidechain
57	BA	1112	G	Sidechain
57	BA	1191	G	Sidechain
57	BA	1215	G	Sidechain
57	BA	1288	U	Sidechain
57	BA	1379	A	Sidechain
57	BA	1416	G	Sidechain
57	BA	1427	A	Sidechain
57	BA	15	G	Sidechain
57	BA	1627	G	Sidechain
57	BA	1633	G	Sidechain
57	BA	1673	U	Sidechain
57	BA	1772	G	Sidechain
57	BA	1801	G	Sidechain
57	BA	1802	A	Sidechain
57	BA	1805	U	Sidechain
57	BA	1807	G	Sidechain
57	BA	1890	A	Sidechain
57	BA	1940	U	Sidechain
57	BA	1952	A	Sidechain
57	BA	1955	U	Sidechain
57	BA	2020	A	Sidechain
57	BA	2031	A	Sidechain
57	BA	2059	A	Sidechain
57	BA	2198	A	Sidechain
57	BA	2267	A	Sidechain
57	BA	2282	G	Sidechain
57	BA	2360	A	Sidechain
57	BA	2387	U	Sidechain
57	BA	2390	U	Sidechain
57	BA	2406	U	Sidechain
57	BA	2414	G	Sidechain
57	BA	2464	C	Sidechain
57	BA	2475	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
57	BA	249	C	Sidechain
57	BA	2495	G	Sidechain
57	BA	2508	G	Sidechain
57	BA	2523	G	Sidechain
57	BA	2542	A	Sidechain
57	BA	2581	G	Sidechain
57	BA	2595	G	Sidechain
57	BA	2665	A	Sidechain
57	BA	2692	C	Sidechain
57	BA	27	G	Sidechain
57	BA	271	A	Sidechain
57	BA	271(K)	U	Sidechain
57	BA	271(Q)	G	Sidechain
57	BA	272	G	Sidechain
57	BA	272(B)	G	Sidechain
57	BA	2739	U	Sidechain
57	BA	2746	U	Sidechain
57	BA	2885	C	Sidechain
57	BA	329	G	Sidechain
57	BA	383	U	Sidechain
57	BA	463	G	Sidechain
57	BA	465	G	Sidechain
57	BA	47	C	Sidechain
57	BA	472	A	Sidechain
57	BA	511	U	Sidechain
57	BA	52	A	Sidechain
57	BA	607	U	Sidechain
57	BA	652	C	Sidechain
57	BA	670	A	Sidechain
57	BA	70	G	Sidechain
57	BA	700	G	Sidechain
57	BA	746	A	Sidechain
57	BA	792	G	Sidechain
57	BA	995	C	Sidechain
58	BB	66	A	Sidechain
38	BR	87	TYR	Sidechain
22	Ba	1077	G	Sidechain
22	Ba	1485	U	Sidechain
22	Ba	1512	U	Sidechain
22	Ba	436	C	Sidechain
22	Ba	575	G	Sidechain
22	Ba	587	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	Ba	760	G	Sidechain
22	Ba	832	C	Sidechain
22	Ba	884	U	Sidechain
22	Ba	9	G	Sidechain
22	Ba	97	G	Sidechain
24	Bv	4	G	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	232/256 (91%)	160 (69%)	45 (19%)	27 (12%)	0	2
1	Bb	232/256 (91%)	160 (69%)	46 (20%)	26 (11%)	0	2
2	Ac	204/239 (85%)	128 (63%)	51 (25%)	25 (12%)	0	1
2	Bc	204/239 (85%)	131 (64%)	49 (24%)	24 (12%)	0	2
3	Ad	206/209 (99%)	142 (69%)	45 (22%)	19 (9%)	1	4
3	Bd	206/209 (99%)	142 (69%)	46 (22%)	18 (9%)	1	5
4	Ae	148/162 (91%)	112 (76%)	24 (16%)	12 (8%)	1	6
4	Be	148/162 (91%)	111 (75%)	25 (17%)	12 (8%)	1	6
5	Af	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	6
5	Bf	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	6
6	Ag	153/156 (98%)	119 (78%)	24 (16%)	10 (6%)	1	9
6	Bg	153/156 (98%)	121 (79%)	22 (14%)	10 (6%)	1	9
7	Ah	136/138 (99%)	106 (78%)	27 (20%)	3 (2%)	6	30
7	Bh	136/138 (99%)	107 (79%)	26 (19%)	3 (2%)	6	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Ai	125/128 (98%)	92 (74%)	22 (18%)	11 (9%)	1	5
8	Bi	125/128 (98%)	90 (72%)	23 (18%)	12 (10%)	0	4
9	Aj	96/105 (91%)	71 (74%)	18 (19%)	7 (7%)	1	7
9	Bj	96/105 (91%)	69 (72%)	20 (21%)	7 (7%)	1	7
10	Ak	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	5	27
10	Bk	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	5	27
11	Al	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
11	Bl	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
12	Am	116/126 (92%)	76 (66%)	21 (18%)	19 (16%)	0	1
12	Bm	116/126 (92%)	74 (64%)	23 (20%)	19 (16%)	0	1
13	An	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
13	Bn	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
14	Ao	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	14
14	Bo	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	14
15	Ap	81/88 (92%)	55 (68%)	21 (26%)	5 (6%)	1	10
15	Bp	81/88 (92%)	56 (69%)	20 (25%)	5 (6%)	1	10
16	Aq	97/105 (92%)	82 (84%)	13 (13%)	2 (2%)	7	31
16	Bq	97/105 (92%)	83 (86%)	11 (11%)	3 (3%)	4	23
17	Ar	68/88 (77%)	47 (69%)	14 (21%)	7 (10%)	0	3
17	Br	68/88 (77%)	47 (69%)	15 (22%)	6 (9%)	1	5
18	As	76/93 (82%)	50 (66%)	14 (18%)	12 (16%)	0	1
18	Bs	76/93 (82%)	49 (64%)	15 (20%)	12 (16%)	0	1
19	At	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
19	Bt	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
20	Au	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	15
20	Bu	22/27 (82%)	15 (68%)	6 (27%)	1 (4%)	2	15
21	Ay	92/95 (97%)	55 (60%)	12 (13%)	25 (27%)	0	0
21	By	92/95 (97%)	58 (63%)	21 (23%)	13 (14%)	0	1
26	AC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	5	27
26	BC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	5	27
27	AD	269/276 (98%)	203 (76%)	37 (14%)	29 (11%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BD	269/276 (98%)	203 (76%)	36 (13%)	30 (11%)	0	2
28	AE	202/206 (98%)	138 (68%)	32 (16%)	32 (16%)	0	1
28	BE	202/206 (98%)	138 (68%)	31 (15%)	33 (16%)	0	1
29	AF	205/210 (98%)	154 (75%)	31 (15%)	20 (10%)	0	3
29	BF	205/210 (98%)	155 (76%)	30 (15%)	20 (10%)	0	3
30	AG	179/182 (98%)	106 (59%)	44 (25%)	29 (16%)	0	1
30	BG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	1
31	AH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
31	BH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
32	AI	143/148 (97%)	84 (59%)	38 (27%)	21 (15%)	0	1
32	BI	143/148 (97%)	85 (59%)	36 (25%)	22 (15%)	0	1
33	AJ	128/173 (74%)	56 (44%)	43 (34%)	29 (23%)	0	0
33	BJ	128/173 (74%)	44 (34%)	38 (30%)	46 (36%)	0	0
34	AN	136/140 (97%)	101 (74%)	20 (15%)	15 (11%)	0	2
34	BN	136/140 (97%)	100 (74%)	20 (15%)	16 (12%)	0	2
35	AO	120/122 (98%)	104 (87%)	10 (8%)	6 (5%)	2	14
35	BO	120/122 (98%)	102 (85%)	13 (11%)	5 (4%)	3	17
36	AP	144/150 (96%)	76 (53%)	35 (24%)	33 (23%)	0	0
36	BP	144/150 (96%)	79 (55%)	32 (22%)	33 (23%)	0	0
37	AQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	11
37	BQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	11
38	AR	115/118 (98%)	85 (74%)	20 (17%)	10 (9%)	1	5
38	BR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	1	5
39	AS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
39	BS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
40	AT	133/146 (91%)	90 (68%)	24 (18%)	19 (14%)	0	1
40	BT	133/146 (91%)	90 (68%)	23 (17%)	20 (15%)	0	1
41	AU	115/118 (98%)	88 (76%)	21 (18%)	6 (5%)	2	13
41	BU	115/118 (98%)	90 (78%)	20 (17%)	5 (4%)	2	16
42	AV	99/101 (98%)	65 (66%)	17 (17%)	17 (17%)	0	1
42	BV	99/101 (98%)	64 (65%)	18 (18%)	17 (17%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AW	111/113 (98%)	89 (80%)	11 (10%)	11 (10%)	0	3
43	BW	111/113 (98%)	90 (81%)	11 (10%)	10 (9%)	1	4
44	AX	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	2	11
44	BX	90/96 (94%)	72 (80%)	11 (12%)	7 (8%)	1	6
45	AY	98/110 (89%)	51 (52%)	18 (18%)	29 (30%)	0	0
45	BY	98/110 (89%)	52 (53%)	16 (16%)	30 (31%)	0	0
46	AZ	182/206 (88%)	115 (63%)	40 (22%)	27 (15%)	0	1
46	BZ	182/206 (88%)	118 (65%)	37 (20%)	27 (15%)	0	1
47	A0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	14
47	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	14
48	A1	91/98 (93%)	74 (81%)	10 (11%)	7 (8%)	1	6
48	B1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	8
49	A2	69/72 (96%)	44 (64%)	16 (23%)	9 (13%)	0	1
49	B2	69/72 (96%)	50 (72%)	13 (19%)	6 (9%)	1	5
50	A3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	2	12
50	B3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	2	12
51	A4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
51	B4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
52	A5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
52	B5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
53	A6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0
53	B6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0
54	A7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	B7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	A8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
55	B8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
56	A9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
56	B9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	12016/13122 (92%)	8475 (70%)	2157 (18%)	1384 (12%)	0	2

All (1384) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ab	15	VAL
1	Ab	18	GLY
1	Ab	26	PRO
1	Ab	63	MET
1	Ab	80	ILE
1	Ab	95	GLN
1	Ab	194	PRO
1	Ab	195	ASP
1	Ab	238	LEU
1	Ab	239	VAL
2	Ac	4	LYS
2	Ac	12	LEU
2	Ac	45	LYS
2	Ac	46	GLU
2	Ac	47	LEU
3	Ad	4	TYR
3	Ad	5	ILE
3	Ad	129	ASN
3	Ad	196	LEU
5	Af	40	VAL
5	Af	43	LEU
5	Af	62	TRP
7	Ah	2	LEU
8	Ai	89	ASN
8	Ai	103	THR
8	Ai	105	ASP
9	Aj	36	GLY
9	Aj	51	ARG
9	Aj	57	LYS
10	Ak	25	TYR
11	Al	91	LYS
11	Al	115	LYS
12	Am	4	ILE
12	Am	5	ALA
12	Am	12	ASN
12	Am	63	THR
12	Am	66	LEU
12	Am	83	ASP
12	Am	107	ALA
12	Am	113	PRO
12	Am	117	VAL
13	An	15	LYS
13	An	16	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	An	52	GLN
18	As	10	PHE
18	As	26	GLY
18	As	28	LYS
19	At	11	SER
19	At	71	THR
19	At	74	LYS
19	At	99	LEU
20	Au	3	LYS
21	Ay	3	TYR
21	Ay	9	GLU
21	Ay	20	SER
21	Ay	31	VAL
21	Ay	36	SER
21	Ay	37	PRO
21	Ay	40	GLU
21	Ay	47	MET
21	Ay	48	PRO
21	Ay	56	ARG
21	Ay	59	GLY
21	Ay	71	VAL
21	Ay	78	VAL
21	Ay	85	GLU
21	Ay	94	ILE
27	AD	25	THR
27	AD	27	THR
27	AD	34	VAL
27	AD	35	LYS
27	AD	225	ALA
27	AD	239	ARG
27	AD	267	SER
27	AD	268	ARG
27	AD	271	ILE
28	AE	53	PRO
28	AE	54	GLN
28	AE	64	LYS
28	AE	66	HIS
28	AE	68	ALA
28	AE	72	VAL
28	AE	77	ILE
28	AE	83	ASP
28	AE	88	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	AE	89	ASP
28	AE	118	LYS
28	AE	131	ALA
28	AE	186	GLY
28	AE	203	LYS
29	AF	3	GLU
29	AF	21	ALA
29	AF	27	GLU
29	AF	59	TYR
29	AF	89	VAL
29	AF	132	VAL
29	AF	133	ASN
29	AF	134	GLY
30	AG	49	ASP
30	AG	50	ALA
30	AG	75	LYS
30	AG	82	LEU
30	AG	96	ARG
30	AG	104	GLU
30	AG	110	ALA
30	AG	118	ARG
30	AG	122	PRO
30	AG	126	ASP
30	AG	159	VAL
31	AH	8	PRO
31	AH	13	LYS
31	AH	24	VAL
31	AH	83	TYR
31	AH	92	ILE
31	AH	154	PRO
31	AH	155	SER
31	AH	156	ALA
31	AH	157	TYR
31	AH	159	GLU
32	AI	15	VAL
32	AI	71	ILE
32	AI	83	ALA
32	AI	85	GLU
32	AI	88	ILE
32	AI	104	GLN
32	AI	105	HIS
32	AI	120	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	AI	132	PRO
32	AI	135	GLU
32	AI	143	SER
33	AJ	17	LEU
33	AJ	33	PRO
33	AJ	53	VAL
33	AJ	54	ALA
33	AJ	68	LEU
33	AJ	90	ALA
33	AJ	105	PRO
33	AJ	112	LEU
33	AJ	120	LYS
34	AN	58	ASP
34	AN	134	ARG
35	AO	29	ASN
36	AP	9	ASN
36	AP	14	LYS
36	AP	17	LYS
36	AP	19	VAL
36	AP	25	SER
36	AP	31	ALA
36	AP	35	HIS
36	AP	47	ASP
36	AP	58	THR
36	AP	103	ALA
36	AP	108	LYS
36	AP	111	ARG
36	AP	147	LEU
36	AP	148	LEU
37	AQ	2	LEU
37	AQ	19	GLY
37	AQ	27	VAL
37	AQ	134	ARG
37	AQ	135	ASP
38	AR	8	ARG
38	AR	45	ARG
39	AS	23	ARG
39	AS	24	LEU
39	AS	35	ILE
39	AS	59	LYS
39	AS	82	ILE
39	AS	94	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	AS	97	ARG
40	AT	2	ASN
40	AT	24	PRO
40	AT	26	ASP
40	AT	27	THR
40	AT	28	VAL
40	AT	30	VAL
40	AT	33	LYS
40	AT	58	ASN
40	AT	80	SER
40	AT	107	ASP
41	AU	91	ASP
41	AU	93	LYS
42	AV	16	PRO
42	AV	19	LYS
42	AV	46	VAL
42	AV	53	GLU
43	AW	11	ARG
43	AW	111	HIS
44	AX	12	VAL
45	AY	3	VAL
45	AY	7	VAL
45	AY	27	VAL
45	AY	42	VAL
45	AY	60	PHE
45	AY	77	PRO
45	AY	78	ALA
46	AZ	6	LYS
46	AZ	31	ARG
46	AZ	65	GLN
46	AZ	123	ASP
46	AZ	134	PRO
46	AZ	136	PHE
46	AZ	146	ILE
46	AZ	152	ALA
48	A1	52	ARG
48	A1	58	ILE
49	A2	45	SER
49	A2	48	HIS
49	A2	70	GLN
50	A3	3	ARG
50	A3	38	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	A4	8	LYS
51	A4	26	SER
51	A4	38	LYS
51	A4	43	TYR
51	A4	44	THR
51	A4	48	ARG
52	A5	35	GLU
52	A5	36	CYS
52	A5	49	CYS
52	A5	53	ALA
53	A6	18	ARG
53	A6	19	ARG
53	A6	27	LYS
53	A6	28	ARG
53	A6	31	PRO
55	A8	33	ASN
55	A8	34	TRP
1	Bb	15	VAL
1	Bb	18	GLY
1	Bb	26	PRO
1	Bb	63	MET
1	Bb	80	ILE
1	Bb	95	GLN
1	Bb	194	PRO
1	Bb	195	ASP
1	Bb	238	LEU
1	Bb	239	VAL
2	Bc	4	LYS
2	Bc	12	LEU
2	Bc	45	LYS
2	Bc	46	GLU
2	Bc	47	LEU
3	Bd	4	TYR
3	Bd	5	ILE
3	Bd	129	ASN
3	Bd	196	LEU
5	Bf	40	VAL
5	Bf	43	LEU
5	Bf	62	TRP
7	Bh	2	LEU
8	Bi	89	ASN
8	Bi	101	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	Bi	103	THR
8	Bi	105	ASP
9	Bj	36	GLY
9	Bj	51	ARG
9	Bj	57	LYS
10	Bk	25	TYR
11	Bl	91	LYS
11	Bl	115	LYS
12	Bm	4	ILE
12	Bm	5	ALA
12	Bm	12	ASN
12	Bm	21	TYR
12	Bm	63	THR
12	Bm	66	LEU
12	Bm	69	GLU
12	Bm	83	ASP
12	Bm	107	ALA
12	Bm	113	PRO
12	Bm	117	VAL
13	Bn	15	LYS
13	Bn	16	PHE
13	Bn	52	GLN
18	Bs	10	PHE
18	Bs	26	GLY
18	Bs	28	LYS
19	Bt	11	SER
19	Bt	71	THR
19	Bt	74	LYS
19	Bt	99	LEU
20	Bu	3	LYS
21	By	36	SER
21	By	48	PRO
21	By	49	ASP
21	By	94	ILE
27	BD	25	THR
27	BD	27	THR
27	BD	34	VAL
27	BD	35	LYS
27	BD	239	ARG
27	BD	267	SER
27	BD	268	ARG
27	BD	271	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BE	53	PRO
28	BE	54	GLN
28	BE	64	LYS
28	BE	66	HIS
28	BE	68	ALA
28	BE	72	VAL
28	BE	77	ILE
28	BE	83	ASP
28	BE	88	GLY
28	BE	89	ASP
28	BE	118	LYS
28	BE	131	ALA
28	BE	186	GLY
28	BE	203	LYS
29	BF	3	GLU
29	BF	21	ALA
29	BF	27	GLU
29	BF	59	TYR
29	BF	89	VAL
29	BF	132	VAL
29	BF	133	ASN
29	BF	134	GLY
30	BG	6	ALA
30	BG	43	LEU
30	BG	47	LYS
30	BG	75	LYS
30	BG	81	LYS
30	BG	82	LEU
30	BG	87	PRO
30	BG	96	ARG
30	BG	110	ALA
30	BG	112	PRO
30	BG	115	ARG
30	BG	143	GLU
31	BH	8	PRO
31	BH	13	LYS
31	BH	24	VAL
31	BH	83	TYR
31	BH	92	ILE
31	BH	154	PRO
31	BH	155	SER
31	BH	156	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	BH	157	TYR
31	BH	159	GLU
32	BI	15	VAL
32	BI	71	ILE
32	BI	83	ALA
32	BI	85	GLU
32	BI	88	ILE
32	BI	104	GLN
32	BI	105	HIS
32	BI	120	ILE
32	BI	132	PRO
32	BI	135	GLU
32	BI	143	SER
33	BJ	32	LEU
33	BJ	33	PRO
33	BJ	51	LEU
33	BJ	59	ILE
33	BJ	69	PRO
33	BJ	70	GLU
33	BJ	80	VAL
33	BJ	81	VAL
33	BJ	82	PHE
33	BJ	83	TYR
33	BJ	85	ASP
33	BJ	86	PRO
33	BJ	87	VAL
33	BJ	100	ASN
33	BJ	101	PRO
33	BJ	105	PRO
33	BJ	120	LYS
33	BJ	123	GLU
33	BJ	124	ALA
33	BJ	125	LEU
34	BN	58	ASP
34	BN	134	ARG
35	BO	29	ASN
36	BP	9	ASN
36	BP	14	LYS
36	BP	17	LYS
36	BP	19	VAL
36	BP	25	SER
36	BP	31	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BP	35	HIS
36	BP	47	ASP
36	BP	58	THR
36	BP	103	ALA
36	BP	108	LYS
36	BP	111	ARG
36	BP	147	LEU
36	BP	148	LEU
37	BQ	2	LEU
37	BQ	19	GLY
37	BQ	27	VAL
37	BQ	134	ARG
37	BQ	135	ASP
38	BR	8	ARG
38	BR	45	ARG
39	BS	23	ARG
39	BS	24	LEU
39	BS	35	ILE
39	BS	59	LYS
39	BS	82	ILE
39	BS	92	TYR
39	BS	94	TYR
39	BS	97	ARG
40	BT	2	ASN
40	BT	24	PRO
40	BT	26	ASP
40	BT	28	VAL
40	BT	30	VAL
40	BT	33	LYS
40	BT	58	ASN
40	BT	80	SER
40	BT	107	ASP
41	BU	91	ASP
41	BU	93	LYS
42	BV	16	PRO
42	BV	19	LYS
42	BV	46	VAL
42	BV	53	GLU
43	BW	11	ARG
43	BW	111	HIS
44	BX	12	VAL
45	BY	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	BY	7	VAL
45	BY	27	VAL
45	BY	42	VAL
45	BY	60	PHE
45	BY	77	PRO
45	BY	78	ALA
45	BY	90	LEU
45	BY	91	GLU
46	BZ	31	ARG
46	BZ	65	GLN
46	BZ	112	ARG
46	BZ	121	HIS
46	BZ	122	ARG
46	BZ	128	VAL
46	BZ	136	PHE
46	BZ	146	ILE
46	BZ	148	ASP
46	BZ	152	ALA
46	BZ	166	SER
48	B1	30	VAL
48	B1	58	ILE
48	B1	85	LEU
49	B2	45	SER
49	B2	47	ASN
50	B3	3	ARG
50	B3	38	GLU
51	B4	8	LYS
51	B4	26	SER
51	B4	38	LYS
51	B4	43	TYR
51	B4	44	THR
51	B4	48	ARG
52	B5	35	GLU
52	B5	36	CYS
52	B5	49	CYS
52	B5	53	ALA
53	B6	18	ARG
53	B6	19	ARG
53	B6	27	LYS
53	B6	28	ARG
53	B6	31	PRO
55	B8	33	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	B8	34	TRP
1	Ab	13	ALA
1	Ab	154	LEU
1	Ab	165	VAL
1	Ab	217	ARG
2	Ac	20	SER
2	Ac	52	LEU
2	Ac	54	ARG
2	Ac	61	ALA
2	Ac	74	GLY
2	Ac	145	GLY
2	Ac	154	SER
2	Ac	156	ARG
2	Ac	165	THR
3	Ad	3	ARG
3	Ad	30	LYS
3	Ad	47	ARG
3	Ad	110	PHE
3	Ad	171	GLY
4	Ae	129	ILE
6	Ag	7	ALA
7	Ah	37	ARG
8	Ai	12	GLU
8	Ai	41	VAL
8	Ai	42	ARG
8	Ai	95	LYS
9	Aj	52	GLY
9	Aj	59	SER
10	Ak	117	ASN
11	Al	27	LEU
11	Al	46	LYS
11	Al	89	ARG
11	Al	90	VAL
11	Al	92	ASP
12	Am	7	VAL
12	Am	21	TYR
12	Am	67	GLU
12	Am	100	GLY
14	Ao	87	ILE
15	Ap	49	LEU
15	Ap	78	GLY
16	Aq	33	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Aq	34	LYS
17	Ar	28	GLU
17	Ar	45	SER
18	As	29	ARG
18	As	80	TYR
19	At	50	GLU
19	At	100	ILE
19	At	103	GLY
21	Ay	38	ARG
21	Ay	49	ASP
21	Ay	57	SER
26	AC	174	ALA
27	AD	32	SER
27	AD	36	PRO
27	AD	58	HIS
27	AD	127	VAL
27	AD	169	GLU
28	AE	2	LYS
28	AE	57	LYS
28	AE	69	LYS
28	AE	71	GLY
28	AE	90	THR
28	AE	130	GLY
28	AE	185	LYS
29	AF	86	GLY
29	AF	128	ALA
30	AG	14	GLU
30	AG	48	GLU
30	AG	97	ASP
30	AG	117	PHE
30	AG	127	GLY
30	AG	129	GLY
30	AG	142	PRO
31	AH	14	GLY
31	AH	45	VAL
31	AH	110	SER
31	AH	138	LYS
31	AH	160	LYS
31	AH	165	ALA
32	AI	6	LEU
32	AI	76	THR
32	AI	91	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	AI	99	GLU
32	AI	115	ALA
33	AJ	7	VAL
33	AJ	56	ASN
33	AJ	59	ILE
33	AJ	80	VAL
33	AJ	106	GLN
33	AJ	113	GLN
33	AJ	129	PRO
34	AN	4	TYR
34	AN	42	TRP
34	AN	133	GLN
35	AO	48	PRO
35	AO	98	VAL
36	AP	18	ARG
36	AP	34	GLY
36	AP	89	ALA
36	AP	98	GLU
36	AP	104	GLY
36	AP	106	LEU
36	AP	107	LYS
36	AP	141	ALA
37	AQ	62	GLY
38	AR	58	GLY
38	AR	86	ARG
38	AR	117	VAL
39	AS	13	ARG
39	AS	57	LYS
39	AS	90	GLY
39	AS	92	TYR
39	AS	102	ALA
39	AS	104	GLY
39	AS	107	GLU
40	AT	3	ARG
40	AT	17	THR
40	AT	35	LYS
41	AU	32	PHE
41	AU	89	GLU
42	AV	22	VAL
42	AV	31	ALA
42	AV	35	LEU
42	AV	48	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	AW	29	LEU
43	AW	63	ASP
44	AX	91	ALA
45	AY	5	MET
45	AY	24	VAL
45	AY	26	LYS
45	AY	48	ALA
45	AY	80	GLY
45	AY	90	LEU
45	AY	91	GLU
46	AZ	5	LEU
46	AZ	42	VAL
46	AZ	81	ARG
46	AZ	114	GLY
46	AZ	154	ASP
46	AZ	166	SER
46	AZ	168	GLU
48	A1	84	GLY
49	A2	18	PRO
49	A2	19	VAL
49	A2	47	ASN
51	A4	16	CYS
51	A4	40	HIS
51	A4	49	PHE
51	A4	50	VAL
53	A6	44	ARG
55	A8	31	HIS
55	A8	43	GLN
1	Bb	13	ALA
1	Bb	165	VAL
1	Bb	217	ARG
2	Bc	20	SER
2	Bc	52	LEU
2	Bc	54	ARG
2	Bc	61	ALA
2	Bc	74	GLY
2	Bc	145	GLY
2	Bc	154	SER
2	Bc	156	ARG
2	Bc	165	THR
3	Bd	3	ARG
3	Bd	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Bd	47	ARG
3	Bd	110	PHE
3	Bd	171	GLY
4	Be	129	ILE
4	Be	153	LYS
6	Bg	7	ALA
7	Bh	37	ARG
8	Bi	12	GLU
8	Bi	41	VAL
8	Bi	42	ARG
8	Bi	95	LYS
9	Bj	52	GLY
9	Bj	59	SER
10	Bk	117	ASN
11	Bl	27	LEU
11	Bl	46	LYS
11	Bl	89	ARG
11	Bl	90	VAL
11	Bl	92	ASP
11	Bl	121	GLY
12	Bm	7	VAL
12	Bm	67	GLU
12	Bm	100	GLY
14	Bo	87	ILE
15	Bp	49	LEU
15	Bp	78	GLY
16	Bq	33	GLY
16	Bq	34	LYS
17	Br	28	GLU
17	Br	45	SER
18	Bs	29	ARG
18	Bs	80	TYR
19	Bt	50	GLU
19	Bt	100	ILE
19	Bt	103	GLY
21	By	13	LYS
21	By	20	SER
21	By	78	VAL
26	BC	174	ALA
27	BD	32	SER
27	BD	36	PRO
27	BD	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	BD	127	VAL
27	BD	225	ALA
28	BE	2	LYS
28	BE	57	LYS
28	BE	63	LEU
28	BE	69	LYS
28	BE	71	GLY
28	BE	90	THR
28	BE	185	LYS
29	BF	86	GLY
30	BG	10	LYS
30	BG	50	ALA
30	BG	126	ASP
30	BG	155	MET
31	BH	14	GLY
31	BH	45	VAL
31	BH	110	SER
31	BH	138	LYS
31	BH	160	LYS
31	BH	165	ALA
32	BI	6	LEU
32	BI	76	THR
32	BI	91	SER
32	BI	99	GLU
32	BI	115	ALA
33	BJ	30	GLN
33	BJ	47	ASN
33	BJ	50	ARG
33	BJ	62	ALA
33	BJ	77	PRO
33	BJ	88	ALA
33	BJ	89	ALA
33	BJ	108	LYS
33	BJ	109	SER
33	BJ	122	VAL
33	BJ	129	PRO
34	BN	42	TRP
34	BN	133	GLN
35	BO	48	PRO
35	BO	98	VAL
36	BP	18	ARG
36	BP	34	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BP	89	ALA
36	BP	98	GLU
36	BP	104	GLY
36	BP	106	LEU
36	BP	107	LYS
36	BP	141	ALA
37	BQ	62	GLY
38	BR	58	GLY
38	BR	86	ARG
38	BR	117	VAL
39	BS	13	ARG
39	BS	57	LYS
39	BS	90	GLY
39	BS	102	ALA
39	BS	104	GLY
39	BS	107	GLU
40	BT	3	ARG
40	BT	17	THR
40	BT	27	THR
40	BT	35	LYS
41	BU	32	PHE
41	BU	89	GLU
42	BV	22	VAL
42	BV	31	ALA
42	BV	35	LEU
42	BV	48	GLY
42	BV	78	LYS
43	BW	29	LEU
43	BW	59	VAL
43	BW	63	ASP
44	BX	91	ALA
45	BY	5	MET
45	BY	18	GLY
45	BY	24	VAL
45	BY	26	LYS
45	BY	48	ALA
45	BY	80	GLY
46	BZ	78	LYS
46	BZ	81	ARG
46	BZ	119	GLU
46	BZ	120	ILE
46	BZ	134	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	B1	53	VAL
48	B1	84	GLY
49	B2	42	GLY
51	B4	40	HIS
51	B4	49	PHE
51	B4	50	VAL
53	B6	44	ARG
55	B8	31	HIS
55	B8	43	GLN
1	Ab	20	GLU
1	Ab	106	LYS
1	Ab	143	GLU
1	Ab	159	PRO
2	Ac	26	LYS
2	Ac	81	GLY
3	Ad	18	LYS
3	Ad	42	GLN
3	Ad	44	GLY
3	Ad	153	ARG
3	Ad	178	VAL
4	Ae	8	GLU
4	Ae	21	ALA
4	Ae	70	PRO
4	Ae	128	PRO
4	Ae	136	MET
4	Ae	153	LYS
6	Ag	6	ARG
6	Ag	14	PRO
6	Ag	54	THR
6	Ag	66	VAL
6	Ag	81	GLY
6	Ag	90	GLU
11	Al	51	ALA
12	Am	29	ARG
12	Am	69	GLU
12	Am	106	ASN
13	An	5	ALA
13	An	28	GLY
14	Ao	24	SER
17	Ar	87	ARG
18	As	45	VAL
19	At	48	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	At	98	PRO
21	Ay	10	ARG
21	Ay	84	SER
26	AC	209	PHE
27	AD	12	SER
27	AD	26	LYS
27	AD	33	LEU
27	AD	42	GLY
27	AD	246	PRO
28	AE	52	LEU
28	AE	63	LEU
29	AF	14	PRO
29	AF	16	GLY
29	AF	25	PRO
29	AF	84	VAL
29	AF	90	PHE
30	AG	6	ALA
30	AG	43	LEU
30	AG	84	LYS
30	AG	87	PRO
31	AH	55	PRO
31	AH	59	ARG
31	AH	158	HIS
33	AJ	47	ASN
33	AJ	70	GLU
33	AJ	100	ASN
33	AJ	104	ILE
33	AJ	128	LEU
34	AN	57	ALA
35	AO	5	GLN
35	AO	26	LYS
36	AP	39	LYS
36	AP	40	SER
36	AP	52	GLU
36	AP	57	THR
36	AP	149	GLU
38	AR	5	LYS
38	AR	106	GLY
39	AS	100	ALA
40	AT	12	SER
40	AT	32	TYR
40	AT	126	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	AV	2	PHE
42	AV	18	LEU
42	AV	28	GLU
42	AV	49	THR
42	AV	50	PRO
42	AV	78	LYS
42	AV	79	VAL
43	AW	6	ILE
43	AW	35	ILE
43	AW	59	VAL
44	AX	4	ALA
45	AY	18	GLY
45	AY	96	ILE
46	AZ	22	GLY
46	AZ	108	PRO
47	A0	20	ARG
47	A0	74	ARG
48	A1	85	LEU
51	A4	28	LYS
52	A5	4	HIS
52	A5	38	ALA
1	Bb	20	GLU
1	Bb	106	LYS
1	Bb	143	GLU
1	Bb	154	LEU
1	Bb	159	PRO
2	Bc	26	LYS
2	Bc	81	GLY
3	Bd	18	LYS
3	Bd	44	GLY
3	Bd	178	VAL
4	Be	8	GLU
4	Be	70	PRO
4	Be	71	LEU
4	Be	128	PRO
4	Be	136	MET
4	Be	148	VAL
6	Bg	6	ARG
6	Bg	14	PRO
6	Bg	54	THR
6	Bg	66	VAL
6	Bg	81	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	Bg	90	GLU
11	Bl	51	ALA
12	Bm	29	ARG
12	Bm	106	ASN
13	Bn	5	ALA
13	Bn	28	GLY
14	Bo	24	SER
17	Br	87	ARG
18	Bs	45	VAL
19	Bt	98	PRO
21	By	30	LEU
21	By	34	LEU
21	By	40	GLU
21	By	84	SER
26	BC	209	PHE
27	BD	12	SER
27	BD	26	LYS
27	BD	33	LEU
27	BD	42	GLY
27	BD	156	ALA
27	BD	169	GLU
27	BD	246	PRO
28	BE	52	LEU
28	BE	75	VAL
28	BE	130	GLY
29	BF	14	PRO
29	BF	16	GLY
29	BF	25	PRO
29	BF	69	HIS
29	BF	84	VAL
29	BF	128	ALA
30	BG	7	LEU
30	BG	8	LYS
30	BG	122	PRO
30	BG	129	GLY
30	BG	146	TYR
31	BH	55	PRO
31	BH	59	ARG
31	BH	71	LEU
31	BH	158	HIS
33	BJ	22	GLY
33	BJ	43	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	BJ	56	ASN
33	BJ	57	THR
33	BJ	74	LEU
33	BJ	84	GLU
33	BJ	97	ALA
33	BJ	112	LEU
34	BN	4	TYR
34	BN	57	ALA
35	BO	5	GLN
35	BO	26	LYS
36	BP	39	LYS
36	BP	40	SER
36	BP	52	GLU
36	BP	149	GLU
38	BR	5	LYS
38	BR	106	GLY
40	BT	32	TYR
40	BT	126	ALA
42	BV	2	PHE
42	BV	18	LEU
42	BV	28	GLU
42	BV	49	THR
42	BV	50	PRO
43	BW	6	ILE
43	BW	35	ILE
44	BX	4	ALA
46	BZ	12	GLY
46	BZ	77	ASP
46	BZ	93	ASP
46	BZ	168	GLU
46	BZ	170	THR
47	B0	20	ARG
47	B0	74	ARG
48	B1	76	ARG
49	B2	44	LEU
49	B2	68	ARG
51	B4	16	CYS
51	B4	28	LYS
52	B5	4	HIS
52	B5	38	ALA
1	Ab	135	GLN
1	Ab	204	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ac	181	ASN
4	Ae	71	LEU
4	Ae	72	GLN
4	Ae	148	VAL
8	Ai	11	LYS
8	Ai	70	LYS
9	Aj	86	MET
11	Al	26	ALA
11	Al	28	LYS
12	Am	41	PRO
13	An	23	ARG
13	An	24	CYS
13	An	60	SER
17	Ar	31	LEU
17	Ar	55	ARG
18	As	25	LYS
18	As	70	LYS
18	As	73	GLU
19	At	97	ALA
27	AD	3	VAL
27	AD	24	ILE
27	AD	156	ALA
27	AD	241	PRO
27	AD	245	PRO
28	AE	58	ARG
28	AE	75	VAL
29	AF	69	HIS
29	AF	115	ALA
30	AG	10	LYS
30	AG	112	PRO
31	AH	81	GLU
31	AH	137	ASP
32	AI	16	GLY
32	AI	133	HIS
33	AJ	114	GLY
33	AJ	125	LEU
34	AN	126	PRO
34	AN	127	ASP
34	AN	135	PRO
35	AO	14	THR
36	AP	10	PRO
36	AP	48	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	AR	102	GLU
39	AS	15	ARG
39	AS	37	ALA
39	AS	85	VAL
39	AS	88	ASP
39	AS	89	ARG
40	AT	25	GLY
43	AW	56	ALA
43	AW	65	LEU
45	AY	9	LYS
45	AY	31	LEU
45	AY	39	VAL
45	AY	53	PRO
45	AY	81	LYS
45	AY	82	PRO
46	AZ	45	ASP
46	AZ	151	HIS
48	A1	28	GLY
48	A1	30	VAL
51	A4	4	GLY
51	A4	33	VAL
53	A6	16	CYS
53	A6	20	ASN
1	Bb	135	GLN
1	Bb	204	ASN
2	Bc	66	VAL
2	Bc	181	ASN
3	Bd	42	GLN
3	Bd	153	ARG
4	Be	21	ALA
8	Bi	11	LYS
8	Bi	70	LYS
11	Bl	26	ALA
11	Bl	28	LYS
12	Bm	41	PRO
12	Bm	65	LYS
13	Bn	23	ARG
13	Bn	24	CYS
13	Bn	60	SER
15	Bp	39	TYR
17	Br	55	ARG
18	Bs	25	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	Bs	70	LYS
18	Bs	73	GLU
19	Bt	48	LYS
19	Bt	61	SER
19	Bt	97	ALA
21	By	6	ASP
27	BD	3	VAL
27	BD	45	ASN
27	BD	241	PRO
27	BD	245	PRO
28	BE	58	ARG
28	BE	189	PRO
28	BE	201	THR
29	BF	90	PHE
29	BF	115	ALA
30	BG	28	VAL
30	BG	105	LYS
30	BG	142	PRO
31	BH	81	GLU
31	BH	137	ASP
32	BI	16	GLY
32	BI	133	HIS
33	BJ	23	SER
33	BJ	90	ALA
33	BJ	102	LYS
33	BJ	103	GLY
34	BN	126	PRO
34	BN	127	ASP
34	BN	135	PRO
36	BP	48	PRO
36	BP	57	THR
38	BR	4	LEU
38	BR	102	GLU
39	BS	37	ALA
39	BS	85	VAL
39	BS	88	ASP
39	BS	100	ALA
40	BT	25	GLY
40	BT	41	ARG
42	BV	79	VAL
43	BW	15	ARG
43	BW	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	BY	31	LEU
45	BY	39	VAL
45	BY	53	PRO
45	BY	81	LYS
45	BY	96	ILE
46	BZ	154	ASP
49	B2	17	SER
51	B4	4	GLY
51	B4	33	VAL
53	B6	16	CYS
53	B6	20	ASN
1	Ab	150	SER
1	Ab	236	TYR
2	Ac	66	VAL
2	Ac	75	VAL
2	Ac	129	ALA
2	Ac	168	ALA
3	Ad	37	PRO
3	Ad	53	ASP
4	Ae	108	ALA
4	Ae	137	GLU
5	Af	29	ALA
7	Ah	91	ARG
8	Ai	21	PRO
11	Al	22	SER
11	Al	121	GLY
12	Am	38	GLY
12	Am	118	ALA
14	Ao	85	LEU
15	Ap	39	TYR
17	Ar	25	THR
19	At	61	SER
21	Ay	29	LYS
21	Ay	76	ILE
27	AD	45	ASN
27	AD	244	ARG
28	AE	189	PRO
28	AE	201	THR
29	AF	11	VAL
30	AG	36	LYS
31	AH	85	LYS
31	AH	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	AI	87	LYS
32	AI	114	LEU
33	AJ	20	ALA
33	AJ	42	GLN
33	AJ	58	LEU
33	AJ	77	PRO
34	AN	60	ILE
34	AN	77	GLY
36	AP	146	VAL
37	AQ	20	ALA
38	AR	4	LEU
39	AS	53	SER
39	AS	96	GLY
40	AT	41	ARG
41	AU	90	VAL
43	AW	93	ALA
44	AX	11	PRO
45	AY	29	GLU
45	AY	56	PRO
45	AY	66	PRO
46	AZ	14	LYS
46	AZ	41	LEU
46	AZ	47	VAL
46	AZ	122	ARG
47	A0	42	GLY
48	A1	53	VAL
49	A2	17	SER
49	A2	58	ALA
55	A8	41	ILE
1	Bb	83	MET
1	Bb	84	GLU
1	Bb	150	SER
2	Bc	75	VAL
2	Bc	168	ALA
3	Bd	53	ASP
4	Be	72	GLN
4	Be	108	ALA
4	Be	137	GLU
5	Bf	29	ALA
5	Bf	96	PRO
9	Bj	86	MET
10	Bk	105	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Bl	22	SER
14	Bo	85	LEU
17	Br	25	THR
17	Br	31	LEU
27	BD	24	ILE
27	BD	244	ARG
29	BF	11	VAL
30	BG	32	PRO
30	BG	97	ASP
30	BG	139	LEU
31	BH	85	LYS
31	BH	126	PRO
32	BI	114	LEU
33	BJ	14	LYS
33	BJ	68	LEU
34	BN	77	GLY
36	BP	10	PRO
36	BP	146	VAL
37	BQ	20	ALA
37	BQ	53	ALA
39	BS	15	ARG
39	BS	53	SER
39	BS	89	ARG
39	BS	96	GLY
40	BT	12	SER
41	BU	90	VAL
43	BW	93	ALA
44	BX	11	PRO
44	BX	22	ALA
44	BX	48	LYS
45	BY	9	LYS
45	BY	29	GLU
45	BY	56	PRO
45	BY	66	PRO
45	BY	67	LEU
45	BY	82	PRO
46	BZ	111	VAL
46	BZ	129	SER
47	B0	55	ARG
55	B8	41	ILE
1	Ab	83	MET
1	Ab	84	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ab	131	PRO
1	Ab	230	VAL
2	Ac	15	THR
2	Ac	167	TRP
3	Ad	164	ALA
5	Af	51	PRO
5	Af	96	PRO
6	Ag	9	VAL
10	Ak	105	VAL
21	Ay	6	ASP
21	Ay	87	TYR
27	AD	28	GLU
27	AD	196	VAL
29	AF	9	ILE
29	AF	24	LEU
30	AG	24	GLY
30	AG	41	GLN
30	AG	114	ILE
36	AP	122	PRO
40	AT	86	ILE
41	AU	61	TRP
42	AV	29	PRO
43	AW	15	ARG
44	AX	13	LEU
45	AY	22	GLY
47	A0	17	GLN
53	A6	23	THR
1	Bb	230	VAL
2	Bc	15	THR
2	Bc	167	TRP
3	Bd	37	PRO
5	Bf	51	PRO
6	Bg	9	VAL
8	Bi	21	PRO
12	Bm	38	GLY
27	BD	28	GLU
28	BE	61	ARG
28	BE	187	ALA
29	BF	9	ILE
29	BF	24	LEU
30	BG	46	ALA
30	BG	121	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	BI	14	ASP
32	BI	87	LYS
34	BN	56	ASN
34	BN	60	ILE
36	BP	122	PRO
40	BT	91	ARG
44	BX	13	LEU
46	BZ	135	GLU
46	BZ	165	VAL
46	BZ	169	GLU
47	B0	42	GLY
50	B3	2	PRO
53	B6	23	THR
1	Ab	130	ARG
3	Ad	56	VAL
5	Af	6	VAL
8	Ai	44	VAL
9	Aj	90	LEU
14	Ao	86	GLY
15	Ap	53	VAL
27	AD	123	ALA
28	AE	55	ASN
28	AE	61	ARG
34	AN	125	GLY
38	AR	83	ILE
39	AS	91	PRO
46	AZ	15	PRO
46	AZ	120	ILE
50	A3	2	PRO
1	Bb	130	ARG
1	Bb	131	PRO
3	Bd	56	VAL
9	Bj	90	LEU
14	Bo	86	GLY
15	Bp	53	VAL
18	Bs	59	PRO
21	By	67	ILE
28	BE	55	ASN
28	BE	56	PRO
34	BN	36	GLY
34	BN	125	GLY
36	BP	109	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	BR	83	ILE
40	BT	86	ILE
42	BV	29	PRO
2	Ac	174	PRO
3	Ad	7	PRO
18	As	9	VAL
19	At	101	GLY
21	Ay	86	VAL
26	AC	52	PRO
28	AE	56	PRO
31	AH	99	VAL
33	AJ	69	PRO
45	AY	38	ILE
45	AY	58	GLY
8	Bi	44	VAL
18	Bs	9	VAL
27	BD	123	ALA
27	BD	196	VAL
31	BH	99	VAL
39	BS	91	PRO
55	B8	53	PRO
2	Ac	195	VAL
6	Ag	88	PRO
18	As	59	PRO
28	AE	175	VAL
32	AI	90	GLY
34	AN	129	PRO
36	AP	109	GLY
37	AQ	47	ILE
49	A2	6	VAL
51	A4	5	ILE
53	A6	48	VAL
2	Bc	174	PRO
3	Bd	7	PRO
5	Bf	81	ILE
6	Bg	88	PRO
16	Bq	30	PRO
26	BC	52	PRO
27	BD	11	PRO
32	BI	90	GLY
33	BJ	104	ILE
36	BP	11	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	BV	54	GLY
45	BY	22	GLY
45	BY	38	ILE
45	BY	58	GLY
53	B6	48	VAL
5	Af	81	ILE
6	Ag	17	VAL
15	Ap	66	PRO
17	Ar	37	VAL
18	As	67	VAL
28	AE	86	PRO
30	AG	111	LEU
31	AH	49	VAL
36	AP	11	GLY
45	AY	37	VAL
46	AZ	130	PRO
46	AZ	137	ILE
2	Bc	195	VAL
5	Bf	6	VAL
6	Bg	17	VAL
18	Bs	67	VAL
19	Bt	101	GLY
28	BE	86	PRO
31	BH	49	VAL
34	BN	129	PRO
51	B4	5	ILE
13	An	13	THR
31	AH	76	VAL
33	AJ	107	VAL
34	AN	5	VAL
34	AN	36	GLY
42	AV	54	GLY
55	A8	53	PRO
7	Bh	6	ILE
13	Bn	13	THR
15	Bp	66	PRO
28	BE	175	VAL
34	BN	5	VAL
45	BY	37	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	202/220 (92%)	189 (94%)	13 (6%)	17	46
1	Bb	202/220 (92%)	189 (94%)	13 (6%)	17	46
2	Ac	160/188 (85%)	143 (89%)	17 (11%)	6	25
2	Bc	160/188 (85%)	143 (89%)	17 (11%)	6	25
3	Ad	180/181 (99%)	157 (87%)	23 (13%)	4	18
3	Bd	180/181 (99%)	156 (87%)	24 (13%)	4	17
4	Ae	115/123 (94%)	107 (93%)	8 (7%)	15	43
4	Be	115/123 (94%)	106 (92%)	9 (8%)	12	38
5	Af	90/90 (100%)	87 (97%)	3 (3%)	38	66
5	Bf	90/90 (100%)	87 (97%)	3 (3%)	38	66
6	Ag	126/127 (99%)	119 (94%)	7 (6%)	21	52
6	Bg	126/127 (99%)	119 (94%)	7 (6%)	21	52
7	Ah	119/119 (100%)	109 (92%)	10 (8%)	11	35
7	Bh	119/119 (100%)	109 (92%)	10 (8%)	11	35
8	Ai	98/99 (99%)	87 (89%)	11 (11%)	6	23
8	Bi	98/99 (99%)	86 (88%)	12 (12%)	5	20
9	Aj	88/92 (96%)	80 (91%)	8 (9%)	9	31
9	Bj	88/92 (96%)	80 (91%)	8 (9%)	9	31
10	Ak	90/99 (91%)	87 (97%)	3 (3%)	38	66
10	Bk	90/99 (91%)	88 (98%)	2 (2%)	52	74
11	Al	104/109 (95%)	87 (84%)	17 (16%)	2	10
11	Bl	104/109 (95%)	88 (85%)	16 (15%)	2	12
12	Am	94/101 (93%)	78 (83%)	16 (17%)	2	9
12	Bm	94/101 (93%)	75 (80%)	19 (20%)	1	5
13	An	49/50 (98%)	47 (96%)	2 (4%)	30	61
13	Bn	49/50 (98%)	47 (96%)	2 (4%)	30	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	Ao	79/80 (99%)	74 (94%)	5 (6%)	18	47
14	Bo	79/80 (99%)	74 (94%)	5 (6%)	18	47
15	Ap	72/74 (97%)	69 (96%)	3 (4%)	30	60
15	Bp	72/74 (97%)	69 (96%)	3 (4%)	30	60
16	Aq	94/97 (97%)	91 (97%)	3 (3%)	39	67
16	Bq	94/97 (97%)	91 (97%)	3 (3%)	39	67
17	Ar	61/77 (79%)	58 (95%)	3 (5%)	25	56
17	Br	61/77 (79%)	58 (95%)	3 (5%)	25	56
18	As	69/80 (86%)	61 (88%)	8 (12%)	5	22
18	Bs	69/80 (86%)	61 (88%)	8 (12%)	5	22
19	At	76/82 (93%)	68 (90%)	8 (10%)	7	25
19	Bt	76/82 (93%)	68 (90%)	8 (10%)	7	25
20	Au	19/22 (86%)	19 (100%)	0	100	100
20	Bu	19/22 (86%)	19 (100%)	0	100	100
21	Ay	84/85 (99%)	64 (76%)	20 (24%)	0	2
21	By	83/85 (98%)	72 (87%)	11 (13%)	4	17
26	AC	99/181 (55%)	96 (97%)	3 (3%)	41	68
26	BC	99/181 (55%)	96 (97%)	3 (3%)	41	68
27	AD	213/218 (98%)	182 (85%)	31 (15%)	3	14
27	BD	213/218 (98%)	181 (85%)	32 (15%)	3	13
28	AE	165/166 (99%)	144 (87%)	21 (13%)	4	19
28	BE	165/166 (99%)	144 (87%)	21 (13%)	4	19
29	AF	165/166 (99%)	141 (86%)	24 (14%)	3	14
29	BF	165/166 (99%)	142 (86%)	23 (14%)	3	16
30	AG	155/156 (99%)	134 (86%)	21 (14%)	4	16
30	BG	155/156 (99%)	131 (84%)	24 (16%)	2	12
31	AH	137/148 (93%)	127 (93%)	10 (7%)	14	41
31	BH	137/148 (93%)	128 (93%)	9 (7%)	16	46
32	AI	122/124 (98%)	99 (81%)	23 (19%)	1	6
32	BI	122/124 (98%)	99 (81%)	23 (19%)	1	6
34	AN	117/119 (98%)	101 (86%)	16 (14%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BN	117/119 (98%)	101 (86%)	16 (14%)	3	16
35	AO	100/100 (100%)	93 (93%)	7 (7%)	15	43
35	BO	100/100 (100%)	93 (93%)	7 (7%)	15	43
36	AP	112/116 (97%)	89 (80%)	23 (20%)	1	4
36	BP	112/116 (97%)	87 (78%)	25 (22%)	1	3
37	AQ	110/111 (99%)	101 (92%)	9 (8%)	11	36
37	BQ	110/111 (99%)	100 (91%)	10 (9%)	9	31
38	AR	100/101 (99%)	85 (85%)	15 (15%)	3	13
38	BR	100/101 (99%)	84 (84%)	16 (16%)	2	11
39	AS	77/88 (88%)	66 (86%)	11 (14%)	3	15
39	BS	77/88 (88%)	67 (87%)	10 (13%)	4	17
40	AT	118/127 (93%)	95 (80%)	23 (20%)	1	5
40	BT	118/127 (93%)	95 (80%)	23 (20%)	1	5
41	AU	92/94 (98%)	81 (88%)	11 (12%)	5	20
41	BU	92/94 (98%)	81 (88%)	11 (12%)	5	20
42	AV	82/82 (100%)	65 (79%)	17 (21%)	1	4
42	BV	82/82 (100%)	65 (79%)	17 (21%)	1	4
43	AW	91/92 (99%)	83 (91%)	8 (9%)	10	33
43	BW	91/92 (99%)	83 (91%)	8 (9%)	10	33
44	AX	74/78 (95%)	66 (89%)	8 (11%)	6	24
44	BX	74/78 (95%)	66 (89%)	8 (11%)	6	24
45	AY	84/91 (92%)	71 (84%)	13 (16%)	2	12
45	BY	84/91 (92%)	72 (86%)	12 (14%)	3	15
46	AZ	162/179 (90%)	142 (88%)	20 (12%)	4	20
46	BZ	162/179 (90%)	136 (84%)	26 (16%)	2	11
47	A0	66/67 (98%)	58 (88%)	8 (12%)	5	20
47	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
48	A1	78/83 (94%)	66 (85%)	12 (15%)	2	12
48	B1	78/83 (94%)	69 (88%)	9 (12%)	5	22
49	A2	66/67 (98%)	61 (92%)	5 (8%)	13	39
49	B2	66/67 (98%)	54 (82%)	12 (18%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	A3	51/52 (98%)	47 (92%)	4 (8%)	12	38
50	B3	51/52 (98%)	47 (92%)	4 (8%)	12	38
51	A4	51/63 (81%)	36 (71%)	15 (29%)	0	1
51	B4	51/63 (81%)	36 (71%)	15 (29%)	0	1
52	A5	47/52 (90%)	42 (89%)	5 (11%)	6	25
52	B5	47/52 (90%)	42 (89%)	5 (11%)	6	25
53	A6	49/52 (94%)	41 (84%)	8 (16%)	2	10
53	B6	49/52 (94%)	40 (82%)	9 (18%)	1	7
54	A7	40/42 (95%)	36 (90%)	4 (10%)	7	27
54	B7	40/42 (95%)	36 (90%)	4 (10%)	7	27
55	A8	53/55 (96%)	40 (76%)	13 (24%)	0	2
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	1
56	A9	34/34 (100%)	32 (94%)	2 (6%)	19	49
56	B9	34/34 (100%)	32 (94%)	2 (6%)	19	49
All	All	9957/10598 (94%)	8789 (88%)	1168 (12%)	5	21

All (1168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ab	15	VAL
1	Ab	17	PHE
1	Ab	24	TRP
1	Ab	36	ARG
1	Ab	69	LEU
1	Ab	137	ARG
1	Ab	140	HIS
1	Ab	145	LEU
1	Ab	155	LEU
1	Ab	172	ILE
1	Ab	196	LEU
1	Ab	204	ASN
1	Ab	221	LEU
2	Ac	3	ASN
2	Ac	5	ILE
2	Ac	6	HIS
2	Ac	16	ARG
2	Ac	18	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Ac	29	TYR
2	Ac	34	LEU
2	Ac	36	ASP
2	Ac	37	GLN
2	Ac	82	GLU
2	Ac	94	LEU
2	Ac	107	GLN
2	Ac	127	ARG
2	Ac	131	ARG
2	Ac	152	ILE
2	Ac	167	TRP
2	Ac	193	TYR
3	Ad	3	ARG
3	Ad	9	CYS
3	Ad	10	ARG
3	Ad	11	LEU
3	Ad	15	GLU
3	Ad	26	CYS
3	Ad	36	ARG
3	Ad	38	TYR
3	Ad	49	ARG
3	Ad	53	ASP
3	Ad	58	LEU
3	Ad	59	ARG
3	Ad	86	LYS
3	Ad	97	LEU
3	Ad	110	PHE
3	Ad	129	ASN
3	Ad	131	ARG
3	Ad	132	ARG
3	Ad	135	LEU
3	Ad	162	LEU
3	Ad	168	ARG
3	Ad	196	LEU
3	Ad	200	GLU
4	Ae	10	MET
4	Ae	12	LEU
4	Ae	20	GLN
4	Ae	31	LEU
4	Ae	55	VAL
4	Ae	56	GLN
4	Ae	79	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Ae	101	ILE
5	Af	63	TYR
5	Af	69	GLU
5	Af	80	ARG
6	Ag	21	VAL
6	Ag	88	PRO
6	Ag	111	ARG
6	Ag	114	ARG
6	Ag	124	LEU
6	Ag	140	ASP
6	Ag	151	TYR
7	Ah	1	MET
7	Ah	25	ASP
7	Ah	26	VAL
7	Ah	50	ARG
7	Ah	52	ASP
7	Ah	60	ARG
7	Ah	65	TYR
7	Ah	102	ARG
7	Ah	112	LEU
7	Ah	119	LEU
8	Ai	3	GLN
8	Ai	10	ARG
8	Ai	78	LYS
8	Ai	88	TYR
8	Ai	95	LYS
8	Ai	105	ASP
8	Ai	112	LYS
8	Ai	114	TYR
8	Ai	121	ARG
8	Ai	125	TYR
8	Ai	128	ARG
9	Aj	4	ILE
9	Aj	22	LYS
9	Aj	46	ARG
9	Aj	49	VAL
9	Aj	50	ILE
9	Aj	62	HIS
9	Aj	68	HIS
9	Aj	96	ILE
10	Ak	29	ILE
10	Ak	124	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	Ak	126	ARG
11	Al	7	ILE
11	Al	20	LYS
11	Al	27	LEU
11	Al	41	ARG
11	Al	42	THR
11	Al	47	LYS
11	Al	53	ARG
11	Al	55	VAL
11	Al	62	SER
11	Al	66	VAL
11	Al	67	THR
11	Al	85	ILE
11	Al	89	ARG
11	Al	92	ASP
11	Al	97	ARG
11	Al	102	ARG
11	Al	126	LYS
12	Am	47	ASP
12	Am	48	LEU
12	Am	56	LEU
12	Am	64	TRP
12	Am	65	LYS
12	Am	66	LEU
12	Am	69	GLU
12	Am	70	LEU
12	Am	77	ASN
12	Am	79	LYS
12	Am	82	MET
12	Am	92	HIS
12	Am	93	ARG
12	Am	98	VAL
12	Am	108	ARG
12	Am	115	LYS
13	An	33	VAL
13	An	44	LEU
14	Ao	37	ASN
14	Ao	65	ARG
14	Ao	82	ILE
14	Ao	85	LEU
14	Ao	88	ARG
15	Ap	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	Ap	2	VAL
15	Ap	69	THR
16	Aq	38	ARG
16	Aq	59	ILE
16	Aq	98	LEU
17	Ar	31	LEU
17	Ar	44	LEU
17	Ar	65	ILE
18	As	5	LEU
18	As	6	LYS
18	As	7	LYS
18	As	15	LEU
18	As	29	ARG
18	As	33	THR
18	As	37	ARG
18	As	70	LYS
19	At	10	LEU
19	At	24	LEU
19	At	26	ASN
19	At	36	LEU
19	At	41	ILE
19	At	73	HIS
19	At	75	ASN
19	At	93	GLU
21	Ay	5	LEU
21	Ay	6	ASP
21	Ay	7	PHE
21	Ay	8	ASP
21	Ay	9	GLU
21	Ay	10	ARG
21	Ay	14	GLU
21	Ay	21	THR
21	Ay	34	LEU
21	Ay	43	LYS
21	Ay	48	PRO
21	Ay	56	ARG
21	Ay	57	SER
21	Ay	61	ARG
21	Ay	64	TYR
21	Ay	68	ASP
21	Ay	73	VAL
21	Ay	83	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	Ay	89	GLU
21	Ay	93	ARG
26	AC	39	ASP
26	AC	53	ARG
26	AC	185	LYS
27	AD	10	THR
27	AD	24	ILE
27	AD	26	LYS
27	AD	35	LYS
27	AD	37	LEU
27	AD	43	ARG
27	AD	46	GLN
27	AD	49	ILE
27	AD	61	LEU
27	AD	65	ILE
27	AD	71	ASP
27	AD	72	LYS
27	AD	94	LEU
27	AD	95	LEU
27	AD	98	VAL
27	AD	103	ARG
27	AD	104	TYR
27	AD	106	ILE
27	AD	122	ASP
27	AD	131	LEU
27	AD	166	GLN
27	AD	192	THR
27	AD	198	ASN
27	AD	200	ASP
27	AD	221	VAL
27	AD	228	PRO
27	AD	229	VAL
27	AD	257	LEU
27	AD	259	THR
27	AD	260	ARG
27	AD	271	ILE
28	AE	24	THR
28	AE	33	VAL
28	AE	49	LEU
28	AE	55	ASN
28	AE	63	LEU
28	AE	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	AE	67	PHE
28	AE	78	LEU
28	AE	79	ARG
28	AE	82	ARG
28	AE	87	GLU
28	AE	101	ARG
28	AE	113	PHE
28	AE	119	ARG
28	AE	144	ARG
28	AE	169	ASN
28	AE	181	LEU
28	AE	197	ILE
28	AE	200	GLU
28	AE	202	LYS
28	AE	203	LYS
29	AF	23	ASP
29	AF	28	ILE
29	AF	33	LEU
29	AF	38	ARG
29	AF	57	VAL
29	AF	65	TRP
29	AF	66	PRO
29	AF	67	GLN
29	AF	74	ARG
29	AF	83	PHE
29	AF	106	ARG
29	AF	110	LEU
29	AF	125	LEU
29	AF	129	PHE
29	AF	157	VAL
29	AF	158	THR
29	AF	160	ASN
29	AF	164	ARG
29	AF	165	ARG
29	AF	170	LEU
29	AF	183	VAL
29	AF	188	ARG
29	AF	192	LEU
29	AF	200	GLU
30	AG	5	VAL
30	AG	16	ARG
30	AG	22	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	AG	33	ARG
30	AG	36	LYS
30	AG	40	ASN
30	AG	49	ASP
30	AG	66	GLN
30	AG	67	LYS
30	AG	77	ILE
30	AG	80	PHE
30	AG	83	ARG
30	AG	91	ARG
30	AG	96	ARG
30	AG	97	ASP
30	AG	111	LEU
30	AG	113	ARG
30	AG	125	PHE
30	AG	130	ASN
30	AG	143	GLU
30	AG	145	THR
31	AH	9	ILE
31	AH	53	GLU
31	AH	54	ARG
31	AH	83	TYR
31	AH	89	ILE
31	AH	105	LEU
31	AH	153	LYS
31	AH	157	TYR
31	AH	163	TYR
31	AH	170	ARG
32	AI	1	MET
32	AI	9	LEU
32	AI	12	LEU
32	AI	31	LEU
32	AI	71	ILE
32	AI	74	ASN
32	AI	85	GLU
32	AI	86	THR
32	AI	89	TYR
32	AI	91	SER
32	AI	92	VAL
32	AI	93	THR
32	AI	99	GLU
32	AI	103	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	AI	105	HIS
32	AI	107	VAL
32	AI	109	ILE
32	AI	110	ASP
32	AI	123	LEU
32	AI	130	TYR
32	AI	138	ILE
32	AI	139	GLN
32	AI	140	LEU
34	AN	4	TYR
34	AN	23	LEU
34	AN	28	THR
34	AN	32	THR
34	AN	33	LEU
34	AN	34	LEU
34	AN	37	LYS
34	AN	39	ARG
34	AN	43	THR
34	AN	48	MET
34	AN	56	ASN
34	AN	60	ILE
34	AN	87	LEU
34	AN	121	LYS
34	AN	127	ASP
34	AN	130	HIS
35	AO	7	TYR
35	AO	8	LEU
35	AO	24	VAL
35	AO	32	TYR
35	AO	89	ASN
35	AO	98	VAL
35	AO	108	GLU
36	AP	13	ASN
36	AP	16	ARG
36	AP	18	ARG
36	AP	32	THR
36	AP	39	LYS
36	AP	41	ARG
36	AP	42	SER
36	AP	45	LEU
36	AP	47	ASP
36	AP	57	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	AP	59	LEU
36	AP	61	ARG
36	AP	64	LYS
36	AP	81	GLN
36	AP	85	LEU
36	AP	91	PHE
36	AP	98	GLU
36	AP	108	LYS
36	AP	110	TYR
36	AP	112	LEU
36	AP	114	ILE
36	AP	119	GLU
36	AP	135	LEU
37	AQ	18	LYS
37	AQ	45	GLN
37	AQ	55	VAL
37	AQ	67	ARG
37	AQ	75	THR
37	AQ	110	THR
37	AQ	134	ARG
37	AQ	135	ASP
37	AQ	137	TYR
38	AR	2	ARG
38	AR	4	LEU
38	AR	8	ARG
38	AR	12	ARG
38	AR	15	SER
38	AR	18	LEU
38	AR	28	LEU
38	AR	65	LEU
38	AR	67	LEU
38	AR	71	GLN
38	AR	76	VAL
38	AR	79	LEU
38	AR	94	TYR
38	AR	99	LYS
38	AR	113	LEU
39	AS	11	LYS
39	AS	12	PHE
39	AS	36	TYR
39	AS	40	ILE
39	AS	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	AS	73	LEU
39	AS	89	ARG
39	AS	92	TYR
39	AS	97	ARG
39	AS	101	LEU
39	AS	106	ARG
40	AT	3	ARG
40	AT	13	ARG
40	AT	14	TYR
40	AT	24	PRO
40	AT	32	TYR
40	AT	38	ASN
40	AT	41	ARG
40	AT	50	ILE
40	AT	51	ARG
40	AT	58	ASN
40	AT	59	THR
40	AT	65	LYS
40	AT	78	LEU
40	AT	82	LEU
40	AT	93	ARG
40	AT	96	ARG
40	AT	99	LEU
40	AT	100	TYR
40	AT	101	PHE
40	AT	107	ASP
40	AT	108	ARG
40	AT	122	ASP
40	AT	128	GLU
41	AU	14	HIS
41	AU	19	LYS
41	AU	52	ARG
41	AU	59	ARG
41	AU	60	LEU
41	AU	66	ASN
41	AU	74	LEU
41	AU	83	LEU
41	AU	101	ARG
41	AU	108	GLU
41	AU	112	ARG
42	AV	14	VAL
42	AV	16	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	AV	18	LEU
42	AV	19	LYS
42	AV	21	ARG
42	AV	22	VAL
42	AV	33	VAL
42	AV	37	VAL
42	AV	39	LEU
42	AV	40	LEU
42	AV	46	VAL
42	AV	47	VAL
42	AV	66	ARG
42	AV	82	ARG
42	AV	91	TYR
42	AV	95	LEU
42	AV	99	ILE
43	AW	11	ARG
43	AW	51	LEU
43	AW	57	ASN
43	AW	60	ASN
43	AW	70	TYR
43	AW	76	VAL
43	AW	100	THR
43	AW	107	LEU
44	AX	27	THR
44	AX	57	LEU
44	AX	63	LYS
44	AX	68	ARG
44	AX	70	LEU
44	AX	80	ILE
44	AX	81	VAL
44	AX	83	VAL
45	AY	2	ARG
45	AY	6	HIS
45	AY	7	VAL
45	AY	9	LYS
45	AY	28	LYS
45	AY	29	GLU
45	AY	32	PRO
45	AY	53	PRO
45	AY	60	PHE
45	AY	77	PRO
45	AY	83	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	AY	89	PHE
45	AY	90	LEU
46	AZ	6	LYS
46	AZ	24	LEU
46	AZ	27	VAL
46	AZ	28	MET
46	AZ	34	ASN
46	AZ	41	LEU
46	AZ	53	ILE
46	AZ	61	LEU
46	AZ	63	ASP
46	AZ	74	VAL
46	AZ	81	ARG
46	AZ	90	VAL
46	AZ	98	MET
46	AZ	112	ARG
46	AZ	123	ASP
46	AZ	124	ILE
46	AZ	155	LEU
46	AZ	162	GLU
46	AZ	166	SER
46	AZ	169	GLU
47	A0	5	LYS
47	A0	11	ARG
47	A0	14	ARG
47	A0	20	ARG
47	A0	36	ILE
47	A0	41	ARG
47	A0	64	ASP
47	A0	84	LEU
48	A1	11	ARG
48	A1	19	GLN
48	A1	25	LYS
48	A1	39	LYS
48	A1	40	ARG
48	A1	41	ARG
48	A1	46	LEU
48	A1	58	ILE
48	A1	61	ARG
48	A1	72	GLU
48	A1	73	LEU
48	A1	82	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	A2	2	LYS
49	A2	19	VAL
49	A2	52	ASP
49	A2	53	LEU
49	A2	64	LEU
50	A3	8	LEU
50	A3	20	LYS
50	A3	31	LEU
50	A3	35	ARG
51	A4	1	MET
51	A4	5	ILE
51	A4	10	VAL
51	A4	13	ARG
51	A4	20	ASN
51	A4	25	TYR
51	A4	30	GLU
51	A4	32	TYR
51	A4	34	GLU
51	A4	42	PHE
51	A4	44	THR
51	A4	49	PHE
51	A4	51	ASP
51	A4	53	GLU
51	A4	55	ARG
52	A5	23	HIS
52	A5	25	LEU
52	A5	44	THR
52	A5	52	TYR
52	A5	55	ARG
53	A6	9	LEU
53	A6	10	LEU
53	A6	11	LEU
53	A6	18	ARG
53	A6	30	THR
53	A6	34	LEU
53	A6	39	TYR
53	A6	42	TRP
54	A7	1	MET
54	A7	4	THR
54	A7	8	ASN
54	A7	41	ARG
55	A8	4	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	A8	8	LYS
55	A8	30	ARG
55	A8	31	HIS
55	A8	32	LEU
55	A8	33	ASN
55	A8	34	TRP
55	A8	44	LYS
55	A8	47	LYS
55	A8	49	VAL
55	A8	56	GLU
55	A8	61	LEU
55	A8	64	TYR
56	A9	1	MET
56	A9	17	ILE
1	Bb	15	VAL
1	Bb	17	PHE
1	Bb	24	TRP
1	Bb	36	ARG
1	Bb	69	LEU
1	Bb	137	ARG
1	Bb	140	HIS
1	Bb	145	LEU
1	Bb	155	LEU
1	Bb	172	ILE
1	Bb	196	LEU
1	Bb	204	ASN
1	Bb	221	LEU
2	Bc	3	ASN
2	Bc	5	ILE
2	Bc	6	HIS
2	Bc	16	ARG
2	Bc	18	TRP
2	Bc	29	TYR
2	Bc	34	LEU
2	Bc	36	ASP
2	Bc	37	GLN
2	Bc	82	GLU
2	Bc	94	LEU
2	Bc	107	GLN
2	Bc	127	ARG
2	Bc	131	ARG
2	Bc	152	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Bc	167	TRP
2	Bc	193	TYR
3	Bd	3	ARG
3	Bd	9	CYS
3	Bd	10	ARG
3	Bd	11	LEU
3	Bd	12	CYS
3	Bd	15	GLU
3	Bd	26	CYS
3	Bd	36	ARG
3	Bd	38	TYR
3	Bd	49	ARG
3	Bd	53	ASP
3	Bd	58	LEU
3	Bd	59	ARG
3	Bd	86	LYS
3	Bd	97	LEU
3	Bd	110	PHE
3	Bd	129	ASN
3	Bd	131	ARG
3	Bd	132	ARG
3	Bd	135	LEU
3	Bd	162	LEU
3	Bd	168	ARG
3	Bd	196	LEU
3	Bd	200	GLU
4	Be	6	PHE
4	Be	10	MET
4	Be	12	LEU
4	Be	20	GLN
4	Be	31	LEU
4	Be	55	VAL
4	Be	56	GLN
4	Be	79	GLU
4	Be	101	ILE
5	Bf	63	TYR
5	Bf	69	GLU
5	Bf	80	ARG
6	Bg	21	VAL
6	Bg	88	PRO
6	Bg	111	ARG
6	Bg	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	Bg	124	LEU
6	Bg	140	ASP
6	Bg	151	TYR
7	Bh	1	MET
7	Bh	25	ASP
7	Bh	26	VAL
7	Bh	50	ARG
7	Bh	52	ASP
7	Bh	60	ARG
7	Bh	65	TYR
7	Bh	102	ARG
7	Bh	112	LEU
7	Bh	119	LEU
8	Bi	3	GLN
8	Bi	10	ARG
8	Bi	78	LYS
8	Bi	88	TYR
8	Bi	95	LYS
8	Bi	104	ARG
8	Bi	105	ASP
8	Bi	112	LYS
8	Bi	114	TYR
8	Bi	121	ARG
8	Bi	125	TYR
8	Bi	128	ARG
9	Bj	4	ILE
9	Bj	22	LYS
9	Bj	46	ARG
9	Bj	49	VAL
9	Bj	50	ILE
9	Bj	62	HIS
9	Bj	68	HIS
9	Bj	96	ILE
10	Bk	29	ILE
10	Bk	126	ARG
11	Bl	7	ILE
11	Bl	20	LYS
11	Bl	27	LEU
11	Bl	41	ARG
11	Bl	42	THR
11	Bl	47	LYS
11	Bl	53	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Bl	55	VAL
11	Bl	62	SER
11	Bl	66	VAL
11	Bl	67	THR
11	Bl	89	ARG
11	Bl	92	ASP
11	Bl	97	ARG
11	Bl	102	ARG
11	Bl	126	LYS
12	Bm	47	ASP
12	Bm	48	LEU
12	Bm	56	LEU
12	Bm	64	TRP
12	Bm	65	LYS
12	Bm	66	LEU
12	Bm	69	GLU
12	Bm	70	LEU
12	Bm	71	ARG
12	Bm	73	GLU
12	Bm	77	ASN
12	Bm	79	LYS
12	Bm	82	MET
12	Bm	92	HIS
12	Bm	93	ARG
12	Bm	98	VAL
12	Bm	106	ASN
12	Bm	108	ARG
12	Bm	115	LYS
13	Bn	33	VAL
13	Bn	44	LEU
14	Bo	37	ASN
14	Bo	65	ARG
14	Bo	82	ILE
14	Bo	85	LEU
14	Bo	88	ARG
15	Bp	1	MET
15	Bp	2	VAL
15	Bp	69	THR
16	Bq	38	ARG
16	Bq	59	ILE
16	Bq	98	LEU
17	Br	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Br	44	LEU
17	Br	65	ILE
18	Bs	5	LEU
18	Bs	6	LYS
18	Bs	7	LYS
18	Bs	15	LEU
18	Bs	29	ARG
18	Bs	33	THR
18	Bs	37	ARG
18	Bs	70	LYS
19	Bt	10	LEU
19	Bt	24	LEU
19	Bt	26	ASN
19	Bt	36	LEU
19	Bt	41	ILE
19	Bt	73	HIS
19	Bt	75	ASN
19	Bt	93	GLU
21	By	5	LEU
21	By	7	PHE
21	By	29	LYS
21	By	34	LEU
21	By	47	MET
21	By	48	PRO
21	By	49	ASP
21	By	56	ARG
21	By	61	ARG
21	By	63	VAL
21	By	85	GLU
26	BC	39	ASP
26	BC	53	ARG
26	BC	185	LYS
27	BD	10	THR
27	BD	24	ILE
27	BD	26	LYS
27	BD	35	LYS
27	BD	37	LEU
27	BD	43	ARG
27	BD	46	GLN
27	BD	49	ILE
27	BD	61	LEU
27	BD	65	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	BD	71	ASP
27	BD	72	LYS
27	BD	73	VAL
27	BD	94	LEU
27	BD	95	LEU
27	BD	98	VAL
27	BD	103	ARG
27	BD	104	TYR
27	BD	106	ILE
27	BD	122	ASP
27	BD	131	LEU
27	BD	166	GLN
27	BD	192	THR
27	BD	198	ASN
27	BD	200	ASP
27	BD	221	VAL
27	BD	228	PRO
27	BD	229	VAL
27	BD	257	LEU
27	BD	259	THR
27	BD	260	ARG
27	BD	271	ILE
28	BE	24	THR
28	BE	33	VAL
28	BE	49	LEU
28	BE	55	ASN
28	BE	63	LEU
28	BE	64	LYS
28	BE	67	PHE
28	BE	78	LEU
28	BE	79	ARG
28	BE	82	ARG
28	BE	87	GLU
28	BE	101	ARG
28	BE	113	PHE
28	BE	119	ARG
28	BE	144	ARG
28	BE	169	ASN
28	BE	181	LEU
28	BE	197	ILE
28	BE	200	GLU
28	BE	202	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BE	203	LYS
29	BF	23	ASP
29	BF	28	ILE
29	BF	33	LEU
29	BF	38	ARG
29	BF	57	VAL
29	BF	66	PRO
29	BF	67	GLN
29	BF	74	ARG
29	BF	83	PHE
29	BF	106	ARG
29	BF	110	LEU
29	BF	125	LEU
29	BF	129	PHE
29	BF	157	VAL
29	BF	158	THR
29	BF	160	ASN
29	BF	164	ARG
29	BF	165	ARG
29	BF	170	LEU
29	BF	183	VAL
29	BF	188	ARG
29	BF	192	LEU
29	BF	200	GLU
30	BG	3	LEU
30	BG	12	TYR
30	BG	21	ARG
30	BG	22	ARG
30	BG	33	ARG
30	BG	43	LEU
30	BG	58	GLN
30	BG	63	ILE
30	BG	64	THR
30	BG	67	LYS
30	BG	71	THR
30	BG	77	ILE
30	BG	80	PHE
30	BG	83	ARG
30	BG	87	PRO
30	BG	93	THR
30	BG	113	ARG
30	BG	115	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	BG	123	ASN
30	BG	126	ASP
30	BG	143	GLU
30	BG	147	ASP
30	BG	159	VAL
30	BG	164	GLU
31	BH	9	ILE
31	BH	53	GLU
31	BH	54	ARG
31	BH	83	TYR
31	BH	89	ILE
31	BH	153	LYS
31	BH	157	TYR
31	BH	163	TYR
31	BH	170	ARG
32	BI	1	MET
32	BI	9	LEU
32	BI	12	LEU
32	BI	31	LEU
32	BI	71	ILE
32	BI	74	ASN
32	BI	85	GLU
32	BI	86	THR
32	BI	89	TYR
32	BI	91	SER
32	BI	92	VAL
32	BI	93	THR
32	BI	99	GLU
32	BI	103	ARG
32	BI	105	HIS
32	BI	107	VAL
32	BI	109	ILE
32	BI	110	ASP
32	BI	123	LEU
32	BI	130	TYR
32	BI	138	ILE
32	BI	139	GLN
32	BI	140	LEU
34	BN	4	TYR
34	BN	23	LEU
34	BN	28	THR
34	BN	32	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	BN	34	LEU
34	BN	37	LYS
34	BN	39	ARG
34	BN	43	THR
34	BN	48	MET
34	BN	56	ASN
34	BN	60	ILE
34	BN	87	LEU
34	BN	119	ARG
34	BN	121	LYS
34	BN	127	ASP
34	BN	130	HIS
35	BO	7	TYR
35	BO	8	LEU
35	BO	24	VAL
35	BO	32	TYR
35	BO	89	ASN
35	BO	98	VAL
35	BO	108	GLU
36	BP	13	ASN
36	BP	16	ARG
36	BP	18	ARG
36	BP	32	THR
36	BP	39	LYS
36	BP	41	ARG
36	BP	42	SER
36	BP	45	LEU
36	BP	47	ASP
36	BP	57	THR
36	BP	59	LEU
36	BP	61	ARG
36	BP	64	LYS
36	BP	67	MET
36	BP	81	GLN
36	BP	85	LEU
36	BP	91	PHE
36	BP	98	GLU
36	BP	105	LEU
36	BP	108	LYS
36	BP	110	TYR
36	BP	112	LEU
36	BP	114	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BP	119	GLU
36	BP	135	LEU
37	BQ	18	LYS
37	BQ	45	GLN
37	BQ	55	VAL
37	BQ	58	PHE
37	BQ	67	ARG
37	BQ	75	THR
37	BQ	110	THR
37	BQ	134	ARG
37	BQ	135	ASP
37	BQ	137	TYR
38	BR	2	ARG
38	BR	4	LEU
38	BR	8	ARG
38	BR	12	ARG
38	BR	15	SER
38	BR	18	LEU
38	BR	28	LEU
38	BR	65	LEU
38	BR	67	LEU
38	BR	71	GLN
38	BR	76	VAL
38	BR	79	LEU
38	BR	94	TYR
38	BR	95	THR
38	BR	99	LYS
38	BR	113	LEU
39	BS	11	LYS
39	BS	12	PHE
39	BS	36	TYR
39	BS	40	ILE
39	BS	44	LYS
39	BS	89	ARG
39	BS	92	TYR
39	BS	97	ARG
39	BS	101	LEU
39	BS	106	ARG
40	BT	3	ARG
40	BT	13	ARG
40	BT	14	TYR
40	BT	24	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	BT	32	TYR
40	BT	38	ASN
40	BT	41	ARG
40	BT	50	ILE
40	BT	51	ARG
40	BT	58	ASN
40	BT	59	THR
40	BT	65	LYS
40	BT	78	LEU
40	BT	82	LEU
40	BT	93	ARG
40	BT	96	ARG
40	BT	99	LEU
40	BT	100	TYR
40	BT	101	PHE
40	BT	107	ASP
40	BT	108	ARG
40	BT	122	ASP
40	BT	128	GLU
41	BU	14	HIS
41	BU	19	LYS
41	BU	52	ARG
41	BU	59	ARG
41	BU	60	LEU
41	BU	66	ASN
41	BU	74	LEU
41	BU	83	LEU
41	BU	101	ARG
41	BU	108	GLU
41	BU	112	ARG
42	BV	14	VAL
42	BV	16	PRO
42	BV	18	LEU
42	BV	19	LYS
42	BV	21	ARG
42	BV	22	VAL
42	BV	33	VAL
42	BV	37	VAL
42	BV	39	LEU
42	BV	40	LEU
42	BV	46	VAL
42	BV	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	BV	66	ARG
42	BV	82	ARG
42	BV	91	TYR
42	BV	95	LEU
42	BV	99	ILE
43	BW	11	ARG
43	BW	51	LEU
43	BW	57	ASN
43	BW	60	ASN
43	BW	70	TYR
43	BW	76	VAL
43	BW	100	THR
43	BW	107	LEU
44	BX	27	THR
44	BX	57	LEU
44	BX	63	LYS
44	BX	68	ARG
44	BX	70	LEU
44	BX	80	ILE
44	BX	81	VAL
44	BX	83	VAL
45	BY	2	ARG
45	BY	6	HIS
45	BY	7	VAL
45	BY	9	LYS
45	BY	28	LYS
45	BY	29	GLU
45	BY	32	PRO
45	BY	53	PRO
45	BY	60	PHE
45	BY	77	PRO
45	BY	89	PHE
45	BY	90	LEU
46	BZ	13	GLU
46	BZ	16	SER
46	BZ	23	LYS
46	BZ	31	ARG
46	BZ	38	TYR
46	BZ	39	VAL
46	BZ	41	LEU
46	BZ	61	LEU
46	BZ	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	BZ	87	ASP
46	BZ	96	VAL
46	BZ	103	ARG
46	BZ	112	ARG
46	BZ	127	LYS
46	BZ	131	ARG
46	BZ	132	ASN
46	BZ	136	PHE
46	BZ	145	GLU
46	BZ	151	HIS
46	BZ	155	LEU
46	BZ	158	PRO
46	BZ	163	LEU
46	BZ	169	GLU
46	BZ	175	VAL
46	BZ	177	PRO
46	BZ	179	ASP
47	B0	5	LYS
47	B0	11	ARG
47	B0	14	ARG
47	B0	20	ARG
47	B0	36	ILE
47	B0	41	ARG
47	B0	64	ASP
47	B0	84	LEU
48	B1	20	ARG
48	B1	40	ARG
48	B1	41	ARG
48	B1	45	ASN
48	B1	46	LEU
48	B1	59	THR
48	B1	73	LEU
48	B1	76	ARG
48	B1	82	LEU
49	B2	2	LYS
49	B2	7	ARG
49	B2	16	LEU
49	B2	17	SER
49	B2	30	ARG
49	B2	32	LEU
49	B2	34	GLU
49	B2	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	B2	53	LEU
49	B2	64	LEU
49	B2	68	ARG
49	B2	70	GLN
50	B3	8	LEU
50	B3	20	LYS
50	B3	31	LEU
50	B3	35	ARG
51	B4	1	MET
51	B4	5	ILE
51	B4	10	VAL
51	B4	13	ARG
51	B4	20	ASN
51	B4	25	TYR
51	B4	30	GLU
51	B4	32	TYR
51	B4	34	GLU
51	B4	42	PHE
51	B4	44	THR
51	B4	49	PHE
51	B4	51	ASP
51	B4	53	GLU
51	B4	55	ARG
52	B5	23	HIS
52	B5	25	LEU
52	B5	44	THR
52	B5	52	TYR
52	B5	55	ARG
53	B6	9	LEU
53	B6	10	LEU
53	B6	11	LEU
53	B6	15	GLU
53	B6	18	ARG
53	B6	30	THR
53	B6	34	LEU
53	B6	39	TYR
53	B6	42	TRP
54	B7	1	MET
54	B7	4	THR
54	B7	8	ASN
54	B7	41	ARG
55	B8	4	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	B8	8	LYS
55	B8	16	ILE
55	B8	30	ARG
55	B8	31	HIS
55	B8	32	LEU
55	B8	33	ASN
55	B8	34	TRP
55	B8	44	LYS
55	B8	46	ARG
55	B8	47	LYS
55	B8	49	VAL
55	B8	56	GLU
55	B8	61	LEU
55	B8	64	TYR
56	B9	1	MET
56	B9	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (314) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ab	37	ASN
1	Ab	40	HIS
1	Ab	78	GLN
1	Ab	135	GLN
1	Ab	146	GLN
1	Ab	204	ASN
2	Ac	69	HIS
2	Ac	107	GLN
2	Ac	123	GLN
2	Ac	170	GLN
2	Ac	181	ASN
3	Ad	42	GLN
3	Ad	62	GLN
3	Ad	77	ASN
3	Ad	129	ASN
3	Ad	161	ASN
3	Ad	201	GLN
4	Ae	20	GLN
4	Ae	72	GLN
4	Ae	73	ASN
4	Ae	78	HIS
5	Af	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Af	18	GLN
5	Af	27	GLN
5	Af	32	ASN
5	Af	64	GLN
5	Af	100	ASN
6	Ag	13	GLN
6	Ag	28	ASN
6	Ag	68	ASN
6	Ag	84	ASN
6	Ag	106	GLN
6	Ag	148	ASN
8	Ai	3	GLN
8	Ai	31	GLN
8	Ai	58	HIS
8	Ai	124	GLN
9	Aj	56	HIS
9	Aj	78	ASN
9	Aj	84	GLN
10	Ak	13	GLN
10	Ak	26	ASN
10	Ak	78	GLN
10	Ak	116	HIS
10	Ak	117	ASN
11	Al	8	ASN
11	Al	9	GLN
11	Al	49	ASN
11	Al	75	HIS
12	Am	101	GLN
14	Ao	37	ASN
14	Ao	46	HIS
15	Ap	76	GLN
16	Aq	16	GLN
17	Ar	36	ASN
18	As	14	HIS
18	As	23	ASN
18	As	65	ASN
19	At	16	HIS
19	At	26	ASN
19	At	42	GLN
19	At	75	ASN
26	AC	189	ASN
27	AD	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	AD	96	HIS
27	AD	126	GLN
27	AD	166	GLN
27	AD	186	HIS
27	AD	198	ASN
27	AD	227	ASN
28	AE	48	GLN
28	AE	54	GLN
28	AE	55	ASN
28	AE	129	HIS
28	AE	143	ASN
28	AE	169	ASN
28	AE	192	ASN
29	AF	69	HIS
29	AF	75	HIS
29	AF	133	ASN
29	AF	160	ASN
29	AF	169	ASN
30	AG	27	ASN
30	AG	40	ASN
30	AG	108	ASN
30	AG	123	ASN
31	AH	65	HIS
31	AH	74	ASN
31	AH	139	GLN
31	AH	147	ASN
32	AI	28	ASN
32	AI	43	ASN
32	AI	74	ASN
32	AI	104	GLN
32	AI	139	GLN
34	AN	38	HIS
34	AN	45	ASN
34	AN	56	ASN
34	AN	128	HIS
35	AO	5	GLN
35	AO	13	ASN
35	AO	82	ASN
35	AO	88	ASN
36	AP	13	ASN
36	AP	84	ASN
36	AP	128	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	AQ	12	GLN
37	AQ	45	GLN
38	AR	23	ASN
38	AR	24	GLN
38	AR	53	HIS
38	AR	71	GLN
39	AS	34	HIS
40	AT	38	ASN
40	AT	43	GLN
40	AT	58	ASN
40	AT	90	GLN
40	AT	123	GLN
41	AU	44	ASN
41	AU	49	HIS
41	AU	66	ASN
42	AV	11	GLN
43	AW	34	ASN
43	AW	57	ASN
43	AW	61	ASN
43	AW	62	HIS
43	AW	102	HIS
44	AX	31	HIS
44	AX	41	ASN
44	AX	55	ASN
46	AZ	34	ASN
46	AZ	118	GLN
47	A0	12	ASN
47	A0	29	GLN
47	A0	70	GLN
48	A1	19	GLN
48	A1	45	ASN
48	A1	47	GLN
49	A2	46	GLN
49	A2	47	ASN
49	A2	70	GLN
50	A3	19	GLN
50	A3	32	GLN
50	A3	46	ASN
50	A3	52	HIS
51	A4	20	ASN
51	A4	40	HIS
52	A5	4	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	A5	43	HIS
53	A6	32	ASN
53	A6	46	HIS
54	A7	8	ASN
55	A8	31	HIS
55	A8	33	ASN
56	A9	32	HIS
56	A9	34	GLN
1	Bb	37	ASN
1	Bb	40	HIS
1	Bb	78	GLN
1	Bb	135	GLN
1	Bb	146	GLN
1	Bb	204	ASN
2	Bc	69	HIS
2	Bc	107	GLN
2	Bc	123	GLN
2	Bc	170	GLN
2	Bc	181	ASN
3	Bd	42	GLN
3	Bd	62	GLN
3	Bd	77	ASN
3	Bd	129	ASN
3	Bd	161	ASN
3	Bd	201	GLN
4	Be	20	GLN
4	Be	72	GLN
4	Be	73	ASN
4	Be	78	HIS
5	Bf	7	ASN
5	Bf	18	GLN
5	Bf	27	GLN
5	Bf	32	ASN
5	Bf	64	GLN
5	Bf	100	ASN
6	Bg	13	GLN
6	Bg	28	ASN
6	Bg	68	ASN
6	Bg	84	ASN
6	Bg	106	GLN
6	Bg	148	ASN
8	Bi	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	Bi	31	GLN
8	Bi	58	HIS
8	Bi	124	GLN
9	Bj	78	ASN
9	Bj	84	GLN
10	Bk	13	GLN
10	Bk	26	ASN
10	Bk	78	GLN
10	Bk	117	ASN
11	Bl	8	ASN
11	Bl	9	GLN
11	Bl	49	ASN
11	Bl	75	HIS
12	Bm	101	GLN
14	Bo	37	ASN
14	Bo	46	HIS
15	Bp	76	GLN
16	Bq	16	GLN
17	Br	36	ASN
18	Bs	14	HIS
18	Bs	23	ASN
18	Bs	65	ASN
19	Bt	16	HIS
19	Bt	26	ASN
19	Bt	42	GLN
19	Bt	75	ASN
21	By	25	GLN
21	By	65	GLN
26	BC	189	ASN
27	BD	58	HIS
27	BD	96	HIS
27	BD	126	GLN
27	BD	166	GLN
27	BD	186	HIS
27	BD	198	ASN
27	BD	227	ASN
28	BE	35	GLN
28	BE	48	GLN
28	BE	54	GLN
28	BE	55	ASN
28	BE	129	HIS
28	BE	143	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	BE	169	ASN
28	BE	192	ASN
29	BF	69	HIS
29	BF	75	HIS
29	BF	133	ASN
29	BF	160	ASN
29	BF	169	ASN
30	BG	40	ASN
30	BG	58	GLN
30	BG	66	GLN
31	BH	65	HIS
31	BH	74	ASN
31	BH	139	GLN
31	BH	147	ASN
32	BI	28	ASN
32	BI	43	ASN
32	BI	74	ASN
32	BI	104	GLN
32	BI	139	GLN
34	BN	38	HIS
34	BN	45	ASN
34	BN	56	ASN
34	BN	128	HIS
35	BO	5	GLN
35	BO	13	ASN
35	BO	82	ASN
35	BO	88	ASN
36	BP	13	ASN
36	BP	84	ASN
36	BP	128	HIS
37	BQ	12	GLN
37	BQ	45	GLN
38	BR	23	ASN
38	BR	24	GLN
38	BR	53	HIS
38	BR	71	GLN
39	BS	34	HIS
40	BT	38	ASN
40	BT	43	GLN
40	BT	58	ASN
40	BT	90	GLN
40	BT	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	BU	14	HIS
41	BU	44	ASN
41	BU	49	HIS
41	BU	66	ASN
42	BV	11	GLN
43	BW	34	ASN
43	BW	57	ASN
43	BW	61	ASN
43	BW	62	HIS
43	BW	102	HIS
44	BX	31	HIS
44	BX	41	ASN
44	BX	55	ASN
46	BZ	55	HIS
46	BZ	132	ASN
46	BZ	151	HIS
47	B0	12	ASN
47	B0	29	GLN
47	B0	70	GLN
48	B1	45	ASN
48	B1	56	GLN
49	B2	9	GLN
49	B2	47	ASN
49	B2	65	ASN
50	B3	19	GLN
50	B3	32	GLN
50	B3	46	ASN
50	B3	52	HIS
51	B4	6	HIS
51	B4	20	ASN
51	B4	40	HIS
52	B5	4	HIS
52	B5	43	HIS
53	B6	32	ASN
53	B6	46	HIS
54	B7	8	ASN
55	B8	31	HIS
55	B8	33	ASN
56	B9	32	HIS
56	B9	34	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	208 (13%)	0
22	Ba	1503/1504 (99%)	209 (13%)	0
23	Ax	11/25 (44%)	5 (45%)	0
23	Bx	11/25 (44%)	5 (45%)	0
24	Av	76/77 (98%)	18 (23%)	0
24	Bv	76/77 (98%)	14 (18%)	0
25	Aw	76/77 (98%)	9 (11%)	0
25	Bw	76/77 (98%)	10 (13%)	0
57	AA	2847/2848 (99%)	491 (17%)	61 (2%)
57	BA	2847/2848 (99%)	486 (17%)	64 (2%)
58	AB	118/119 (99%)	18 (15%)	1 (0%)
58	BB	118/119 (99%)	18 (15%)	1 (0%)
All	All	9262/9300 (99%)	1491 (16%)	127 (1%)

All (1491) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	Aa	9	G
22	Aa	31	G
22	Aa	32	A
22	Aa	39	G
22	Aa	47	C
22	Aa	48	C
22	Aa	51	A
22	Aa	60	A
22	Aa	61	G
22	Aa	79	G
22	Aa	80	G
22	Aa	81	U
22	Aa	84	U
22	Aa	89	C
22	Aa	90	U
22	Aa	97	G
22	Aa	116	A
22	Aa	120	A
22	Aa	121	C
22	Aa	131	C
22	Aa	150	C
22	Aa	172	A
22	Aa	195	A
22	Aa	197	A
22	Aa	203	U
22	Aa	204	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Aa	220	G
22	Aa	244	U
22	Aa	247	G
22	Aa	251	G
22	Aa	266	G
22	Aa	267	C
22	Aa	289	G
22	Aa	321	A
22	Aa	328	C
22	Aa	329	A
22	Aa	332	G
22	Aa	345	C
22	Aa	352	C
22	Aa	353	A
22	Aa	354	G
22	Aa	367	U
22	Aa	372	C
22	Aa	397	A
22	Aa	398	C
22	Aa	412	A
22	Aa	413	G
22	Aa	414	A
22	Aa	422	C
22	Aa	423	G
22	Aa	428	G
22	Aa	429	U
22	Aa	430	A
22	Aa	435	C
22	Aa	437	U
22	Aa	439	A
22	Aa	452	A
22	Aa	461	A
22	Aa	484	G
22	Aa	485	G
22	Aa	496	A
22	Aa	498	U
22	Aa	509	A
22	Aa	510	A
22	Aa	511	C
22	Aa	518	C
22	Aa	527	G
22	Aa	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Aa	533	A
22	Aa	534	U
22	Aa	547	A
22	Aa	559	A
22	Aa	561	U
22	Aa	562	C
22	Aa	572	A
22	Aa	573	A
22	Aa	575	G
22	Aa	576	G
22	Aa	577	G
22	Aa	630	G
22	Aa	631	G
22	Aa	632	A
22	Aa	633	G
22	Aa	653	A
22	Aa	665	A
22	Aa	687	A
22	Aa	688	G
22	Aa	703	G
22	Aa	724	G
22	Aa	731	G
22	Aa	749	C
22	Aa	755	G
22	Aa	777	A
22	Aa	794	A
22	Aa	816	A
22	Aa	817	C
22	Aa	818	G
22	Aa	821	G
22	Aa	828	A
22	Aa	833	U
22	Aa	839	U
22	Aa	840	C
22	Aa	841	U
22	Aa	848	C
22	Aa	859	A
22	Aa	885	G
22	Aa	902	G
22	Aa	913	A
22	Aa	914	A
22	Aa	926	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Aa	927	G
22	Aa	934	C
22	Aa	935	A
22	Aa	960	U
22	Aa	961	U
22	Aa	966	G
22	Aa	968	A
22	Aa	969	A
22	Aa	971	G
22	Aa	974	A
22	Aa	975	A
22	Aa	976	G
22	Aa	977	A
22	Aa	978	A
22	Aa	980	C
22	Aa	991	U
22	Aa	992	U
22	Aa	993	G
22	Aa	1001(A)	G
22	Aa	1026	G
22	Aa	1030	C
22	Aa	1050	G
22	Aa	1054	C
22	Aa	1055	A
22	Aa	1065	U
22	Aa	1066	C
22	Aa	1068	G
22	Aa	1081	G
22	Aa	1094	G
22	Aa	1095	U
22	Aa	1101	A
22	Aa	1108	G
22	Aa	1117	G
22	Aa	1124	G
22	Aa	1125	U
22	Aa	1126	U
22	Aa	1129	C
22	Aa	1131	G
22	Aa	1136	U
22	Aa	1137	C
22	Aa	1138	G
22	Aa	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Aa	1146	A
22	Aa	1152	A
22	Aa	1159	U
22	Aa	1182	G
22	Aa	1194	U
22	Aa	1196	U
22	Aa	1197	G
22	Aa	1201	A
22	Aa	1202	G
22	Aa	1212	U
22	Aa	1213	A
22	Aa	1225	A
22	Aa	1226	C
22	Aa	1238	A
22	Aa	1249	C
22	Aa	1255	G
22	Aa	1256	A
22	Aa	1257	U
22	Aa	1280	A
22	Aa	1281	U
22	Aa	1282	C
22	Aa	1286	A
22	Aa	1287	A
22	Aa	1294	G
22	Aa	1300	G
22	Aa	1301	U
22	Aa	1302	U
22	Aa	1305	G
22	Aa	1317	C
22	Aa	1320	C
22	Aa	1322	C
22	Aa	1323	G
22	Aa	1331	G
22	Aa	1346	A
22	Aa	1347	G
22	Aa	1363	C
22	Aa	1364	U
22	Aa	1397	C
22	Aa	1419	G
22	Aa	1442	G
22	Aa	1442(A)	G
22	Aa	1442(B)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Aa	1443	G
22	Aa	1452	C
22	Aa	1492	A
22	Aa	1497	G
22	Aa	1498	U
22	Aa	1499	A
22	Aa	1504	G
22	Aa	1505	G
22	Aa	1506	U
22	Aa	1507	A
22	Aa	1517	G
22	Aa	1520	G
22	Aa	1529	G
22	Aa	1530	G
23	Ax	14	A
23	Ax	19	OMU
23	Ax	21	OMG
23	Ax	22	A
23	Ax	24	A
24	Av	3	C
24	Av	4	G
24	Av	5	G
24	Av	7	G
24	Av	8	U
24	Av	9	G
24	Av	17(A)	U
24	Av	18	G
24	Av	19	G
24	Av	20	U
24	Av	21	A
24	Av	47	U
24	Av	48	C
24	Av	49	G
24	Av	65	C
24	Av	73	A
24	Av	75	C
24	Av	76	A
25	Aw	5	G
25	Aw	8	U
25	Aw	16	C
25	Aw	17(A)	U
25	Aw	18	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Aw	19	G
25	Aw	20	U
25	Aw	47	U
25	Aw	48	C
57	AA	10	G
57	AA	34	C
57	AA	35	G
57	AA	45	C
57	AA	49	A
57	AA	50	U
57	AA	55	G
57	AA	71	A
57	AA	72	U
57	AA	75	G
57	AA	88	G
57	AA	90	U
57	AA	94	C
57	AA	95	G
57	AA	100	G
57	AA	102	G
57	AA	118	A
57	AA	119	A
57	AA	120	U
57	AA	129	C
57	AA	139(A)	G
57	AA	141	A
57	AA	146	G
57	AA	154(A)	C
57	AA	155	U
57	AA	156	U
57	AA	171	G
57	AA	174	C
57	AA	181	A
57	AA	182	A
57	AA	196	A
57	AA	197	A
57	AA	199	A
57	AA	204	A
57	AA	205	G
57	AA	215	G
57	AA	216	A
57	AA	221	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	222	A
57	AA	228	A
57	AA	229	A
57	AA	230	U
57	AA	233	A
57	AA	248	G
57	AA	252	G
57	AA	269	U
57	AA	271(J)	C
57	AA	271(N)	U
57	AA	271(O)	C
57	AA	271(P)	C
57	AA	271(R)	G
57	AA	271(Y)	U
57	AA	272	G
57	AA	272(B)	G
57	AA	272(H)	C
57	AA	272(I)	U
57	AA	274	G
57	AA	276	A
57	AA	277	C
57	AA	299	A
57	AA	311	A
57	AA	329	G
57	AA	330	A
57	AA	332	A
57	AA	333	G
57	AA	352	G
57	AA	353	G
57	AA	356	G
57	AA	363(B)	G
57	AA	363(F)	A
57	AA	365	C
57	AA	372	G
57	AA	386	G
57	AA	388	G
57	AA	405	U
57	AA	406	G
57	AA	411	G
57	AA	412	A
57	AA	428	A
57	AA	444	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	448	U
57	AA	454	A
57	AA	456	C
57	AA	457	A
57	AA	470	A
57	AA	475	U
57	AA	481	G
57	AA	494	G
57	AA	505	A
57	AA	508	G
57	AA	509	C
57	AA	528	A
57	AA	530	G
57	AA	531	C
57	AA	532	A
57	AA	533	G
57	AA	544	G
57	AA	547	A
57	AA	563	G
57	AA	573	G
57	AA	575	A
57	AA	586	A
57	AA	588	U
57	AA	603	A
57	AA	604	G
57	AA	607	U
57	AA	613	G
57	AA	614(B)	G
57	AA	615	G
57	AA	620	G
57	AA	622	G
57	AA	627	A
57	AA	637	A
57	AA	645	C
57	AA	646	A
57	AA	651	G
57	AA	653	A
57	AA	654	A
57	AA	654(C)	G
57	AA	654(I)	C
57	AA	654(J)	A
57	AA	654(K)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	654(L)	G
57	AA	654(M)	C
57	AA	654(T)	C
57	AA	655	A
57	AA	669	G
57	AA	670	A
57	AA	673	C
57	AA	686	G
57	AA	708	C
57	AA	717	G
57	AA	722	A
57	AA	730	C
57	AA	753	C
57	AA	764	A
57	AA	765	G
57	AA	775	G
57	AA	776	G
57	AA	782	A
57	AA	784	A
57	AA	785	G
57	AA	790	C
57	AA	791	C
57	AA	792	G
57	AA	805	G
57	AA	812	C
57	AA	819	A
57	AA	827	U
57	AA	828	U
57	AA	830	G
57	AA	848	G
57	AA	856	C
57	AA	859	G
57	AA	869	G
57	AA	878	A
57	AA	890	A
57	AA	896	A
57	AA	897	C
57	AA	904	C
57	AA	910	A
57	AA	917	A
57	AA	932	G
57	AA	941	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	945	A
57	AA	946	G
57	AA	958	U
57	AA	959	A
57	AA	961	C
57	AA	965	C
57	AA	974	G
57	AA	975	C
57	AA	983	A
57	AA	991	C
57	AA	996	A
57	AA	1012	U
57	AA	1013	C
57	AA	1015	G
57	AA	1022	G
57	AA	1023	U
57	AA	1025	G
57	AA	1026	U
57	AA	1039	G
57	AA	1041	C
57	AA	1045	A
57	AA	1046	A
57	AA	1047	G
57	AA	1049	C
57	AA	1052	C
57	AA	1053	C
57	AA	1106	A
57	AA	1110	G
57	AA	1112	G
57	AA	1113	U
57	AA	1114	G
57	AA	1116	C
57	AA	1130	U
57	AA	1135	C
57	AA	1136	G
57	AA	1142	U
57	AA	1155	A
57	AA	1171	G
57	AA	1173	G
57	AA	1174	A
57	AA	1175	U
57	AA	1176	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	1178	C
57	AA	1195	G
57	AA	1205	U
57	AA	1210	A
57	AA	1211	U
57	AA	1212	G
57	AA	1221	C
57	AA	1247	A
57	AA	1250	G
57	AA	1253	A
57	AA	1256	G
57	AA	1265	A
57	AA	1271	G
57	AA	1272	A
57	AA	1273	U
57	AA	1281	G
57	AA	1300	U
57	AA	1301	A
57	AA	1314	C
57	AA	1319	G
57	AA	1321	A
57	AA	1332	G
57	AA	1345	C
57	AA	1349	A
57	AA	1359	A
57	AA	1368	G
57	AA	1378	A
57	AA	1379	A
57	AA	1380	G
57	AA	1384	A
57	AA	1385	G
57	AA	1386	C
57	AA	1407	C
57	AA	1416	G
57	AA	1417	C
57	AA	1419	A
57	AA	1420	U
57	AA	1421	G
57	AA	1427	A
57	AA	1428	C
57	AA	1437	C
57	AA	1445	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	1449	A
57	AA	1450	G
57	AA	1460	A
57	AA	1461	G
57	AA	1467	C
57	AA	1471	A
57	AA	1475	G
57	AA	1478	G
57	AA	1481	U
57	AA	1482	G
57	AA	1485	G
57	AA	1488	G
57	AA	1490	A
57	AA	1493	C
57	AA	1494	A
57	AA	1495	A
57	AA	1497	U
57	AA	1501	C
57	AA	1502	C
57	AA	1505	C
57	AA	1509	C
57	AA	1509(A)	A
57	AA	1528(A)	A
57	AA	1537	G
57	AA	1539	G
57	AA	1541	G
57	AA	1542	A
57	AA	1544	A
57	AA	1554	A
57	AA	1558	A
57	AA	1559	G
57	AA	1566	A
57	AA	1569	A
57	AA	1578	U
57	AA	1579	A
57	AA	1584	C
57	AA	1586	A
57	AA	1588	C
57	AA	1591	G
57	AA	1603	A
57	AA	1608	A
57	AA	1609	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	1616	A
57	AA	1617	C
57	AA	1618	A
57	AA	1640	C
57	AA	1648	C
57	AA	1653	G
57	AA	1654	A
57	AA	1674	G
57	AA	1694	C
57	AA	1696	G
57	AA	1718	G
57	AA	1722	A
57	AA	1739	U
57	AA	1740	G
57	AA	1742	G
57	AA	1746	G
57	AA	1748	G
57	AA	1763	G
57	AA	1764	G
57	AA	1773	A
57	AA	1780	A
57	AA	1791	A
57	AA	1799	G
57	AA	1800	C
57	AA	1801	G
57	AA	1816	G
57	AA	1820	U
57	AA	1821	A
57	AA	1835	G
57	AA	1846	G
57	AA	1847	A
57	AA	1848	A
57	AA	1858	G
57	AA	1865	G
57	AA	1866	C
57	AA	1878	G
57	AA	1881	C
57	AA	1882	C
57	AA	1885	A
57	AA	1888	G
57	AA	1889	A
57	AA	1900	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	1906	G
57	AA	1912	A
57	AA	1913	A
57	AA	1929	G
57	AA	1930	G
57	AA	1936	A
57	AA	1938	A
57	AA	1948	G
57	AA	1955	U
57	AA	1963	U
57	AA	1967	C
57	AA	1969	A
57	AA	1970	A
57	AA	1971	A
57	AA	1972	A
57	AA	1982	C
57	AA	1987	G
57	AA	1992	G
57	AA	1993	U
57	AA	1997	G
57	AA	2023	G
57	AA	2031	A
57	AA	2033	A
57	AA	2034	U
57	AA	2036	C
57	AA	2043	C
57	AA	2055	C
57	AA	2056	G
57	AA	2060	A
57	AA	2061	G
57	AA	2062	A
57	AA	2069	G
57	AA	2100	G
57	AA	2103	C
57	AA	2104	G
57	AA	2116	G
57	AA	2118	U
57	AA	2127	G
57	AA	2131	G
57	AA	2133	G
57	AA	2159	G
57	AA	2172	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	2173	A
57	AA	2177	C
57	AA	2179	C
57	AA	2185	C
57	AA	2187	G
57	AA	2190	G
57	AA	2192	G
57	AA	2193	G
57	AA	2198	A
57	AA	2199	A
57	AA	2200	C
57	AA	2207	G
57	AA	2208	A
57	AA	2218	U
57	AA	2225	A
57	AA	2226	C
57	AA	2238	G
57	AA	2239	G
57	AA	2275	C
57	AA	2283	C
57	AA	2287	A
57	AA	2288	A
57	AA	2302	G
57	AA	2305	A
57	AA	2307	G
57	AA	2308	G
57	AA	2309	A
57	AA	2311	A
57	AA	2313	C
57	AA	2316	C
57	AA	2319	G
57	AA	2320	A
57	AA	2334	G
57	AA	2336	A
57	AA	2347	C
57	AA	2350	C
57	AA	2360	A
57	AA	2361	A
57	AA	2383	G
57	AA	2385	C
57	AA	2400	G
57	AA	2402	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	2406	U
57	AA	2423	U
57	AA	2425	A
57	AA	2429	G
57	AA	2430	A
57	AA	2435	A
57	AA	2439	A
57	AA	2441	C
57	AA	2448	A
57	AA	2459	A
57	AA	2465	C
57	AA	2469	A
57	AA	2470	G
57	AA	2472	G
57	AA	2476	A
57	AA	2477	C
57	AA	2478	A
57	AA	2482	G
57	AA	2484	G
57	AA	2491	U
57	AA	2502	G
57	AA	2505	G
57	AA	2518	A
57	AA	2524	G
57	AA	2529	G
57	AA	2531	A
57	AA	2542	A
57	AA	2543	G
57	AA	2554	U
57	AA	2566	A
57	AA	2567	G
57	AA	2573	C
57	AA	2586	C
57	AA	2602	A
57	AA	2611	U
57	AA	2612	C
57	AA	2615	U
57	AA	2630	G
57	AA	2657	A
57	AA	2673	G
57	AA	2690	C
57	AA	2691	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	2702	U
57	AA	2703	C
57	AA	2712	U
57	AA	2712(A)	A
57	AA	2713	A
57	AA	2720	U
57	AA	2726	U
57	AA	2733	A
57	AA	2752	C
57	AA	2758	A
57	AA	2762	G
57	AA	2765	A
57	AA	2766	G
57	AA	2778	A
57	AA	2779	U
57	AA	2790	A
57	AA	2791	C
57	AA	2794	C
57	AA	2799	C
57	AA	2801(A)	A
57	AA	2802	G
57	AA	2803	C
57	AA	2804	C
57	AA	2808	U
57	AA	2818	G
57	AA	2820	A
57	AA	2821	A
57	AA	2833	G
57	AA	2834	G
57	AA	2849	U
57	AA	2872	G
57	AA	2892	A
57	AA	2893	G
58	AB	8	U
58	AB	13	A
58	AB	15	A
58	AB	16	G
58	AB	22	U
58	AB	24	G
58	AB	41	U
58	AB	42	C
58	AB	45	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	AB	52	A
58	AB	53	A
58	AB	67	G
58	AB	73	A
58	AB	81	G
58	AB	82	G
58	AB	88	C
58	AB	110	G
58	AB	113	G
22	Ba	9	G
22	Ba	31	G
22	Ba	32	A
22	Ba	39	G
22	Ba	47	C
22	Ba	48	C
22	Ba	50	A
22	Ba	51	A
22	Ba	54	C
22	Ba	60	A
22	Ba	61	G
22	Ba	79	G
22	Ba	80	G
22	Ba	81	U
22	Ba	84	U
22	Ba	89	C
22	Ba	90	U
22	Ba	97	G
22	Ba	116	A
22	Ba	120	A
22	Ba	121	C
22	Ba	131	C
22	Ba	150	C
22	Ba	172	A
22	Ba	195	A
22	Ba	197	A
22	Ba	203	U
22	Ba	204	U
22	Ba	220	G
22	Ba	244	U
22	Ba	247	G
22	Ba	251	G
22	Ba	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Ba	267	C
22	Ba	289	G
22	Ba	321	A
22	Ba	328	C
22	Ba	329	A
22	Ba	332	G
22	Ba	345	C
22	Ba	352	C
22	Ba	353	A
22	Ba	354	G
22	Ba	367	U
22	Ba	372	C
22	Ba	397	A
22	Ba	398	C
22	Ba	412	A
22	Ba	413	G
22	Ba	414	A
22	Ba	422	C
22	Ba	423	G
22	Ba	428	G
22	Ba	429	U
22	Ba	430	A
22	Ba	435	C
22	Ba	437	U
22	Ba	439	A
22	Ba	452	A
22	Ba	461	A
22	Ba	484	G
22	Ba	485	G
22	Ba	496	A
22	Ba	498	U
22	Ba	509	A
22	Ba	510	A
22	Ba	511	C
22	Ba	518	C
22	Ba	527	G
22	Ba	532	A
22	Ba	533	A
22	Ba	534	U
22	Ba	547	A
22	Ba	559	A
22	Ba	561	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Ba	562	C
22	Ba	572	A
22	Ba	573	A
22	Ba	575	G
22	Ba	576	G
22	Ba	577	G
22	Ba	630	G
22	Ba	631	G
22	Ba	632	A
22	Ba	633	G
22	Ba	653	A
22	Ba	665	A
22	Ba	687	A
22	Ba	688	G
22	Ba	703	G
22	Ba	724	G
22	Ba	731	G
22	Ba	749	C
22	Ba	755	G
22	Ba	777	A
22	Ba	794	A
22	Ba	817	C
22	Ba	818	G
22	Ba	821	G
22	Ba	828	A
22	Ba	833	U
22	Ba	839	U
22	Ba	840	C
22	Ba	841	U
22	Ba	848	C
22	Ba	859	A
22	Ba	885	G
22	Ba	902	G
22	Ba	913	A
22	Ba	914	A
22	Ba	926	G
22	Ba	927	G
22	Ba	934	C
22	Ba	935	A
22	Ba	960	U
22	Ba	961	U
22	Ba	966	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Ba	968	A
22	Ba	969	A
22	Ba	974	A
22	Ba	975	A
22	Ba	976	G
22	Ba	977	A
22	Ba	978	A
22	Ba	980	C
22	Ba	991	U
22	Ba	992	U
22	Ba	993	G
22	Ba	1001(A)	G
22	Ba	1026	G
22	Ba	1030	C
22	Ba	1050	G
22	Ba	1054	C
22	Ba	1055	A
22	Ba	1065	U
22	Ba	1066	C
22	Ba	1068	G
22	Ba	1081	G
22	Ba	1094	G
22	Ba	1095	U
22	Ba	1101	A
22	Ba	1108	G
22	Ba	1117	G
22	Ba	1124	G
22	Ba	1125	U
22	Ba	1126	U
22	Ba	1129	C
22	Ba	1131	G
22	Ba	1136	U
22	Ba	1137	C
22	Ba	1138	G
22	Ba	1139	G
22	Ba	1146	A
22	Ba	1152	A
22	Ba	1159	U
22	Ba	1182	G
22	Ba	1196	U
22	Ba	1197	G
22	Ba	1198	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Ba	1201	A
22	Ba	1202	G
22	Ba	1212	U
22	Ba	1213	A
22	Ba	1225	A
22	Ba	1227	A
22	Ba	1238	A
22	Ba	1249	C
22	Ba	1255	G
22	Ba	1256	A
22	Ba	1257	U
22	Ba	1280	A
22	Ba	1281	U
22	Ba	1282	C
22	Ba	1286	A
22	Ba	1287	A
22	Ba	1294	G
22	Ba	1300	G
22	Ba	1301	U
22	Ba	1302	U
22	Ba	1305	G
22	Ba	1317	C
22	Ba	1320	C
22	Ba	1322	C
22	Ba	1323	G
22	Ba	1331	G
22	Ba	1346	A
22	Ba	1347	G
22	Ba	1363	C
22	Ba	1364	U
22	Ba	1419	G
22	Ba	1439	C
22	Ba	1442	G
22	Ba	1442(A)	G
22	Ba	1442(B)	A
22	Ba	1443	G
22	Ba	1447	A
22	Ba	1452	C
22	Ba	1487	G
22	Ba	1497	G
22	Ba	1499	A
22	Ba	1502	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	Ba	1504	G
22	Ba	1505	G
22	Ba	1506	U
22	Ba	1517	G
22	Ba	1519	A
22	Ba	1520	G
22	Ba	1529	G
22	Ba	1530	G
23	Bx	14	A
23	Bx	19	OMU
23	Bx	20	A2M
23	Bx	21	OMG
23	Bx	22	A
24	Bv	3	C
24	Bv	5	G
24	Bv	17(A)	U
24	Bv	18	G
24	Bv	19	G
24	Bv	20	U
24	Bv	21	A
24	Bv	47	U
24	Bv	48	C
24	Bv	61	C
24	Bv	65	C
24	Bv	73	A
24	Bv	75	C
24	Bv	76	A
25	Bw	5	G
25	Bw	7	G
25	Bw	8	U
25	Bw	9	G
25	Bw	17(A)	U
25	Bw	18	G
25	Bw	19	G
25	Bw	20	U
25	Bw	47	U
25	Bw	48	C
57	BA	10	G
57	BA	34	C
57	BA	35	G
57	BA	45	C
57	BA	49	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	50	U
57	BA	55	G
57	BA	71	A
57	BA	72	U
57	BA	75	G
57	BA	88	G
57	BA	90	U
57	BA	94	C
57	BA	95	G
57	BA	100	G
57	BA	102	G
57	BA	118	A
57	BA	119	A
57	BA	120	U
57	BA	129	C
57	BA	139(A)	G
57	BA	141	A
57	BA	146	G
57	BA	154(A)	C
57	BA	155	U
57	BA	156	U
57	BA	171	G
57	BA	174	C
57	BA	181	A
57	BA	182	A
57	BA	196	A
57	BA	197	A
57	BA	204	A
57	BA	205	G
57	BA	215	G
57	BA	216	A
57	BA	221	A
57	BA	222	A
57	BA	228	A
57	BA	229	A
57	BA	230	U
57	BA	233	A
57	BA	248	G
57	BA	252	G
57	BA	269	U
57	BA	271(J)	C
57	BA	271(N)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	271(O)	C
57	BA	271(P)	C
57	BA	271(R)	G
57	BA	271(Y)	U
57	BA	272	G
57	BA	272(B)	G
57	BA	272(H)	C
57	BA	272(I)	U
57	BA	274	G
57	BA	276	A
57	BA	277	C
57	BA	299	A
57	BA	311	A
57	BA	329	G
57	BA	330	A
57	BA	332	A
57	BA	333	G
57	BA	352	G
57	BA	353	G
57	BA	356	G
57	BA	363(B)	G
57	BA	363(F)	A
57	BA	365	C
57	BA	372	G
57	BA	386	G
57	BA	388	G
57	BA	405	U
57	BA	406	G
57	BA	411	G
57	BA	412	A
57	BA	428	A
57	BA	444	C
57	BA	448	U
57	BA	456	C
57	BA	457	A
57	BA	470	A
57	BA	475	U
57	BA	481	G
57	BA	494	G
57	BA	505	A
57	BA	508	G
57	BA	509	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	528	A
57	BA	531	C
57	BA	532	A
57	BA	533	G
57	BA	544	G
57	BA	547	A
57	BA	563	G
57	BA	573	G
57	BA	575	A
57	BA	586	A
57	BA	588	U
57	BA	603	A
57	BA	604	G
57	BA	607	U
57	BA	613	G
57	BA	614(B)	G
57	BA	615	G
57	BA	622	G
57	BA	627	A
57	BA	637	A
57	BA	645	C
57	BA	646	A
57	BA	651	G
57	BA	653	A
57	BA	654	A
57	BA	654(C)	G
57	BA	654(I)	C
57	BA	654(J)	A
57	BA	654(K)	C
57	BA	654(L)	G
57	BA	654(M)	C
57	BA	654(T)	C
57	BA	655	A
57	BA	669	G
57	BA	673	C
57	BA	686	G
57	BA	708	C
57	BA	717	G
57	BA	722	A
57	BA	730	C
57	BA	753	C
57	BA	764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	765	G
57	BA	775	G
57	BA	776	G
57	BA	782	A
57	BA	784	A
57	BA	785	G
57	BA	790	C
57	BA	791	C
57	BA	792	G
57	BA	805	G
57	BA	812	C
57	BA	819	A
57	BA	827	U
57	BA	828	U
57	BA	830	G
57	BA	848	G
57	BA	856	C
57	BA	859	G
57	BA	878	A
57	BA	890	A
57	BA	896	A
57	BA	897	C
57	BA	904	C
57	BA	910	A
57	BA	917	A
57	BA	932	G
57	BA	941	A
57	BA	945	A
57	BA	946	G
57	BA	958	U
57	BA	959	A
57	BA	961	C
57	BA	965	C
57	BA	974	G
57	BA	975	C
57	BA	983	A
57	BA	991	C
57	BA	996	A
57	BA	1012	U
57	BA	1013	C
57	BA	1015	G
57	BA	1022	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	1023	U
57	BA	1025	G
57	BA	1026	U
57	BA	1039	G
57	BA	1041	C
57	BA	1045	A
57	BA	1046	A
57	BA	1047	G
57	BA	1049	C
57	BA	1052	C
57	BA	1053	C
57	BA	1106	A
57	BA	1110	G
57	BA	1112	G
57	BA	1113	U
57	BA	1114	G
57	BA	1116	C
57	BA	1130	U
57	BA	1135	C
57	BA	1136	G
57	BA	1142	U
57	BA	1155	A
57	BA	1171	G
57	BA	1173	G
57	BA	1174	A
57	BA	1175	U
57	BA	1176	G
57	BA	1178	C
57	BA	1195	G
57	BA	1205	U
57	BA	1210	A
57	BA	1211	U
57	BA	1212	G
57	BA	1221	C
57	BA	1247	A
57	BA	1250	G
57	BA	1253	A
57	BA	1256	G
57	BA	1265	A
57	BA	1271	G
57	BA	1272	A
57	BA	1273	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	1281	G
57	BA	1286	A
57	BA	1300	U
57	BA	1301	A
57	BA	1314	C
57	BA	1319	G
57	BA	1321	A
57	BA	1332	G
57	BA	1345	C
57	BA	1349	A
57	BA	1359	A
57	BA	1368	G
57	BA	1378	A
57	BA	1379	A
57	BA	1380	G
57	BA	1384	A
57	BA	1385	G
57	BA	1386	C
57	BA	1407	C
57	BA	1416	G
57	BA	1417	C
57	BA	1419	A
57	BA	1420	U
57	BA	1421	G
57	BA	1427	A
57	BA	1428	C
57	BA	1437	C
57	BA	1445	A
57	BA	1449	A
57	BA	1450	G
57	BA	1460	A
57	BA	1461	G
57	BA	1467	C
57	BA	1471	A
57	BA	1475	G
57	BA	1478	G
57	BA	1481	U
57	BA	1482	G
57	BA	1485	G
57	BA	1488	G
57	BA	1490	A
57	BA	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	1494	A
57	BA	1495	A
57	BA	1497	U
57	BA	1501	C
57	BA	1502	C
57	BA	1505	C
57	BA	1509	C
57	BA	1509(A)	A
57	BA	1528(A)	A
57	BA	1537	G
57	BA	1539	G
57	BA	1541	G
57	BA	1542	A
57	BA	1544	A
57	BA	1554	A
57	BA	1558	A
57	BA	1559	G
57	BA	1566	A
57	BA	1569	A
57	BA	1578	U
57	BA	1579	A
57	BA	1584	C
57	BA	1586	A
57	BA	1588	C
57	BA	1591	G
57	BA	1603	A
57	BA	1608	A
57	BA	1609	A
57	BA	1616	A
57	BA	1617	C
57	BA	1618	A
57	BA	1640	C
57	BA	1648	C
57	BA	1653	G
57	BA	1654	A
57	BA	1674	G
57	BA	1694	C
57	BA	1696	G
57	BA	1718	G
57	BA	1722	A
57	BA	1739	U
57	BA	1740	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	1742	G
57	BA	1746	G
57	BA	1748	G
57	BA	1763	G
57	BA	1764	G
57	BA	1773	A
57	BA	1780	A
57	BA	1791	A
57	BA	1799	G
57	BA	1800	C
57	BA	1801	G
57	BA	1816	G
57	BA	1820	U
57	BA	1821	A
57	BA	1835	G
57	BA	1846	G
57	BA	1847	A
57	BA	1848	A
57	BA	1858	G
57	BA	1865	G
57	BA	1866	C
57	BA	1878	G
57	BA	1881	C
57	BA	1882	C
57	BA	1885	A
57	BA	1888	G
57	BA	1889	A
57	BA	1900	A
57	BA	1906	G
57	BA	1912	A
57	BA	1913	A
57	BA	1929	G
57	BA	1930	G
57	BA	1936	A
57	BA	1938	A
57	BA	1948	G
57	BA	1955	U
57	BA	1963	U
57	BA	1967	C
57	BA	1969	A
57	BA	1970	A
57	BA	1971	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	1972	A
57	BA	1982	C
57	BA	1987	G
57	BA	1992	G
57	BA	1993	U
57	BA	1997	G
57	BA	2023	G
57	BA	2031	A
57	BA	2033	A
57	BA	2034	U
57	BA	2036	C
57	BA	2043	C
57	BA	2055	C
57	BA	2056	G
57	BA	2060	A
57	BA	2061	G
57	BA	2062	A
57	BA	2069	G
57	BA	2100	G
57	BA	2103	C
57	BA	2104	G
57	BA	2116	G
57	BA	2118	U
57	BA	2127	G
57	BA	2131	G
57	BA	2133	G
57	BA	2159	G
57	BA	2172	U
57	BA	2173	A
57	BA	2177	C
57	BA	2179	C
57	BA	2185	C
57	BA	2187	G
57	BA	2190	G
57	BA	2192	G
57	BA	2193	G
57	BA	2198	A
57	BA	2199	A
57	BA	2200	C
57	BA	2207	G
57	BA	2208	A
57	BA	2218	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	2225	A
57	BA	2226	C
57	BA	2238	G
57	BA	2239	G
57	BA	2275	C
57	BA	2283	C
57	BA	2287	A
57	BA	2288	A
57	BA	2302	G
57	BA	2305	A
57	BA	2307	G
57	BA	2308	G
57	BA	2309	A
57	BA	2311	A
57	BA	2313	C
57	BA	2316	C
57	BA	2319	G
57	BA	2320	A
57	BA	2334	G
57	BA	2336	A
57	BA	2347	C
57	BA	2350	C
57	BA	2360	A
57	BA	2361	A
57	BA	2383	G
57	BA	2385	C
57	BA	2400	G
57	BA	2402	C
57	BA	2406	U
57	BA	2423	U
57	BA	2425	A
57	BA	2429	G
57	BA	2430	A
57	BA	2435	A
57	BA	2439	A
57	BA	2441	C
57	BA	2448	A
57	BA	2459	A
57	BA	2465	C
57	BA	2469	A
57	BA	2470	G
57	BA	2472	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	2476	A
57	BA	2477	C
57	BA	2478	A
57	BA	2482	G
57	BA	2484	G
57	BA	2491	U
57	BA	2502	G
57	BA	2505	G
57	BA	2518	A
57	BA	2524	G
57	BA	2529	G
57	BA	2531	A
57	BA	2542	A
57	BA	2543	G
57	BA	2554	U
57	BA	2566	A
57	BA	2567	G
57	BA	2573	C
57	BA	2586	C
57	BA	2602	A
57	BA	2609	U
57	BA	2611	U
57	BA	2612	C
57	BA	2615	U
57	BA	2630	G
57	BA	2657	A
57	BA	2673	G
57	BA	2690	C
57	BA	2691	C
57	BA	2702	U
57	BA	2703	C
57	BA	2712	U
57	BA	2712(A)	A
57	BA	2713	A
57	BA	2720	U
57	BA	2726	U
57	BA	2733	A
57	BA	2752	C
57	BA	2758	A
57	BA	2762	G
57	BA	2765	A
57	BA	2778	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	2779	U
57	BA	2790	A
57	BA	2791	C
57	BA	2794	C
57	BA	2799	C
57	BA	2801(A)	A
57	BA	2802	G
57	BA	2803	C
57	BA	2804	C
57	BA	2808	U
57	BA	2818	G
57	BA	2820	A
57	BA	2821	A
57	BA	2833	G
57	BA	2834	G
57	BA	2849	U
57	BA	2872	G
57	BA	2892	A
57	BA	2893	G
58	BB	8	U
58	BB	13	A
58	BB	15	A
58	BB	16	G
58	BB	22	U
58	BB	24	G
58	BB	41	U
58	BB	42	C
58	BB	45	A
58	BB	52	A
58	BB	53	A
58	BB	67	G
58	BB	73	A
58	BB	81	G
58	BB	82	G
58	BB	88	C
58	BB	110	G
58	BB	113	G

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	AA	49	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	71	A
57	AA	74	A
57	AA	79	G
57	AA	119	A
57	AA	128	C
57	AA	197	A
57	AA	221	A
57	AA	266	G
57	AA	272	G
57	AA	331	A
57	AA	332	A
57	AA	366	C
57	AA	387	U
57	AA	438	G
57	AA	474	G
57	AA	587	C
57	AA	603	A
57	AA	614(C)	A
57	AA	669	G
57	AA	752	A
57	AA	764	A
57	AA	790	C
57	AA	858	U
57	AA	904	C
57	AA	1022	G
57	AA	1210	A
57	AA	1286	A
57	AA	1378	A
57	AA	1427	A
57	AA	1490	A
57	AA	1494	A
57	AA	1541	G
57	AA	1558	A
57	AA	1603	A
57	AA	1608	A
57	AA	1652	A
57	AA	1653	G
57	AA	1799	G
57	AA	1819	A
57	AA	1820	U
57	AA	1846	G
57	AA	1885	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	AA	1948	G
57	AA	1970	A
57	AA	1992	G
57	AA	2033	A
57	AA	2036	C
57	AA	2126	A
57	AA	2171	A
57	AA	2191	G
57	AA	2225	A
57	AA	2282	G
57	AA	2311	A
57	AA	2405	G
57	AA	2422	A
57	AA	2439	A
57	AA	2481	G
57	AA	2611	U
57	AA	2689	U
57	AA	2873	A
58	AB	66	A
57	BA	49	A
57	BA	71	A
57	BA	74	A
57	BA	79	G
57	BA	119	A
57	BA	128	C
57	BA	146	G
57	BA	197	A
57	BA	221	A
57	BA	266	G
57	BA	272	G
57	BA	331	A
57	BA	332	A
57	BA	366	C
57	BA	387	U
57	BA	438	G
57	BA	474	G
57	BA	587	C
57	BA	603	A
57	BA	614(C)	A
57	BA	669	G
57	BA	752	A
57	BA	764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	BA	790	C
57	BA	858	U
57	BA	904	C
57	BA	1022	G
57	BA	1197	G
57	BA	1210	A
57	BA	1281	G
57	BA	1286	A
57	BA	1378	A
57	BA	1427	A
57	BA	1490	A
57	BA	1494	A
57	BA	1541	G
57	BA	1558	A
57	BA	1603	A
57	BA	1608	A
57	BA	1652	A
57	BA	1653	G
57	BA	1799	G
57	BA	1819	A
57	BA	1820	U
57	BA	1846	G
57	BA	1885	A
57	BA	1948	G
57	BA	1970	A
57	BA	1992	G
57	BA	2033	A
57	BA	2036	C
57	BA	2126	A
57	BA	2171	A
57	BA	2191	G
57	BA	2225	A
57	BA	2282	G
57	BA	2311	A
57	BA	2405	G
57	BA	2422	A
57	BA	2439	A
57	BA	2481	G
57	BA	2611	U
57	BA	2689	U
57	BA	2873	A
58	BB	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	A2M	Bx	20	23	18,25,26	0.63	0	18,36,39	1.21	3 (16%)
23	A2M	Ax	20	23	18,25,26	0.63	0	18,36,39	1.10	1 (5%)
23	OMG	Ax	21	23	18,26,27	1.17	1 (5%)	20,38,41	2.71	5 (25%)
24	5MU	Bv	54	24	15,22,23	1.15	3 (20%)	16,32,35	3.74	1 (6%)
23	OMU	Ax	19	23	14,22,23	1.14	1 (7%)	14,31,34	1.26	1 (7%)
23	OMG	Bx	21	23	18,26,27	1.11	2 (11%)	20,38,41	2.67	6 (30%)
24	5MU	Av	54	24	15,22,23	1.19	2 (13%)	16,32,35	3.71	1 (6%)
23	OMU	Bx	19	23	14,22,23	1.23	2 (14%)	14,31,34	1.20	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A2M	Bx	20	23	-	0/5/27/28	0/3/3/3
23	A2M	Ax	20	23	-	1/5/27/28	0/3/3/3
23	OMG	Ax	21	23	-	2/5/27/28	0/3/3/3
24	5MU	Bv	54	24	-	0/5/25/26	0/2/2/2
23	OMU	Ax	19	23	-	2/7/27/28	0/2/2/2
23	OMG	Bx	21	23	-	0/5/27/28	0/3/3/3
24	5MU	Av	54	24	-	0/5/25/26	0/2/2/2
23	OMU	Bx	19	23	-	3/7/27/28	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Ax	21	OMG	C6-N1	3.88	1.39	1.33
23	Bx	21	OMG	C6-N1	3.66	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Av	54	5MU	C4-N3	3.46	1.39	1.33
23	Bx	19	OMU	C4-N3	3.27	1.38	1.33
23	Ax	19	OMU	C4-N3	3.08	1.38	1.33
24	Bv	54	5MU	C4-N3	3.08	1.38	1.33
23	Bx	21	OMG	C8-N7	-2.12	1.30	1.34
24	Bv	54	5MU	C4-C5	2.11	1.46	1.41
23	Bx	19	OMU	C6-N1	2.06	1.38	1.35
24	Av	54	5MU	C6-C5	-2.03	1.34	1.40
24	Bv	54	5MU	C6-C5	-2.03	1.34	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Bv	54	5MU	C4-N3-C2	14.65	127.51	115.14
24	Av	54	5MU	C4-N3-C2	14.47	127.36	115.14
23	Bx	21	OMG	C5-C6-N1	-8.71	111.52	123.43
23	Ax	21	OMG	C5-C6-N1	-8.67	111.57	123.43
23	Ax	21	OMG	C6-N1-C2	5.86	125.23	115.93
23	Bx	21	OMG	C6-N1-C2	5.85	125.23	115.93
23	Ax	19	OMU	C5-C4-N3	-3.83	114.87	123.31
23	Bx	19	OMU	C5-C4-N3	-3.83	114.88	123.31
23	Bx	21	OMG	C2-N3-C4	-3.03	111.90	115.36
23	Ax	21	OMG	C2-N3-C4	-2.90	112.05	115.36
23	Ax	21	OMG	N3-C2-N1	-2.59	123.77	127.22
23	Bx	20	A2M	O3'-C3'-C2'	2.57	118.46	111.17
23	Bx	21	OMG	N3-C2-N1	-2.55	123.83	127.22
23	Ax	21	OMG	C6-C5-C4	-2.34	118.57	120.80
23	Ax	20	A2M	C5-C6-N6	2.30	123.85	120.35
23	Bx	21	OMG	CM2-O2'-C2'	-2.27	108.57	114.52
23	Bx	20	A2M	C5-C6-N6	2.21	123.71	120.35
23	Bx	21	OMG	C6-C5-C4	-2.16	118.73	120.80
23	Bx	20	A2M	CM'-O2'-C2'	-2.10	109.02	114.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Ax	19	OMU	C2'-C1'-N1-C6
23	Ax	19	OMU	O4'-C1'-N1-C6
23	Bx	19	OMU	C2'-C1'-N1-C6
23	Bx	19	OMU	O4'-C1'-N1-C6
23	Ax	21	OMG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Ax	21	OMG	C3'-C4'-C5'-O5'
23	Bx	19	OMU	C4'-C5'-O5'-P
23	Ax	20	A2M	C3'-C2'-O2'-CM'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1072 ligands modelled in this entry, 1072 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ab	234/256 (91%)	0.43	21 (8%) 9 9	119, 151, 187, 193	0
1	Bb	234/256 (91%)	0.50	18 (7%) 13 12	117, 151, 186, 193	0
2	Ac	206/239 (86%)	0.60	17 (8%) 11 11	116, 147, 171, 173	0
2	Bc	206/239 (86%)	0.63	21 (10%) 6 6	115, 147, 171, 174	0
3	Ad	208/209 (99%)	0.16	3 (1%) 75 75	94, 123, 145, 154	0
3	Bd	208/209 (99%)	0.34	8 (3%) 40 37	94, 124, 146, 155	0
4	Ae	150/162 (92%)	0.21	4 (2%) 54 52	90, 114, 142, 160	0
4	Be	150/162 (92%)	0.33	7 (4%) 31 29	91, 114, 143, 161	0
5	Af	101/101 (100%)	0.16	4 (3%) 38 36	103, 127, 143, 167	0
5	Bf	101/101 (100%)	0.16	4 (3%) 38 36	100, 126, 143, 167	0
6	Ag	155/156 (99%)	0.57	19 (12%) 4 3	119, 141, 173, 189	0
6	Bg	155/156 (99%)	0.77	23 (14%) 2 2	120, 141, 173, 189	0
7	Ah	138/138 (100%)	0.17	2 (1%) 75 75	99, 118, 133, 143	0
7	Bh	138/138 (100%)	0.48	6 (4%) 35 34	100, 118, 133, 144	0
8	Ai	127/128 (99%)	1.23	30 (23%) 0 1	121, 162, 182, 190	0
8	Bi	127/128 (99%)	1.17	32 (25%) 0 0	121, 162, 182, 189	0
9	Aj	98/105 (93%)	1.58	33 (33%) 0 0	118, 165, 185, 187	0
9	Bj	98/105 (93%)	1.50	29 (29%) 0 0	116, 164, 184, 188	0
10	Ak	119/129 (92%)	0.42	10 (8%) 11 10	89, 121, 156, 176	0
10	Bk	119/129 (92%)	0.50	13 (10%) 5 5	91, 120, 155, 175	0
11	Al	124/132 (93%)	0.30	5 (4%) 38 36	81, 101, 133, 169	0
11	Bl	124/132 (93%)	0.43	9 (7%) 15 15	83, 102, 134, 169	0
12	Am	118/126 (93%)	0.56	14 (11%) 4 4	115, 147, 161, 169	0
12	Bm	118/126 (93%)	0.77	18 (15%) 2 2	115, 146, 161, 168	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
13	An	60/61 (98%)	0.93	8 (13%)	3	3	127, 140, 158, 161	0
13	Bn	60/61 (98%)	0.69	3 (5%)	28	27	125, 140, 157, 160	0
14	Ao	88/89 (98%)	0.28	3 (3%)	45	43	87, 114, 138, 146	0
14	Bo	88/89 (98%)	0.17	1 (1%)	80	81	88, 114, 138, 146	0
15	Ap	83/88 (94%)	0.51	4 (4%)	30	28	96, 114, 135, 162	0
15	Bp	83/88 (94%)	0.73	10 (12%)	4	3	97, 116, 136, 163	0
16	Aq	99/105 (94%)	0.24	2 (2%)	65	64	89, 112, 125, 133	0
16	Bq	99/105 (94%)	0.34	6 (6%)	21	20	92, 112, 125, 133	0
17	Ar	70/88 (79%)	0.69	6 (8%)	10	10	98, 125, 147, 153	0
17	Br	70/88 (79%)	0.54	5 (7%)	16	16	98, 123, 147, 153	0
18	As	78/93 (83%)	1.10	18 (23%)	0	1	135, 151, 180, 185	0
18	Bs	78/93 (83%)	1.15	17 (21%)	0	1	135, 151, 180, 185	0
19	At	99/106 (93%)	0.60	9 (9%)	9	9	105, 123, 157, 161	0
19	Bt	99/106 (93%)	0.50	3 (3%)	50	49	107, 124, 158, 162	0
20	Au	24/27 (88%)	3.00	15 (62%)	0	0	113, 141, 162, 175	0
20	Bu	24/27 (88%)	2.50	12 (50%)	0	0	113, 141, 162, 174	0
21	Ay	94/95 (98%)	0.80	15 (15%)	1	2	67, 133, 155, 159	0
21	By	94/95 (98%)	0.89	9 (9%)	8	8	112, 136, 154, 169	0
22	Aa	1504/1504 (100%)	0.07	28 (1%)	66	65	70, 123, 196, 208	0
22	Ba	1504/1504 (100%)	0.05	33 (2%)	62	60	70, 124, 196, 208	0
23	Ax	9/25 (36%)	1.25	3 (33%)	0	0	102, 161, 194, 201	0
23	Bx	9/25 (36%)	1.29	4 (44%)	0	0	100, 159, 202, 204	0
24	Av	76/77 (98%)	-0.33	1 (1%)	77	77	93, 120, 159, 176	0
24	Bv	76/77 (98%)	-0.27	1 (1%)	77	77	82, 113, 154, 168	0
25	Aw	77/77 (100%)	1.36	19 (24%)	0	0	135, 202, 204, 205	0
25	Bw	77/77 (100%)	1.54	17 (22%)	0	1	134, 203, 205, 207	0
26	AC	120/229 (52%)	3.11	82 (68%)	0	0	167, 186, 194, 195	0
26	BC	120/229 (52%)	3.73	89 (74%)	0	0	166, 186, 194, 195	0
27	AD	271/276 (98%)	0.08	3 (1%)	80	81	58, 81, 109, 137	0
27	BD	271/276 (98%)	0.02	3 (1%)	80	81	55, 79, 108, 137	0
28	AE	204/206 (99%)	0.21	7 (3%)	45	43	62, 88, 143, 161	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	BE	204/206 (99%)	0.27	7 (3%)	45	43	59, 87, 143, 160	0
29	AF	207/210 (98%)	0.15	6 (2%)	51	50	61, 93, 150, 182	0
29	BF	207/210 (98%)	0.16	11 (5%)	26	24	55, 90, 150, 182	0
30	AG	181/182 (99%)	0.48	19 (10%)	6	6	113, 140, 165, 181	0
30	BG	181/182 (99%)	0.49	18 (9%)	7	7	102, 133, 164, 183	0
31	AH	164/180 (91%)	1.20	44 (26%)	0	0	103, 134, 154, 175	0
31	BH	164/180 (91%)	0.46	13 (7%)	12	12	96, 131, 151, 176	0
32	AI	145/148 (97%)	1.91	45 (31%)	0	0	91, 163, 180, 185	0
32	BI	145/148 (97%)	1.44	37 (25%)	0	0	90, 163, 181, 186	0
33	AJ	130/173 (75%)	4.47	99 (76%)	0	0	180, 195, 199, 201	0
33	BJ	130/173 (75%)	2.72	74 (56%)	0	0	167, 185, 194, 197	0
34	AN	138/140 (98%)	0.27	5 (3%)	42	40	76, 98, 133, 153	0
34	BN	138/140 (98%)	0.13	3 (2%)	62	60	73, 95, 132, 152	0
35	AO	122/122 (100%)	-0.07	0	100	100	65, 84, 106, 133	0
35	BO	122/122 (100%)	-0.04	0	100	100	64, 83, 106, 131	0
36	AP	146/150 (97%)	0.64	10 (6%)	17	17	63, 112, 139, 175	0
36	BP	146/150 (97%)	0.52	9 (6%)	20	20	62, 111, 139, 173	0
37	AQ	140/141 (99%)	0.10	2 (1%)	75	75	76, 99, 132, 153	0
37	BQ	140/141 (99%)	0.23	3 (2%)	63	62	74, 99, 131, 153	0
38	AR	117/118 (99%)	0.15	2 (1%)	70	68	70, 90, 119, 144	0
38	BR	117/118 (99%)	0.31	3 (2%)	56	53	67, 89, 119, 143	0
39	AS	98/112 (87%)	0.97	18 (18%)	1	1	115, 139, 161, 162	0
39	BS	98/112 (87%)	1.42	29 (29%)	0	0	112, 138, 161, 163	0
40	AT	135/146 (92%)	0.14	9 (6%)	17	17	78, 103, 154, 185	0
40	BT	135/146 (92%)	0.22	10 (7%)	14	14	78, 103, 154, 185	0
41	AU	117/118 (99%)	0.12	4 (3%)	45	43	67, 88, 124, 155	0
41	BU	117/118 (99%)	0.03	1 (0%)	84	84	63, 84, 123, 156	0
42	AV	101/101 (100%)	0.33	7 (6%)	16	16	62, 114, 136, 151	0
42	BV	101/101 (100%)	0.27	3 (2%)	50	49	59, 110, 135, 151	0
43	AW	113/113 (100%)	0.15	1 (0%)	84	84	67, 83, 110, 183	0
43	BW	113/113 (100%)	0.18	2 (1%)	68	67	65, 81, 108, 183	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AX	92/96 (95%)	0.13	2 (2%) 62 60	74, 93, 115, 124	0
44	BX	92/96 (95%)	0.12	0 100 100	66, 90, 113, 125	0
45	AY	100/110 (90%)	1.61	31 (31%) 0 0	85, 122, 162, 169	0
45	BY	100/110 (90%)	0.72	14 (14%) 2 2	84, 120, 162, 168	0
46	AZ	184/206 (89%)	0.38	14 (7%) 13 13	109, 138, 158, 192	0
46	BZ	184/206 (89%)	0.17	6 (3%) 46 44	96, 128, 152, 187	0
47	A0	84/85 (98%)	0.82	13 (15%) 2 2	87, 104, 152, 185	0
47	B0	84/85 (98%)	1.06	12 (14%) 2 2	86, 102, 153, 185	0
48	A1	93/98 (94%)	0.17	2 (2%) 62 60	68, 93, 132, 144	0
48	B1	93/98 (94%)	0.35	4 (4%) 35 34	60, 87, 133, 146	0
49	A2	71/72 (98%)	0.13	1 (1%) 75 75	89, 124, 144, 163	0
49	B2	71/72 (98%)	0.06	4 (5%) 24 23	60, 90, 134, 169	0
50	A3	59/60 (98%)	0.86	5 (8%) 10 10	79, 100, 124, 169	0
50	B3	59/60 (98%)	0.39	1 (1%) 70 68	75, 98, 121, 169	0
51	A4	57/71 (80%)	0.21	3 (5%) 26 24	153, 167, 183, 186	0
51	B4	57/71 (80%)	1.06	10 (17%) 1 1	154, 167, 182, 187	0
52	A5	55/60 (91%)	-0.04	3 (5%) 25 23	55, 91, 137, 144	0
52	B5	55/60 (91%)	-0.06	1 (1%) 68 67	54, 89, 137, 145	0
53	A6	50/54 (92%)	2.86	30 (60%) 0 0	128, 155, 169, 182	0
53	B6	50/54 (92%)	2.73	29 (58%) 0 0	128, 154, 169, 182	0
54	A7	47/49 (95%)	0.38	2 (4%) 35 34	58, 70, 95, 144	0
54	B7	47/49 (95%)	0.17	1 (2%) 63 62	53, 66, 91, 144	0
55	A8	63/65 (96%)	0.61	6 (9%) 8 8	70, 91, 118, 155	0
55	B8	63/65 (96%)	0.47	1 (1%) 72 70	70, 89, 117, 155	0
56	A9	37/37 (100%)	2.59	22 (59%) 0 0	109, 121, 141, 144	0
56	B9	37/37 (100%)	2.93	27 (72%) 0 0	105, 120, 141, 144	0
57	AA	2848/2848 (100%)	-0.05	79 (2%) 53 51	56, 90, 194, 209	0
57	BA	2848/2848 (100%)	0.09	79 (2%) 53 51	53, 87, 195, 208	0
58	AB	119/119 (100%)	-0.17	1 (0%) 86 86	96, 140, 176, 197	0
58	BB	119/119 (100%)	-0.03	0 100 100	94, 139, 175, 197	0
All	All	21494/22422 (95%)	0.38	1683 (7%) 13 12	53, 114, 186, 209	0

All (1683) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	AJ	63	LEU	17.7
33	AJ	85	ASP	17.5
26	BC	177	GLY	15.2
33	AJ	84	GLU	14.8
32	BI	88	ILE	14.6
33	AJ	64	LYS	13.8
32	BI	84	GLY	13.2
57	BA	277	C	13.0
26	BC	176	VAL	12.9
26	BC	174	ALA	12.8
33	AJ	70	GLU	12.7
47	B0	3	HIS	12.6
22	Aa	82	U	12.5
33	AJ	68	LEU	12.4
32	AI	144	VAL	12.2
36	AP	150	ALA	12.1
22	Aa	83	U	12.1
33	AJ	12	THR	12.1
6	Ag	82	GLY	12.0
57	BA	654(E)	G	11.9
22	Aa	89	C	11.5
33	AJ	67	GLY	11.5
32	AI	119	PRO	11.5
26	AC	229	SER	11.2
32	AI	65	ALA	11.1
33	AJ	73	GLY	11.0
33	AJ	69	PRO	11.0
57	AA	654(F)	C	10.7
32	AI	145	VAL	10.6
26	BC	173	HIS	10.5
26	BC	44	VAL	10.3
33	AJ	7	VAL	10.0
33	BJ	68	LEU	10.0
32	AI	111	PRO	10.0
57	AA	654(E)	G	9.9
57	AA	654(I)	C	9.9
22	Ba	89	C	9.9
33	AJ	72	ASP	9.7
53	A6	13	CYS	9.6
33	AJ	11	ALA	9.5
57	AA	654(D)	G	9.4
26	BC	172	ILE	9.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	AC	175	PRO	9.2
57	AA	2802	G	9.1
10	Ak	128	ALA	9.1
33	AJ	16	ASN	9.0
56	A9	1	MET	9.0
26	AC	176	VAL	8.9
33	AJ	13	LEU	8.9
22	Aa	81	U	8.8
22	Aa	80	G	8.7
32	AI	121	LYS	8.7
56	B9	1	MET	8.7
32	AI	118	LYS	8.7
32	BI	90	GLY	8.7
26	BC	42	VAL	8.6
33	AJ	62	ALA	8.6
20	Au	18	TYR	8.5
26	BC	178	LYS	8.5
50	A3	1	MET	8.5
26	BC	209	PHE	8.4
57	AA	2795	G	8.4
26	AC	172	ILE	8.4
45	AY	59	GLY	8.4
33	BJ	72	ASP	8.4
57	AA	654(H)	G	8.3
33	AJ	78	SER	8.3
10	Bk	129	SER	8.2
57	AA	654(K)	C	8.1
51	B4	56	VAL	8.1
22	Aa	84	U	8.0
57	AA	654(G)	C	8.0
25	Bw	34	C	8.0
10	Ak	129	SER	8.0
26	AC	173	HIS	8.0
39	BS	54	LEU	7.9
32	AI	97	ILE	7.9
26	AC	177	GLY	7.9
33	AJ	122	VAL	7.9
33	BJ	69	PRO	7.8
26	BC	171	ALA	7.8
33	AJ	99	SER	7.8
33	AJ	17	LEU	7.8
32	AI	61	ARG	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	AA	654(L)	G	7.7
33	BJ	73	GLY	7.7
57	BA	654(S)	G	7.7
33	BJ	36	GLU	7.7
26	AC	34	ALA	7.7
6	Ag	83	ALA	7.7
56	A9	37	GLY	7.7
57	BA	654(K)	C	7.6
57	BA	654(F)	C	7.5
6	Bg	83	ALA	7.5
6	Ag	81	GLY	7.4
33	BJ	43	ALA	7.4
33	AJ	40	LEU	7.4
57	BA	654(H)	G	7.3
20	Bu	18	TYR	7.3
26	BC	179	ALA	7.3
33	AJ	52	PHE	7.3
33	AJ	66	LEU	7.3
33	BJ	53	VAL	7.3
57	BA	2802	G	7.3
26	BC	175	PRO	7.2
51	B4	1	MET	7.2
32	BI	92	VAL	7.2
33	AJ	100	ASN	7.2
18	As	81	ARG	7.2
22	Ba	1030	C	7.2
33	BJ	110	GLY	7.1
32	AI	86	THR	7.1
52	A5	2	ALA	7.1
45	AY	58	GLY	7.0
6	Bg	84	ASN	7.0
33	BJ	75	GLN	7.0
31	BH	42	ARG	7.0
26	AC	228	HIS	7.0
33	AJ	8	GLU	7.0
33	AJ	86	PRO	7.0
45	AY	44	ILE	6.9
25	Aw	17	C	6.9
33	AJ	103	GLY	6.9
33	AJ	25	PHE	6.9
33	BJ	12	THR	6.8
33	AJ	60	ARG	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	AC	188	ASP	6.7
57	BA	654(G)	C	6.7
53	A6	21	TYR	6.7
32	AI	58	LEU	6.7
57	BA	654(D)	G	6.7
28	AE	204	ALA	6.7
33	AJ	44	LEU	6.7
26	AC	193	PHE	6.7
6	Bg	81	GLY	6.6
26	BC	170	GLY	6.6
57	BA	1534	U	6.6
57	AA	654(S)	G	6.6
42	BV	36	PRO	6.5
31	AH	96	ALA	6.5
32	AI	122	GLU	6.5
33	AJ	10	LEU	6.5
49	B2	70	GLN	6.5
53	A6	42	TRP	6.5
26	BC	166	ASN	6.4
53	A6	14	THR	6.4
29	AF	1	MET	6.3
53	B6	49	HIS	6.3
33	BJ	103	GLY	6.3
57	BA	654(I)	C	6.3
26	AC	212	SER	6.3
53	A6	45	LYS	6.3
47	B0	5	LYS	6.3
51	B4	57	GLU	6.3
33	AJ	77	PRO	6.2
56	B9	34	GLN	6.2
18	Bs	81	ARG	6.2
33	AJ	65	GLU	6.1
53	B6	19	ARG	6.1
57	BA	2799	C	6.1
26	BC	190	ILE	6.1
22	Ba	80	G	6.1
33	BJ	108	LYS	6.1
30	AG	2	PRO	6.1
33	BJ	67	GLY	6.1
33	BJ	40	LEU	6.0
1	Bb	96	ARG	6.0
32	AI	109	ILE	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	A9	12	ASP	6.0
26	AC	189	ASN	6.0
6	Bg	82	GLY	5.9
26	AC	181	PHE	5.9
31	BH	45	VAL	5.9
33	BJ	11	ALA	5.9
33	AJ	80	VAL	5.9
33	AJ	83	TYR	5.9
25	Bw	17(A)	U	5.9
57	BA	2795	G	5.9
30	BG	49	ASP	5.9
33	BJ	52	PHE	5.9
45	AY	45	VAL	5.8
26	BC	2	PRO	5.8
33	BJ	84	GLU	5.8
45	AY	60	PHE	5.8
33	AJ	26	LEU	5.8
26	BC	181	PHE	5.8
57	AA	2796	U	5.8
33	AJ	101	PRO	5.7
26	BC	180	SER	5.7
26	BC	25	GLU	5.7
33	BJ	35	LYS	5.7
9	Bj	5	ARG	5.7
47	B0	6	GLY	5.7
26	BC	208	THR	5.7
26	AC	182	PRO	5.7
26	BC	14	LYS	5.7
47	B0	4	LYS	5.7
9	Aj	33	GLN	5.7
53	B6	42	TRP	5.7
20	Bu	24	ARG	5.7
6	Bg	85	TYR	5.6
26	BC	219	MET	5.6
53	B6	20	ASN	5.6
22	Aa	88	A	5.6
26	BC	40	GLU	5.6
57	AA	2139	C	5.6
9	Bj	98	ILE	5.6
9	Bj	71	LEU	5.6
33	BJ	88	ALA	5.6
8	Bi	8	GLY	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	AJ	102	LYS	5.6
32	AI	68	LEU	5.5
33	AJ	74	LEU	5.5
26	BC	203	GLU	5.5
57	AA	2794	C	5.5
32	BI	56	LYS	5.5
53	B6	26	ASN	5.5
33	AJ	18	GLU	5.5
12	Am	75	ALA	5.5
56	B9	7	VAL	5.5
53	B6	37	ARG	5.5
26	AC	42	VAL	5.5
22	Ba	88	A	5.5
26	BC	27	ALA	5.5
33	AJ	79	ALA	5.5
33	BJ	8	GLU	5.4
33	AJ	110	GLY	5.4
10	Bk	128	ALA	5.4
32	BI	70	GLU	5.4
57	AA	2801(A)	A	5.4
45	AY	57	GLN	5.4
33	BJ	76	GLY	5.3
57	AA	2154	G	5.3
22	Ba	1030(B)	C	5.3
33	BJ	48	GLY	5.3
2	Ac	177	THR	5.3
13	Bn	2	ALA	5.3
26	BC	41	THR	5.3
12	Am	119	GLY	5.3
18	Bs	40	ILE	5.3
39	BS	108	GLY	5.3
9	Bj	10	GLY	5.3
31	BH	44	VAL	5.3
33	BJ	109	SER	5.2
33	AJ	37	THR	5.2
33	AJ	5	ARG	5.2
20	Au	5	ASP	5.2
2	Bc	193	TYR	5.2
32	BI	59	ALA	5.2
33	BJ	101	PRO	5.2
57	AA	1534	U	5.2
57	AA	654(V)	A	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	AA	654(J)	A	5.1
33	AJ	75	GLN	5.1
57	BA	1535	A	5.1
25	Bw	17	C	5.1
22	Ba	1286	A	5.1
47	B0	42	GLY	5.1
53	A6	46	HIS	5.1
13	Bn	8	GLU	5.1
26	BC	46	ALA	5.1
33	AJ	115	GLN	5.0
57	AA	654(N)	G	5.0
53	A6	29	ASN	5.0
32	AI	72	LEU	5.0
32	AI	132	PRO	5.0
26	AC	209	PHE	5.0
26	AC	23	ILE	5.0
49	B2	72	ALA	5.0
26	AC	210	LEU	5.0
6	Bg	5	ARG	5.0
33	BJ	70	GLU	5.0
21	Ay	84	SER	5.0
22	Ba	82	U	5.0
6	Ag	84	ASN	5.0
26	BC	39	ASP	5.0
57	AA	1535	A	5.0
47	A0	8	GLY	4.9
6	Bg	156	TRP	4.9
47	B0	85	ALA	4.9
53	A6	20	ASN	4.9
1	Bb	132	LYS	4.9
30	AG	47	LYS	4.9
57	AA	2803	C	4.9
33	BJ	46	GLN	4.9
26	BC	32	GLU	4.9
1	Ab	130	ARG	4.9
32	BI	71	ILE	4.9
8	Ai	7	THR	4.9
18	As	79	THR	4.9
9	Bj	65	LEU	4.9
6	Ag	85	TYR	4.9
9	Aj	74	ILE	4.8
26	AC	41	THR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	BA	276	A	4.8
26	AC	203	GLU	4.8
41	AU	118	GLY	4.8
26	BC	217	THR	4.8
26	AC	221	PRO	4.8
33	BJ	37	THR	4.8
40	AT	39	ARG	4.8
56	B9	12	ASP	4.8
33	AJ	114	GLY	4.8
8	Ai	82	ALA	4.7
26	BC	36	ALA	4.7
26	AC	46	ALA	4.7
39	BS	36	TYR	4.7
26	AC	187	ALA	4.7
25	Aw	20	U	4.7
30	BG	35	GLU	4.7
20	Au	9	ARG	4.7
51	B4	17	GLY	4.7
57	AA	2138	C	4.7
26	BC	30	VAL	4.7
33	AJ	132	ASP	4.6
57	AA	2799	C	4.6
12	Am	84	ILE	4.6
20	Au	22	ARG	4.6
53	B6	13	CYS	4.6
26	BC	4	HIS	4.6
6	Ag	86	GLN	4.6
33	AJ	59	ILE	4.6
26	AC	27	ALA	4.6
57	AA	2894	G	4.6
32	AI	85	GLU	4.6
8	Ai	9	ARG	4.6
12	Bm	102	ARG	4.6
37	AQ	140	ALA	4.6
26	AC	8	TYR	4.6
33	AJ	6	ASN	4.6
26	AC	174	ALA	4.6
32	BI	80	PRO	4.6
57	AA	229	A	4.6
26	BC	43	GLU	4.6
26	AC	24	ASP	4.6
32	AI	120	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	BY	2	ARG	4.5
32	BI	120	ILE	4.5
31	AH	129	THR	4.5
39	BS	53	SER	4.5
6	Ag	156	TRP	4.5
26	BC	200	HIS	4.5
6	Bg	80	VAL	4.5
57	BA	1509	C	4.5
4	Ae	31	LEU	4.5
33	BJ	56	ASN	4.5
33	BJ	106	GLN	4.5
32	AI	81	VAL	4.5
26	AC	204	GLY	4.5
12	Am	7	VAL	4.5
31	AH	29	PRO	4.5
22	Ba	81	U	4.5
8	Ai	8	GLY	4.5
26	BC	31	LYS	4.5
56	A9	13	LYS	4.5
20	Au	2	GLY	4.5
21	Ay	16	ARG	4.5
19	Bt	106	ALA	4.5
56	B9	18	ARG	4.4
28	BE	54	GLN	4.4
6	Bg	78	ARG	4.4
22	Ba	90	U	4.4
36	AP	149	GLU	4.4
33	AJ	113	GLN	4.4
33	AJ	121	ASP	4.4
13	An	17	LYS	4.4
25	Bw	35	A	4.4
57	BA	2117	A	4.4
26	AC	4	HIS	4.4
8	Bi	15	ALA	4.4
33	BJ	92	THR	4.4
53	B6	40	CYS	4.4
9	Aj	34	VAL	4.4
22	Aa	1030(B)	C	4.4
26	BC	48	LEU	4.4
53	A6	49	HIS	4.4
53	A6	52	VAL	4.3
45	AY	50	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	AC	200	HIS	4.3
56	A9	35	ARG	4.3
57	AA	1509	C	4.3
53	A6	26	ASN	4.3
33	AJ	41	ARG	4.3
26	AC	171	ALA	4.3
6	Ag	80	VAL	4.3
45	AY	62	GLU	4.3
31	AH	168	PRO	4.3
32	BI	130	TYR	4.3
33	AJ	49	ALA	4.3
33	AJ	116	ILE	4.3
17	Br	54	ARG	4.3
56	A9	25	VAL	4.3
30	BG	50	ALA	4.3
57	BA	2801	A	4.3
33	AJ	32	LEU	4.3
25	Aw	17(A)	U	4.2
6	Bg	86	GLN	4.2
9	Bj	8	LEU	4.2
30	BG	2	PRO	4.2
33	BJ	17	LEU	4.2
29	AF	11	VAL	4.2
57	AA	2147	G	4.2
57	BA	2796	U	4.2
39	BS	60	GLY	4.2
12	Bm	98	VAL	4.2
39	BS	24	LEU	4.2
26	BC	192	ALA	4.2
33	BJ	20	ALA	4.2
29	BF	24	LEU	4.2
25	Aw	16	C	4.2
9	Aj	39	PRO	4.2
39	BS	107	GLU	4.2
53	B6	14	THR	4.2
26	BC	167	ASP	4.2
6	Bg	4	ARG	4.2
53	B6	23	THR	4.2
57	AA	2113	U	4.2
26	BC	220	GLY	4.2
26	AC	197	LEU	4.2
57	BA	654(V)	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	B5	2	ALA	4.2
33	BJ	4	LYS	4.2
10	Ak	12	ARG	4.1
47	B0	7	LEU	4.1
10	Bk	12	ARG	4.1
57	BA	654(N)	G	4.1
45	AY	46	LYS	4.1
12	Bm	84	ILE	4.1
57	BA	654(J)	A	4.1
18	Bs	69	HIS	4.1
26	BC	24	ASP	4.1
29	BF	133	ASN	4.1
1	Bb	127	ILE	4.1
26	AC	227	PRO	4.1
30	AG	48	GLU	4.1
53	A6	39	TYR	4.1
26	BC	186	LEU	4.1
32	BI	105	HIS	4.1
8	Bi	7	THR	4.1
20	Au	25	LYS	4.1
32	AI	127	VAL	4.1
32	BI	63	ALA	4.1
26	BC	198	GLU	4.1
32	AI	112	LYS	4.1
22	Ba	1024	G	4.1
57	AA	2155	G	4.1
57	AA	2169	A	4.0
33	BJ	7	VAL	4.0
17	Ar	23	LYS	4.0
33	BJ	45	LYS	4.0
41	BU	118	GLY	4.0
32	AI	100	ALA	4.0
56	A9	34	GLN	4.0
22	Ba	1030(A)	G	4.0
57	BA	508	G	4.0
8	Ai	5	TYR	4.0
20	Au	8	THR	4.0
20	Au	14	TRP	4.0
31	AH	18	GLU	4.0
53	A6	12	GLU	4.0
57	BA	2793	G	4.0
1	Ab	135	GLN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	AT	1	MET	4.0
57	AA	2158	A	4.0
2	Ac	189	ALA	4.0
22	Ba	204	U	4.0
57	AA	2131	G	4.0
39	AS	54	LEU	4.0
56	A9	14	CYS	3.9
26	BC	35	THR	3.9
32	BI	66	GLU	3.9
53	B6	35	GLU	3.9
30	BG	34	LEU	3.9
33	BJ	49	ALA	3.9
57	AA	2793	G	3.9
45	AY	55	TYR	3.9
56	B9	37	GLY	3.9
45	AY	48	ALA	3.9
53	A6	40	CYS	3.9
15	Bp	13	HIS	3.9
51	B4	32	TYR	3.9
26	BC	188	ASP	3.9
33	BJ	105	PRO	3.9
53	B6	31	PRO	3.9
53	B6	9	LEU	3.9
40	BT	1	MET	3.9
53	B6	39	TYR	3.9
26	AC	190	ILE	3.9
26	BC	191	ARG	3.9
53	A6	18	ARG	3.8
26	BC	38	PHE	3.8
9	Bj	73	ASP	3.8
8	Bi	92	TYR	3.8
26	AC	170	GLY	3.8
53	A6	50	ARG	3.8
30	AG	75	LYS	3.8
26	AC	40	GLU	3.8
20	Au	24	ARG	3.8
32	BI	108	THR	3.8
53	A6	23	THR	3.8
57	AA	2132	U	3.8
32	AI	91	SER	3.8
57	AA	2145	C	3.8
33	AJ	76	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	Ba	1531	A	3.8
32	BI	134	PRO	3.8
57	AA	2310	A	3.8
2	Ac	91	LEU	3.8
30	AG	50	ALA	3.8
32	BI	67	ARG	3.8
57	BA	2116	G	3.8
21	Ay	77	SER	3.8
8	Ai	10	ARG	3.8
46	AZ	97	GLU	3.8
53	A6	31	PRO	3.8
26	BC	229	SER	3.8
32	AI	143	SER	3.8
57	AA	654(C)	G	3.8
3	Bd	204	ILE	3.8
2	Ac	207	VAL	3.8
11	Al	28	LYS	3.8
53	A6	19	ARG	3.8
29	AF	12	LEU	3.8
26	AC	199	ALA	3.7
26	BC	201	LYS	3.7
43	BW	113	LYS	3.7
30	AG	86	MET	3.7
30	AG	25	TYR	3.7
30	BG	86	MET	3.7
8	Ai	125	TYR	3.7
26	AC	35	THR	3.7
36	BP	149	GLU	3.7
32	BI	119	PRO	3.7
9	Aj	8	LEU	3.7
26	AC	180	SER	3.7
33	BJ	44	LEU	3.7
31	AH	101	ARG	3.7
32	BI	85	GLU	3.7
8	Bi	128	ARG	3.7
31	AH	115	VAL	3.7
51	B4	47	GLN	3.7
56	B9	30	PRO	3.7
20	Bu	25	LYS	3.7
56	B9	29	ASN	3.7
28	AE	76	ARG	3.7
56	B9	8	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BC	5	GLY	3.6
25	Bw	27	U	3.6
57	AA	508	G	3.6
9	Bj	4	ILE	3.6
21	By	87	TYR	3.6
57	AA	654	A	3.6
57	AA	2801	A	3.6
57	AA	2896	C	3.6
9	Aj	29	ARG	3.6
33	AJ	93	LEU	3.6
11	Bl	128	ALA	3.6
18	As	52	TYR	3.6
26	AC	39	ASP	3.6
28	BE	76	ARG	3.6
33	AJ	109	SER	3.6
33	AJ	111	LEU	3.6
11	Al	128	ALA	3.6
33	AJ	53	VAL	3.6
39	BS	23	ARG	3.6
12	Bm	7	VAL	3.6
40	BT	39	ARG	3.6
9	Aj	10	GLY	3.6
39	AS	104	GLY	3.6
33	BJ	132	ASP	3.6
7	Bh	129	VAL	3.6
40	BT	92	GLY	3.6
39	BS	49	VAL	3.6
19	At	101	GLY	3.6
9	Aj	9	ARG	3.6
26	AC	198	GLU	3.6
32	AI	135	GLU	3.6
57	BA	2896	C	3.6
33	AJ	81	VAL	3.5
53	B6	22	ALA	3.5
6	Ag	3	ARG	3.5
9	Aj	7	LYS	3.5
26	AC	3	LYS	3.5
5	Af	8	ILE	3.5
9	Aj	76	ASN	3.5
33	AJ	108	LYS	3.5
57	BA	654(Q)	C	3.5
31	AH	44	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	Bu	23	PRO	3.5
31	AH	170	ARG	3.5
10	Ak	11	LYS	3.5
10	Bk	11	LYS	3.5
18	As	5	LEU	3.5
30	AG	49	ASP	3.5
32	BI	143	SER	3.5
39	AS	33	LYS	3.5
8	Bi	87	GLN	3.5
26	AC	183	PRO	3.5
28	AE	54	GLN	3.5
21	Ay	60	TYR	3.5
32	AI	128	LEU	3.5
47	A0	7	LEU	3.5
8	Bi	46	ALA	3.5
45	AY	47	LYS	3.5
26	AC	219	MET	3.5
10	Ak	127	LYS	3.5
33	BJ	32	LEU	3.5
9	Aj	70	ARG	3.5
25	Aw	56	C	3.5
57	AA	654(M)	C	3.5
57	BA	2178	C	3.5
5	Af	101	ALA	3.5
32	BI	94	ALA	3.5
40	BT	2	ASN	3.5
12	Am	103	THR	3.5
2	Ac	155	GLY	3.5
1	Ab	231	GLU	3.4
26	BC	34	ALA	3.5
22	Ba	1001(A)	G	3.4
33	BJ	13	LEU	3.4
17	Ar	43	PHE	3.4
2	Bc	207	VAL	3.4
31	AH	105	LEU	3.4
57	BA	2804	C	3.4
32	AI	16	GLY	3.4
36	BP	51	PHE	3.4
56	B9	32	HIS	3.4
36	BP	110	TYR	3.4
26	AC	48	LEU	3.4
26	BC	29	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	Bi	126	SER	3.4
53	B6	18	ARG	3.4
1	Bb	122	PHE	3.4
8	Bi	105	ASP	3.4
31	BH	167	GLU	3.4
12	Bm	117	VAL	3.4
25	Bw	36	U	3.4
26	BC	26	ALA	3.4
26	AC	33	LEU	3.4
2	Bc	179	ARG	3.4
45	AY	79	CYS	3.4
31	AH	45	VAL	3.4
53	A6	22	ALA	3.4
22	Ba	1002	G	3.4
22	Ba	84	U	3.4
57	AA	156	U	3.4
39	BS	59	LYS	3.4
57	AA	2140	C	3.4
57	BA	2145	C	3.4
29	BF	1	MET	3.4
45	AY	28	LYS	3.4
56	B9	33	LYS	3.4
22	Ba	1027	C	3.4
57	AA	888	C	3.4
57	AA	2146	C	3.4
57	BA	654(P)	C	3.4
12	Bm	4	ILE	3.4
56	B9	10	ILE	3.4
9	Bj	95	GLU	3.4
57	BA	2114	A	3.4
56	A9	30	PRO	3.4
57	AA	2157	G	3.4
57	BA	2138	C	3.4
31	AH	158	HIS	3.4
32	AI	123	LEU	3.3
26	AC	196	ALA	3.3
55	B8	48	PHE	3.3
33	AJ	31	GLY	3.3
38	BR	118	GLU	3.3
33	AJ	42	GLN	3.3
26	AC	44	VAL	3.3
1	Ab	116	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	Bu	22	ARG	3.3
29	AF	10	PRO	3.3
26	AC	194	ILE	3.3
9	Aj	99	LYS	3.3
12	Am	102	ARG	3.3
26	AC	185	LYS	3.3
57	BA	654(L)	G	3.3
31	AH	95	ARG	3.3
31	AH	169	VAL	3.3
18	Bs	10	PHE	3.3
39	BS	82	ILE	3.3
47	B0	2	ALA	3.3
8	Bi	21	PRO	3.3
21	Ay	95	LEU	3.3
8	Ai	105	ASP	3.3
9	Bj	64	GLU	3.3
10	Ak	90	GLY	3.3
21	Ay	87	TYR	3.3
33	AJ	28	ASN	3.3
47	A0	3	HIS	3.3
22	Aa	1027	C	3.3
26	BC	8	TYR	3.3
33	BJ	50	ARG	3.3
8	Ai	14	VAL	3.3
31	AH	128	PRO	3.3
32	AI	108	THR	3.3
1	Ab	214	ILE	3.3
9	Bj	7	LYS	3.3
57	BA	2801(A)	A	3.3
22	Aa	1036	G	3.3
22	Ba	93	G	3.3
57	AA	2125	G	3.3
57	AA	2133	G	3.3
32	AI	79	ILE	3.3
26	BC	202	PRO	3.3
8	Ai	20	ARG	3.3
33	BJ	131	MET	3.3
56	B9	9	ARG	3.3
13	An	2	ALA	3.3
18	As	71	LEU	3.3
21	By	95	LEU	3.3
56	B9	25	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	BC	204	GLY	3.2
26	BC	212	SER	3.2
47	A0	26	TYR	3.2
19	At	106	ALA	3.2
26	BC	197	LEU	3.2
31	AH	88	LEU	3.2
4	Be	135	THR	3.2
9	Aj	28	ARG	3.2
22	Aa	1001(A)	G	3.2
22	Ba	1033	G	3.2
26	BC	49	GLY	3.2
53	B6	53	LYS	3.2
2	Ac	201	TYR	3.2
36	BP	15	ARG	3.2
31	AH	40	GLU	3.2
20	Bu	14	TRP	3.2
45	BY	63	LYS	3.2
57	BA	2113	U	3.2
26	BC	33	LEU	3.2
8	Bi	86	VAL	3.2
8	Ai	128	ARG	3.2
53	A6	47	THR	3.2
8	Ai	79	LEU	3.2
29	BF	156	LEU	3.2
26	BC	57	GLN	3.2
32	AI	62	LYS	3.2
50	B3	1	MET	3.2
1	Bb	136	VAL	3.2
39	AS	59	LYS	3.2
22	Ba	1031	G	3.2
40	AT	115	ARG	3.2
32	AI	4	ILE	3.2
56	B9	15	LYS	3.2
57	BA	2794	C	3.2
22	Ba	1257	U	3.2
33	BJ	66	LEU	3.2
19	Bt	56	MET	3.2
22	Aa	1002	G	3.2
43	BW	112	GLY	3.2
2	Ac	206	GLU	3.2
57	BA	2139	C	3.2
39	AS	58	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	Bi	54	ASP	3.2
21	Ay	83	ARG	3.1
34	AN	1	MET	3.1
26	AC	22	THR	3.1
2	Ac	103	VAL	3.1
45	AY	85	VAL	3.1
33	BJ	42	GLN	3.1
51	A4	57	GLU	3.1
53	A6	25	LYS	3.1
2	Bc	22	TRP	3.1
33	AJ	46	GLN	3.1
57	BA	1536	C	3.1
3	Bd	134	ASP	3.1
45	AY	39	VAL	3.1
46	AZ	5	LEU	3.1
48	B1	85	LEU	3.1
57	BA	2310	A	3.1
31	AH	111	HIS	3.1
20	Au	17	THR	3.1
1	Ab	128	GLU	3.1
9	Bj	72	VAL	3.1
31	BH	169	VAL	3.1
33	AJ	112	LEU	3.1
8	Ai	127	LYS	3.1
31	AH	54	ARG	3.1
17	Br	31	LEU	3.1
56	B9	14	CYS	3.1
17	Ar	54	ARG	3.1
26	BC	45	HIS	3.1
30	AG	22	ARG	3.1
40	BT	36	GLU	3.1
18	Bs	39	THR	3.1
23	Bx	24	A	3.1
50	A3	2	PRO	3.1
9	Aj	96	ILE	3.1
57	BA	2141	G	3.1
39	AS	73	LEU	3.1
57	BA	1174	A	3.1
30	BG	48	GLU	3.1
26	AC	201	LYS	3.1
32	AI	20	ASP	3.1
33	BJ	77	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	B9	28	GLU	3.1
53	A6	41	PRO	3.1
57	BA	2115	G	3.1
33	BJ	80	VAL	3.1
2	Bc	127	ARG	3.1
15	Ap	29	ASP	3.0
53	B6	29	ASN	3.0
9	Bj	100	THR	3.0
27	AD	262	ARG	3.0
34	BN	3	THR	3.0
33	BJ	74	LEU	3.0
12	Am	97	PRO	3.0
22	Aa	1026	G	3.0
31	AH	112	PRO	3.0
10	Ak	13	GLN	3.0
56	A9	4	ARG	3.0
26	AC	208	THR	3.0
1	Ab	156	LYS	3.0
33	AJ	96	PHE	3.0
46	BZ	88	PHE	3.0
5	Bf	8	ILE	3.0
45	AY	6	HIS	3.0
26	AC	166	ASN	3.0
57	BA	654(C)	G	3.0
57	BA	2137	C	3.0
7	Bh	131	GLY	3.0
46	AZ	4	ARG	3.0
53	B6	51	GLU	3.0
32	BI	114	LEU	3.0
8	Ai	37	PHE	3.0
1	Bb	128	GLU	3.0
2	Bc	149	ALA	3.0
30	BG	75	LYS	3.0
18	Bs	74	PHE	3.0
39	BS	87	PHE	3.0
51	B4	55	ARG	3.0
26	AC	205	ALA	3.0
33	AJ	104	ILE	3.0
33	AJ	130	THR	3.0
18	As	28	LYS	3.0
22	Aa	1286	A	3.0
25	Bw	37	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	BI	98	ALA	3.0
18	Bs	45	VAL	3.0
33	BJ	111	LEU	3.0
4	Be	9	LYS	3.0
11	Bl	28	LYS	3.0
57	BA	2132	U	3.0
20	Bu	19	GLY	3.0
2	Ac	53	ALA	3.0
25	Aw	34	C	3.0
26	AC	55	SER	3.0
26	AC	213	VAL	3.0
45	AY	49	VAL	3.0
56	A9	33	LYS	3.0
22	Aa	1257	U	3.0
8	Bi	4	TYR	3.0
18	Bs	5	LEU	3.0
1	Bb	232	PRO	3.0
22	Ba	1003	G	2.9
3	Bd	96	LEU	2.9
56	B9	16	VAL	2.9
32	BI	87	LYS	2.9
33	BJ	64	LYS	2.9
19	At	9	ASN	2.9
1	Bb	134	GLU	2.9
33	AJ	131	MET	2.9
34	AN	3	THR	2.9
37	BQ	33	GLY	2.9
1	Ab	123	ALA	2.9
15	Bp	35	LYS	2.9
32	AI	3	VAL	2.9
7	Bh	25	ASP	2.9
30	BG	26	GLN	2.9
39	AS	34	HIS	2.9
57	BA	2803	C	2.9
22	Aa	1024	G	2.9
2	Bc	168	ALA	2.9
30	AG	160	VAL	2.9
30	BG	103	LEU	2.9
33	AJ	24	PHE	2.9
51	B4	18	CYS	2.9
20	Bu	3	LYS	2.9
12	Am	100	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	Ba	83	U	2.9
9	Aj	32	ALA	2.9
28	BE	204	ALA	2.9
10	Bk	127	LYS	2.9
52	A5	3	LYS	2.9
26	BC	196	ALA	2.9
33	AJ	56	ASN	2.9
33	AJ	105	PRO	2.9
9	Bj	99	LYS	2.9
2	Bc	101	LEU	2.9
6	Bg	26	PHE	2.9
57	BA	2135	A	2.9
10	Bk	42	TRP	2.9
4	Ae	29	GLY	2.9
8	Bi	93	ARG	2.9
21	By	62	LEU	2.9
8	Ai	15	ALA	2.9
34	AN	72	TYR	2.9
57	AA	1536	C	2.9
57	BA	2805	G	2.9
22	Aa	1447	A	2.9
39	AS	61	ASN	2.9
39	BS	61	ASN	2.9
57	BA	2169	A	2.9
6	Bg	3	ARG	2.9
53	B6	28	ARG	2.9
8	Bi	96	LEU	2.9
32	AI	87	LYS	2.9
33	BJ	26	LEU	2.9
33	BJ	16	ASN	2.9
10	Bk	21	ILE	2.9
19	At	92	LEU	2.9
20	Bu	17	THR	2.9
2	Ac	184	TYR	2.9
33	BJ	83	TYR	2.9
9	Bj	59	SER	2.9
28	AE	69	LYS	2.9
33	AJ	33	PRO	2.9
32	AI	93	THR	2.9
8	Ai	13	ALA	2.9
20	Bu	9	ARG	2.8
46	AZ	156	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	A0	4	LYS	2.8
16	Bq	98	LEU	2.8
29	BF	20	LEU	2.8
31	AH	52	VAL	2.8
45	AY	61	ILE	2.8
4	Be	24	ARG	2.8
8	Ai	4	TYR	2.8
26	AC	169	THR	2.8
53	B6	21	TYR	2.8
47	B0	52	GLY	2.8
8	Ai	98	PRO	2.8
2	Ac	19	GLU	2.8
47	A0	2	ALA	2.8
56	A9	36	GLN	2.8
53	B6	47	THR	2.8
2	Ac	87	LEU	2.8
45	BY	98	VAL	2.8
8	Ai	36	TYR	2.8
9	Aj	31	GLY	2.8
1	Ab	132	LYS	2.8
18	As	41	VAL	2.8
25	Bw	26	G	2.8
45	BY	47	LYS	2.8
56	B9	4	ARG	2.8
57	BA	654(O)	G	2.8
30	AG	137	GLU	2.8
57	BA	2164	C	2.8
2	Bc	200	ALA	2.8
30	BG	36	LYS	2.8
39	AS	48	LEU	2.8
9	Bj	33	GLN	2.8
20	Au	10	ARG	2.8
26	AC	186	LEU	2.8
42	AV	65	GLY	2.8
26	BC	18	ASN	2.8
33	AJ	82	PHE	2.8
30	AG	127	GLY	2.8
31	AH	123	PHE	2.8
33	BJ	6	ASN	2.8
40	AT	2	ASN	2.8
12	Bm	5	ALA	2.8
57	AA	2135	A	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	Aj	69	ASN	2.8
22	Aa	1030(A)	G	2.8
23	Ax	23	A	2.8
45	AY	3	VAL	2.8
9	Bj	9	ARG	2.8
27	AD	83	GLU	2.8
31	AH	85	LYS	2.8
46	AZ	60	GLU	2.8
56	B9	13	LYS	2.8
1	Bb	227	GLY	2.8
3	Ad	123	HIS	2.8
22	Aa	1117	G	2.8
32	BI	89	TYR	2.8
26	BC	215	VAL	2.8
9	Aj	3	LYS	2.8
31	AH	83	TYR	2.8
57	AA	654(P)	C	2.8
31	AH	58	GLU	2.7
33	BJ	18	GLU	2.7
57	AA	2897	U	2.7
26	AC	12	LEU	2.7
5	Bf	7	ASN	2.7
19	At	103	GLY	2.7
33	AJ	92	THR	2.7
34	AN	73	THR	2.7
26	BC	56	ASP	2.7
13	An	25	VAL	2.7
29	AF	128	ALA	2.7
39	AS	105	ALA	2.7
57	AA	2893	G	2.7
2	Bc	206	GLU	2.7
32	BI	78	THR	2.7
18	Bs	29	ARG	2.7
19	At	104	LEU	2.7
39	BS	48	LEU	2.7
53	A6	6	ARG	2.7
1	Ab	122	PHE	2.7
26	BC	222	SER	2.7
25	Aw	22	G	2.7
26	AC	28	ARG	2.7
57	AA	2792	G	2.7
57	AA	2805	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	BA	2143	C	2.7
9	Bj	35	SER	2.7
26	AC	52	PRO	2.7
26	BC	211	ARG	2.7
33	BJ	63	LEU	2.7
2	Bc	169	ALA	2.7
10	Bk	19	ALA	2.7
23	Bx	13	A	2.7
6	Bg	79	ARG	2.7
16	Aq	59	ILE	2.7
26	BC	50	ILE	2.7
25	Aw	55	U	2.7
33	AJ	106	GLN	2.7
8	Bi	119	ALA	2.7
21	By	11	ALA	2.7
32	AI	131	LYS	2.7
33	BJ	27	VAL	2.7
25	Aw	72	A	2.7
25	Aw	19	G	2.7
2	Ac	205	GLY	2.7
9	Bj	63	PHE	2.7
57	AA	1026	U	2.7
13	An	50	LYS	2.7
26	AC	49	GLY	2.7
48	A1	85	LEU	2.7
12	Bm	119	GLY	2.7
26	AC	211	ARG	2.7
53	B6	8	LYS	2.7
54	B7	47	ARG	2.7
56	B9	22	ARG	2.7
11	Bl	68	ALA	2.7
33	AJ	97	ALA	2.7
38	AR	11	ASN	2.7
17	Br	78	LEU	2.7
9	Aj	71	LEU	2.7
57	AA	2123	G	2.7
31	AH	17	VAL	2.7
26	BC	10	ALA	2.7
28	BE	57	LYS	2.7
36	AP	147	LEU	2.7
8	Ai	33	PHE	2.7
5	Af	90	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	Bw	45	G	2.7
26	BC	52	PRO	2.7
8	Ai	62	TYR	2.6
8	Bi	106	ALA	2.7
28	AE	151	TYR	2.6
33	AJ	54	ALA	2.7
9	Aj	85	LEU	2.6
39	AS	26	LEU	2.6
29	BF	23	ASP	2.6
25	Bw	61	C	2.6
33	AJ	45	LYS	2.6
1	Ab	92	TYR	2.6
2	Bc	87	LEU	2.6
2	Bc	201	TYR	2.6
14	Ao	52	SER	2.6
22	Ba	1030(C)	G	2.6
57	AA	275	G	2.6
33	BJ	47	ASN	2.6
30	AG	177	GLY	2.6
31	AH	131	VAL	2.6
22	Aa	1531	A	2.6
21	By	15	TRP	2.6
57	AA	2112	G	2.6
30	AG	128	ARG	2.6
2	Bc	91	LEU	2.6
56	A9	26	ILE	2.6
11	Bl	32	PHE	2.6
5	Af	34	GLY	2.6
11	Bl	33	ARG	2.6
57	AA	2164	C	2.6
49	B2	43	GLN	2.6
11	Bl	64	TYR	2.6
42	AV	94	LEU	2.6
22	Ba	1026	G	2.6
22	Ba	1032	G	2.6
36	AP	27	HIS	2.6
8	Ai	65	VAL	2.6
9	Bj	34	VAL	2.6
26	AC	191	ARG	2.6
33	AJ	27	VAL	2.6
33	BJ	115	GLN	2.6
22	Ba	1138	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	AI	19	VAL	2.6
4	Be	31	LEU	2.6
51	B4	31	ILE	2.6
11	Bl	19	ARG	2.6
24	Bv	1	C	2.6
27	BD	262	ARG	2.6
6	Bg	34	GLY	2.6
39	BS	84	GLN	2.6
25	Aw	18	G	2.6
56	B9	5	ALA	2.6
26	BC	182	PRO	2.6
47	A0	68	GLU	2.6
39	BS	34	HIS	2.6
16	Bq	100	LYS	2.6
25	Aw	33	U	2.6
31	BH	170	ARG	2.6
32	BI	91	SER	2.6
31	AH	50	VAL	2.6
33	AJ	48	GLY	2.6
18	As	36	ARG	2.6
33	AJ	71	LEU	2.6
1	Ab	70	PHE	2.6
13	An	55	GLY	2.6
27	AD	26	LYS	2.6
31	AH	53	GLU	2.6
56	A9	15	LYS	2.6
45	AY	43	ASN	2.6
56	B9	21	GLY	2.6
8	Bi	56	LEU	2.6
18	Bs	37	ARG	2.6
45	BY	84	ARG	2.6
56	A9	9	ARG	2.6
30	BG	66	GLN	2.6
45	AY	65	ALA	2.6
56	A9	5	ALA	2.6
39	AS	43	GLU	2.6
45	BY	45	VAL	2.6
46	BZ	96	VAL	2.6
47	B0	8	GLY	2.6
9	Aj	5	ARG	2.6
1	Ab	131	PRO	2.6
55	A8	48	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	BS	51	ALA	2.5
6	Ag	78	ARG	2.5
15	Bp	30	GLY	2.5
22	Aa	90	U	2.5
25	Bw	50	U	2.5
36	AP	15	ARG	2.5
9	Aj	19	SER	2.5
57	BA	654(T)	C	2.5
9	Aj	90	LEU	2.5
39	BS	58	LEU	2.5
45	BY	53	PRO	2.5
26	AC	216	THR	2.5
45	BY	28	LYS	2.5
45	BY	60	PHE	2.5
56	A9	11	CYS	2.5
32	BI	64	GLU	2.5
23	Ax	13	A	2.5
29	AF	24	LEU	2.5
8	Bi	33	PHE	2.5
26	BC	23	ILE	2.5
46	BZ	133	ILE	2.5
26	BC	21	TYR	2.5
30	BG	25	TYR	2.5
39	AS	23	ARG	2.5
39	AS	37	ALA	2.5
8	Ai	19	LEU	2.5
8	Bi	98	PRO	2.5
26	BC	193	PHE	2.5
23	Bx	23	A	2.5
9	Aj	68	HIS	2.5
47	A0	85	ALA	2.5
2	Bc	151	VAL	2.5
2	Bc	198	VAL	2.5
12	Am	117	VAL	2.5
33	BJ	102	LYS	2.5
21	Ay	89	GLU	2.5
33	AJ	36	GLU	2.5
40	BT	11	GLU	2.5
26	AC	45	HIS	2.5
23	Ax	22	A	2.5
36	BP	64	LYS	2.5
57	BA	2140	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	Bj	96	ILE	2.5
32	BI	52	ARG	2.5
2	Bc	166	GLU	2.5
9	Bj	94	VAL	2.5
10	Ak	89	ALA	2.5
10	Bk	80	VAL	2.5
20	Au	3	LYS	2.5
42	AV	36	PRO	2.5
22	Ba	202	U	2.5
52	A5	45	VAL	2.5
26	BC	226	ASN	2.5
9	Bj	79	ARG	2.5
39	AS	87	PHE	2.5
18	As	38	SER	2.5
18	As	78	ARG	2.5
40	AT	91	ARG	2.5
57	BA	2159	G	2.5
57	AA	2111	C	2.5
26	BC	207	GLY	2.5
26	BC	210	LEU	2.5
39	BS	33	LYS	2.5
57	AA	1173	G	2.5
9	Bj	61	GLU	2.5
26	BC	13	GLU	2.5
25	Aw	21	A	2.5
26	AC	2	PRO	2.5
56	A9	24	TYR	2.5
4	Ae	45	PHE	2.5
15	Ap	19	ILE	2.5
12	Bm	94	ARG	2.5
8	Bi	19	LEU	2.5
22	Ba	1023	G	2.5
26	BC	187	ALA	2.5
33	AJ	51	LEU	2.5
57	BA	2894	G	2.5
8	Ai	95	LYS	2.5
5	Bf	88	VAL	2.5
57	AA	155	U	2.5
8	Bi	61	ALA	2.5
18	As	80	TYR	2.5
33	BJ	62	ALA	2.5
9	Aj	4	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	Aw	6	G	2.5
39	BS	89	ARG	2.5
40	AT	106	SER	2.5
53	A6	37	ARG	2.5
57	BA	352	G	2.5
57	BA	1176	G	2.5
1	Bb	7	VAL	2.4
33	AJ	55	LYS	2.4
8	Bi	82	ALA	2.4
33	AJ	118	THR	2.4
12	Bm	113	PRO	2.4
19	At	45	GLN	2.4
3	Ad	152	SER	2.4
8	Ai	126	SER	2.4
7	Ah	107	LEU	2.4
28	BE	75	VAL	2.4
6	Bg	18	TYR	2.4
18	Bs	78	ARG	2.4
22	Ba	1447	A	2.4
57	BA	2144	U	2.4
9	Aj	38	ILE	2.4
26	AC	50	ILE	2.4
26	AC	31	LYS	2.4
1	Ab	163	PHE	2.4
9	Aj	75	ILE	2.4
9	Bj	22	LYS	2.4
21	Ay	13	LYS	2.4
53	A6	51	GLU	2.4
17	Br	32	ARG	2.4
26	AC	220	GLY	2.4
43	AW	112	GLY	2.4
49	B2	69	ARG	2.4
50	A3	29	ARG	2.4
20	Au	21	TYR	2.4
20	Bu	21	TYR	2.4
27	BD	35	LYS	2.4
31	AH	89	ILE	2.4
31	BH	85	LYS	2.4
8	Ai	87	GLN	2.4
31	AH	87	LEU	2.4
28	AE	132	HIS	2.4
57	AA	2115	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	AA	2318	G	2.4
6	Ag	26	PHE	2.4
33	AJ	34	ALA	2.4
26	AC	32	GLU	2.4
33	BJ	95	GLN	2.4
11	Bl	61	THR	2.4
32	AI	101	LEU	2.4
40	AT	27	THR	2.4
53	B6	46	HIS	2.4
10	Ak	42	TRP	2.4
37	BQ	140	ALA	2.4
39	AS	82	ILE	2.4
39	BS	52	SER	2.4
9	Aj	100	THR	2.4
20	Au	23	PRO	2.4
39	BS	28	VAL	2.4
48	A1	71	TYR	2.4
53	B6	50	ARG	2.4
57	AA	2804	C	2.4
57	BA	2174	C	2.4
9	Aj	65	LEU	2.4
14	Ao	60	VAL	2.4
32	BI	75	LEU	2.4
46	AZ	150	LEU	2.4
34	BN	1	MET	2.4
9	Bj	70	ARG	2.4
26	BC	51	ASP	2.4
31	BH	102	ALA	2.4
53	A6	54	ILE	2.4
9	Aj	44	VAL	2.4
33	AJ	107	VAL	2.4
57	BA	888	C	2.4
18	Bs	47	HIS	2.4
15	Bp	6	LEU	2.4
7	Bh	61	VAL	2.4
31	AH	49	VAL	2.4
25	Bw	75	C	2.4
6	Bg	90	GLU	2.4
12	Bm	8	GLU	2.4
2	Bc	192	THR	2.4
26	BC	205	ALA	2.4
1	Bb	40	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Be	89	ILE	2.4
6	Ag	153	HIS	2.4
39	BS	11	LYS	2.4
15	Bp	59	TRP	2.4
31	BH	103	LEU	2.4
1	Ab	136	VAL	2.4
1	Bb	152	PHE	2.4
30	BG	95	ARG	2.4
45	AY	2	ARG	2.4
57	BA	2112	G	2.4
14	Bo	84	LYS	2.4
19	At	48	LYS	2.4
21	Ay	80	LYS	2.4
39	BS	35	ILE	2.4
46	AZ	164	ALA	2.4
32	BI	133	HIS	2.4
33	AJ	57	THR	2.4
21	By	86	VAL	2.3
47	A0	5	LYS	2.3
2	Ac	77	ILE	2.3
31	AH	102	ALA	2.3
57	AA	2153	G	2.3
32	AI	5	LEU	2.3
6	Ag	79	ARG	2.3
11	Al	33	ARG	2.3
33	AJ	50	ARG	2.3
33	AJ	4	LYS	2.3
56	A9	31	LYS	2.3
53	B6	24	GLU	2.3
21	Ay	88	SER	2.3
47	A0	9	SER	2.3
21	By	94	ILE	2.3
1	Ab	36	ARG	2.3
1	Ab	155	LEU	2.3
7	Bh	127	LEU	2.3
4	Be	98	THR	2.3
8	Bi	103	THR	2.3
28	BE	69	LYS	2.3
30	AG	81	LYS	2.3
57	AA	2159	G	2.3
57	BA	2121	G	2.3
57	BA	2125	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	A6	24	GLU	2.3
3	Ad	158	ILE	2.3
7	Bh	119	LEU	2.3
15	Bp	17	TYR	2.3
16	Bq	43	LEU	2.3
26	BC	9	ARG	2.3
37	BQ	10	ARG	2.3
56	B9	17	ILE	2.3
57	BA	229	A	2.3
33	AJ	35	LYS	2.3
26	AC	217	THR	2.3
46	AZ	28	MET	2.3
21	Ay	10	ARG	2.3
4	Ae	30	ALA	2.3
17	Ar	76	LEU	2.3
25	Bw	10	G	2.3
30	AG	43	LEU	2.3
32	BI	116	LEU	2.3
33	BJ	51	LEU	2.3
57	AA	2165	G	2.3
57	BA	654(M)	C	2.3
31	BH	43	VAL	2.3
45	BY	85	VAL	2.3
25	Aw	35	A	2.3
57	BA	2173	A	2.3
46	AZ	98	MET	2.3
21	Ay	93	ARG	2.3
26	AC	218	THR	2.3
8	Bi	81	ILE	2.3
31	AH	92	ILE	2.3
1	Bb	28	PHE	2.3
30	AG	89	GLY	2.3
21	By	89	GLU	2.3
39	BS	43	GLU	2.3
18	As	40	ILE	2.3
32	BI	110	ASP	2.3
46	AZ	96	VAL	2.3
6	Ag	4	ARG	2.3
25	Bw	1	C	2.3
26	AC	184	GLU	2.3
2	Ac	124	ILE	2.3
12	Bm	64	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	AA	2156	G	2.3
57	BA	2189	U	2.3
4	Be	45	PHE	2.3
36	AP	127	ALA	2.3
38	AR	2	ARG	2.3
9	Bj	3	LYS	2.3
11	Al	127	GLU	2.3
27	BD	26	LYS	2.3
32	BI	137	PRO	2.3
17	Ar	51	LEU	2.3
26	BC	12	LEU	2.3
57	AA	654(T)	C	2.3
31	AH	51	ARG	2.3
36	AP	91	PHE	2.3
12	Bm	112	GLY	2.3
42	AV	24	LYS	2.3
57	BA	2134	A	2.3
45	BY	5	MET	2.3
31	AH	56	SER	2.3
10	Bk	89	ALA	2.3
38	BR	105	ARG	2.3
26	BC	22	THR	2.3
26	BC	184	GLU	2.3
3	Bd	120	LEU	2.3
31	AH	55	PRO	2.3
18	As	29	ARG	2.3
56	A9	10	ILE	2.3
30	AG	23	PHE	2.3
36	AP	51	PHE	2.3
36	BP	27	HIS	2.3
45	AY	89	PHE	2.3
54	A7	18	PHE	2.3
25	Aw	32	C	2.3
21	By	47	MET	2.3
20	Bu	12	LYS	2.3
1	Bb	197	VAL	2.3
2	Bc	128	PHE	2.3
47	B0	57	PHE	2.3
15	Ap	48	TRP	2.2
47	A0	76	GLY	2.2
33	BJ	10	LEU	2.2
1	Ab	127	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Bc	147	LYS	2.2
15	Bp	19	ILE	2.2
22	Aa	1006	C	2.2
22	Aa	1129	C	2.2
18	As	45	VAL	2.2
18	As	75	ALA	2.2
46	AZ	186	GLU	2.2
6	Ag	5	ARG	2.2
11	Al	19	ARG	2.2
47	A0	74	ARG	2.2
57	AA	654(O)	G	2.2
51	B4	10	VAL	2.2
2	Bc	189	ALA	2.2
29	BF	207	GLY	2.2
34	BN	68	GLU	2.2
12	Am	88	ARG	2.2
31	AH	38	SER	2.2
46	BZ	4	ARG	2.2
17	Ar	88	LYS	2.2
33	BJ	91	LYS	2.2
34	AN	85	ILE	2.2
46	AZ	171	ILE	2.2
57	BA	654	A	2.2
28	BE	198	VAL	2.2
53	B6	41	PRO	2.2
26	AC	5	GLY	2.2
33	BJ	19	ARG	2.2
46	AZ	112	ARG	2.2
39	AS	57	LYS	2.2
53	A6	53	LYS	2.2
22	Aa	1030	C	2.2
33	BJ	99	SER	2.2
39	BS	32	LEU	2.2
45	AY	24	VAL	2.2
22	Aa	1035	A	2.2
32	AI	1	MET	2.2
8	Bi	104	ARG	2.2
49	A2	66	GLU	2.2
5	Bf	101	ALA	2.2
16	Aq	44	ALA	2.2
26	BC	216	THR	2.2
33	AJ	124	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	A8	35	GLN	2.2
47	A0	75	LEU	2.2
21	Ay	15	TRP	2.2
9	Bj	38	ILE	2.2
22	Aa	92	C	2.2
6	Bg	22	LEU	2.2
17	Br	56	THR	2.2
1	Bb	163	PHE	2.2
40	AT	3	ARG	2.2
28	AE	150	VAL	2.2
8	Bi	94	ALA	2.2
38	BR	3	HIS	2.2
57	BA	2170	A	2.2
18	As	16	LEU	2.2
36	BP	70	GLN	2.2
45	BY	50	ARG	2.2
56	B9	31	LYS	2.2
39	AS	39	ILE	2.2
22	Ba	220	G	2.2
25	Bw	5	G	2.2
57	BA	2151	G	2.2
30	BG	106	LEU	2.2
32	BI	74	ASN	2.2
40	BT	27	THR	2.2
42	AV	5	VAL	2.2
42	BV	21	ARG	2.2
31	BH	155	SER	2.2
33	AJ	20	ALA	2.2
55	A8	64	TYR	2.2
13	An	60	SER	2.2
57	AA	2141	G	2.2
1	Bb	229	VAL	2.2
9	Aj	72	VAL	2.2
29	BF	137	LYS	2.2
48	B1	31	GLY	2.2
30	BG	107	LEU	2.1
8	Ai	106	ALA	2.1
25	Aw	28	C	2.1
13	An	32	SER	2.1
57	AA	157	U	2.1
2	Ac	198	VAL	2.1
3	Bd	31	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	Bg	53	LYS	2.1
12	Am	80	ARG	2.1
21	Ay	23	ARG	2.1
26	AC	30	VAL	2.1
50	A3	6	VAL	2.1
15	Bp	38	TYR	2.1
18	Bs	79	THR	2.1
26	BC	11	LEU	2.1
31	AH	61	HIS	2.1
32	AI	12	LEU	2.1
36	BP	106	LEU	2.1
57	BA	278	A	2.1
6	Ag	77	SER	2.1
8	Bi	65	VAL	2.1
10	Bk	82	VAL	2.1
13	Bn	17	LYS	2.1
26	BC	28	ARG	2.1
45	AY	56	PRO	2.1
45	BY	86	ARG	2.1
10	Bk	98	LEU	2.1
26	AC	21	TYR	2.1
44	AX	69	TYR	2.1
2	Ac	179	ARG	2.1
11	Bl	127	GLU	2.1
12	Bm	27	LYS	2.1
22	Ba	1030(D)	A	2.1
23	Bx	22	A	2.1
32	BI	117	GLU	2.1
46	BZ	80	ARG	2.1
56	B9	19	ARG	2.1
15	Bp	2	VAL	2.1
51	A4	56	VAL	2.1
56	A9	23	VAL	2.1
12	Bm	97	PRO	2.1
55	A8	37	SER	2.1
18	Bs	71	LEU	2.1
25	Bw	74	C	2.1
57	AA	2179	C	2.1
57	BA	2118	U	2.1
12	Bm	87	TYR	2.1
31	AH	30	LYS	2.1
48	B1	58	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	Bi	90	PRO	2.1
33	BJ	86	PRO	2.1
36	AP	138	LEU	2.1
10	Bk	50	TYR	2.1
18	As	9	VAL	2.1
26	AC	215	VAL	2.1
39	BS	68	GLN	2.1
31	BH	100	GLY	2.1
1	Ab	31	TYR	2.1
12	Am	118	ALA	2.1
57	AA	352	G	2.1
24	Av	1	C	2.1
26	AC	226	ASN	2.1
18	Bs	30	LEU	2.1
19	At	89	ARG	2.1
40	BT	115	ARG	2.1
56	A9	19	ARG	2.1
32	AI	96	ASP	2.1
39	BS	55	ALA	2.1
6	Bg	66	VAL	2.1
42	AV	93	GLU	2.1
18	Bs	46	GLY	2.1
29	BF	25	PRO	2.1
3	Bd	207	TYR	2.1
10	Ak	50	TYR	2.1
53	B6	12	GLU	2.1
1	Bb	133	LYS	2.1
33	BJ	87	VAL	2.1
6	Ag	94	ARG	2.1
8	Bi	102	LEU	2.1
15	Bp	71	ARG	2.1
16	Bq	75	ARG	2.1
19	Bt	59	ALA	2.1
30	BG	164	GLU	2.1
31	BH	164	TYR	2.1
40	AT	135	ALA	2.1
57	BA	2155	G	2.1
31	AH	42	ARG	2.1
40	BT	29	ARG	2.1
45	AY	86	ARG	2.1
30	BG	100	TRP	2.1
33	BJ	9	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	AP	128	HIS	2.1
1	Ab	90	MET	2.1
6	Ag	144	MET	2.1
25	Aw	47	U	2.1
57	BA	271(K)	U	2.1
6	Bg	155	ARG	2.1
18	Bs	73	GLU	2.1
56	B9	24	TYR	2.1
37	AQ	5	ARG	2.1
45	AY	84	ARG	2.1
3	Bd	135	LEU	2.1
33	BJ	31	GLY	2.1
13	An	8	GLU	2.1
26	AC	26	ALA	2.1
36	BP	30	THR	2.1
33	AJ	94	VAL	2.1
42	AV	16	PRO	2.1
12	Bm	85	GLY	2.1
55	A8	4	MET	2.1
53	A6	28	ARG	2.0
57	BA	2123	G	2.0
57	BA	2152	G	2.0
8	Ai	103	THR	2.0
31	AH	37	VAL	2.0
45	AY	92	ASN	2.0
45	AY	100	ALA	2.0
25	Bw	47	U	2.0
30	AG	90	LEU	2.0
33	BJ	25	PHE	2.0
42	BV	19	LYS	2.0
1	Bb	130	ARG	2.0
26	AC	57	GLN	2.0
6	Ag	113	GLU	2.0
12	Am	8	GLU	2.0
16	Bq	78	GLU	2.0
25	Aw	62	C	2.0
8	Bi	50	LEU	2.0
32	BI	109	ILE	2.0
40	BT	6	LEU	2.0
8	Ai	70	LYS	2.0
12	Bm	36	LYS	2.0
55	A8	29	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Bd	165	MET	2.0
48	B1	60	PHE	2.0
29	BF	172	TRP	2.0
46	BZ	11	GLU	2.0
41	AU	86	ALA	2.0
44	AX	51	VAL	2.0
15	Ap	6	LEU	2.0
16	Bq	6	LEU	2.0
45	AY	63	LYS	2.0
50	A3	28	LEU	2.0
58	AB	88	C	2.0
6	Bg	72	ARG	2.0
8	Bi	9	ARG	2.0
9	Bj	37	PRO	2.0
18	As	42	PRO	2.0
41	AU	58	ARG	2.0
41	AU	89	GLU	2.0
6	Bg	131	LYS	2.0
9	Aj	18	ALA	2.0
31	AH	103	LEU	2.0
32	AI	114	LEU	2.0
33	AJ	126	ALA	2.0
39	BS	76	LYS	2.0
20	Au	16	GLY	2.0
7	Ah	9	MET	2.0
32	AI	78	THR	2.0
33	BJ	133	GLU	2.0
51	A4	47	GLN	2.0
9	Aj	55	LYS	2.0
53	B6	45	LYS	2.0
12	Am	96	LEU	2.0
29	BF	12	LEU	2.0
22	Ba	1036	G	2.0
57	AA	2127	G	2.0
8	Ai	49	PRO	2.0
22	Aa	1001	A	2.0
33	BJ	130	THR	2.0
45	BY	92	ASN	2.0
54	A7	1	MET	2.0
22	Aa	1260	C	2.0
1	Ab	96	ARG	2.0
14	Ao	56	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	AH	113	VAL	2.0
46	AZ	125	LEU	2.0
47	B0	41	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	OMG	Ax	21	24/25	0.78	0.33	174,180,182,184	0
23	A2M	Ax	20	23/24	0.85	0.28	160,168,169,173	0
23	OMU	Bx	19	21/22	0.86	0.29	129,157,162,162	0
23	OMU	Ax	19	21/22	0.89	0.23	133,158,162,164	0
23	OMG	Bx	21	24/25	0.89	0.27	177,182,184,186	0
23	A2M	Bx	20	23/24	0.91	0.22	161,170,172,175	0
24	5MU	Av	54	21/22	0.93	0.15	139,140,144,145	0
24	5MU	Bv	54	21/22	0.93	0.15	121,125,138,138	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	AA	3239	1/1	0.17	1.07	113,113,113,113	0
60	MG	Aa	1665	1/1	0.20	0.72	88,88,88,88	0
60	MG	Ba	1712	1/1	0.29	0.59	96,96,96,96	0
60	MG	BA	2945	1/1	0.29	0.69	149,149,149,149	0
60	MG	Ba	1647	1/1	0.33	0.91	148,148,148,148	0
60	MG	BA	3206	1/1	0.33	0.58	78,78,78,78	0
60	MG	BA	3258	1/1	0.34	0.99	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1645	1/1	0.37	1.25	89,89,89,89	0
60	MG	Aa	1674	1/1	0.37	0.27	108,108,108,108	0
60	MG	Aa	1706	1/1	0.40	0.50	91,91,91,91	0
60	MG	Ba	1698	1/1	0.40	0.62	123,123,123,123	1
60	MG	AA	2968	1/1	0.41	0.67	73,73,73,73	0
60	MG	AA	3261	1/1	0.41	0.71	110,110,110,110	0
60	MG	BA	2902	1/1	0.41	0.36	129,129,129,129	0
60	MG	AA	3134	1/1	0.42	0.40	98,98,98,98	0
60	MG	AA	3187	1/1	0.42	0.32	98,98,98,98	0
60	MG	Ba	1713	1/1	0.42	0.37	105,105,105,105	0
60	MG	Bw	101	1/1	0.42	0.31	140,140,140,140	1
60	MG	Aw	101	1/1	0.43	0.85	95,95,95,95	1
60	MG	Aa	1699	1/1	0.43	0.35	125,125,125,125	1
60	MG	Ba	1728	1/1	0.45	1.09	113,113,113,113	0
60	MG	BA	3191	1/1	0.45	0.70	116,116,116,116	0
60	MG	Aa	1689	1/1	0.47	0.20	57,57,57,57	1
60	MG	Aa	1727	1/1	0.47	0.61	90,90,90,90	1
60	MG	Am	201	1/1	0.48	0.86	88,88,88,88	0
60	MG	Ba	1664	1/1	0.48	0.55	88,88,88,88	0
60	MG	Aa	1641	1/1	0.49	0.84	87,87,87,87	0
60	MG	BA	3135	1/1	0.51	0.46	146,146,146,146	0
60	MG	AA	2954	1/1	0.51	0.26	103,103,103,103	0
60	MG	AA	3249	1/1	0.52	1.15	109,109,109,109	0
60	MG	AA	3165	1/1	0.52	0.48	83,83,83,83	0
60	MG	AA	3069	1/1	0.52	0.93	87,87,87,87	0
60	MG	Aa	1614	1/1	0.52	0.29	88,88,88,88	0
60	MG	BA	3265	1/1	0.52	0.83	104,104,104,104	0
60	MG	Ba	1737	1/1	0.54	0.34	101,101,101,101	0
60	MG	BA	3148	1/1	0.54	0.49	82,82,82,82	0
60	MG	AA	3146	1/1	0.54	1.05	87,87,87,87	0
60	MG	Ba	1643	1/1	0.56	0.86	95,95,95,95	0
60	MG	Ba	1699	1/1	0.56	1.55	113,113,113,113	0
60	MG	BA	3261	1/1	0.56	0.69	95,95,95,95	0
60	MG	A7	101	1/1	0.56	0.65	73,73,73,73	0
60	MG	Aa	1610	1/1	0.57	0.91	117,117,117,117	0
60	MG	Ba	1646	1/1	0.57	1.35	122,122,122,122	0
60	MG	AA	3262	1/1	0.57	0.57	94,94,94,94	0
60	MG	Bm	202	1/1	0.57	0.99	97,97,97,97	0
60	MG	Aa	1616	1/1	0.57	0.72	123,123,123,123	0
60	MG	AA	3208	1/1	0.58	0.33	72,72,72,72	0
60	MG	Ba	1676	1/1	0.59	0.75	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1631	1/1	0.60	1.27	101,101,101,101	0
60	MG	AA	3253	1/1	0.60	1.36	87,87,87,87	0
60	MG	Ba	1660	1/1	0.60	0.54	127,127,127,127	0
60	MG	Aa	1658	1/1	0.60	0.52	105,105,105,105	0
60	MG	BA	3180	1/1	0.60	0.56	92,92,92,92	0
60	MG	BA	3182	1/1	0.61	0.48	140,140,140,140	0
60	MG	BA	3149	1/1	0.61	1.31	126,126,126,126	0
60	MG	AA	3144	1/1	0.61	0.39	85,85,85,85	0
60	MG	BA	2938	1/1	0.62	1.11	104,104,104,104	0
60	MG	AA	3211	1/1	0.62	0.14	97,97,97,97	0
60	MG	AA	3176	1/1	0.62	0.45	84,84,84,84	0
60	MG	AA	3149	1/1	0.62	1.36	109,109,109,109	0
60	MG	Ba	1601	1/1	0.62	0.22	77,77,77,77	0
60	MG	AA	3092	1/1	0.62	0.32	112,112,112,112	0
60	MG	AA	2959	1/1	0.63	0.31	77,77,77,77	0
60	MG	Aa	1715	1/1	0.63	0.22	84,84,84,84	0
60	MG	BA	3147	1/1	0.64	0.38	67,67,67,67	0
60	MG	Ba	1695	1/1	0.64	0.91	148,148,148,148	0
60	MG	Aa	1630	1/1	0.64	0.76	89,89,89,89	0
60	MG	AA	3002	1/1	0.64	0.71	84,84,84,84	0
60	MG	BA	2937	1/1	0.64	0.25	70,70,70,70	0
60	MG	AA	3225	1/1	0.64	0.58	71,71,71,71	0
60	MG	AA	3150	1/1	0.64	0.39	81,81,81,81	0
60	MG	BA	3071	1/1	0.64	1.32	113,113,113,113	0
60	MG	BA	3080	1/1	0.64	0.28	79,79,79,79	0
60	MG	AB	202	1/1	0.64	0.61	103,103,103,103	0
60	MG	BA	3154	1/1	0.65	0.54	164,164,164,164	0
60	MG	AQ	201	1/1	0.65	1.07	105,105,105,105	0
60	MG	BA	3074	1/1	0.65	0.65	97,97,97,97	0
60	MG	B0	101	1/1	0.65	0.66	104,104,104,104	0
60	MG	AA	3241	1/1	0.65	0.91	100,100,100,100	0
60	MG	AA	3247	1/1	0.65	0.31	92,92,92,92	0
60	MG	AA	3194	1/1	0.65	0.82	108,108,108,108	0
60	MG	AA	3207	1/1	0.65	0.71	122,122,122,122	0
60	MG	BA	3162	1/1	0.66	0.45	86,86,86,86	0
60	MG	AA	3103	1/1	0.66	0.54	103,103,103,103	0
60	MG	AA	3204	1/1	0.66	0.24	84,84,84,84	0
60	MG	Aa	1651	1/1	0.66	0.70	84,84,84,84	0
60	MG	AA	3257	1/1	0.66	0.46	75,75,75,75	0
60	MG	Ba	1740	1/1	0.66	0.25	93,93,93,93	0
60	MG	BA	2965	1/1	0.66	0.61	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1601	1/1	0.66	0.34	93,93,93,93	0
60	MG	BA	3011	1/1	0.67	1.35	81,81,81,81	0
60	MG	Aa	1713	1/1	0.67	1.62	149,149,149,149	0
60	MG	Ba	1718	1/1	0.67	0.34	75,75,75,75	0
60	MG	BA	3237	1/1	0.67	1.20	98,98,98,98	0
60	MG	Ba	1688	1/1	0.67	0.24	90,90,90,90	1
60	MG	BA	3119	1/1	0.67	0.25	79,79,79,79	0
60	MG	Aa	1730	1/1	0.67	0.77	104,104,104,104	0
60	MG	Ba	1670	1/1	0.68	0.59	132,132,132,132	0
60	MG	Ba	1717	1/1	0.68	1.03	99,99,99,99	0
60	MG	Aa	1681	1/1	0.68	0.51	86,86,86,86	0
60	MG	AA	3237	1/1	0.68	0.81	88,88,88,88	0
60	MG	Aa	1700	1/1	0.68	0.48	84,84,84,84	1
60	MG	BA	3253	1/1	0.68	0.46	72,72,72,72	0
60	MG	Ba	1648	1/1	0.68	0.71	145,145,145,145	0
60	MG	AA	3112	1/1	0.68	1.15	114,114,114,114	0
60	MG	Aa	1633	1/1	0.68	0.46	71,71,71,71	0
60	MG	AA	2946	1/1	0.69	0.41	116,116,116,116	0
60	MG	Aa	1618	1/1	0.69	0.55	73,73,73,73	1
60	MG	AA	3264	1/1	0.69	0.77	101,101,101,101	0
60	MG	BA	3246	1/1	0.69	0.43	107,107,107,107	0
60	MG	BA	3088	1/1	0.69	0.52	113,113,113,113	0
60	MG	AA	3067	1/1	0.69	0.47	66,66,66,66	0
60	MG	BA	3126	1/1	0.69	0.77	154,154,154,154	0
60	MG	AA	2925	1/1	0.69	0.50	92,92,92,92	0
60	MG	AA	3157	1/1	0.70	0.11	123,123,123,123	0
60	MG	AA	3209	1/1	0.70	1.10	108,108,108,108	0
60	MG	AA	3267	1/1	0.70	0.37	89,89,89,89	0
60	MG	BA	3150	1/1	0.70	1.22	104,104,104,104	0
60	MG	AA	3260	1/1	0.71	0.72	104,104,104,104	0
60	MG	BA	3173	1/1	0.71	0.45	91,91,91,91	0
60	MG	AA	3114	1/1	0.71	0.34	84,84,84,84	0
60	MG	Ba	1734	1/1	0.71	0.12	138,138,138,138	0
60	MG	BA	2947	1/1	0.71	0.35	68,68,68,68	0
60	MG	BA	3136	1/1	0.71	1.06	109,109,109,109	0
60	MG	BA	3219	1/1	0.71	0.53	88,88,88,88	0
60	MG	BA	3138	1/1	0.71	0.24	61,61,61,61	0
60	MG	Ba	1612	1/1	0.71	0.38	100,100,100,100	0
60	MG	Ba	1706	1/1	0.71	0.53	131,131,131,131	0
60	MG	Ba	1673	1/1	0.71	0.16	83,83,83,83	0
60	MG	Ba	1616	1/1	0.71	0.23	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	Bm	201	1/1	0.71	0.18	103,103,103,103	0
60	MG	BA	3049	1/1	0.72	0.97	82,82,82,82	0
60	MG	AA	3016	1/1	0.72	1.19	82,82,82,82	0
60	MG	BA	3239	1/1	0.72	0.40	88,88,88,88	0
60	MG	AA	3224	1/1	0.72	0.53	86,86,86,86	0
60	MG	AA	3138	1/1	0.72	1.37	115,115,115,115	0
60	MG	Aa	1652	1/1	0.72	1.01	91,91,91,91	0
60	MG	BA	3259	1/1	0.72	0.34	99,99,99,99	0
59	ZN	B4	101	1/1	0.72	0.10	203,203,203,203	0
60	MG	AA	3086	1/1	0.72	0.29	94,94,94,94	0
60	MG	BA	3065	1/1	0.73	0.77	66,66,66,66	0
60	MG	AA	3143	1/1	0.73	0.98	72,72,72,72	0
60	MG	AA	2917	1/1	0.73	0.67	99,99,99,99	0
60	MG	BA	3146	1/1	0.73	0.36	112,112,112,112	0
60	MG	Aa	1637	1/1	0.73	1.21	99,99,99,99	0
60	MG	AA	3168	1/1	0.73	0.42	84,84,84,84	0
60	MG	AA	3040	1/1	0.73	0.49	82,82,82,82	0
60	MG	Ba	1602	1/1	0.73	0.39	73,73,73,73	0
60	MG	Aa	1611	1/1	0.74	1.01	82,82,82,82	0
60	MG	BA	3109	1/1	0.74	0.84	83,83,83,83	0
60	MG	AA	3219	1/1	0.74	0.66	94,94,94,94	0
60	MG	AA	3087	1/1	0.74	0.63	81,81,81,81	0
60	MG	AA	3053	1/1	0.74	0.32	79,79,79,79	0
60	MG	Aa	1723	1/1	0.74	0.78	98,98,98,98	0
60	MG	BA	3175	1/1	0.74	0.78	91,91,91,91	0
60	MG	AA	3106	1/1	0.74	0.41	75,75,75,75	0
60	MG	Aa	1714	1/1	0.74	0.54	111,111,111,111	0
60	MG	Ba	1610	1/1	0.74	0.62	87,87,87,87	0
60	MG	Ba	1716	1/1	0.75	0.67	102,102,102,102	0
60	MG	BA	3172	1/1	0.75	0.35	45,45,45,45	0
60	MG	AA	3236	1/1	0.75	1.19	90,90,90,90	0
60	MG	AX	101	1/1	0.75	1.11	96,96,96,96	1
60	MG	BA	2976	1/1	0.75	1.30	93,93,93,93	0
60	MG	BA	3255	1/1	0.75	0.64	74,74,74,74	0
60	MG	BA	3129	1/1	0.75	0.61	75,75,75,75	0
60	MG	BA	3075	1/1	0.75	0.33	56,56,56,56	0
60	MG	AA	2970	1/1	0.75	0.20	67,67,67,67	0
60	MG	BA	3209	1/1	0.75	0.22	107,107,107,107	0
60	MG	BA	3244	1/1	0.76	1.20	89,89,89,89	0
60	MG	BA	3204	1/1	0.76	0.57	92,92,92,92	0
60	MG	BA	2955	1/1	0.76	0.22	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AF	301	1/1	0.76	0.24	87,87,87,87	0
60	MG	Aa	1677	1/1	0.76	1.32	82,82,82,82	0
60	MG	BA	3229	1/1	0.76	0.60	101,101,101,101	0
60	MG	BA	2984	1/1	0.76	0.77	69,69,69,69	0
60	MG	BA	3264	1/1	0.76	0.31	68,68,68,68	0
60	MG	BA	3102	1/1	0.76	0.16	81,81,81,81	0
60	MG	Aa	1697	1/1	0.77	0.27	129,129,129,129	0
60	MG	AA	3248	1/1	0.77	0.47	141,141,141,141	0
60	MG	BA	2946	1/1	0.77	0.24	74,74,74,74	0
60	MG	Ba	1665	1/1	0.77	1.00	80,80,80,80	0
60	MG	AA	3266	1/1	0.77	0.44	73,73,73,73	0
60	MG	Ba	1621	1/1	0.77	0.33	84,84,84,84	0
60	MG	AA	2951	1/1	0.77	0.30	61,61,61,61	0
60	MG	Ba	1680	1/1	0.77	0.86	134,134,134,134	0
60	MG	BA	3231	1/1	0.77	0.48	105,105,105,105	0
60	MG	Ba	1682	1/1	0.77	0.69	113,113,113,113	0
60	MG	BA	3036	1/1	0.77	0.63	73,73,73,73	0
60	MG	Ba	1739	1/1	0.77	0.80	82,82,82,82	0
60	MG	AA	3136	1/1	0.77	0.31	88,88,88,88	0
60	MG	AA	3255	1/1	0.77	0.32	70,70,70,70	0
60	MG	BF	301	1/1	0.77	0.18	87,87,87,87	0
60	MG	BA	3157	1/1	0.77	0.76	78,78,78,78	0
60	MG	AA	2937	1/1	0.77	0.24	63,63,63,63	0
60	MG	AA	3171	1/1	0.77	0.26	68,68,68,68	0
60	MG	BA	3086	1/1	0.77	0.43	65,65,65,65	0
60	MG	AA	3242	1/1	0.77	0.46	78,78,78,78	0
60	MG	AA	3222	1/1	0.78	0.47	67,67,67,67	0
60	MG	AA	3102	1/1	0.78	0.82	92,92,92,92	0
60	MG	AA	2975	1/1	0.78	1.60	97,97,97,97	0
60	MG	BA	2958	1/1	0.78	1.17	100,100,100,100	0
60	MG	AA	3142	1/1	0.78	0.25	65,65,65,65	0
60	MG	Av	102	1/1	0.78	0.12	107,107,107,107	0
60	MG	AA	3206	1/1	0.78	0.60	75,75,75,75	0
60	MG	Ba	1640	1/1	0.78	1.20	105,105,105,105	0
60	MG	BB	203	1/1	0.78	0.70	79,79,79,79	0
60	MG	AA	3186	1/1	0.79	0.14	74,74,74,74	0
60	MG	AA	3156	1/1	0.79	0.38	83,83,83,83	0
60	MG	Ba	1613	1/1	0.79	0.35	101,101,101,101	0
60	MG	BA	2921	1/1	0.79	0.77	77,77,77,77	0
60	MG	BA	2998	1/1	0.79	0.60	59,59,59,59	0
60	MG	Aa	1623	1/1	0.79	1.12	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	3030	1/1	0.79	0.85	94,94,94,94	0
60	MG	Aa	1604	1/1	0.79	0.31	82,82,82,82	0
60	MG	Bq	201	1/1	0.79	0.36	116,116,116,116	0
60	MG	AA	3139	1/1	0.79	0.68	90,90,90,90	0
60	MG	AA	3084	1/1	0.79	0.41	84,84,84,84	0
60	MG	AA	3185	1/1	0.80	0.47	95,95,95,95	0
60	MG	BA	3222	1/1	0.80	0.34	109,109,109,109	0
60	MG	BA	3226	1/1	0.80	0.35	50,50,50,50	0
60	MG	AA	3268	1/1	0.80	0.71	102,102,102,102	0
60	MG	Bv	104	1/1	0.80	1.58	118,118,118,118	1
60	MG	BA	3235	1/1	0.80	0.52	90,90,90,90	0
60	MG	AB	201	1/1	0.80	0.38	69,69,69,69	0
60	MG	AA	3075	1/1	0.80	0.48	104,104,104,104	0
60	MG	AA	3050	1/1	0.80	0.52	87,87,87,87	0
60	MG	Aa	1735	1/1	0.80	0.33	80,80,80,80	1
60	MG	BA	3032	1/1	0.80	0.81	88,88,88,88	0
60	MG	Aa	1646	1/1	0.80	1.32	81,81,81,81	0
60	MG	Ba	1644	1/1	0.80	0.46	109,109,109,109	0
60	MG	AA	3015	1/1	0.80	1.00	103,103,103,103	0
60	MG	Ba	1732	1/1	0.80	0.65	135,135,135,135	0
60	MG	BA	3263	1/1	0.80	0.57	66,66,66,66	0
60	MG	AA	3152	1/1	0.80	1.01	113,113,113,113	0
60	MG	BA	3208	1/1	0.80	0.79	97,97,97,97	0
60	MG	AA	3230	1/1	0.80	1.16	94,94,94,94	0
60	MG	Ba	1657	1/1	0.81	0.69	109,109,109,109	0
60	MG	Ba	1617	1/1	0.81	0.56	69,69,69,69	1
60	MG	BA	2925	1/1	0.81	0.26	82,82,82,82	0
60	MG	BA	2932	1/1	0.81	0.53	87,87,87,87	0
60	MG	Ba	1661	1/1	0.81	0.88	98,98,98,98	0
60	MG	BA	3234	1/1	0.81	0.62	116,116,116,116	0
60	MG	AA	3212	1/1	0.81	0.42	79,79,79,79	0
60	MG	Ba	1625	1/1	0.81	1.38	113,113,113,113	0
60	MG	AA	2980	1/1	0.81	1.01	97,97,97,97	0
60	MG	Ba	1636	1/1	0.81	1.17	91,91,91,91	0
60	MG	BA	3245	1/1	0.81	0.31	80,80,80,80	0
60	MG	AA	2988	1/1	0.81	1.15	89,89,89,89	0
60	MG	AA	3179	1/1	0.81	0.50	76,76,76,76	0
60	MG	Aa	1671	1/1	0.81	0.40	113,113,113,113	0
60	MG	AA	3167	1/1	0.81	0.22	84,84,84,84	0
60	MG	Aa	1736	1/1	0.81	0.14	126,126,126,126	0
60	MG	BA	3200	1/1	0.81	1.37	98,98,98,98	0
60	MG	BA	3130	1/1	0.81	0.55	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	3192	1/1	0.81	0.65	59,59,59,59	0
60	MG	AA	3238	1/1	0.81	0.70	74,74,74,74	0
60	MG	Ba	1655	1/1	0.81	0.39	66,66,66,66	0
60	MG	BA	2951	1/1	0.82	0.56	90,90,90,90	0
60	MG	Aa	1717	1/1	0.82	0.17	90,90,90,90	0
60	MG	Aa	1719	1/1	0.82	0.79	92,92,92,92	0
60	MG	BA	2961	1/1	0.82	0.36	60,60,60,60	0
60	MG	BA	3210	1/1	0.82	0.78	93,93,93,93	0
60	MG	Aa	1622	1/1	0.82	0.26	101,101,101,101	0
60	MG	BA	2973	1/1	0.82	0.57	61,61,61,61	0
60	MG	Ba	1637	1/1	0.82	0.53	103,103,103,103	0
60	MG	Ba	1605	1/1	0.82	0.61	99,99,99,99	0
60	MG	Ba	1707	1/1	0.82	0.47	100,100,100,100	0
60	MG	AA	3099	1/1	0.82	0.63	78,78,78,78	0
60	MG	Ba	1667	1/1	0.82	0.63	91,91,91,91	0
60	MG	BA	3236	1/1	0.82	0.29	64,64,64,64	0
60	MG	Ba	1715	1/1	0.82	0.17	121,121,121,121	0
60	MG	Ba	1668	1/1	0.82	0.65	80,80,80,80	0
60	MG	BA	3153	1/1	0.82	0.82	73,73,73,73	0
60	MG	BA	3053	1/1	0.82	1.04	70,70,70,70	0
60	MG	AA	3170	1/1	0.82	0.25	82,82,82,82	0
60	MG	BA	2935	1/1	0.82	0.75	124,124,124,124	0
60	MG	Aa	1725	1/1	0.82	0.81	88,88,88,88	0
60	MG	Ba	1720	1/1	0.82	0.98	123,123,123,123	0
60	MG	BA	2943	1/1	0.82	0.54	79,79,79,79	0
60	MG	BA	3082	1/1	0.82	0.22	71,71,71,71	0
60	MG	AB	203	1/1	0.82	0.57	71,71,71,71	0
60	MG	AA	2978	1/1	0.82	0.39	100,100,100,100	0
60	MG	Aa	1682	1/1	0.82	0.34	97,97,97,97	0
60	MG	BA	3202	1/1	0.82	0.31	65,65,65,65	0
60	MG	AA	3163	1/1	0.83	0.62	89,89,89,89	0
60	MG	BA	3228	1/1	0.83	0.87	82,82,82,82	0
60	MG	AA	2940	1/1	0.83	0.61	102,102,102,102	0
60	MG	BA	3167	1/1	0.83	0.48	74,74,74,74	0
60	MG	BA	3118	1/1	0.83	0.53	82,82,82,82	0
60	MG	AA	2964	1/1	0.83	0.55	76,76,76,76	0
60	MG	AA	3246	1/1	0.83	0.95	103,103,103,103	0
60	MG	BA	3179	1/1	0.83	0.52	90,90,90,90	0
60	MG	Ba	1702	1/1	0.83	0.57	110,110,110,110	0
60	MG	Ba	1704	1/1	0.83	1.21	108,108,108,108	0
60	MG	BA	3184	1/1	0.83	0.36	83,83,83,83	0
60	MG	Ba	1705	1/1	0.83	0.20	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3248	1/1	0.83	0.22	64,64,64,64	0
60	MG	AA	3226	1/1	0.83	0.27	91,91,91,91	0
60	MG	Ba	1743	1/1	0.83	0.82	90,90,90,90	0
60	MG	Ba	1622	1/1	0.83	0.98	88,88,88,88	0
60	MG	Ba	1672	1/1	0.83	0.59	106,106,106,106	0
60	MG	AA	3151	1/1	0.83	0.28	88,88,88,88	0
60	MG	AA	3108	1/1	0.83	0.39	69,69,69,69	0
60	MG	AA	3137	1/1	0.83	0.71	95,95,95,95	0
60	MG	Aa	1695	1/1	0.83	0.55	97,97,97,97	0
60	MG	BA	2975	1/1	0.83	0.71	93,93,93,93	0
60	MG	Ba	1686	1/1	0.84	0.11	79,79,79,79	0
60	MG	BA	3207	1/1	0.84	0.26	90,90,90,90	0
60	MG	Aa	1707	1/1	0.84	0.64	79,79,79,79	0
60	MG	Ba	1690	1/1	0.84	0.46	67,67,67,67	0
60	MG	Ba	1692	1/1	0.84	0.63	99,99,99,99	0
60	MG	BA	3140	1/1	0.84	0.88	60,60,60,60	0
60	MG	BA	3143	1/1	0.84	2.37	90,90,90,90	0
60	MG	BA	3225	1/1	0.84	0.41	99,99,99,99	0
60	MG	AA	3223	1/1	0.84	0.81	75,75,75,75	0
60	MG	Aa	1626	1/1	0.84	0.77	85,85,85,85	0
60	MG	BX	101	1/1	0.84	0.65	59,59,59,59	1
60	MG	AA	2973	1/1	0.84	0.38	82,82,82,82	0
60	MG	AA	3188	1/1	0.84	0.24	91,91,91,91	0
60	MG	Aa	1656	1/1	0.84	0.12	67,67,67,67	0
60	MG	AA	3231	1/1	0.84	1.03	107,107,107,107	0
60	MG	BA	3069	1/1	0.84	0.40	72,72,72,72	0
60	MG	AA	3162	1/1	0.84	0.45	126,126,126,126	0
60	MG	Aa	1644	1/1	0.84	1.01	100,100,100,100	0
60	MG	AA	3141	1/1	0.84	0.18	54,54,54,54	0
60	MG	Aa	1701	1/1	0.84	1.09	96,96,96,96	0
60	MG	AA	3105	1/1	0.84	1.44	92,92,92,92	0
60	MG	Aa	1662	1/1	0.84	0.56	76,76,76,76	0
60	MG	AA	3245	1/1	0.84	0.55	71,71,71,71	0
60	MG	A7	102	1/1	0.84	0.47	98,98,98,98	0
60	MG	BA	3183	1/1	0.84	0.28	67,67,67,67	0
60	MG	Ba	1641	1/1	0.84	0.68	92,92,92,92	0
60	MG	Ba	1677	1/1	0.84	0.45	152,152,152,152	1
60	MG	AA	3081	1/1	0.84	0.28	89,89,89,89	0
60	MG	Aa	1741	1/1	0.84	1.01	88,88,88,88	0
60	MG	Ba	1684	1/1	0.84	0.51	76,76,76,76	0
60	MG	AA	2971	1/1	0.85	0.17	77,77,77,77	0
60	MG	Ba	1650	1/1	0.85	0.81	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3061	1/1	0.85	0.32	64,64,64,64	0
60	MG	BA	3233	1/1	0.85	0.60	109,109,109,109	0
60	MG	BA	3131	1/1	0.85	0.71	89,89,89,89	0
60	MG	AA	3227	1/1	0.85	0.47	110,110,110,110	0
60	MG	Ba	1656	1/1	0.85	1.15	80,80,80,80	0
60	MG	AA	2942	1/1	0.85	0.20	65,65,65,65	0
60	MG	B7	102	1/1	0.85	0.34	80,80,80,80	0
60	MG	Ba	1721	1/1	0.85	0.63	108,108,108,108	0
60	MG	Ba	1725	1/1	0.85	0.76	72,72,72,72	1
60	MG	BA	3081	1/1	0.85	0.36	106,106,106,106	0
60	MG	BA	3247	1/1	0.85	0.32	99,99,99,99	0
60	MG	Aa	1676	1/1	0.85	0.13	120,120,120,120	0
60	MG	AA	3091	1/1	0.85	0.61	104,104,104,104	0
60	MG	AA	2977	1/1	0.85	0.60	69,69,69,69	0
60	MG	BA	3096	1/1	0.85	0.16	49,49,49,49	0
60	MG	BA	3101	1/1	0.85	0.86	64,64,64,64	0
60	MG	BA	3217	1/1	0.85	0.67	76,76,76,76	0
60	MG	AA	2902	1/1	0.85	0.31	131,131,131,131	0
60	MG	Ba	1711	1/1	0.85	0.71	117,117,117,117	0
60	MG	Aa	1709	1/1	0.85	0.21	92,92,92,92	0
60	MG	AA	3254	1/1	0.85	0.34	84,84,84,84	0
60	MG	AA	2944	1/1	0.86	0.68	82,82,82,82	0
60	MG	BA	3121	1/1	0.86	1.26	82,82,82,82	0
60	MG	AA	2979	1/1	0.86	0.72	71,71,71,71	0
60	MG	BA	3177	1/1	0.86	0.67	66,66,66,66	0
60	MG	AA	2935	1/1	0.86	0.50	90,90,90,90	0
60	MG	AA	3183	1/1	0.86	0.37	79,79,79,79	0
60	MG	Ba	1741	1/1	0.86	0.52	81,81,81,81	0
60	MG	AA	2985	1/1	0.86	0.39	44,44,44,44	0
60	MG	AA	3101	1/1	0.86	0.28	92,92,92,92	0
60	MG	AA	2948	1/1	0.86	0.16	80,80,80,80	0
60	MG	Ba	1694	1/1	0.86	0.35	112,112,112,112	0
60	MG	AA	3140	1/1	0.86	0.53	107,107,107,107	0
60	MG	AA	3074	1/1	0.86	0.39	87,87,87,87	0
60	MG	Aa	1642	1/1	0.86	0.65	102,102,102,102	0
60	MG	Ba	1723	1/1	0.86	0.64	89,89,89,89	0
60	MG	AA	2919	1/1	0.86	0.31	49,49,49,49	0
60	MG	Aa	1743	1/1	0.86	0.63	80,80,80,80	0
60	MG	BA	2985	1/1	0.86	0.44	64,64,64,64	0
60	MG	BA	3260	1/1	0.86	0.24	93,93,93,93	0
60	MG	Ba	1731	1/1	0.86	0.25	103,103,103,103	0
60	MG	BA	3262	1/1	0.86	0.58	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3006	1/1	0.86	0.56	107,107,107,107	0
60	MG	AA	2961	1/1	0.86	1.12	99,99,99,99	0
60	MG	BA	3164	1/1	0.86	0.46	78,78,78,78	0
60	MG	BA	3023	1/1	0.86	0.63	54,54,54,54	0
60	MG	BA	3211	1/1	0.87	0.43	81,81,81,81	0
60	MG	BA	3213	1/1	0.87	1.01	81,81,81,81	0
60	MG	AA	3059	1/1	0.87	0.27	90,90,90,90	0
60	MG	AA	3062	1/1	0.87	0.17	62,62,62,62	0
60	MG	Aa	1686	1/1	0.87	0.55	74,74,74,74	0
60	MG	BA	3151	1/1	0.87	1.49	105,105,105,105	0
60	MG	Ba	1652	1/1	0.87	0.80	80,80,80,80	0
60	MG	BA	2980	1/1	0.87	1.08	80,80,80,80	0
60	MG	BA	3097	1/1	0.87	0.18	65,65,65,65	0
60	MG	BA	3158	1/1	0.87	0.50	61,61,61,61	0
60	MG	BA	2901	1/1	0.87	0.42	122,122,122,122	0
60	MG	Aa	1648	1/1	0.87	0.44	118,118,118,118	0
60	MG	BA	2919	1/1	0.87	0.18	40,40,40,40	0
60	MG	BA	3111	1/1	0.87	0.53	99,99,99,99	0
60	MG	BA	3116	1/1	0.87	0.72	99,99,99,99	0
60	MG	Aa	1649	1/1	0.87	0.14	88,88,88,88	0
60	MG	BA	3240	1/1	0.87	0.28	73,73,73,73	0
60	MG	AA	2932	1/1	0.87	0.39	79,79,79,79	0
60	MG	AA	3078	1/1	0.87	0.87	94,94,94,94	0
60	MG	BA	3125	1/1	0.87	0.42	68,68,68,68	0
60	MG	AA	2952	1/1	0.87	0.27	81,81,81,81	0
60	MG	Ba	1633	1/1	0.87	0.77	71,71,71,71	0
60	MG	BA	3250	1/1	0.87	0.94	97,97,97,97	0
60	MG	AA	3120	1/1	0.87	0.59	90,90,90,90	0
60	MG	BA	3190	1/1	0.87	0.21	98,98,98,98	0
60	MG	AA	3028	1/1	0.87	0.26	53,53,53,53	0
60	MG	BA	3132	1/1	0.87	0.49	73,73,73,73	0
60	MG	Aa	1722	1/1	0.87	0.71	110,110,110,110	0
60	MG	Aa	1731	1/1	0.87	0.46	82,82,82,82	0
60	MG	Aa	1734	1/1	0.87	0.65	125,125,125,125	0
60	MG	AA	2903	1/1	0.87	0.22	98,98,98,98	0
60	MG	Ba	1675	1/1	0.87	0.08	69,69,69,69	0
60	MG	Ba	1606	1/1	0.87	0.52	101,101,101,101	0
60	MG	AA	3057	1/1	0.87	1.26	73,73,73,73	0
60	MG	Aa	1602	1/1	0.88	0.19	108,108,108,108	0
60	MG	AA	3164	1/1	0.88	0.20	81,81,81,81	0
60	MG	Ba	1708	1/1	0.88	0.08	139,139,139,139	0
60	MG	AA	3083	1/1	0.88	0.45	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3178	1/1	0.88	0.98	71,71,71,71	0
60	MG	AA	3135	1/1	0.88	0.49	89,89,89,89	0
60	MG	Ba	1628	1/1	0.88	0.32	79,79,79,79	0
60	MG	BA	2959	1/1	0.88	0.17	62,62,62,62	0
60	MG	AA	2938	1/1	0.88	1.08	95,95,95,95	0
60	MG	Ba	1687	1/1	0.88	0.19	69,69,69,69	1
60	MG	BA	3185	1/1	0.88	0.14	66,66,66,66	0
60	MG	BA	3189	1/1	0.88	0.89	62,62,62,62	0
60	MG	AA	3036	1/1	0.88	0.78	99,99,99,99	0
60	MG	Ba	1689	1/1	0.88	0.43	82,82,82,82	0
60	MG	Aa	1693	1/1	0.88	0.71	65,65,65,65	0
60	MG	AA	3175	1/1	0.88	0.63	54,54,54,54	0
60	MG	AA	3259	1/1	0.88	0.51	65,65,65,65	0
60	MG	BA	3251	1/1	0.88	1.00	78,78,78,78	0
60	MG	AA	3010	1/1	0.88	0.26	94,94,94,94	0
60	MG	BA	3099	1/1	0.88	0.88	97,97,97,97	0
60	MG	AA	3155	1/1	0.88	0.83	72,72,72,72	0
60	MG	Aa	1710	1/1	0.88	0.08	128,128,128,128	0
60	MG	BA	3103	1/1	0.88	0.28	63,63,63,63	0
60	MG	AA	2962	1/1	0.88	0.16	53,53,53,53	0
60	MG	AA	3221	1/1	0.88	0.26	59,59,59,59	0
60	MG	BA	3029	1/1	0.88	0.60	49,49,49,49	0
60	MG	BA	3117	1/1	0.88	0.82	106,106,106,106	0
60	MG	AA	3118	1/1	0.88	0.60	59,59,59,59	0
60	MG	Ba	1738	1/1	0.88	0.38	77,77,77,77	0
60	MG	Aa	1738	1/1	0.89	0.49	78,78,78,78	0
60	MG	BA	3221	1/1	0.89	0.65	66,66,66,66	0
60	MG	AA	3182	1/1	0.89	0.32	82,82,82,82	0
60	MG	AA	3076	1/1	0.89	0.56	92,92,92,92	0
60	MG	BA	2963	1/1	0.89	0.90	91,91,91,91	0
60	MG	AA	2930	1/1	0.89	0.18	38,38,38,38	0
60	MG	Aa	1690	1/1	0.89	0.23	96,96,96,96	1
60	MG	Bv	101	1/1	0.89	0.56	71,71,71,71	1
60	MG	BA	3232	1/1	0.89	0.35	82,82,82,82	0
60	MG	AA	3119	1/1	0.89	0.25	143,143,143,143	0
60	MG	AA	3033	1/1	0.89	0.77	68,68,68,68	0
60	MG	Ba	1710	1/1	0.89	0.44	81,81,81,81	0
60	MG	AA	3129	1/1	0.89	0.35	112,112,112,112	0
60	MG	Aa	1659	1/1	0.89	0.25	70,70,70,70	0
60	MG	AA	2956	1/1	0.89	0.77	111,111,111,111	0
60	MG	AA	2957	1/1	0.89	0.31	83,83,83,83	0
60	MG	BA	3243	1/1	0.89	0.75	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3018	1/1	0.89	0.39	51,51,51,51	0
60	MG	Aa	1745	1/1	0.89	0.45	70,70,70,70	0
60	MG	Aa	1678	1/1	0.89	1.24	111,111,111,111	1
60	MG	Av	104	1/1	0.89	0.49	88,88,88,88	1
60	MG	AA	3001	1/1	0.89	0.42	68,68,68,68	0
60	MG	AA	3063	1/1	0.89	0.33	47,47,47,47	0
60	MG	AA	3252	1/1	0.89	0.64	85,85,85,85	0
60	MG	BA	3252	1/1	0.89	0.26	72,72,72,72	0
60	MG	AA	2909	1/1	0.89	0.38	46,46,46,46	0
60	MG	Ba	1654	1/1	0.89	1.19	97,97,97,97	0
60	MG	Ba	1730	1/1	0.89	0.40	64,64,64,64	0
60	MG	AA	3173	1/1	0.89	0.13	72,72,72,72	0
60	MG	Aa	1687	1/1	0.89	0.55	51,51,51,51	1
60	MG	Ba	1733	1/1	0.89	0.18	100,100,100,100	1
60	MG	BA	3079	1/1	0.89	0.36	79,79,79,79	0
60	MG	Aa	1663	1/1	0.89	0.23	68,68,68,68	0
60	MG	BA	2952	1/1	0.89	0.23	87,87,87,87	0
60	MG	AA	3178	1/1	0.89	1.09	86,86,86,86	0
60	MG	BA	3083	1/1	0.89	0.57	73,73,73,73	0
60	MG	BA	2970	1/1	0.90	1.14	104,104,104,104	0
60	MG	AA	3115	1/1	0.90	0.59	108,108,108,108	0
60	MG	BA	3087	1/1	0.90	0.49	74,74,74,74	0
60	MG	AA	2939	1/1	0.90	0.16	53,53,53,53	0
60	MG	BA	3155	1/1	0.90	0.23	77,77,77,77	1
60	MG	BA	3093	1/1	0.90	0.18	71,71,71,71	0
60	MG	Aa	1653	1/1	0.90	0.94	71,71,71,71	0
60	MG	AA	3235	1/1	0.90	0.21	102,102,102,102	0
60	MG	BA	2981	1/1	0.90	0.51	45,45,45,45	0
60	MG	AA	3205	1/1	0.90	0.52	58,58,58,58	0
60	MG	BA	3170	1/1	0.90	0.17	58,58,58,58	0
60	MG	Ba	1618	1/1	0.90	0.36	56,56,56,56	0
60	MG	AA	2972	1/1	0.90	0.37	75,75,75,75	0
60	MG	BA	3000	1/1	0.90	0.15	61,61,61,61	0
60	MG	AA	3147	1/1	0.90	0.84	66,66,66,66	0
60	MG	AA	3121	1/1	0.90	0.45	83,83,83,83	0
60	MG	AA	3100	1/1	0.90	0.29	64,64,64,64	0
60	MG	BA	3241	1/1	0.90	0.55	106,106,106,106	0
60	MG	Ba	1662	1/1	0.90	0.20	68,68,68,68	0
60	MG	AA	3210	1/1	0.90	1.01	99,99,99,99	0
60	MG	Ba	1632	1/1	0.90	0.21	81,81,81,81	0
60	MG	BA	3034	1/1	0.90	0.58	78,78,78,78	0
60	MG	Aa	1679	1/1	0.90	0.24	131,131,131,131	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3186	1/1	0.90	0.18	70,70,70,70	0
60	MG	AA	3004	1/1	0.90	0.07	84,84,84,84	0
60	MG	AA	3153	1/1	0.90	0.70	92,92,92,92	0
60	MG	BA	2949	1/1	0.90	0.21	63,63,63,63	0
60	MG	BA	3197	1/1	0.90	0.23	58,58,58,58	0
60	MG	Aa	1655	1/1	0.90	1.01	88,88,88,88	0
60	MG	Aa	1603	1/1	0.90	0.24	112,112,112,112	1
60	MG	Aa	1705	1/1	0.90	1.08	50,50,50,50	1
60	MG	BA	3072	1/1	0.90	0.69	75,75,75,75	0
60	MG	AA	3085	1/1	0.90	0.25	86,86,86,86	0
60	MG	Bv	102	1/1	0.90	0.25	54,54,54,54	0
60	MG	Aa	1615	1/1	0.90	0.65	58,58,58,58	0
60	MG	Aa	1729	1/1	0.90	0.43	60,60,60,60	0
60	MG	BA	2964	1/1	0.90	1.34	84,84,84,84	0
60	MG	Ba	1681	1/1	0.90	0.14	71,71,71,71	0
60	MG	AA	3090	1/1	0.91	0.49	86,86,86,86	0
60	MG	BA	3142	1/1	0.91	0.70	61,61,61,61	0
60	MG	BA	2944	1/1	0.91	0.14	86,86,86,86	0
60	MG	AA	3122	1/1	0.91	0.13	101,101,101,101	0
60	MG	Ba	1615	1/1	0.91	0.81	86,86,86,86	0
60	MG	Ba	1693	1/1	0.91	0.18	108,108,108,108	0
60	MG	BA	2948	1/1	0.91	0.58	93,93,93,93	0
60	MG	AA	3154	1/1	0.91	0.68	86,86,86,86	0
60	MG	BA	3223	1/1	0.91	0.26	74,74,74,74	0
60	MG	Ba	1736	1/1	0.91	0.37	88,88,88,88	0
60	MG	BA	3152	1/1	0.91	1.00	92,92,92,92	0
60	MG	Aa	1702	1/1	0.91	0.54	65,65,65,65	0
59	ZN	A4	101	1/1	0.91	0.06	195,195,195,195	0
60	MG	BA	2956	1/1	0.91	0.25	89,89,89,89	0
60	MG	Ba	1619	1/1	0.91	0.31	70,70,70,70	0
60	MG	Aa	1624	1/1	0.91	0.53	86,86,86,86	0
60	MG	BA	3161	1/1	0.91	0.20	51,51,51,51	0
60	MG	AA	3263	1/1	0.91	0.54	94,94,94,94	0
60	MG	AA	3005	1/1	0.91	0.35	64,64,64,64	0
60	MG	AD	301	1/1	0.91	0.29	38,38,38,38	0
60	MG	Aa	1645	1/1	0.91	0.39	83,83,83,83	0
60	MG	Aa	1683	1/1	0.91	0.08	59,59,59,59	0
60	MG	Aa	1640	1/1	0.91	0.52	82,82,82,82	0
60	MG	Ba	1634	1/1	0.91	0.16	83,83,83,83	0
60	MG	A5	101	1/1	0.91	0.59	62,62,62,62	0
60	MG	Aa	1632	1/1	0.91	0.98	86,86,86,86	0
60	MG	B0	102	1/1	0.91	0.24	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1639	1/1	0.91	0.41	68,68,68,68	0
60	MG	Aa	1742	1/1	0.91	0.32	91,91,91,91	0
60	MG	Aa	1728	1/1	0.91	0.38	81,81,81,81	0
60	MG	BA	2909	1/1	0.91	0.27	36,36,36,36	0
60	MG	BA	2917	1/1	0.91	0.50	75,75,75,75	0
60	MG	AA	3048	1/1	0.91	0.37	69,69,69,69	0
60	MG	AA	3217	1/1	0.91	0.56	70,70,70,70	0
60	MG	AA	3116	1/1	0.91	0.62	39,39,39,39	1
60	MG	Ba	1722	1/1	0.91	0.18	106,106,106,106	0
60	MG	AA	3049	1/1	0.91	0.52	64,64,64,64	0
60	MG	Aa	1664	1/1	0.91	0.70	114,114,114,114	0
60	MG	AA	2989	1/1	0.91	0.30	50,50,50,50	0
60	MG	BA	3133	1/1	0.91	0.28	83,83,83,83	0
60	MG	BA	2941	1/1	0.91	0.40	98,98,98,98	0
60	MG	BA	2942	1/1	0.91	0.20	78,78,78,78	0
60	MG	BB	202	1/1	0.91	0.36	55,55,55,55	0
60	MG	BA	3056	1/1	0.91	0.22	53,53,53,53	0
60	MG	AA	3124	1/1	0.92	0.66	63,63,63,63	0
60	MG	BA	3091	1/1	0.92	0.39	66,66,66,66	0
60	MG	BA	2957	1/1	0.92	0.45	38,38,38,38	0
60	MG	BA	3188	1/1	0.92	0.85	90,90,90,90	0
60	MG	BA	3095	1/1	0.92	0.44	61,61,61,61	0
60	MG	AA	2974	1/1	0.92	1.26	85,85,85,85	0
60	MG	AA	3166	1/1	0.92	0.49	94,94,94,94	0
60	MG	Ba	1638	1/1	0.92	0.52	79,79,79,79	0
60	MG	BA	2962	1/1	0.92	0.32	71,71,71,71	0
60	MG	AA	3133	1/1	0.92	0.97	78,78,78,78	0
60	MG	Ba	1742	1/1	0.92	0.41	105,105,105,105	0
60	MG	BA	3205	1/1	0.92	0.39	113,113,113,113	0
60	MG	AA	3029	1/1	0.92	0.40	74,74,74,74	0
60	MG	BA	2967	1/1	0.92	0.14	58,58,58,58	0
60	MG	Aa	1657	1/1	0.92	1.05	93,93,93,93	0
60	MG	BA	2971	1/1	0.92	0.78	63,63,63,63	0
60	MG	AA	2920	1/1	0.92	0.34	45,45,45,45	0
60	MG	AD	302	1/1	0.92	0.49	64,64,64,64	0
60	MG	Aa	1654	1/1	0.92	0.21	93,93,93,93	0
60	MG	BA	3215	1/1	0.92	0.48	61,61,61,61	0
60	MG	Aa	1606	1/1	0.92	1.07	105,105,105,105	0
60	MG	Aa	1692	1/1	0.92	0.30	62,62,62,62	0
60	MG	AA	3233	1/1	0.92	0.19	90,90,90,90	0
60	MG	Aa	1667	1/1	0.92	0.54	100,100,100,100	0
60	MG	B7	101	1/1	0.92	0.37	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1694	1/1	0.92	0.70	107,107,107,107	0
60	MG	BA	3004	1/1	0.92	0.29	45,45,45,45	0
60	MG	AA	2998	1/1	0.92	0.67	51,51,51,51	0
60	MG	Aa	1660	1/1	0.92	0.47	88,88,88,88	0
60	MG	AA	3061	1/1	0.92	0.73	89,89,89,89	0
60	MG	Aa	1696	1/1	0.92	0.15	93,93,93,93	0
60	MG	BA	3026	1/1	0.92	0.55	59,59,59,59	0
60	MG	AA	3148	1/1	0.92	0.73	72,72,72,72	0
60	MG	BA	3144	1/1	0.92	0.67	59,59,59,59	0
60	MG	Aa	1711	1/1	0.92	0.30	61,61,61,61	0
60	MG	Aa	1661	1/1	0.92	0.29	91,91,91,91	0
60	MG	AA	3007	1/1	0.92	0.21	83,83,83,83	0
60	MG	BA	3046	1/1	0.92	0.55	76,76,76,76	0
60	MG	BA	3048	1/1	0.92	0.58	95,95,95,95	0
60	MG	AA	3073	1/1	0.92	0.52	84,84,84,84	0
60	MG	AA	2945	1/1	0.92	0.11	73,73,73,73	0
60	MG	AA	3250	1/1	0.92	0.23	65,65,65,65	0
60	MG	BA	2940	1/1	0.92	0.28	76,76,76,76	0
60	MG	BA	3063	1/1	0.92	0.30	59,59,59,59	0
60	MG	Ba	1620	1/1	0.92	0.13	102,102,102,102	0
60	MG	BA	3066	1/1	0.92	0.24	28,28,28,28	0
60	MG	BA	3067	1/1	0.92	0.41	78,78,78,78	0
60	MG	AA	3013	1/1	0.92	0.85	49,49,49,49	0
60	MG	Aa	1617	1/1	0.92	0.31	66,66,66,66	0
60	MG	Ba	1674	1/1	0.92	0.13	57,57,57,57	0
60	MG	BA	3073	1/1	0.92	0.44	54,54,54,54	0
60	MG	AA	2947	1/1	0.92	0.24	103,103,103,103	0
60	MG	Ba	1729	1/1	0.92	0.31	84,84,84,84	0
60	MG	Ba	1626	1/1	0.92	0.30	92,92,92,92	0
60	MG	Ba	1627	1/1	0.92	0.38	71,71,71,71	0
60	MG	AA	3079	1/1	0.92	0.33	95,95,95,95	0
60	MG	AA	3017	1/1	0.92	0.22	59,59,59,59	0
60	MG	AA	3082	1/1	0.92	0.52	69,69,69,69	0
60	MG	BB	201	1/1	0.92	0.29	50,50,50,50	0
60	MG	BA	2953	1/1	0.92	0.43	100,100,100,100	0
60	MG	AA	3215	1/1	0.92	1.14	89,89,89,89	0
60	MG	BA	3199	1/1	0.93	0.29	89,89,89,89	1
60	MG	AA	3214	1/1	0.93	0.27	57,57,57,57	0
60	MG	AA	2967	1/1	0.93	1.80	96,96,96,96	0
60	MG	AA	2923	1/1	0.93	0.77	75,75,75,75	0
60	MG	Ba	1683	1/1	0.93	0.10	93,93,93,93	0
60	MG	Aq	201	1/1	0.93	0.31	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	2984	1/1	0.93	0.70	79,79,79,79	0
60	MG	BA	3047	1/1	0.93	0.31	57,57,57,57	0
60	MG	Ba	1611	1/1	0.93	0.25	81,81,81,81	0
60	MG	BA	3134	1/1	0.93	0.84	98,98,98,98	0
60	MG	AA	3107	1/1	0.93	0.16	58,58,58,58	0
60	MG	Aa	1638	1/1	0.93	0.31	84,84,84,84	0
60	MG	AA	3159	1/1	0.93	0.23	75,75,75,75	0
60	MG	AA	3054	1/1	0.93	0.43	43,43,43,43	0
60	MG	AA	3258	1/1	0.93	0.68	103,103,103,103	0
60	MG	Aa	1732	1/1	0.93	0.37	58,58,58,58	0
60	MG	AA	3193	1/1	0.93	0.16	85,85,85,85	0
60	MG	BA	3145	1/1	0.93	0.65	62,62,62,62	0
60	MG	Ba	1696	1/1	0.93	0.87	99,99,99,99	0
60	MG	Aa	1716	1/1	0.93	0.10	79,79,79,79	0
60	MG	AA	3200	1/1	0.93	0.39	82,82,82,82	0
60	MG	Ba	1658	1/1	0.93	0.34	84,84,84,84	0
60	MG	AA	3232	1/1	0.93	0.40	70,70,70,70	0
60	MG	Ba	1623	1/1	0.93	0.40	75,75,75,75	0
60	MG	Ba	1624	1/1	0.93	0.24	73,73,73,73	0
60	MG	BQ	201	1/1	0.93	1.22	79,79,79,79	0
60	MG	Ba	1663	1/1	0.93	0.21	86,86,86,86	0
60	MG	AA	2994	1/1	0.93	0.41	69,69,69,69	0
60	MG	Ba	1709	1/1	0.93	0.39	63,63,63,63	0
60	MG	BA	3238	1/1	0.93	0.33	89,89,89,89	0
60	MG	BA	2969	1/1	0.93	0.35	58,58,58,58	0
60	MG	B5	101	1/1	0.93	0.42	43,43,43,43	0
60	MG	AA	3265	1/1	0.93	0.82	83,83,83,83	0
60	MG	BA	3242	1/1	0.93	0.46	73,73,73,73	0
60	MG	AA	3027	1/1	0.93	0.51	57,57,57,57	0
60	MG	BA	3165	1/1	0.93	0.60	73,73,73,73	0
60	MG	BA	3166	1/1	0.93	0.62	54,54,54,54	0
60	MG	AA	2995	1/1	0.93	0.38	82,82,82,82	0
60	MG	AA	2997	1/1	0.93	0.69	44,44,44,44	0
60	MG	BA	2903	1/1	0.93	0.93	91,91,91,91	0
60	MG	Ba	1671	1/1	0.93	0.19	75,75,75,75	0
60	MG	Aa	1672	1/1	0.93	0.30	77,77,77,77	0
60	MG	BA	3098	1/1	0.93	0.56	77,77,77,77	0
60	MG	AA	3031	1/1	0.93	0.23	56,56,56,56	0
60	MG	BA	3100	1/1	0.93	0.17	63,63,63,63	0
60	MG	BA	3256	1/1	0.93	0.51	84,84,84,84	0
60	MG	Aa	1650	1/1	0.93	0.30	53,53,53,53	0
60	MG	BA	2923	1/1	0.93	0.41	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3001	1/1	0.93	0.29	45,45,45,45	0
60	MG	Aa	1720	1/1	0.93	0.58	90,90,90,90	0
60	MG	BA	2929	1/1	0.93	0.23	43,43,43,43	0
60	MG	BA	3112	1/1	0.93	0.32	81,81,81,81	0
60	MG	BA	3113	1/1	0.93	1.18	55,55,55,55	1
60	MG	AA	3132	1/1	0.93	0.62	93,93,93,93	0
60	MG	AA	3213	1/1	0.93	0.83	98,98,98,98	0
60	MG	BA	3019	1/1	0.93	0.42	72,72,72,72	0
60	MG	Ba	1679	1/1	0.93	0.54	67,67,67,67	0
60	MG	Ba	1678	1/1	0.94	0.44	131,131,131,131	0
60	MG	Ba	1635	1/1	0.94	0.65	86,86,86,86	0
60	MG	BA	2939	1/1	0.94	0.15	44,44,44,44	0
60	MG	AA	3097	1/1	0.94	0.48	69,69,69,69	0
60	MG	BA	3038	1/1	0.94	0.37	52,52,52,52	0
60	MG	BA	3045	1/1	0.94	0.49	47,47,47,47	0
60	MG	AA	3234	1/1	0.94	0.14	59,59,59,59	0
60	MG	AA	3130	1/1	0.94	0.46	42,42,42,42	0
60	MG	Aa	1675	1/1	0.94	0.12	58,58,58,58	0
60	MG	Aa	1612	1/1	0.94	0.25	58,58,58,58	0
60	MG	AA	3160	1/1	0.94	0.74	65,65,65,65	0
60	MG	BA	3055	1/1	0.94	0.24	64,64,64,64	0
60	MG	AA	3035	1/1	0.94	0.47	74,74,74,74	0
60	MG	BA	3141	1/1	0.94	0.53	82,82,82,82	0
60	MG	AA	3240	1/1	0.94	0.69	104,104,104,104	0
60	MG	BA	3220	1/1	0.94	0.49	59,59,59,59	0
60	MG	Aa	1609	1/1	0.94	0.13	82,82,82,82	0
60	MG	Aa	1620	1/1	0.94	0.39	79,79,79,79	0
60	MG	AA	3244	1/1	0.94	0.80	98,98,98,98	0
60	MG	Ba	1609	1/1	0.94	0.42	104,104,104,104	0
60	MG	Av	101	1/1	0.94	0.51	65,65,65,65	1
60	MG	Aa	1698	1/1	0.94	0.67	86,86,86,86	0
60	MG	AA	2958	1/1	0.94	0.23	77,77,77,77	0
60	MG	Av	103	1/1	0.94	0.78	69,69,69,69	1
60	MG	Bv	103	1/1	0.94	0.24	110,110,110,110	0
60	MG	AA	3109	1/1	0.94	0.54	73,73,73,73	0
60	MG	Bv	105	1/1	0.94	0.26	95,95,95,95	1
60	MG	Aa	1605	1/1	0.94	0.18	70,70,70,70	0
60	MG	BD	302	1/1	0.94	0.33	53,53,53,53	0
60	MG	Ba	1703	1/1	0.94	0.77	69,69,69,69	1
60	MG	AA	3113	1/1	0.94	0.49	55,55,55,55	0
60	MG	AA	2910	1/1	0.94	0.70	71,71,71,71	0
60	MG	AA	3058	1/1	0.94	0.70	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	2943	1/1	0.94	0.37	77,77,77,77	0
60	MG	BA	3090	1/1	0.94	0.32	47,47,47,47	0
60	MG	AA	3256	1/1	0.94	0.48	74,74,74,74	0
60	MG	BA	3092	1/1	0.94	0.44	83,83,83,83	0
60	MG	BA	3168	1/1	0.94	0.11	87,87,87,87	0
60	MG	Aa	1721	1/1	0.94	1.07	97,97,97,97	0
60	MG	AA	3180	1/1	0.94	0.46	58,58,58,58	0
60	MG	Ba	1666	1/1	0.94	1.17	84,84,84,84	0
60	MG	BA	3249	1/1	0.94	0.60	55,55,55,55	0
60	MG	AA	3181	1/1	0.94	0.30	65,65,65,65	0
60	MG	AA	3089	1/1	0.94	0.24	74,74,74,74	0
60	MG	Ba	1714	1/1	0.94	0.13	90,90,90,90	0
60	MG	BA	2914	1/1	0.94	0.35	32,32,32,32	0
60	MG	BA	3254	1/1	0.94	0.58	56,56,56,56	0
59	ZN	An	101	1/1	0.94	0.20	171,171,171,171	0
60	MG	BA	3181	1/1	0.94	0.37	51,51,51,51	0
60	MG	Aa	1712	1/1	0.94	0.43	86,86,86,86	0
60	MG	Aa	1635	1/1	0.94	0.09	61,61,61,61	0
60	MG	Ba	1629	1/1	0.94	0.29	69,69,69,69	0
60	MG	AA	3228	1/1	0.94	0.22	57,57,57,57	0
60	MG	AA	3095	1/1	0.94	0.28	67,67,67,67	0
60	MG	BA	3013	1/1	0.94	0.28	41,41,41,41	0
60	MG	BA	2930	1/1	0.94	0.11	34,34,34,34	0
60	MG	AA	3128	1/1	0.94	0.37	71,71,71,71	0
60	MG	BA	2934	1/1	0.94	0.52	65,65,65,65	1
60	MG	BA	3194	1/1	0.94	0.19	28,28,28,28	0
60	MG	AA	3190	1/1	0.94	0.39	52,52,52,52	0
60	MG	AA	3077	1/1	0.95	0.58	60,60,60,60	0
60	MG	AA	3243	1/1	0.95	1.47	117,117,117,117	0
60	MG	AA	2924	1/1	0.95	0.23	54,54,54,54	0
60	MG	AA	3009	1/1	0.95	0.25	61,61,61,61	0
60	MG	AA	2960	1/1	0.95	0.43	37,37,37,37	0
60	MG	BA	2966	1/1	0.95	0.59	39,39,39,39	0
60	MG	AA	3012	1/1	0.95	0.57	46,46,46,46	0
60	MG	Aa	1668	1/1	0.95	0.62	84,84,84,84	0
60	MG	AA	3191	1/1	0.95	0.59	102,102,102,102	0
60	MG	AA	2926	1/1	0.95	0.57	62,62,62,62	0
60	MG	AA	3251	1/1	0.95	0.61	68,68,68,68	0
60	MG	AA	2963	1/1	0.95	0.85	65,65,65,65	0
60	MG	Ba	1691	1/1	0.95	0.59	61,61,61,61	0
60	MG	BA	3201	1/1	0.95	0.29	62,62,62,62	0
60	MG	BA	2978	1/1	0.95	0.51	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3104	1/1	0.95	0.19	36,36,36,36	0
60	MG	BA	3107	1/1	0.95	0.36	58,58,58,58	0
60	MG	BA	2979	1/1	0.95	0.47	36,36,36,36	0
60	MG	AA	2928	1/1	0.95	0.29	89,89,89,89	0
60	MG	AA	3199	1/1	0.95	0.44	44,44,44,44	0
60	MG	AA	3022	1/1	0.95	0.36	43,43,43,43	0
60	MG	AA	3202	1/1	0.95	0.44	85,85,85,85	1
60	MG	BA	2986	1/1	0.95	0.45	42,42,42,42	0
60	MG	BA	2988	1/1	0.95	0.56	45,45,45,45	0
60	MG	BA	2995	1/1	0.95	0.52	45,45,45,45	0
60	MG	AA	3024	1/1	0.95	0.45	51,51,51,51	0
60	MG	AA	3145	1/1	0.95	0.64	68,68,68,68	0
60	MG	AA	2965	1/1	0.95	0.22	80,80,80,80	0
60	MG	Ba	1700	1/1	0.95	0.63	113,113,113,113	0
60	MG	Aa	1669	1/1	0.95	0.68	71,71,71,71	0
60	MG	BA	3009	1/1	0.95	0.65	38,38,38,38	0
60	MG	BA	3224	1/1	0.95	0.16	89,89,89,89	0
60	MG	AA	2931	1/1	0.95	0.51	63,63,63,63	0
60	MG	BA	3012	1/1	0.95	1.12	69,69,69,69	0
60	MG	BA	2911	1/1	0.95	0.27	36,36,36,36	0
60	MG	Aa	1703	1/1	0.95	0.32	70,70,70,70	0
60	MG	BA	3230	1/1	0.95	0.16	61,61,61,61	0
60	MG	AA	2933	1/1	0.95	0.82	84,84,84,84	0
60	MG	AA	3032	1/1	0.95	0.21	64,64,64,64	0
60	MG	AA	2934	1/1	0.95	0.34	53,53,53,53	1
60	MG	AA	3034	1/1	0.95	0.23	49,49,49,49	0
60	MG	BA	3031	1/1	0.95	0.53	46,46,46,46	0
60	MG	Ba	1649	1/1	0.95	0.21	52,52,52,52	0
60	MG	BA	2926	1/1	0.95	0.42	58,58,58,58	0
60	MG	Aa	1733	1/1	0.95	0.26	79,79,79,79	0
60	MG	BA	3037	1/1	0.95	0.29	41,41,41,41	0
60	MG	Ba	1651	1/1	0.95	0.47	51,51,51,51	0
60	MG	Aa	1704	1/1	0.95	0.55	86,86,86,86	0
60	MG	BA	2933	1/1	0.95	0.57	84,84,84,84	0
60	MG	AA	3038	1/1	0.95	0.82	95,95,95,95	0
60	MG	Aa	1680	1/1	0.95	0.33	115,115,115,115	0
60	MG	A1	101	1/1	0.95	0.33	70,70,70,70	0
60	MG	Aa	1613	1/1	0.95	0.40	85,85,85,85	0
60	MG	AA	3161	1/1	0.95	0.49	75,75,75,75	0
60	MG	Aa	1643	1/1	0.95	0.17	117,117,117,117	0
60	MG	Aa	1739	1/1	0.95	0.86	100,100,100,100	0
60	MG	AA	2901	1/1	0.95	0.15	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1604	1/1	0.95	0.09	78,78,78,78	0
60	MG	AA	3055	1/1	0.95	0.70	59,59,59,59	0
60	MG	Aa	1708	1/1	0.95	0.36	89,89,89,89	0
60	MG	Aa	1627	1/1	0.95	0.23	84,84,84,84	0
60	MG	AA	2905	1/1	0.95	0.66	45,45,45,45	0
60	MG	AA	2992	1/1	0.95	0.63	61,61,61,61	0
60	MG	BA	3257	1/1	0.95	0.58	63,63,63,63	0
60	MG	Aa	1724	1/1	0.95	0.26	100,100,100,100	0
60	MG	BA	2950	1/1	0.95	0.30	69,69,69,69	0
60	MG	AA	2950	1/1	0.95	0.48	59,59,59,59	0
60	MG	Aa	1684	1/1	0.95	0.55	71,71,71,71	0
60	MG	AA	2911	1/1	0.95	0.30	39,39,39,39	0
60	MG	BA	3176	1/1	0.95	0.54	66,66,66,66	0
60	MG	AA	3072	1/1	0.95	0.26	79,79,79,79	0
60	MG	Aa	1726	1/1	0.95	0.34	57,57,57,57	0
60	MG	BA	3266	1/1	0.95	0.18	80,80,80,80	0
60	MG	Aa	1639	1/1	0.95	0.59	83,83,83,83	0
60	MG	Aa	1619	1/1	0.95	0.47	62,62,62,62	0
60	MG	Aa	1636	1/1	0.95	0.45	62,62,62,62	0
60	MG	AA	2941	1/1	0.96	0.48	68,68,68,68	0
60	MG	AA	2996	1/1	0.96	0.61	62,62,62,62	0
60	MG	AA	3220	1/1	0.96	0.50	47,47,47,47	0
60	MG	BA	3010	1/1	0.96	0.38	28,28,28,28	0
60	MG	BA	3195	1/1	0.96	0.51	57,57,57,57	0
60	MG	AA	2921	1/1	0.96	0.41	59,59,59,59	0
60	MG	AA	3172	1/1	0.96	0.46	58,58,58,58	0
60	MG	Aa	1688	1/1	0.96	0.51	72,72,72,72	0
60	MG	BA	3015	1/1	0.96	0.36	39,39,39,39	0
60	MG	BA	3016	1/1	0.96	0.30	50,50,50,50	0
60	MG	AA	3041	1/1	0.96	0.35	49,49,49,49	0
60	MG	AA	2999	1/1	0.96	0.46	61,61,61,61	0
60	MG	Aa	1647	1/1	0.96	1.12	105,105,105,105	0
60	MG	Ba	1642	1/1	0.96	0.38	83,83,83,83	0
60	MG	BA	3028	1/1	0.96	0.31	44,44,44,44	0
60	MG	Aa	1629	1/1	0.96	0.20	76,76,76,76	0
60	MG	AA	3093	1/1	0.96	0.32	73,73,73,73	0
60	MG	BA	3127	1/1	0.96	0.63	38,38,38,38	0
60	MG	AA	3229	1/1	0.96	0.34	87,87,87,87	0
60	MG	BA	3214	1/1	0.96	0.21	52,52,52,52	0
60	MG	AA	3052	1/1	0.96	0.56	98,98,98,98	0
60	MG	Bx	101	1/1	0.96	0.42	92,92,92,92	0
60	MG	AA	3096	1/1	0.96	0.64	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1718	1/1	0.96	0.56	78,78,78,78	0
60	MG	BA	3044	1/1	0.96	0.48	52,52,52,52	0
60	MG	AA	3184	1/1	0.96	0.56	69,69,69,69	0
60	MG	Ba	1697	1/1	0.96	0.32	98,98,98,98	1
60	MG	AA	2927	1/1	0.96	0.47	50,50,50,50	0
60	MG	BA	3139	1/1	0.96	0.11	67,67,67,67	0
60	MG	Aa	1691	1/1	0.96	0.55	73,73,73,73	0
60	MG	BA	3227	1/1	0.96	0.23	73,73,73,73	0
60	MG	BD	301	1/1	0.96	0.44	39,39,39,39	0
60	MG	AA	3056	1/1	0.96	0.39	48,48,48,48	0
60	MG	AA	2929	1/1	0.96	0.40	68,68,68,68	0
60	MG	AA	3189	1/1	0.96	0.40	73,73,73,73	0
60	MG	BA	3058	1/1	0.96	0.20	60,60,60,60	0
60	MG	BA	3060	1/1	0.96	0.27	51,51,51,51	0
60	MG	AA	2906	1/1	0.96	0.40	38,38,38,38	0
60	MG	AA	2976	1/1	0.96	0.26	85,85,85,85	0
60	MG	BA	3064	1/1	0.96	0.50	44,44,44,44	0
60	MG	Aa	1621	1/1	0.96	0.17	91,91,91,91	0
60	MG	Aa	1666	1/1	0.96	0.80	66,66,66,66	0
60	MG	Aa	1744	1/1	0.96	0.39	114,114,114,114	0
60	MG	BA	3068	1/1	0.96	0.20	91,91,91,91	0
60	MG	AA	2912	1/1	0.96	0.22	56,56,56,56	0
60	MG	BA	2968	1/1	0.96	0.12	63,63,63,63	0
60	MG	AA	2981	1/1	0.96	0.07	54,54,54,54	0
60	MG	AA	3201	1/1	0.96	0.31	70,70,70,70	0
60	MG	BA	3160	1/1	0.96	0.32	73,73,73,73	0
60	MG	AA	3071	1/1	0.96	0.39	87,87,87,87	0
60	MG	BA	2905	1/1	0.96	0.55	31,31,31,31	0
60	MG	BA	3163	1/1	0.96	0.14	87,87,87,87	0
60	MG	BA	2974	1/1	0.96	0.20	118,118,118,118	0
60	MG	AA	3023	1/1	0.96	0.29	96,96,96,96	0
60	MG	BA	2910	1/1	0.96	0.47	70,70,70,70	0
60	MG	AA	2982	1/1	0.96	0.84	83,83,83,83	0
60	MG	AA	3025	1/1	0.96	0.46	39,39,39,39	0
60	MG	BA	3085	1/1	0.96	0.12	72,72,72,72	0
60	MG	AA	2914	1/1	0.96	0.30	37,37,37,37	0
60	MG	AA	2936	1/1	0.96	0.56	33,33,33,33	0
60	MG	AA	2986	1/1	0.96	0.33	86,86,86,86	0
60	MG	BA	3089	1/1	0.96	0.34	61,61,61,61	0
60	MG	AA	2916	1/1	0.96	0.43	35,35,35,35	0
60	MG	Aa	1685	1/1	0.96	0.08	85,85,85,85	0
60	MG	AA	2991	1/1	0.96	0.29	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	2990	1/1	0.96	0.56	56,56,56,56	0
60	MG	BA	3094	1/1	0.96	0.53	39,39,39,39	0
60	MG	AA	3126	1/1	0.96	0.70	49,49,49,49	0
60	MG	BA	2997	1/1	0.96	0.38	49,49,49,49	0
60	MG	Ba	1724	1/1	0.96	0.79	74,74,74,74	0
60	MG	BA	2999	1/1	0.96	0.49	41,41,41,41	0
60	MG	Aa	1673	1/1	0.96	0.17	91,91,91,91	0
60	MG	Aa	1634	1/1	0.96	0.66	56,56,56,56	0
60	MG	AA	3018	1/1	0.97	0.21	46,46,46,46	0
60	MG	BA	2936	1/1	0.97	0.48	40,40,40,40	0
60	MG	BA	3003	1/1	0.97	0.17	73,73,73,73	0
60	MG	AA	3196	1/1	0.97	0.40	59,59,59,59	0
60	MG	BA	3005	1/1	0.97	0.50	57,57,57,57	0
60	MG	AA	3197	1/1	0.97	0.19	34,34,34,34	0
60	MG	BA	3187	1/1	0.97	0.61	68,68,68,68	0
60	MG	BA	3007	1/1	0.97	0.41	56,56,56,56	0
60	MG	AA	3198	1/1	0.97	0.35	73,73,73,73	0
60	MG	AA	3019	1/1	0.97	0.32	48,48,48,48	0
60	MG	AA	3020	1/1	0.97	0.46	63,63,63,63	0
60	MG	BA	3192	1/1	0.97	0.39	43,43,43,43	0
60	MG	BA	3193	1/1	0.97	0.25	44,44,44,44	0
60	MG	Ba	1608	1/1	0.97	0.28	91,91,91,91	0
60	MG	AA	2913	1/1	0.97	0.47	44,44,44,44	0
60	MG	BA	3196	1/1	0.97	0.55	45,45,45,45	0
60	MG	BA	3014	1/1	0.97	0.30	38,38,38,38	0
60	MG	AA	2953	1/1	0.97	0.21	81,81,81,81	0
60	MG	BA	3105	1/1	0.97	0.22	55,55,55,55	0
60	MG	BA	3106	1/1	0.97	0.55	58,58,58,58	0
60	MG	AA	2966	1/1	0.97	0.63	74,74,74,74	0
60	MG	BA	3203	1/1	0.97	0.56	67,67,67,67	0
60	MG	BA	3108	1/1	0.97	0.15	71,71,71,71	0
60	MG	Ba	1653	1/1	0.97	0.13	91,91,91,91	0
60	MG	Aa	1670	1/1	0.97	0.38	70,70,70,70	0
60	MG	BA	3022	1/1	0.97	0.39	33,33,33,33	0
60	MG	AA	3131	1/1	0.97	0.36	75,75,75,75	0
60	MG	BA	3115	1/1	0.97	0.57	50,50,50,50	0
60	MG	AA	3026	1/1	0.97	0.50	43,43,43,43	0
60	MG	AA	2955	1/1	0.97	0.41	60,60,60,60	0
60	MG	BA	3212	1/1	0.97	0.21	36,36,36,36	0
60	MG	AA	2969	1/1	0.97	0.40	36,36,36,36	0
60	MG	Ba	1659	1/1	0.97	0.50	77,77,77,77	0
60	MG	BA	3120	1/1	0.97	0.46	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3216	1/1	0.97	0.45	89,89,89,89	0
60	MG	AA	3169	1/1	0.97	0.72	78,78,78,78	0
60	MG	BA	3033	1/1	0.97	0.43	42,42,42,42	0
60	MG	AA	3003	1/1	0.97	0.54	43,43,43,43	0
60	MG	AA	2915	1/1	0.97	0.45	50,50,50,50	0
60	MG	AA	2907	1/1	0.97	0.38	58,58,58,58	0
60	MG	AA	3065	1/1	0.97	0.54	82,82,82,82	0
60	MG	BA	3040	1/1	0.97	0.46	41,41,41,41	0
60	MG	BA	3043	1/1	0.97	0.51	49,49,49,49	0
60	MG	AA	2987	1/1	0.97	0.57	41,41,41,41	0
60	MG	BA	2960	1/1	0.97	0.54	45,45,45,45	0
60	MG	AA	3068	1/1	0.97	0.51	50,50,50,50	0
60	MG	AA	3177	1/1	0.97	0.45	54,54,54,54	0
60	MG	AA	2908	1/1	0.97	0.28	53,53,53,53	0
60	MG	Ba	1669	1/1	0.97	0.41	55,55,55,55	0
60	MG	BA	3050	1/1	0.97	0.51	34,34,34,34	0
60	MG	BA	3051	1/1	0.97	0.59	38,38,38,38	0
60	MG	AA	3104	1/1	0.97	0.15	64,64,64,64	0
60	MG	Aa	1740	1/1	0.97	0.52	65,65,65,65	0
60	MG	AA	3011	1/1	0.97	0.52	55,55,55,55	0
60	MG	BA	3057	1/1	0.97	0.40	58,58,58,58	0
60	MG	Aa	1607	1/1	0.97	0.29	95,95,95,95	0
60	MG	AA	3037	1/1	0.97	0.45	52,52,52,52	0
60	MG	Ba	1719	1/1	0.97	0.86	85,85,85,85	0
60	MG	AA	2949	1/1	0.97	0.48	63,63,63,63	0
60	MG	BA	2972	1/1	0.97	0.48	79,79,79,79	0
60	MG	BA	2913	1/1	0.97	0.58	47,47,47,47	0
60	MG	AA	3111	1/1	0.97	0.26	91,91,91,91	0
60	MG	BA	2916	1/1	0.97	0.50	28,28,28,28	0
60	MG	AA	2993	1/1	0.97	0.51	57,57,57,57	0
60	MG	BA	2977	1/1	0.97	0.15	74,74,74,74	0
60	MG	BA	3156	1/1	0.97	0.29	64,64,64,64	0
60	MG	BA	3070	1/1	0.97	0.54	96,96,96,96	0
60	MG	Aa	1608	1/1	0.97	0.20	48,48,48,48	0
60	MG	BA	2920	1/1	0.97	0.19	31,31,31,31	0
60	MG	AA	3044	1/1	0.97	0.42	46,46,46,46	0
60	MG	AA	3045	1/1	0.97	0.23	55,55,55,55	0
60	MG	Ba	1726	1/1	0.97	0.54	65,65,65,65	0
60	MG	BA	3076	1/1	0.97	0.53	91,91,91,91	0
60	MG	BA	3078	1/1	0.97	0.60	61,61,61,61	0
60	MG	Ba	1727	1/1	0.97	0.49	44,44,44,44	0
60	MG	BA	2928	1/1	0.97	0.48	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	3080	1/1	0.97	0.57	120,120,120,120	0
60	MG	BA	2989	1/1	0.97	0.34	49,49,49,49	0
60	MG	AA	3046	1/1	0.97	0.87	59,59,59,59	0
60	MG	BA	3084	1/1	0.97	0.47	64,64,64,64	0
60	MG	BA	3174	1/1	0.97	0.59	63,63,63,63	0
60	MG	BA	2993	1/1	0.97	0.62	40,40,40,40	0
60	MG	BA	2994	1/1	0.97	0.57	44,44,44,44	0
60	MG	BA	2931	1/1	0.97	0.55	52,52,52,52	0
60	MG	AA	3047	1/1	0.97	0.44	62,62,62,62	0
59	ZN	A9	101	1/1	0.97	0.07	143,143,143,143	0
60	MG	Ba	1685	1/1	0.97	0.74	42,42,42,42	1
60	MG	AA	3039	1/1	0.98	0.41	50,50,50,50	0
60	MG	AA	2983	1/1	0.98	0.61	43,43,43,43	0
60	MG	BA	3035	1/1	0.98	0.36	43,43,43,43	0
60	MG	BA	2982	1/1	0.98	0.31	53,53,53,53	0
60	MG	BA	2983	1/1	0.98	0.53	37,37,37,37	0
60	MG	AA	3203	1/1	0.98	0.32	79,79,79,79	0
60	MG	AA	3110	1/1	0.98	0.19	59,59,59,59	0
60	MG	BA	3041	1/1	0.98	0.25	42,42,42,42	0
59	ZN	Bn	101	1/1	0.98	0.14	142,142,142,142	0
60	MG	BA	2987	1/1	0.98	0.22	43,43,43,43	0
60	MG	BA	3218	1/1	0.98	0.35	38,38,38,38	0
60	MG	BA	2907	1/1	0.98	0.44	51,51,51,51	0
60	MG	BA	2908	1/1	0.98	0.48	49,49,49,49	0
60	MG	BA	3159	1/1	0.98	0.18	110,110,110,110	0
60	MG	AA	3042	1/1	0.98	0.18	49,49,49,49	0
60	MG	BA	2991	1/1	0.98	0.33	48,48,48,48	0
60	MG	Ba	1735	1/1	0.98	0.15	79,79,79,79	0
60	MG	Ba	1614	1/1	0.98	0.82	60,60,60,60	0
60	MG	BA	2912	1/1	0.98	0.24	39,39,39,39	0
60	MG	AA	3158	1/1	0.98	0.13	104,104,104,104	1
60	MG	AA	3043	1/1	0.98	0.23	63,63,63,63	0
60	MG	BA	2915	1/1	0.98	0.37	32,32,32,32	0
60	MG	AA	3021	1/1	0.98	0.30	42,42,42,42	0
60	MG	BA	3169	1/1	0.98	0.58	58,58,58,58	0
60	MG	BA	3110	1/1	0.98	0.47	46,46,46,46	0
60	MG	BA	3171	1/1	0.98	0.29	38,38,38,38	0
60	MG	AA	2918	1/1	0.98	0.59	42,42,42,42	0
60	MG	BA	3002	1/1	0.98	0.23	38,38,38,38	0
60	MG	BA	2918	1/1	0.98	0.53	32,32,32,32	0
60	MG	BA	3114	1/1	0.98	0.43	36,36,36,36	0
60	MG	BA	3062	1/1	0.98	0.25	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	3060	1/1	0.98	0.38	55,55,55,55	0
60	MG	AA	3098	1/1	0.98	0.49	47,47,47,47	0
59	ZN	Bd	301	1/1	0.98	0.33	103,103,103,103	0
60	MG	AA	3014	1/1	0.98	0.53	51,51,51,51	0
60	MG	BA	3008	1/1	0.98	0.49	34,34,34,34	0
60	MG	BA	2924	1/1	0.98	0.32	43,43,43,43	0
60	MG	BA	3122	1/1	0.98	0.39	51,51,51,51	0
60	MG	BA	3124	1/1	0.98	0.45	45,45,45,45	0
60	MG	Aa	1737	1/1	0.98	0.32	107,107,107,107	0
60	MG	AA	3216	1/1	0.98	0.30	74,74,74,74	0
60	MG	BA	2927	1/1	0.98	0.64	45,45,45,45	0
60	MG	BA	3128	1/1	0.98	0.34	40,40,40,40	0
60	MG	AA	3064	1/1	0.98	0.32	59,59,59,59	0
60	MG	AA	3123	1/1	0.98	0.48	54,54,54,54	0
60	MG	Aa	1628	1/1	0.98	0.32	72,72,72,72	0
60	MG	AA	3125	1/1	0.98	0.44	49,49,49,49	0
60	MG	AA	3195	1/1	0.98	0.33	41,41,41,41	0
60	MG	BA	3077	1/1	0.98	0.36	69,69,69,69	0
60	MG	Ba	1630	1/1	0.98	0.11	53,53,53,53	0
60	MG	BA	3020	1/1	0.98	0.37	47,47,47,47	0
60	MG	BA	3137	1/1	0.98	0.13	94,94,94,94	0
60	MG	BA	3198	1/1	0.98	0.21	70,70,70,70	0
60	MG	AA	3066	1/1	0.98	0.24	55,55,55,55	0
60	MG	AA	3127	1/1	0.98	0.66	44,44,44,44	0
60	MG	BA	3025	1/1	0.98	0.33	69,69,69,69	0
60	MG	Ba	1603	1/1	0.98	0.17	73,73,73,73	1
60	MG	BA	3027	1/1	0.98	0.32	53,53,53,53	0
60	MG	AA	2922	1/1	0.98	0.26	52,52,52,52	0
60	MG	AA	3051	1/1	0.98	0.36	66,66,66,66	0
60	MG	AA	2990	1/1	0.98	0.43	51,51,51,51	0
60	MG	Ba	1607	1/1	0.98	0.12	67,67,67,67	0
60	MG	AA	3070	1/1	0.99	0.33	47,47,47,47	0
60	MG	AA	3006	1/1	0.99	0.28	39,39,39,39	0
60	MG	AA	3000	1/1	0.99	0.17	49,49,49,49	0
60	MG	AA	3174	1/1	0.99	0.42	50,50,50,50	0
60	MG	BA	3059	1/1	0.99	0.51	52,52,52,52	0
60	MG	BA	3030	1/1	0.99	0.27	37,37,37,37	0
60	MG	AA	3008	1/1	0.99	0.33	44,44,44,44	0
60	MG	Aa	1631	1/1	0.99	0.17	52,52,52,52	0
60	MG	BA	3123	1/1	0.99	0.56	37,37,37,37	0
60	MG	AA	3094	1/1	0.99	0.42	65,65,65,65	0
60	MG	AA	3117	1/1	0.99	0.32	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	3218	1/1	0.99	0.34	104,104,104,104	0
60	MG	Aa	1625	1/1	0.99	0.38	61,61,61,61	0
59	ZN	Ad	301	1/1	0.99	0.34	94,94,94,94	0
60	MG	BA	2992	1/1	0.99	0.47	40,40,40,40	0
60	MG	BA	3039	1/1	0.99	0.31	44,44,44,44	0
60	MG	BA	2954	1/1	0.99	0.33	37,37,37,37	0
60	MG	Ba	1701	1/1	0.99	0.32	71,71,71,71	0
60	MG	BA	3042	1/1	0.99	0.60	48,48,48,48	0
59	ZN	B9	101	1/1	0.99	0.06	124,124,124,124	0
60	MG	BA	3017	1/1	0.99	0.38	40,40,40,40	0
60	MG	BA	2996	1/1	0.99	0.24	35,35,35,35	0
60	MG	AA	2904	1/1	0.99	0.14	142,142,142,142	0
60	MG	BA	2904	1/1	0.99	0.12	138,138,138,138	0
60	MG	BA	3021	1/1	0.99	0.68	45,45,45,45	0
60	MG	BA	2922	1/1	0.99	0.20	45,45,45,45	0
60	MG	AA	3088	1/1	0.99	0.31	64,64,64,64	0
60	MG	BA	3024	1/1	0.99	0.28	46,46,46,46	0
60	MG	BA	3052	1/1	0.99	0.52	30,30,30,30	0
60	MG	BA	2906	1/1	0.99	0.41	35,35,35,35	0
60	MG	BA	3054	1/1	0.99	0.52	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.