wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:51 AM EDT

PDB ID	:	4V88 / pdb_00004v88
Title	:	The structure of the eukaryotic ribosome at 3.0 A resolution.
Authors	:	Ben-Shem, A.; Garreau de Loubresse, N.; Melnikov, S.; Jenner, L.; Yusupova, G.; Yusupov, M.
Deposited on	:	2011-10-11
Resolution	:	3.00 Å(reported)

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

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

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

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

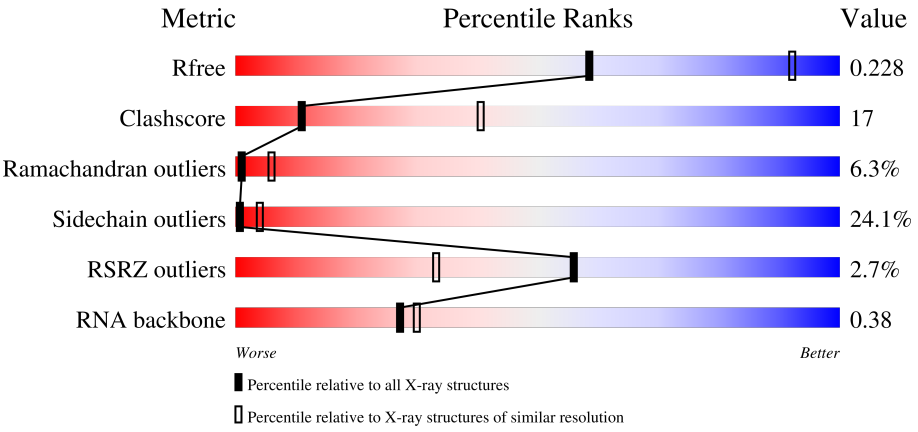
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.00 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.



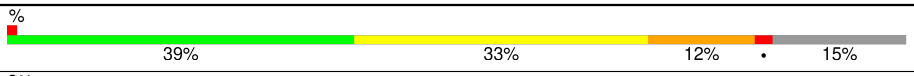
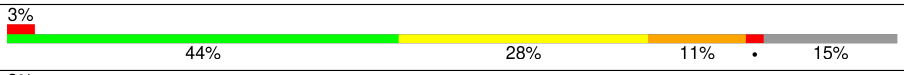
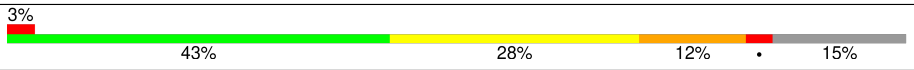
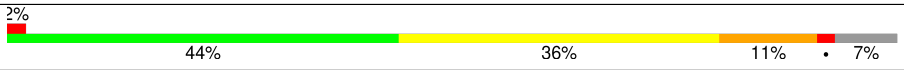
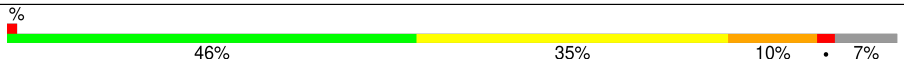
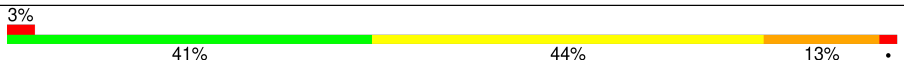
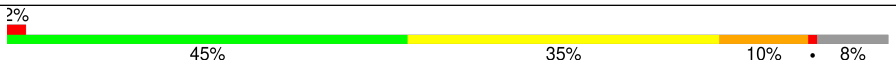
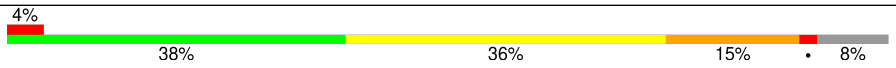
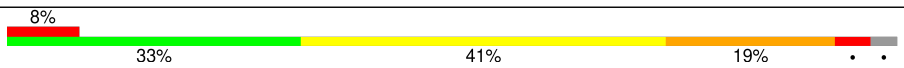
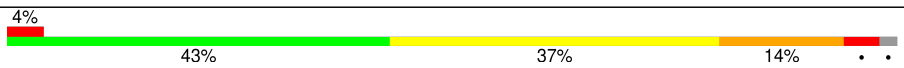
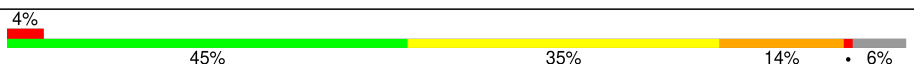
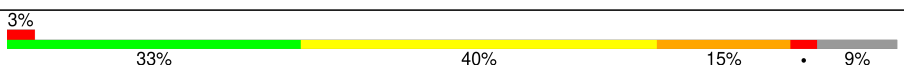
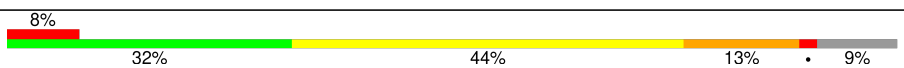
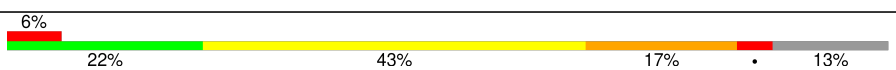
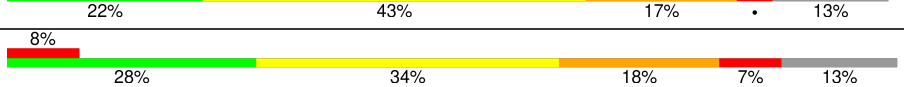
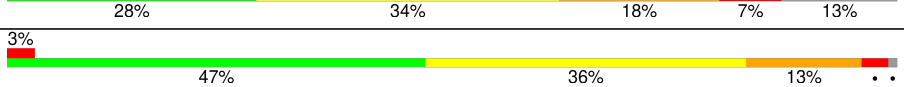
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A2	1800	2% 38% 40% 21%
2	AA	252	7% 27% 33% 19% 18%
2	CA	252	5% 30% 33% 16% 18%
3	AB	255	10% 25% 35% 17% 6% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	CB	255	
4	AC	254	
4	CC	254	
5	AD	240	
5	CD	240	
6	AE	261	
6	CE	261	
7	AF	225	
7	CF	225	
8	AG	236	
8	CG	236	
9	AH	190	
9	CH	190	
10	AI	200	
10	CI	200	
11	AJ	197	
11	CJ	197	
12	AK	105	
12	CK	105	
13	AL	156	
13	CL	156	
14	AM	143	
14	CM	143	
15	AN	151	
15	CN	151	

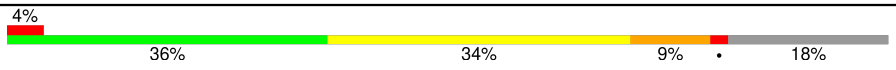
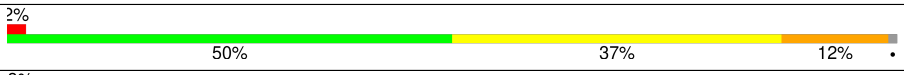
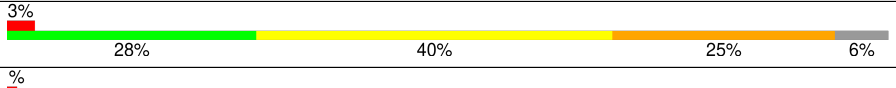
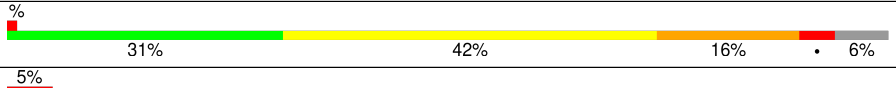
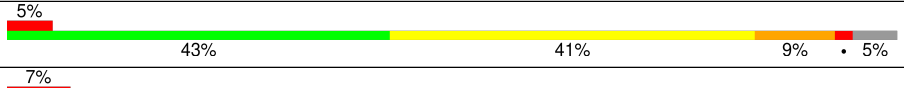
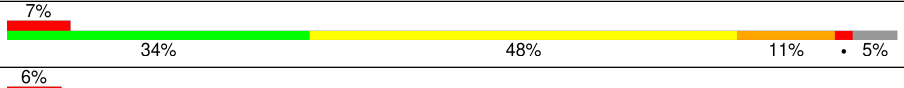
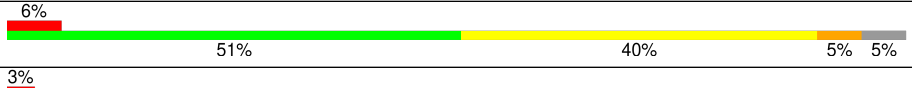
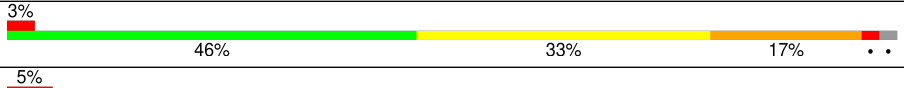
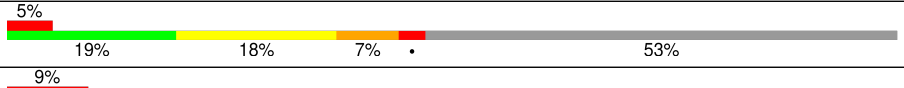
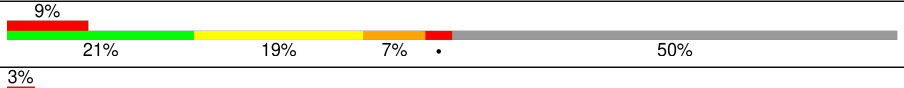
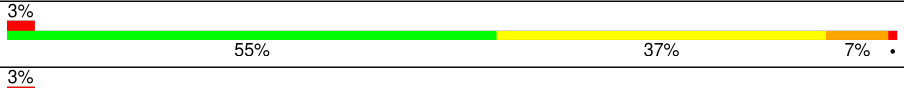
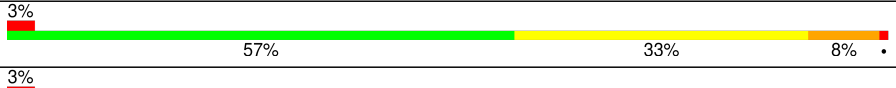
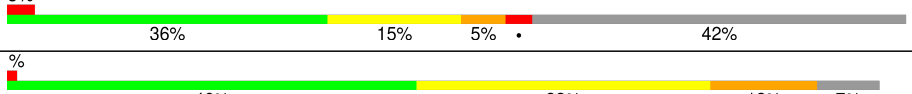
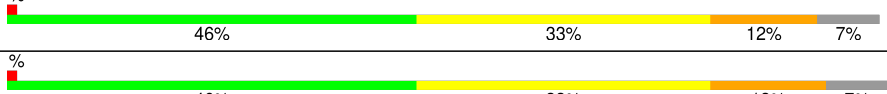
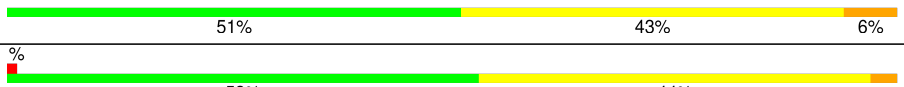
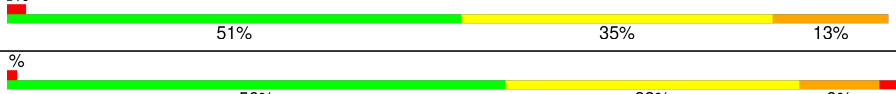
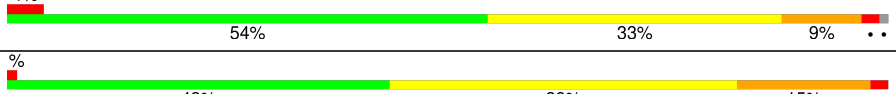
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AO	137	15% 43% 34% 11% • 7%
16	CO	137	% 47% 28% 16% • 7%
17	AP	142	5% 37% 39% 7% • 13%
17	CP	142	11% 38% 41% 14% • 5%
18	AQ	143	9% 37% 41% 18% • •
18	CQ	143	10% 51% 34% 13% • •
19	AR	136	7% 41% 35% 8% • 12%
19	CR	136	8% 36% 36% 12% • 14%
20	AS	146	3% 33% 48% 14% • •
20	CS	146	4% 44% 37% 16% • •
21	AT	144	6% 40% 41% 17% ••
21	CT	144	56% 28% 15% ••
22	AU	121	13% 36% 34% 18% • 12%
22	CU	121	3% 27% 32% 26% 5% 9%
23	AV	87	3% 40% 37% 21% •
23	CV	87	44% 44% 11% •
24	AW	130	2% 45% 35% 17% ••
24	CW	130	% 59% 33% 5% ••
25	AX	145	5% 47% 37% 12% • •
25	CX	145	% 61% 28% 8% ••
26	AY	135	8% 53% 27% 16% ••
26	CY	135	4% 44% 34% 19% ••
27	AZ	108	5% 18% 26% 17% 5% 35%
27	CZ	108	5% 29% 21% 11% • 36%
28	Aa	119	10% 29% 33% 13% 6% 18%

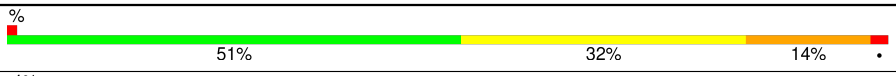
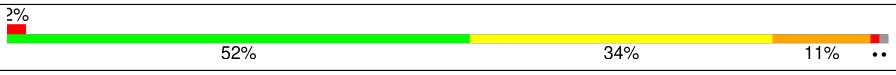
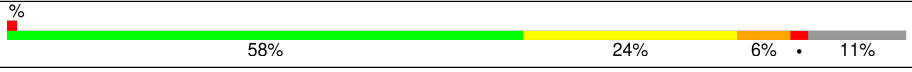
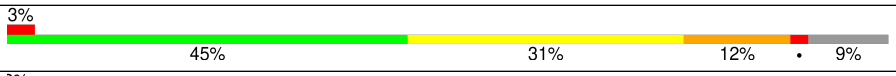
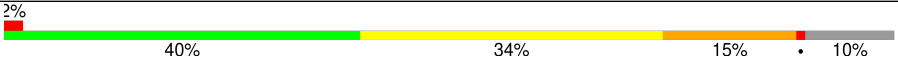
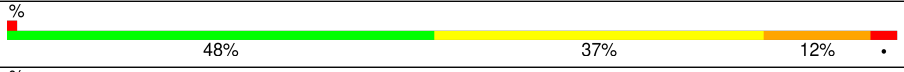
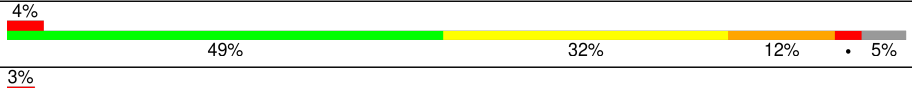
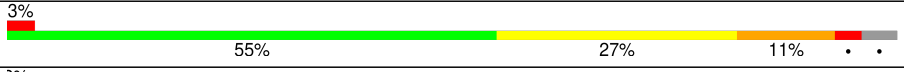
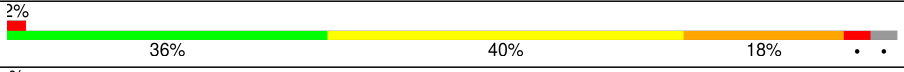
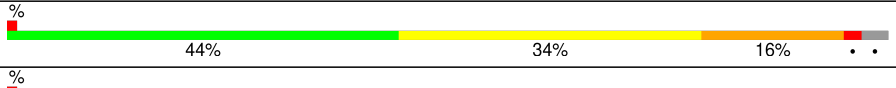
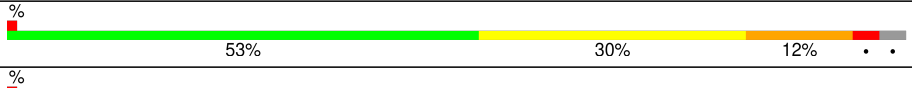
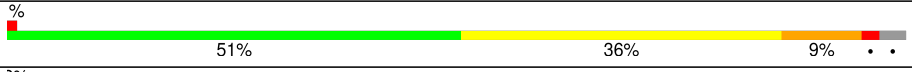
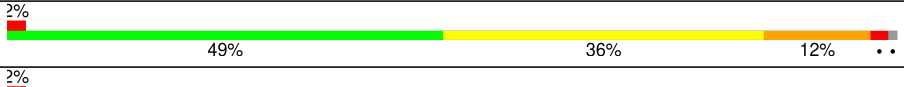
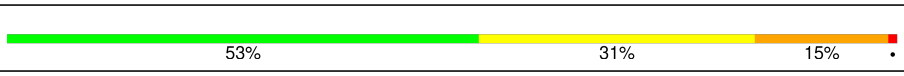
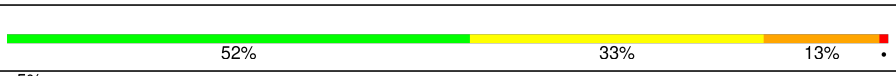
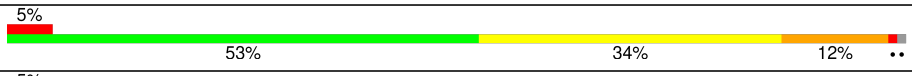
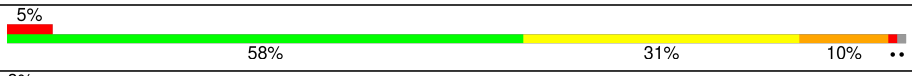
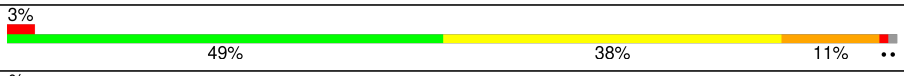
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	Ca	119	
29	Ab	82	
29	Cb	82	
30	Ac	67	
30	Cc	67	
31	Ad	56	
31	Cd	56	
32	Ae	63	
32	Ce	63	
33	Af	152	
33	Cf	152	
34	Ag	319	
34	Cg	319	
35	Ah	273	
36	A1	3396	
36	A5	3396	
37	A3	121	
37	A7	121	
38	A4	158	
38	A8	158	
39	BA	254	
39	DA	254	
40	BB	387	
40	DB	387	
41	BC	362	

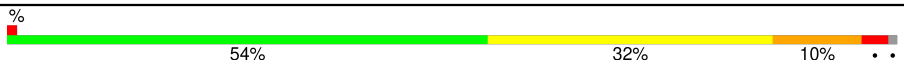
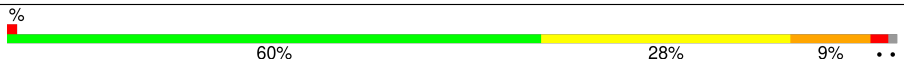
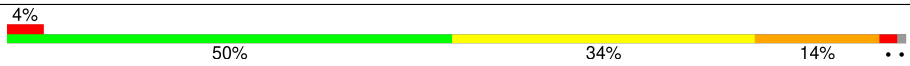
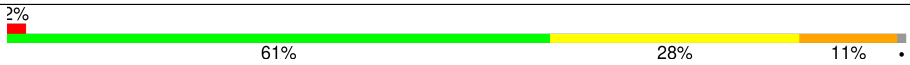
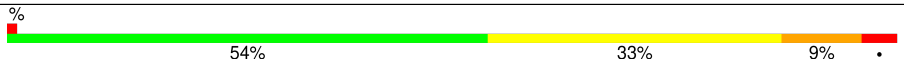
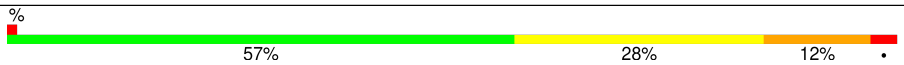
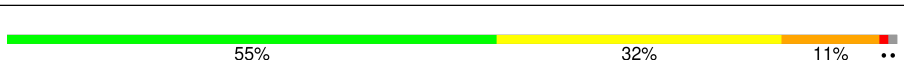
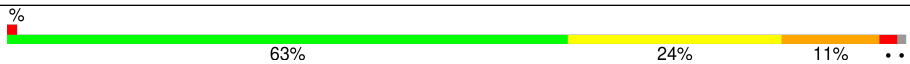
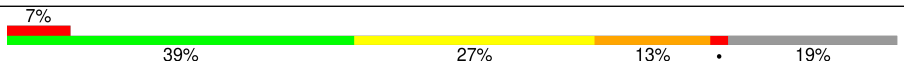
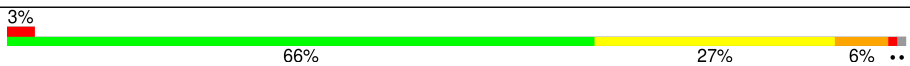
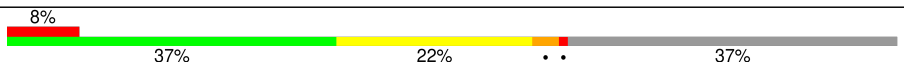
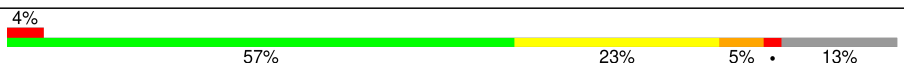
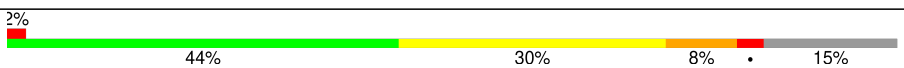
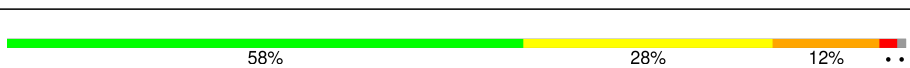
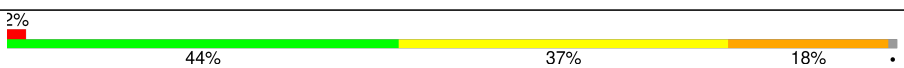
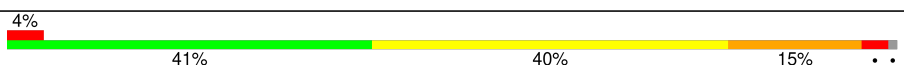
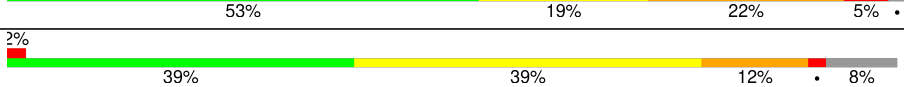
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	DC	362	
42	BD	297	
42	DD	297	
43	BE	176	
43	DE	176	
44	BF	244	
44	DF	244	
45	BG	256	
45	DG	256	
46	BH	191	
46	DH	191	
47	BI	221	
47	DI	221	
48	BJ	174	
48	DJ	174	
49	BL	199	
49	DL	199	
50	BM	138	
50	DM	138	
51	BN	204	
51	DN	204	
52	BO	219	
52	DO	219	
53	BP	184	
53	DP	184	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	BQ	186	
54	DQ	186	
55	BR	189	
55	DR	189	
56	BS	172	
56	DS	172	
57	BT	160	
57	DT	160	
58	BU	121	
58	DU	121	
59	BV	137	
59	DV	137	
60	BW	155	
60	DW	155	
61	BX	142	
61	DX	142	
62	BY	127	
62	DY	127	
63	BZ	136	
63	DZ	136	
64	Ba	149	
64	Da	149	
65	Bb	59	
65	Db	59	
66	Bc	105	

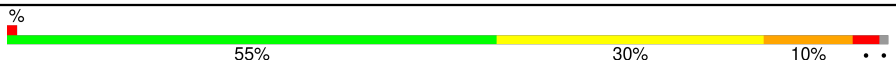
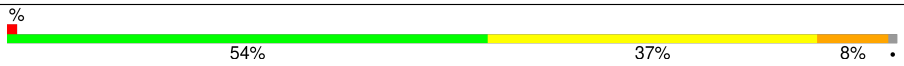
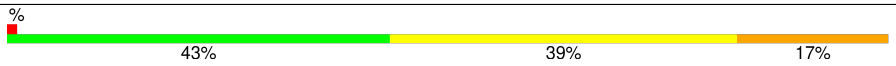
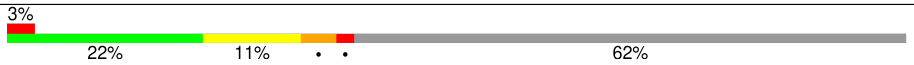
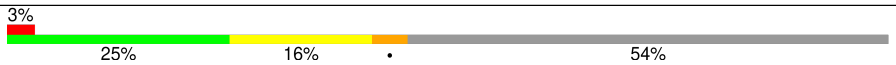
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
66	Dc	105	3% 47% 37% 10% 5%
67	Bd	113	4% 53% 32% 12%
67	Dd	113	54% 29% 12%
68	Be	130	2% 52% 36% 7%
68	De	130	5% 53% 31% 10%
69	Bf	107	% 65% 23% 8%
69	Df	107	57% 34% 7%
70	Bg	121	2% 45% 37% 10% 7%
70	Dg	121	3% 50% 31% 12% 7%
71	Bh	120	2% 52% 29% 16%
71	Dh	120	2% 49% 32% 16%
72	Bi	100	2% 48% 31% 15% 5%
72	Di	100	4% 48% 34% 17%
73	Bj	88	2% 53% 33% 9%
73	Dj	88	2% 45% 44% 9%
74	Bk	78	4% 44% 41% 14%
74	Dk	78	10% 53% 28% 18%
75	Bl	51	2% 37% 45% 16%
75	Dl	51	6% 43% 39% 16%
76	Bm	128	2% 24% 11% 59%
76	Dm	128	2% 23% 12% 5% 59%
77	Bn	25	40% 36% 24%
77	Dn	25	4% 36% 28% 28% 8%
78	Bo	106	48% 35% 13%
78	Do	106	% 61% 27% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Bp	92	
79	Dp	92	
80	A6	1800	
81	Ch	273	
82	DK	155	
83	Dq	312	
84	Dr	47	
85	Ds	46	

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
86	OHX	A1	3414	-	-	X	-
86	OHX	A1	3432	-	-	X	-
86	OHX	A1	3439	-	-	X	-
86	OHX	A1	3452	-	-	X	-
86	OHX	A1	3457	-	-	X	-
86	OHX	A1	3458	-	-	X	-
86	OHX	A1	3463	-	-	X	-
86	OHX	A1	3466	-	-	X	-
86	OHX	A1	3467	-	-	X	-
86	OHX	A1	3471	-	-	X	-
86	OHX	A1	3478	-	-	X	-
86	OHX	A1	3479	-	-	X	-
86	OHX	A1	3481	-	-	X	-
86	OHX	A1	3483	-	-	X	-
86	OHX	A1	3491	-	-	X	-
86	OHX	A1	3496	-	-	X	-
86	OHX	A1	3497	-	-	X	-
86	OHX	A1	3503	-	-	X	-
86	OHX	A1	3506	-	-	X	-
86	OHX	A1	3509	-	-	X	-
86	OHX	A1	3512	-	-	X	-
86	OHX	A1	3516	-	-	X	-
86	OHX	A1	3520	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	A1	3542	-	-	X	-
86	OHX	A1	3549	-	-	X	-
86	OHX	A1	3562	-	-	X	-
86	OHX	A1	3565	-	-	X	-
86	OHX	A1	3574	-	-	X	-
86	OHX	A1	3578	-	-	X	-
86	OHX	A1	3584	-	-	X	-
86	OHX	A1	3591	-	-	X	-
86	OHX	A1	3598	-	-	X	-
86	OHX	A1	3601	-	-	X	-
86	OHX	A1	3602	-	-	X	-
86	OHX	A1	3603	-	-	X	-
86	OHX	A1	3604	-	-	X	-
86	OHX	A1	3607	-	-	X	-
86	OHX	A1	3650	-	-	X	-
86	OHX	A1	3659	-	-	X	-
86	OHX	A1	3667	-	-	X	-
86	OHX	A1	3671	-	-	X	-
86	OHX	A1	3680	-	-	X	-
86	OHX	A1	3687	-	-	X	-
86	OHX	A1	3693	-	-	X	-
86	OHX	A1	3698	-	-	X	-
86	OHX	A1	3706	-	-	X	-
86	OHX	A1	3712	-	-	X	-
86	OHX	A1	3717	-	-	X	-
86	OHX	A1	3718	-	-	X	-
86	OHX	A1	3722	-	-	X	-
86	OHX	A1	3725	-	-	X	-
86	OHX	A1	3735	-	-	X	-
86	OHX	A1	3738	-	-	X	-
86	OHX	A1	3742	-	-	X	-
86	OHX	A1	3744	-	-	X	-
86	OHX	A1	3746	-	-	X	-
86	OHX	A1	3748	-	-	X	-
86	OHX	A1	3750	-	-	X	-
86	OHX	A1	3751	-	-	X	-
86	OHX	A1	3757	-	-	X	-
86	OHX	A1	3762	-	-	X	-
86	OHX	A1	3777	-	-	X	-
86	OHX	A1	3785	-	-	X	-
86	OHX	A1	3788	-	-	X	-
86	OHX	A1	3789	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	A1	3792	-	-	X	-
86	OHX	A1	3795	-	-	X	-
86	OHX	A1	3798	-	-	X	-
86	OHX	A1	3800	-	-	X	-
86	OHX	A1	3802	-	-	X	-
86	OHX	A1	3805	-	-	X	-
86	OHX	A1	3806	-	-	X	-
86	OHX	A1	3811	-	-	X	-
86	OHX	A1	3812	-	-	X	-
86	OHX	A1	3816	-	-	X	-
86	OHX	A2	1907	-	-	X	-
86	OHX	A2	1914	-	-	X	-
86	OHX	A2	1915	-	-	X	-
86	OHX	A2	1918	-	-	X	-
86	OHX	A2	1921	-	-	X	-
86	OHX	A2	1922	-	-	X	-
86	OHX	A2	1940	-	-	X	-
86	OHX	A2	1954	-	-	X	-
86	OHX	A2	1962	-	-	X	-
86	OHX	A2	1964	-	-	X	-
86	OHX	A2	1965	-	-	X	-
86	OHX	A2	1969	-	-	X	-
86	OHX	A2	1970	-	-	X	-
86	OHX	A2	1975	-	-	X	-
86	OHX	A2	1978	-	-	X	-
86	OHX	A2	1983	-	-	X	-
86	OHX	A2	1989	-	-	X	-
86	OHX	A2	2014	-	-	X	-
86	OHX	A2	2017	-	-	X	-
86	OHX	A2	2029	-	-	X	-
86	OHX	A2	2048	-	-	X	-
86	OHX	A2	2052	-	-	X	-
86	OHX	A2	2067	-	-	X	-
86	OHX	A2	2071	-	-	X	-
86	OHX	A2	2074	-	-	X	-
86	OHX	A2	2076	-	-	X	-
86	OHX	A2	2082	-	-	X	-
86	OHX	A2	2086	-	-	X	-
86	OHX	A5	3457	-	-	X	-
86	OHX	A5	3458	-	-	X	-
86	OHX	A5	3461	-	-	X	-
86	OHX	A5	3464	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	A5	3465	-	-	X	-
86	OHX	A5	3470	-	-	X	-
86	OHX	A5	3473	-	-	X	-
86	OHX	A5	3474	-	-	X	-
86	OHX	A5	3477	-	-	X	-
86	OHX	A5	3480	-	-	X	-
86	OHX	A5	3487	-	-	X	-
86	OHX	A5	3489	-	-	X	-
86	OHX	A5	3491	-	-	X	-
86	OHX	A5	3492	-	-	X	-
86	OHX	A5	3509	-	-	X	-
86	OHX	A5	3513	-	-	X	-
86	OHX	A5	3514	-	-	X	-
86	OHX	A5	3515	-	-	X	-
86	OHX	A5	3516	-	-	X	-
86	OHX	A5	3517	-	-	X	-
86	OHX	A5	3518	-	-	X	-
86	OHX	A5	3521	-	-	X	-
86	OHX	A5	3526	-	-	X	-
86	OHX	A5	3532	-	-	X	-
86	OHX	A5	3533	-	-	X	-
86	OHX	A5	3538	-	-	X	-
86	OHX	A5	3542	-	-	X	-
86	OHX	A5	3548	-	-	X	-
86	OHX	A5	3550	-	-	X	-
86	OHX	A5	3569	-	-	X	-
86	OHX	A5	3577	-	-	X	-
86	OHX	A5	3580	-	-	X	-
86	OHX	A5	3581	-	-	X	-
86	OHX	A5	3591	-	-	X	-
86	OHX	A5	3595	-	-	X	-
86	OHX	A5	3598	-	-	X	-
86	OHX	A5	3603	-	-	X	-
86	OHX	A5	3606	-	-	X	-
86	OHX	A5	3607	-	-	X	-
86	OHX	A5	3610	-	-	X	-
86	OHX	A5	3617	-	-	X	-
86	OHX	A5	3640	-	-	X	-
86	OHX	A5	3644	-	-	X	-
86	OHX	A5	3660	-	-	X	-
86	OHX	A5	3662	-	-	X	-
86	OHX	A5	3666	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	A5	3667	-	-	X	-
86	OHX	A5	3680	-	-	X	-
86	OHX	A5	3681	-	-	X	-
86	OHX	A5	3695	-	-	X	-
86	OHX	A5	3699	-	-	X	-
86	OHX	A5	3720	-	-	X	-
86	OHX	A5	3722	-	-	X	-
86	OHX	A5	3723	-	-	X	-
86	OHX	A5	3729	-	-	X	-
86	OHX	A5	3732	-	-	X	-
86	OHX	A5	3734	-	-	X	-
86	OHX	A5	3737	-	-	X	-
86	OHX	A5	3738	-	-	X	-
86	OHX	A5	3739	-	-	X	-
86	OHX	A5	3740	-	-	X	-
86	OHX	A5	3741	-	-	X	-
86	OHX	A5	3743	-	-	X	-
86	OHX	A5	3762	-	-	X	-
86	OHX	A5	3763	-	-	X	-
86	OHX	A5	3772	-	-	X	-
86	OHX	A5	3779	-	-	X	-
86	OHX	A5	3792	-	-	-	X
86	OHX	A5	3795	-	-	X	-
86	OHX	A5	3801	-	-	X	-
86	OHX	A5	3803	-	-	X	-
86	OHX	A5	3807	-	-	X	-
86	OHX	A5	3808	-	-	X	-
86	OHX	A5	3809	-	-	X	-
86	OHX	A5	3810	-	-	X	-
86	OHX	A5	3811	-	-	X	-
86	OHX	A5	3812	-	-	X	-
86	OHX	A5	3813	-	-	X	-
86	OHX	A5	3814	-	-	X	-
86	OHX	A5	3815	-	-	X	-
86	OHX	A5	3820	-	-	X	-
86	OHX	A5	3821	-	-	X	-
86	OHX	A6	1909	-	-	X	-
86	OHX	A6	1915	-	-	X	-
86	OHX	A6	1922	-	-	X	-
86	OHX	A6	1923	-	-	X	-
86	OHX	A6	1933	-	-	X	-
86	OHX	A6	1940	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	A6	1941	-	-	X	-
86	OHX	A6	1956	-	-	X	-
86	OHX	A6	1961	-	-	X	-
86	OHX	A6	1983	-	-	X	-
86	OHX	A6	2002	-	-	X	-
86	OHX	A6	2005	-	-	X	-
86	OHX	A6	2009	-	-	X	-
86	OHX	A6	2016	-	-	X	-
86	OHX	A6	2058	-	-	X	-
86	OHX	A6	2062	-	-	X	-
86	OHX	A6	2068	-	-	X	-
86	OHX	A6	2071	-	-	X	-
86	OHX	A6	2086	-	-	X	-
86	OHX	A6	2090	-	-	X	-
86	OHX	A6	2092	-	-	X	-
86	OHX	A6	2099	-	-	X	-
86	OHX	A6	2100	-	-	X	-
86	OHX	A7	203	-	-	X	-
86	OHX	A7	209	-	-	X	-
86	OHX	A7	211	-	-	X	-
86	OHX	A8	203	-	-	X	-
86	OHX	A8	211	-	-	X	-
86	OHX	A8	218	-	-	X	-
86	OHX	AC	301	-	-	X	-
86	OHX	AP	201	-	-	X	-
86	OHX	Ad	101	-	-	X	-
86	OHX	BA	301	-	-	X	-
86	OHX	BI	303	-	-	X	-
86	OHX	BI	304	-	-	X	-
86	OHX	Bj	101	-	-	X	-
86	OHX	CG	301	-	-	X	-
86	OHX	CG	302	-	-	X	-
86	OHX	CL	201	-	-	X	-
86	OHX	CP	202	-	-	X	-
86	OHX	Cd	101	-	-	X	-
86	OHX	DA	302	-	-	X	-
86	OHX	DG	301	-	-	X	-
87	MG	A1	3829	-	-	-	X
87	MG	A1	3848	-	-	-	X
87	MG	A1	3859	-	-	-	X
87	MG	A1	3879	-	-	-	X
87	MG	A1	3888	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A1	3909	-	-	-	X
87	MG	A1	3919	-	-	-	X
87	MG	A1	3922	-	-	-	X
87	MG	A1	3965	-	-	-	X
87	MG	A1	3977	-	-	-	X
87	MG	A1	4105	-	-	-	X
87	MG	A1	4159	-	-	-	X
87	MG	A1	4190	-	-	-	X
87	MG	A1	4194	-	-	-	X
87	MG	A1	4220	-	-	-	X
87	MG	A1	4255	-	-	-	X
87	MG	A1	4273	-	-	-	X
87	MG	A1	4284	-	-	-	X
87	MG	A1	4465	-	-	-	X
87	MG	A1	4482	-	-	-	X
87	MG	A2	2094	-	-	-	X
87	MG	A2	2097	-	-	-	X
87	MG	A2	2098	-	-	-	X
87	MG	A2	2103	-	-	-	X
87	MG	A2	2121	-	-	-	X
87	MG	A2	2123	-	-	-	X
87	MG	A2	2126	-	-	-	X
87	MG	A2	2128	-	-	-	X
87	MG	A2	2150	-	-	-	X
87	MG	A2	2158	-	-	-	X
87	MG	A2	2159	-	-	-	X
87	MG	A2	2162	-	-	-	X
87	MG	A2	2167	-	-	-	X
87	MG	A2	2191	-	-	-	X
87	MG	A2	2209	-	-	-	X
87	MG	A2	2213	-	-	-	X
87	MG	A2	2242	-	-	-	X
87	MG	A3	220	-	-	-	X
87	MG	A4	226	-	-	-	X
87	MG	A5	3889	-	-	-	X
87	MG	A5	3897	-	-	-	X
87	MG	A5	3921	-	-	-	X
87	MG	A5	3928	-	-	-	X
87	MG	A5	3929	-	-	-	X
87	MG	A5	3979	-	-	-	X
87	MG	A5	3989	-	-	-	X
87	MG	A5	4042	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	MG	A5	4054	-	-	-	X
87	MG	A5	4056	-	-	-	X
87	MG	A5	4175	-	-	-	X
87	MG	A5	4194	-	-	-	X
87	MG	A5	4207	-	-	-	X
87	MG	A5	4249	-	-	-	X
87	MG	A5	4254	-	-	-	X
87	MG	A5	4336	-	-	-	X
87	MG	A5	4341	-	-	-	X
87	MG	A5	4371	-	-	-	X
87	MG	A5	4372	-	-	-	X
87	MG	A5	4412	-	-	-	X
87	MG	A5	4492	-	-	-	X
87	MG	A5	4499	-	-	-	X
87	MG	A5	4530	-	-	-	X
87	MG	A6	2116	-	-	-	X
87	MG	A6	2128	-	-	-	X
87	MG	A6	2141	-	-	-	X
87	MG	A6	2156	-	-	-	X
87	MG	A6	2157	-	-	-	X
87	MG	A6	2168	-	-	-	X
87	MG	A6	2228	-	-	-	X
87	MG	A6	2273	-	-	-	X
87	MG	A8	229	-	-	-	X
87	MG	BP	211	-	-	-	X
87	MG	DB	404	-	-	-	X
87	MG	DB	413	-	-	-	X
87	MG	DC	406	-	-	-	X
88	ZN	Bo	205	-	-	X	-

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 416785 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 RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A2	1781	37835	16910	6661	12482	1782	0	1	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AA	206	1577	1014	278	283	2	0	0	0
			Total	C	N	O	S			
2	CA	206	1583	1017	281	283	2	0	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AB	214	1709	1084	310	311	4	0	0	0
			Total	C	N	O	S			
3	CB	216	1722	1091	312	315	4	0	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AC	217	1635	1047	289	297	2	0	0	0
			Total	C	N	O	S			
4	CC	217	1635	1047	289	297	2	0	0	0

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AD	223	1734	1101	313	314	6	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CD	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AE	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	CE	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AF	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	CF	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AG	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	CG	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AH	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	CH	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AI	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
10	CI	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AJ	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	CJ	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AK	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
12	CK	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AL	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	CL	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AM	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	CM	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AN	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	CN	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AO	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	CO	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AP	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	CP	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AQ	141	Total	C	N	O	0	0	0
			1105	708	203	194			
18	CQ	142	Total	C	N	O	0	0	0
			1111	711	204	196			

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AR	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	CR	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AS	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	CS	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AT	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	CT	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AU	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	CU	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	CV	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	CW	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	CX	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AY	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	CY	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	AZ	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	CZ	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Aa	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	Ca	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Ab	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	Cb	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Ac	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	Cc	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Ad	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	Cd	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Ae	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	Ce	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 33 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Af	71	Total	C	N	O	S	0	0	0
			516	328	93	91	4			
33	Cf	76	Total	C	N	O	S	0	0	0
			544	346	98	96	4			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Af	82	UNK	LYS	SEE REMARK 999	UNP P05759
Af	83	UNK	LYS	SEE REMARK 999	UNP P05759
Af	84	UNK	VAL	SEE REMARK 999	UNP P05759
Af	85	UNK	TYR	SEE REMARK 999	UNP P05759
Af	86	UNK	THR	SEE REMARK 999	UNP P05759
Af	87	UNK	THR	SEE REMARK 999	UNP P05759
Af	88	UNK	PRO	SEE REMARK 999	UNP P05759
Af	89	UNK	LYS	SEE REMARK 999	UNP P05759
Af	90	UNK	LYS	SEE REMARK 999	UNP P05759
Af	91	UNK	ILE	SEE REMARK 999	UNP P05759
Af	92	UNK	LYS	SEE REMARK 999	UNP P05759
Af	93	UNK	HIS	SEE REMARK 999	UNP P05759
Af	94	UNK	LYS	SEE REMARK 999	UNP P05759
Af	95	UNK	HIS	SEE REMARK 999	UNP P05759
Af	96	UNK	LYS	SEE REMARK 999	UNP P05759
Af	97	UNK	LYS	SEE REMARK 999	UNP P05759
Af	98	UNK	VAL	SEE REMARK 999	UNP P05759
Af	99	UNK	LYS	SEE REMARK 999	UNP P05759
Af	100	UNK	LEU	SEE REMARK 999	UNP P05759
Af	101	UNK	ALA	SEE REMARK 999	UNP P05759
Cf	77	UNK	GLY	SEE REMARK 999	UNP P05759
Cf	78	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	79	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	80	UNK	ARG	SEE REMARK 999	UNP P05759
Cf	81	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	82	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	83	UNK	LYS	SEE REMARK 999	UNP P05759

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Cf	84	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	85	UNK	TYR	SEE REMARK 999	UNP P05759
Cf	86	UNK	THR	SEE REMARK 999	UNP P05759
Cf	87	UNK	THR	SEE REMARK 999	UNP P05759
Cf	88	UNK	PRO	SEE REMARK 999	UNP P05759
Cf	89	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	90	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	91	UNK	ILE	SEE REMARK 999	UNP P05759
Cf	92	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	93	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	94	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	95	UNK	HIS	SEE REMARK 999	UNP P05759
Cf	96	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	97	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	98	UNK	VAL	SEE REMARK 999	UNP P05759
Cf	99	UNK	LYS	SEE REMARK 999	UNP P05759
Cf	100	UNK	LEU	SEE REMARK 999	UNP P05759
Cf	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	Ag	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	Cg	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	Ah	159	Total	C	N	O	0	0	0
			1105	653	221	231			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	9	UNK	GLY	SEE REMARK 999	UNP P39015
Ah	10	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	11	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	12	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	13	UNK	GLU	SEE REMARK 999	UNP P39015

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	14	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	15	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	16	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	17	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	18	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	19	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	20	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	151	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	152	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	153	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	154	UNK	TYR	SEE REMARK 999	UNP P39015
Ah	155	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ah	163	UNK	PHE	SEE REMARK 999	UNP P39015
Ah	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ah	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ah	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ah	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ah	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ah	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ah	174	UNK	LEU	SEE REMARK 999	UNP P39015
Ah	175	UNK	ASP	SEE REMARK 999	UNP P39015
Ah	176	UNK	ALA	SEE REMARK 999	UNP P39015

- Molecule 36 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	A1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	A5	3150	Total	C	N	O	P	0	0	0
			67376	30095	12145	21987	3149			

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	A3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	A7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	A4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	A8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BA	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	DA	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BB	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	DB	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BC	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	DC	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BD	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DD	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BE	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	DE	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BF	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	DF	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BG	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	DG	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BH	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	DH	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BI	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
47	DI	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	DJ	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BL	193	Total	C	N	O	0	0	0
			1543	962	315	266			
49	DL	194	Total	C	N	O	0	0	0
			1548	965	316	267			

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BM	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	DM	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BN	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	DN	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A, 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			
52	DO	197	Total	C	N	O	S	0	197	0
			3119	2008	581	528	2			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	BP	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	DP	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BQ	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	DQ	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BR	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	DR	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BS	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	DS	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BT	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	DT	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BU	100	Total	C	N	O	0	0	0
			796	516	131	149			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	DU	98	Total 778	C 505	N 127	O 146	0	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BV	136	Total 1003	C 628	N 189	O 179	S 7	0	0	0
59	DV	136	Total 1003	C 628	N 189	O 179	S 7	0	0	0

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BW	98	Total 699	C 443	N 137	O 118	S 1	0	0	0
60	DW	135	Total 1038	C 651	N 206	O 180	S 1	0	0	0

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	BX	121	Total 964	C 620	N 169	O 173	S 2	0	0	0
61	DX	120	Total 959	C 617	N 168	O 172	S 2	0	0	0

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	BY	126	Total 993	C 625	N 192	O 176	0	0	0
62	DY	126	Total 993	C 625	N 192	O 176	0	0	0

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	BZ	135	Total 1092	C 710	N 202	O 180	0	0	0
63	DZ	135	Total 1092	C 710	N 202	O 180	0	0	0

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Ba	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	Da	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	Bb	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	Db	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	Bc	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	Dc	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	Bd	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	Dd	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	Be	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	De	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	Bf	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	Df	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	Bg	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	Dg	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	Bh	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	Dh	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	Bi	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	Di	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	Bj	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
73	Dj	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	Bk	77	Total	C	N	O	0	0	0
			612	391	115	106			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	Dk	77	Total	C	N	O	0	0	0
			608	388	114	106			

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	Bl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	Dl	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Bm	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	Dm	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Bn	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	Dn	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Bo	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	Do	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Bp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	Dp	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	A6	1795	Total	C	N	O	P	0	1	0
			38021	16989	6669	12567	1796			

- Molecule 81 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	Ch	104	Total	C	N	O	0	0	0
			680	403	140	137			

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	119	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	120	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	121	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	122	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	123	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	124	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	125	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	126	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	127	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	128	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	129	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	130	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	131	UNK	ILE	SEE REMARK 999	UNP P39015
Ch	132	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	133	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	134	UNK	ASP	SEE REMARK 999	UNP P39015
Ch	135	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	136	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	137	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	138	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	139	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	155	UNK	LEU	SEE REMARK 999	UNP P39015
Ch	156	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	157	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	158	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	159	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	160	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	161	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	162	UNK	GLN	SEE REMARK 999	UNP P39015
Ch	163	UNK	PHE	SEE REMARK 999	UNP P39015

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	164	UNK	ASN	SEE REMARK 999	UNP P39015
Ch	165	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	166	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	167	UNK	PRO	SEE REMARK 999	UNP P39015
Ch	168	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	169	UNK	ALA	SEE REMARK 999	UNP P39015
Ch	170	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	171	UNK	LYS	SEE REMARK 999	UNP P39015
Ch	172	UNK	VAL	SEE REMARK 999	UNP P39015
Ch	173	UNK	GLU	SEE REMARK 999	UNP P39015
Ch	174	UNK	LEU	SEE REMARK 999	UNP P39015

- Molecule 82 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
82	DK	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	Dq	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Dq	199	UNK	SER	SEE REMARK 999	UNP P05317
Dq	200	UNK	SER	SEE REMARK 999	UNP P05317
Dq	201	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	202	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	203	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	204	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	205	UNK	THR	SEE REMARK 999	UNP P05317
Dq	206	UNK	ASP	SEE REMARK 999	UNP P05317
Dq	207	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	208	UNK	GLU	SEE REMARK 999	UNP P05317
Dq	209	UNK	LEU	SEE REMARK 999	UNP P05317
Dq	210	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	211	UNK	SER	SEE REMARK 999	UNP P05317
Dq	212	UNK	HIS	SEE REMARK 999	UNP P05317
Dq	213	UNK	PHE	SEE REMARK 999	UNP P05317

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Dq	214	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	215	UNK	SER	SEE REMARK 999	UNP P05317
Dq	216	UNK	ALA	SEE REMARK 999	UNP P05317
Dq	217	UNK	VAL	SEE REMARK 999	UNP P05317
Dq	218	UNK	SER	SEE REMARK 999	UNP P05317
Dq	219	UNK	THR	SEE REMARK 999	UNP P05317
Dq	220	UNK	ILE	SEE REMARK 999	UNP P05317
Dq	221	UNK	ALA	SEE REMARK 999	UNP P05317

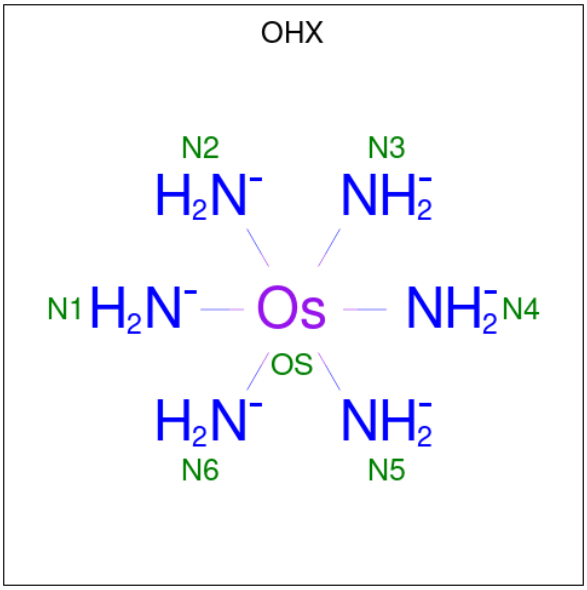
- Molecule 84 is a protein called Ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
84	Dr	47	Total	C	N	O	0	0	0
			235	141	47	47			

- Molecule 85 is a protein called Ribosomal protein P2 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
85	Ds	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	A2	1	Total	N	Os		0	0
			7	6	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	A2	1	Total	N	Os	0	0
			7	6	1		
86	AC	1	Total	N	Os	0	0
			7	6	1		
86	AI	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	AL	1	Total	N	Os	0	0
			7	6	1		
86	AN	1	Total	N	Os	0	0
			7	6	1		
86	AP	1	Total	N	Os	0	0
			7	6	1		
86	Ad	1	Total	N	Os	0	0
			7	6	1		
86	Ag	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A1	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A3	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	A4	1	Total	N	Os	0	0
			7	6	1		
86	BA	1	Total	N	Os	0	0
			7	6	1		
86	BB	1	Total	N	Os	0	0
			7	6	1		
86	BB	1	Total	N	Os	0	0
			7	6	1		
86	BC	1	Total	N	Os	0	0
			7	6	1		
86	BD	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BI	1	Total	N	Os	0	0
			7	6	1		
86	BN	1	Total	N	Os	0	0
			7	6	1		
86	BO	1	Total	N	Os	0	0
			7	6	1		
86	BP	1	Total	N	Os	0	0
			7	6	1		
86	BP	1	Total	N	Os	0	0
			7	6	1		
86	BR	1	Total	N	Os	0	0
			7	6	1		
86	BT	1	Total	N	Os	0	0
			7	6	1		
86	Bb	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	Bf	1	Total	N	Os	0	0
			7	6	1		
86	Bj	1	Total	N	Os	0	0
			7	6	1		
86	Bj	1	Total	N	Os	0	0
			7	6	1		
86	Bj	1	Total	N	Os	0	0
			7	6	1		
86	Bo	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 6	N 5	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0
86	A6	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	A6	1	Total	N	Os	0	0
			7	6	1		
86	CB	1	Total	N	Os	0	0
			7	6	1		
86	CG	1	Total	N	Os	0	0
			7	6	1		
86	CG	1	Total	N	Os	0	0
			7	6	1		
86	CI	1	Total	N	Os	0	0
			7	6	1		
86	CJ	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	CL	1	Total	N	Os	0	0
			7	6	1		
86	CN	1	Total	N	Os	0	0
			7	6	1		
86	CP	1	Total	N	Os	0	0
			7	6	1		
86	CP	1	Total	N	Os	0	0
			7	6	1		
86	CS	1	Total	N	Os	0	0
			7	6	1		
86	CY	1	Total	N	Os	0	0
			7	6	1		
86	CY	1	Total	N	Os	0	0
			7	6	1		
86	Cd	1	Total	N	Os	0	0
			7	6	1		
86	Cg	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A5	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A7	1	Total	N	Os	0	0
			7	6	1		
86	A8	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	A8	1	Total 7	N 6	Os 1	0	0
86	DA	1	Total 7	N 6	Os 1	0	0
86	DB	1	Total 7	N 6	Os 1	0	0
86	DB	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	DC	1	Total	N	Os	0	0
			7	6	1		
86	DC	1	Total	N	Os	0	0
			7	6	1		
86	DD	1	Total	N	Os	0	0
			7	6	1		
86	DG	1	Total	N	Os	0	0
			7	6	1		
86	DH	1	Total	N	Os	0	0
			7	6	1		
86	DI	1	Total	N	Os	0	0
			7	6	1		
86	DI	1	Total	N	Os	0	0
			7	6	1		
86	DJ	1	Total	N	Os	0	0
			7	6	1		
86	DM	1	Total	N	Os	0	0
			7	6	1		
86	DO	1	Total	N	Os	0	0
			7	6	1		
86	DP	1	Total	N	Os	0	0
			7	6	1		
86	DQ	1	Total	N	Os	0	0
			7	6	1		
86	DR	1	Total	N	Os	0	0
			7	6	1		
86	DV	1	Total	N	Os	0	0
			7	6	1		
86	Db	1	Total	N	Os	0	0
			7	6	1		
86	De	1	Total	N	Os	0	0
			7	6	1		
86	Df	1	Total	N	Os	0	0
			7	6	1		
86	Dg	1	Total	N	Os	0	0
			7	6	1		
86	Dh	1	Total	N	Os	0	0
			7	6	1		
86	Dj	1	Total	N	Os	0	0
			7	6	1		
86	Do	1	Total	N	Os	0	0
			7	6	1		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	A2	171	Total Mg 171 171	0	0
87	AB	2	Total Mg 2 2	0	0
87	AC	1	Total Mg 1 1	0	0
87	AE	1	Total Mg 1 1	0	0
87	AI	2	Total Mg 2 2	0	0
87	AJ	1	Total Mg 1 1	0	0
87	AL	2	Total Mg 2 2	0	0
87	AN	1	Total Mg 1 1	0	0
87	AP	1	Total Mg 1 1	0	0
87	AS	2	Total Mg 2 2	0	0
87	AX	1	Total Mg 1 1	0	0
87	Aa	1	Total Mg 1 1	0	0
87	Ad	3	Total Mg 3 3	0	0
87	Af	1	Total Mg 1 1	0	0
87	A1	695	Total Mg 695 695	0	0
87	A3	19	Total Mg 19 19	0	0
87	A4	34	Total Mg 34 34	0	0
87	BA	5	Total Mg 5 5	0	0
87	BB	4	Total Mg 4 4	0	0
87	BC	6	Total Mg 6 6	0	0
87	BD	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	BE	1	Total Mg 1 1	0	0
87	BF	2	Total Mg 2 2	0	0
87	BG	1	Total Mg 1 1	0	0
87	BI	4	Total Mg 4 4	0	0
87	BJ	1	Total Mg 1 1	0	0
87	BL	5	Total Mg 5 5	0	0
87	BN	6	Total Mg 6 6	0	0
87	BO	8	Total Mg 8 8	0	0
87	BP	10	Total Mg 10 10	0	0
87	BQ	4	Total Mg 4 4	0	0
87	BR	4	Total Mg 4 4	0	0
87	BS	2	Total Mg 2 2	0	0
87	BT	1	Total Mg 1 1	0	0
87	BV	5	Total Mg 5 5	0	0
87	BY	2	Total Mg 2 2	0	0
87	Ba	8	Total Mg 8 8	0	0
87	Bd	1	Total Mg 1 1	0	0
87	Be	2	Total Mg 2 2	0	0
87	Bf	1	Total Mg 1 1	0	0
87	Bg	1	Total Mg 1 1	0	0
87	Bj	7	Total Mg 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	Bl	1	Total Mg 1 1	0	0
87	Bm	1	Total Mg 1 1	0	0
87	Bo	3	Total Mg 3 3	0	0
87	A6	239	Total Mg 239 239	0	0
87	CB	1	Total Mg 1 1	0	0
87	CE	1	Total Mg 1 1	0	0
87	CF	2	Total Mg 2 2	0	0
87	CG	2	Total Mg 2 2	0	0
87	CI	2	Total Mg 2 2	0	0
87	CL	3	Total Mg 3 3	0	0
87	CP	1	Total Mg 1 1	0	0
87	CQ	2	Total Mg 2 2	0	0
87	CS	2	Total Mg 2 2	0	0
87	CX	2	Total Mg 2 2	0	0
87	CY	2	Total Mg 2 2	0	0
87	CZ	1	Total Mg 1 1	0	0
87	Ca	1	Total Mg 1 1	0	0
87	Cd	1	Total Mg 1 1	0	0
87	Ch	2	Total Mg 2 2	0	0
87	A5	763	Total Mg 763 763	0	0
87	A7	26	Total Mg 26 26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	A8	20	Total Mg 20 20	0	0
87	DA	4	Total Mg 4 4	0	0
87	DB	13	Total Mg 13 13	0	0
87	DC	5	Total Mg 5 5	0	0
87	DD	7	Total Mg 7 7	0	0
87	DF	4	Total Mg 4 4	0	0
87	DG	1	Total Mg 1 1	0	0
87	DH	2	Total Mg 2 2	0	0
87	DJ	2	Total Mg 2 2	0	0
87	DL	1	Total Mg 1 1	0	0
87	DM	2	Total Mg 2 2	0	0
87	DN	1	Total Mg 1 1	0	0
87	DO	8	Total Mg 8 8	0	0
87	DP	7	Total Mg 7 7	0	0
87	DQ	1	Total Mg 1 1	0	0
87	DR	1	Total Mg 1 1	0	0
87	DS	4	Total Mg 4 4	0	0
87	DT	3	Total Mg 3 3	0	0
87	DV	3	Total Mg 3 3	0	0
87	DW	1	Total Mg 1 1	0	0
87	DY	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	Da	4	Total Mg 4 4	0	0
87	Db	1	Total Mg 1 1	0	0
87	Dd	1	Total Mg 1 1	0	0
87	De	2	Total Mg 2 2	0	0
87	Df	4	Total Mg 4 4	0	0
87	Dg	2	Total Mg 2 2	0	0
87	Dj	3	Total Mg 3 3	0	0
87	Dl	1	Total Mg 1 1	0	0
87	Dm	1	Total Mg 1 1	0	0
87	Dn	1	Total Mg 1 1	0	0
87	Do	1	Total Mg 1 1	0	0
87	Dp	3	Total Mg 3 3	0	0
87	Dq	1	Total Mg 1 1	0	0

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	Aa	1	Total Zn 1 1	0	0
88	Ab	1	Total Zn 1 1	0	0
88	Ad	1	Total Zn 1 1	0	0
88	Af	1	Total Zn 1 1	0	0
88	Bj	1	Total Zn 1 1	0	0
88	Bm	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	Bo	1	Total Zn 1 1	0	0
88	Bp	1	Total Zn 1 1	0	0
88	Ca	1	Total Zn 1 1	0	0
88	Cb	1	Total Zn 1 1	0	0
88	Cd	1	Total Zn 1 1	0	0
88	Cf	1	Total Zn 1 1	0	0
88	Dj	1	Total Zn 1 1	0	0
88	Dm	1	Total Zn 1 1	0	0
88	Do	1	Total Zn 1 1	0	0
88	Dp	1	Total Zn 1 1	0	0

- Molecule 89 is water.

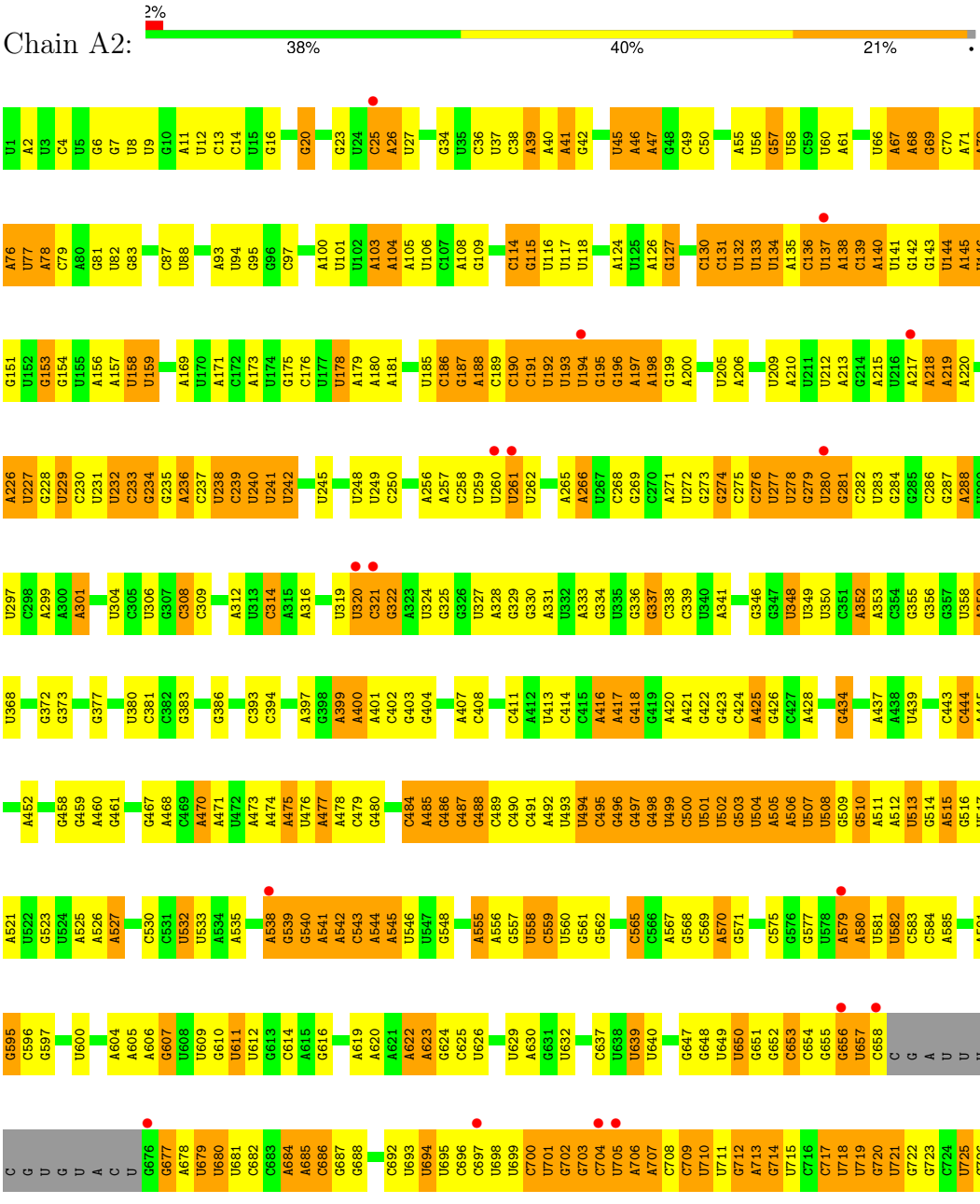
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
89	CI	1	Total O 1 1	0	0
89	DB	1	Total O 1 1	0	0

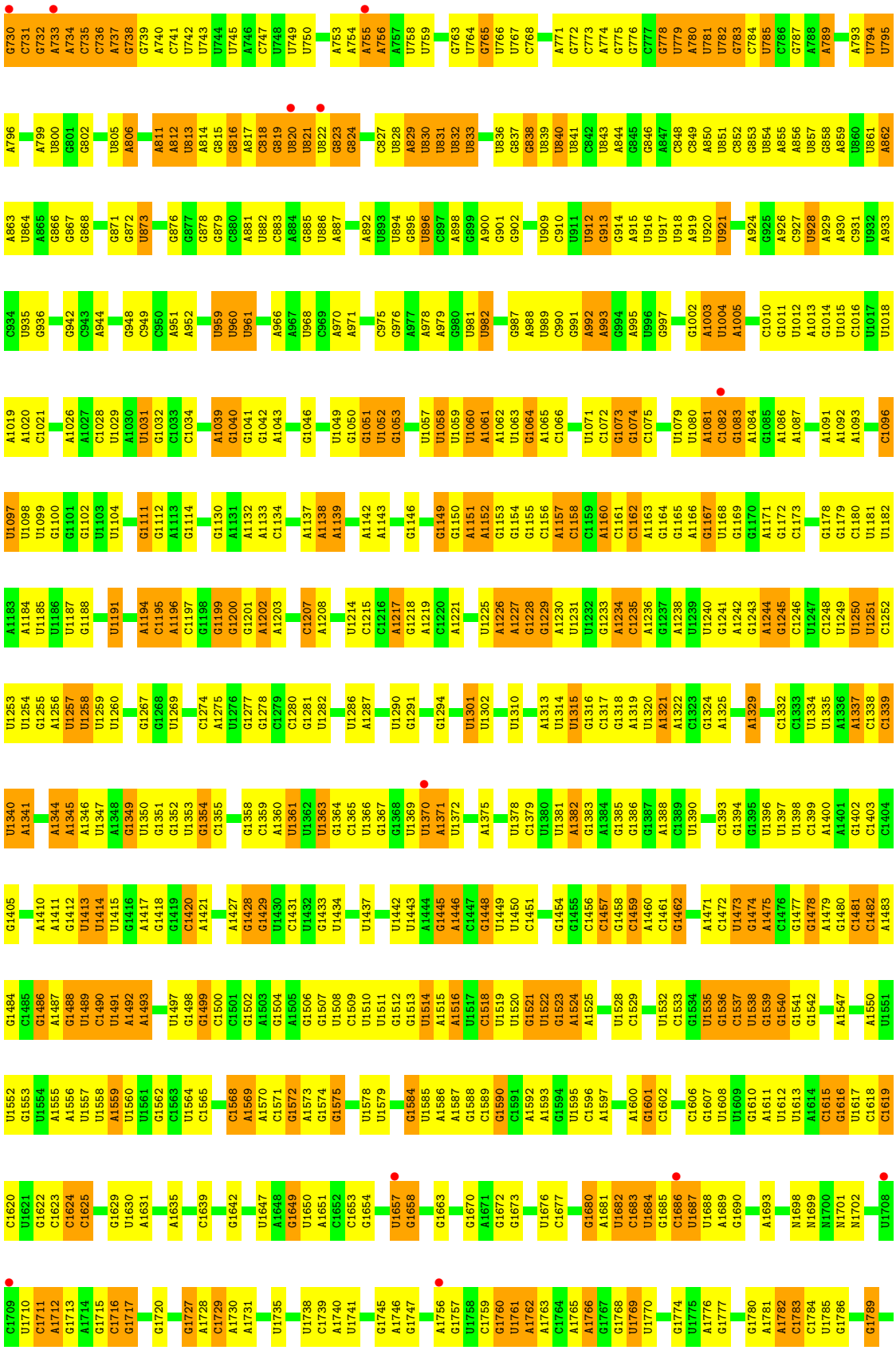
3 Residue-property plots (i)

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

- Molecule 1: 18S RIBOSOMAL RNA

Chain A2:



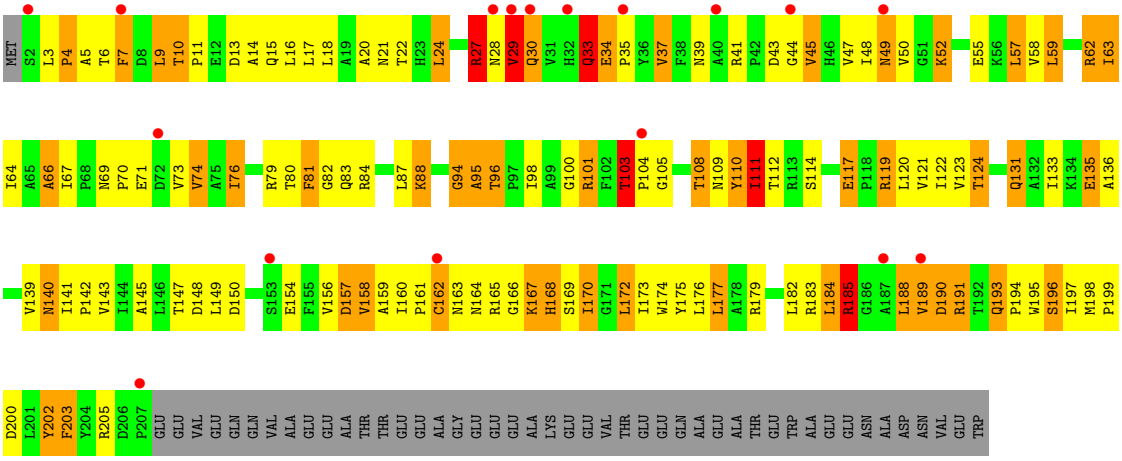




• Molecule 2: 40S ribosomal protein S0-A

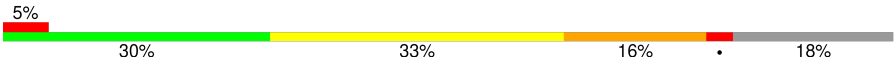
Chain AA:

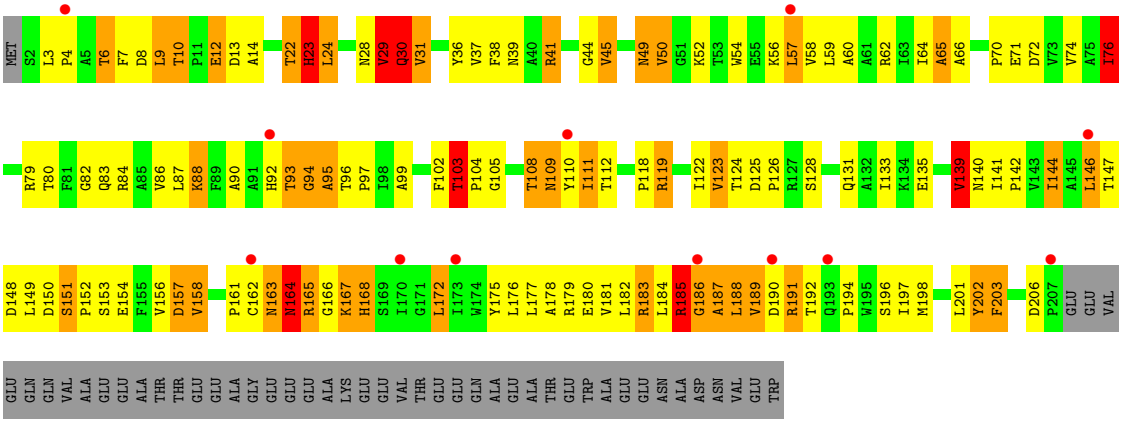




• Molecule 2: 40S ribosomal protein S0-A

Chain CA:

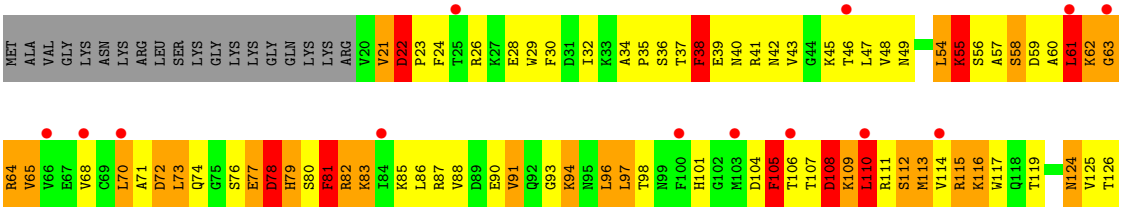


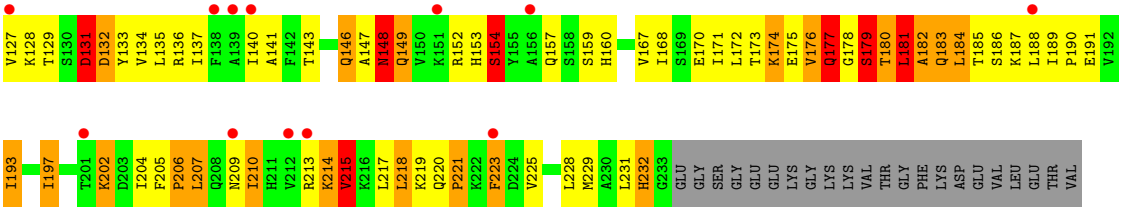


• Molecule 3: 40S ribosomal protein S1-A

Chain AB:

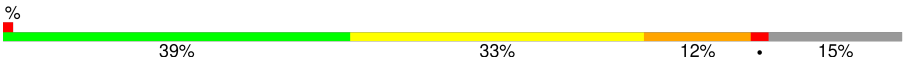


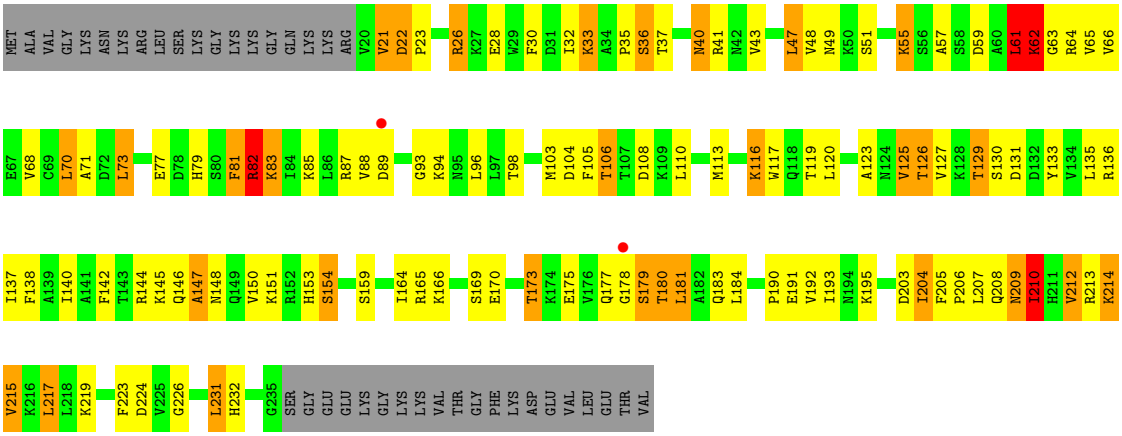




• Molecule 3: 40S ribosomal protein S1-A

Chain CB:

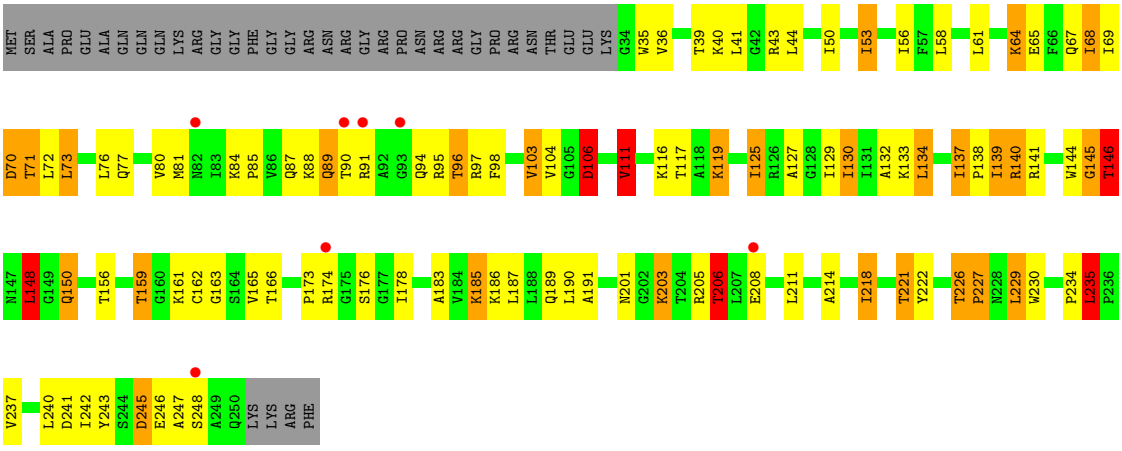




• Molecule 4: 40S ribosomal protein S2

Chain AC:



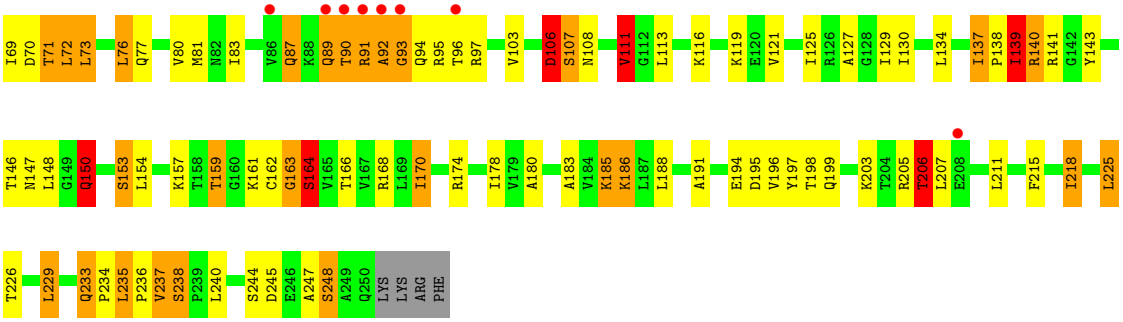


• Molecule 4: 40S ribosomal protein S2

Chain CC:

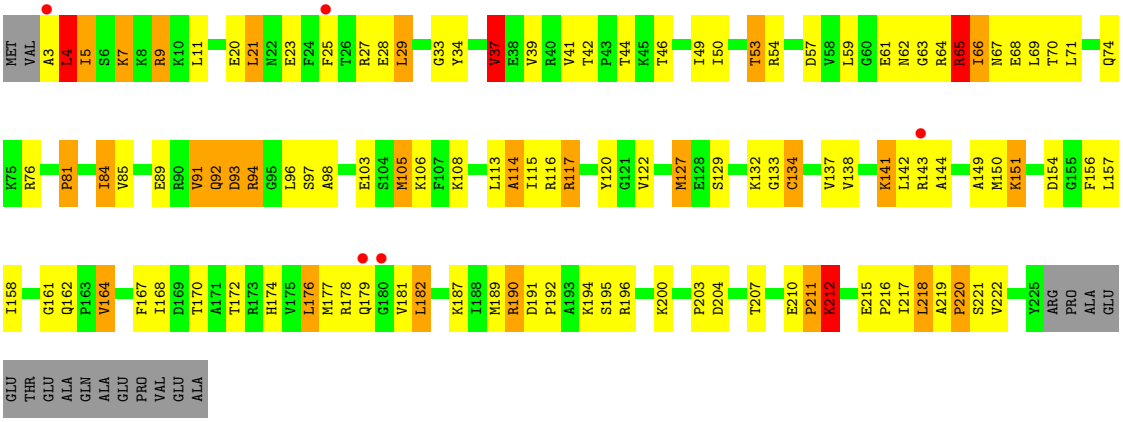






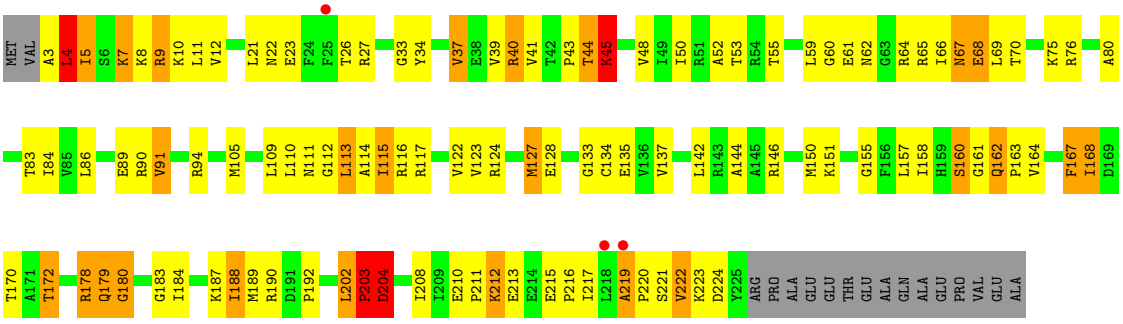
• Molecule 5: 40S ribosomal protein S3





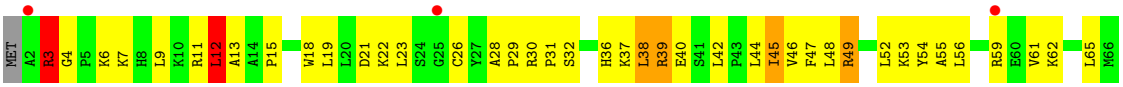
• Molecule 5: 40S ribosomal protein S3

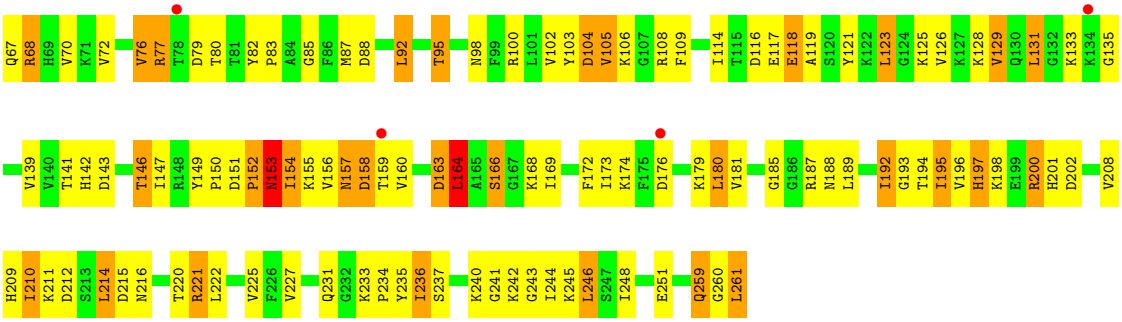




• Molecule 6: 40S ribosomal protein S4-A



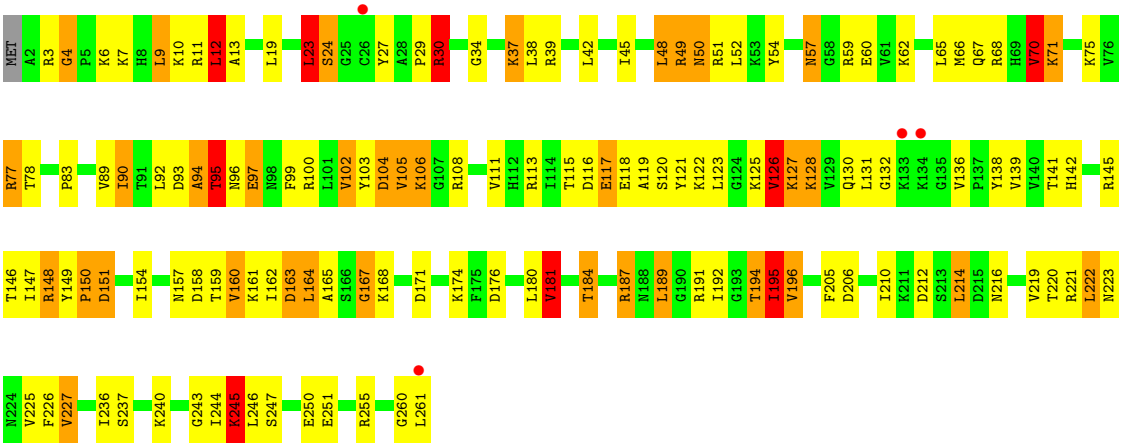




• Molecule 6: 40S ribosomal protein S4-A

Chain CE:

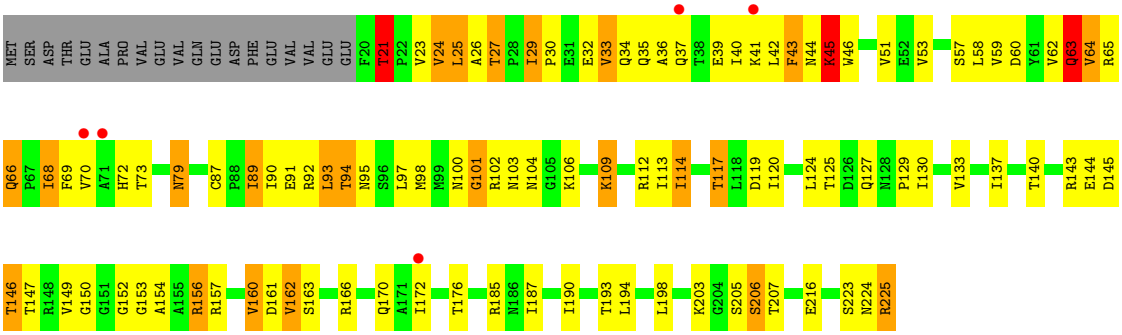




• Molecule 7: 40S ribosomal protein S5

Chain AF:



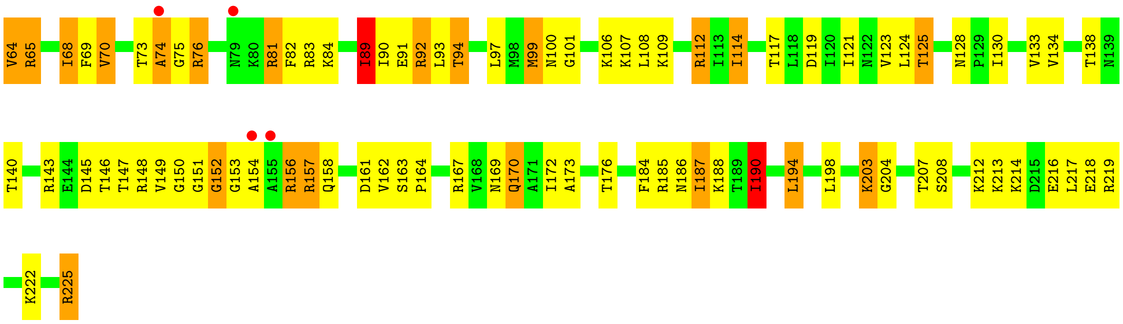


• Molecule 7: 40S ribosomal protein S5

Chain CF:

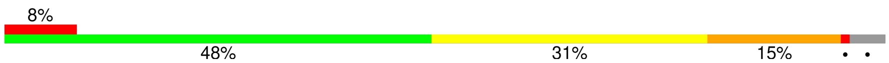


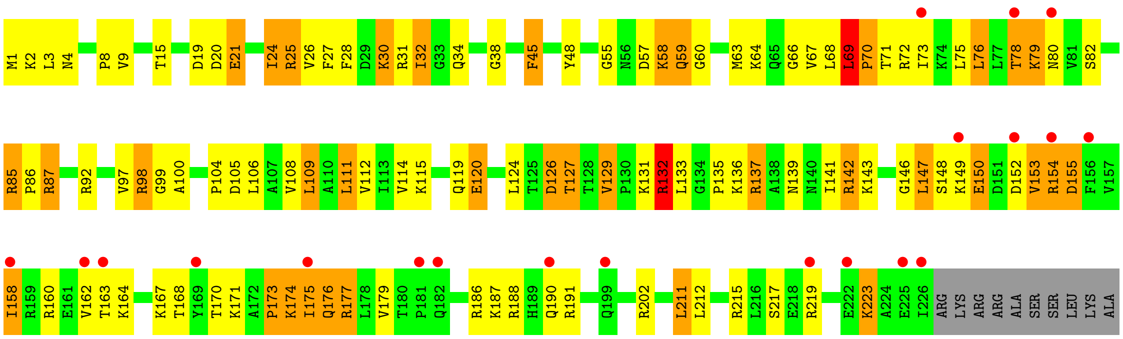




- Molecule 8: 40S ribosomal protein S6-A

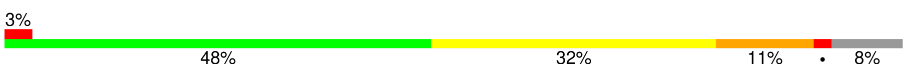
Chain AG:

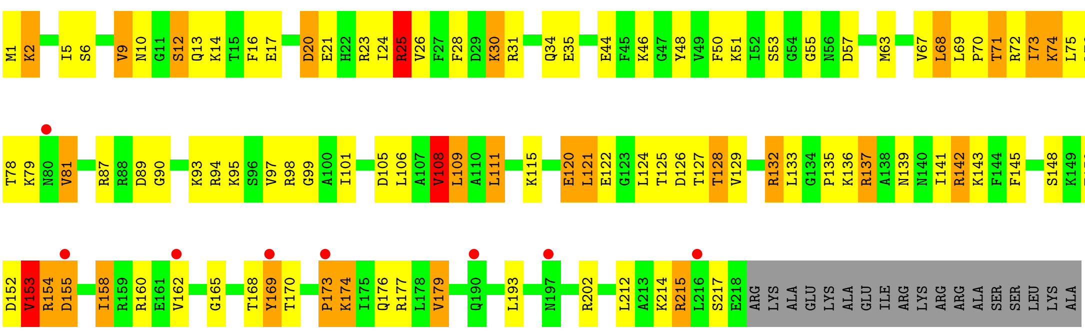




- Molecule 8: 40S ribosomal protein S6-A

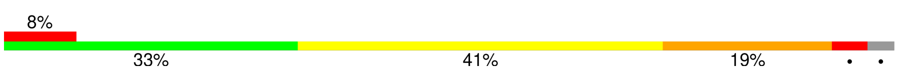
Chain CG:

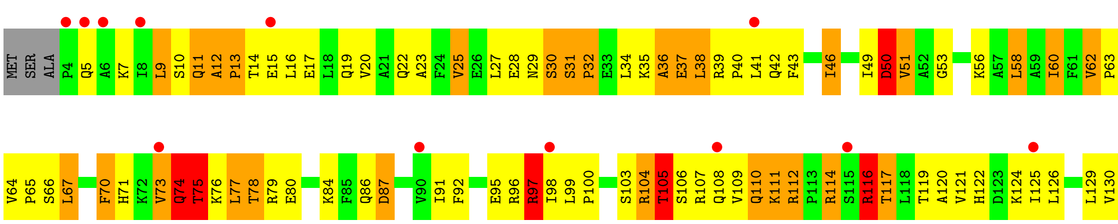


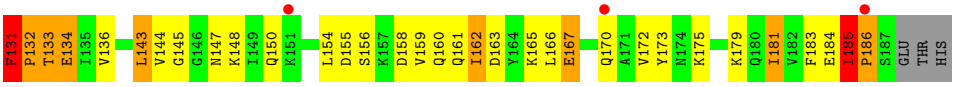


- Molecule 9: 40S ribosomal protein S7-A

Chain AH:



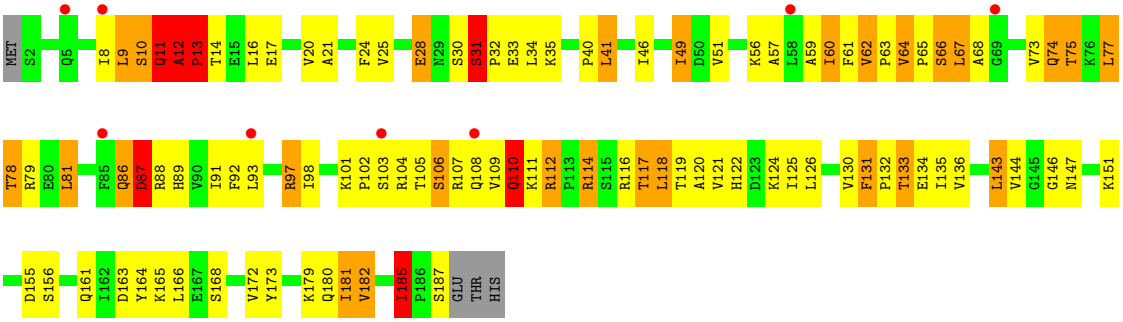




• Molecule 9: 40S ribosomal protein S7-A

Chain CH:

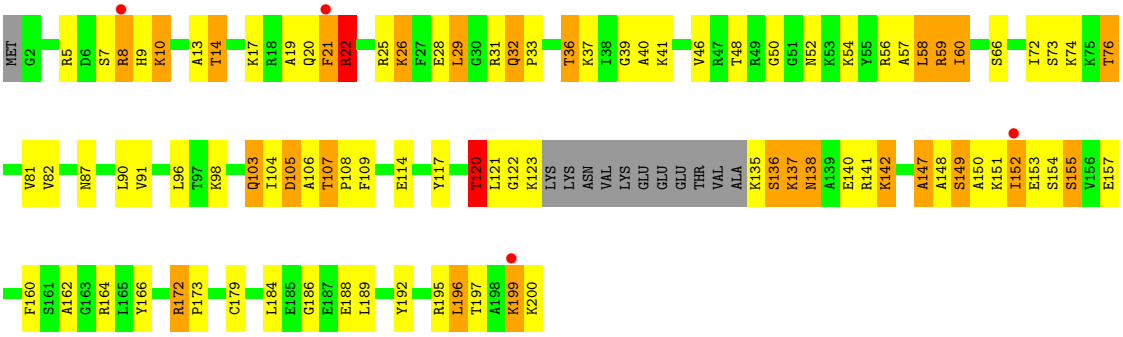




• Molecule 10: 40S ribosomal protein S8-A

Chain AI:

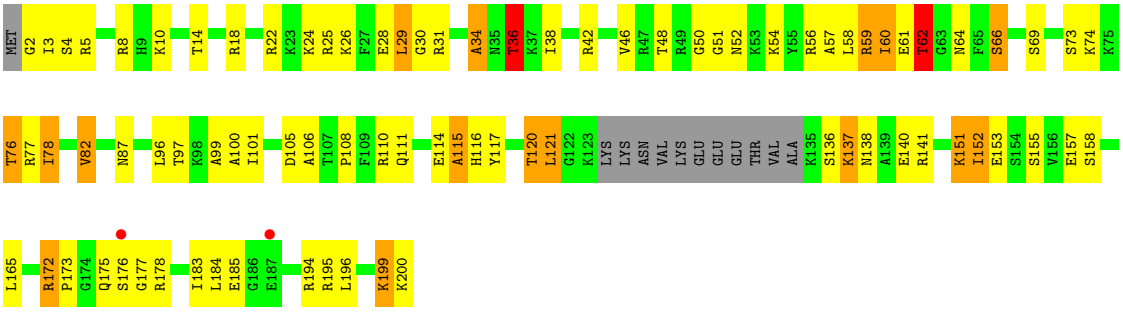




• Molecule 10: 40S ribosomal protein S8-A

Chain CI:

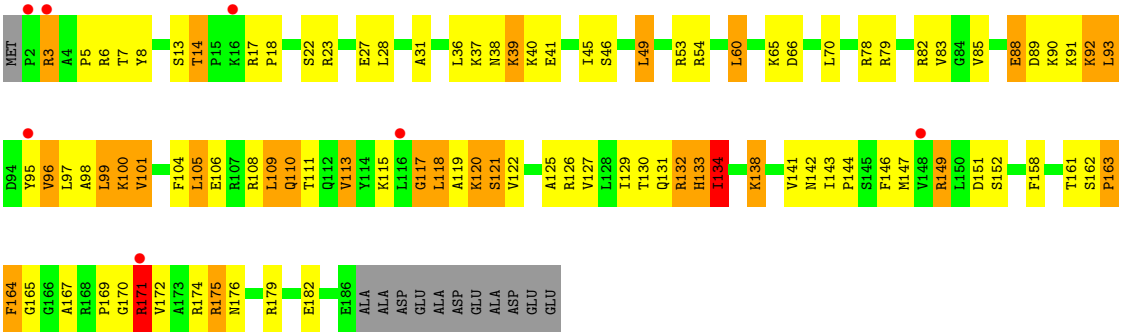




• Molecule 11: 40S ribosomal protein S9-A

Chain AJ:

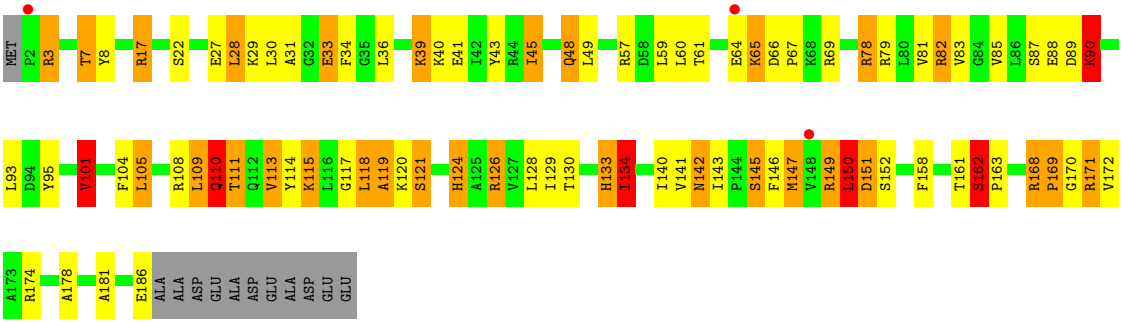




• Molecule 11: 40S ribosomal protein S9-A

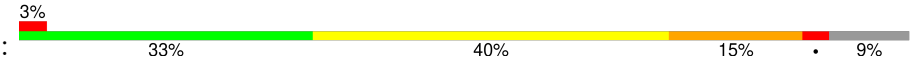
Chain CJ:

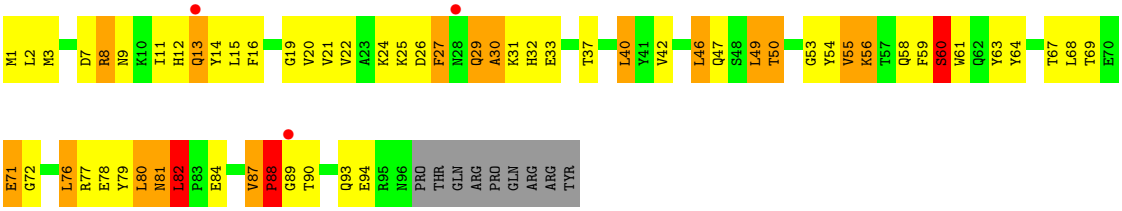




• Molecule 12: 40S ribosomal protein S10-A

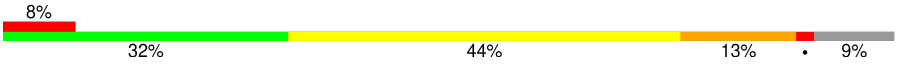
Chain AK:

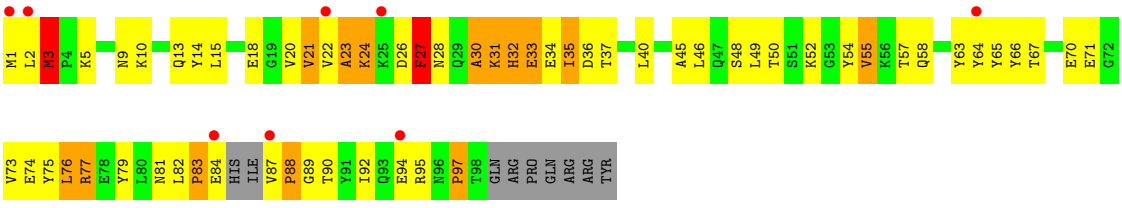




• Molecule 12: 40S ribosomal protein S10-A

Chain CK:

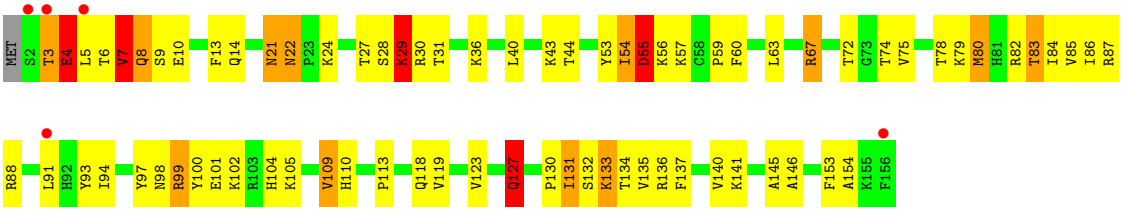




• Molecule 13: 40S ribosomal protein S11-A

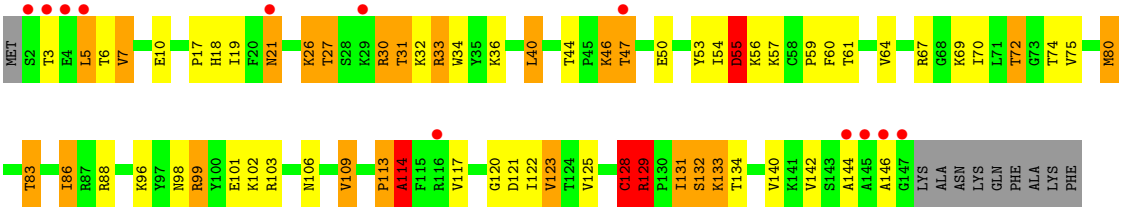
Chain AL:



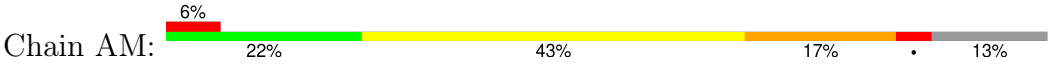


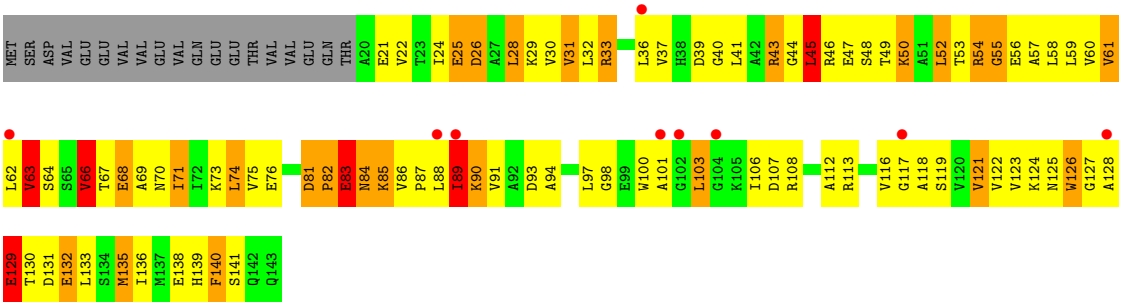
• Molecule 13: 40S ribosomal protein S11-A



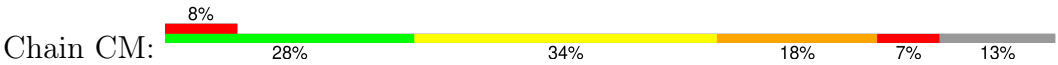


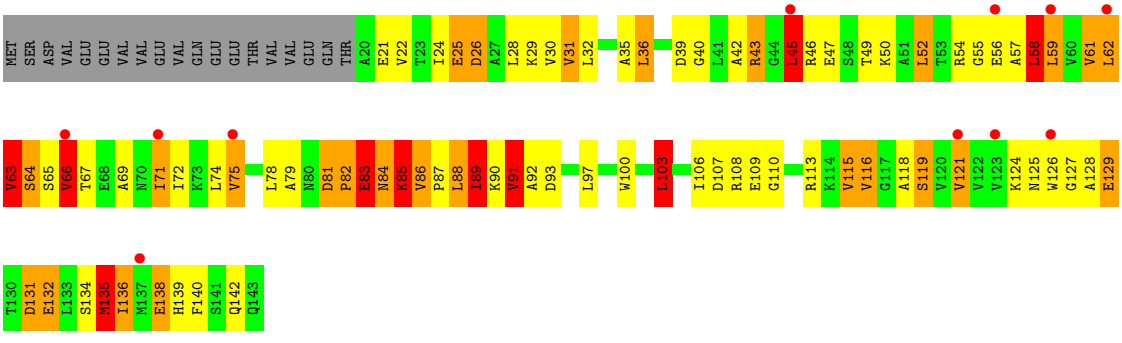
• Molecule 14: 40S ribosomal protein S12





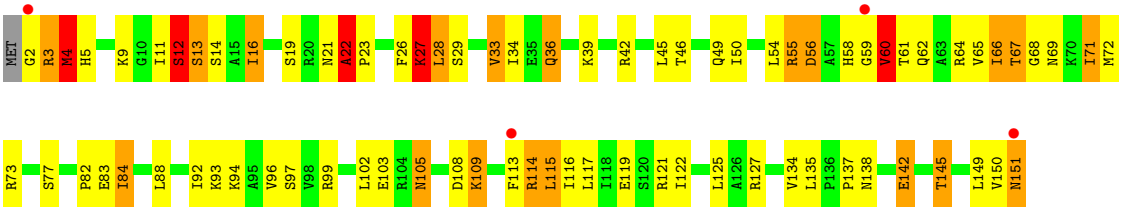
• Molecule 14: 40S ribosomal protein S12

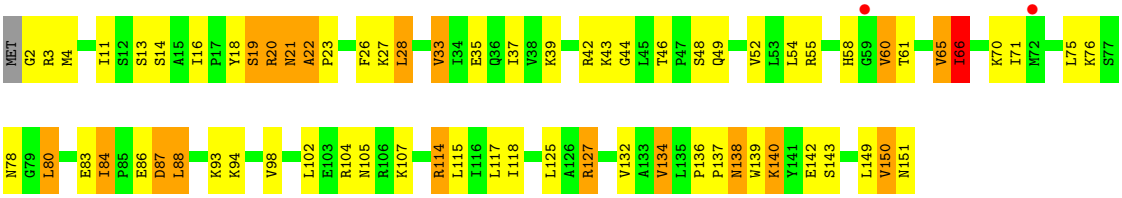




• Molecule 15: 40S ribosomal protein S13







• Molecule 15: 40S ribosomal protein S13

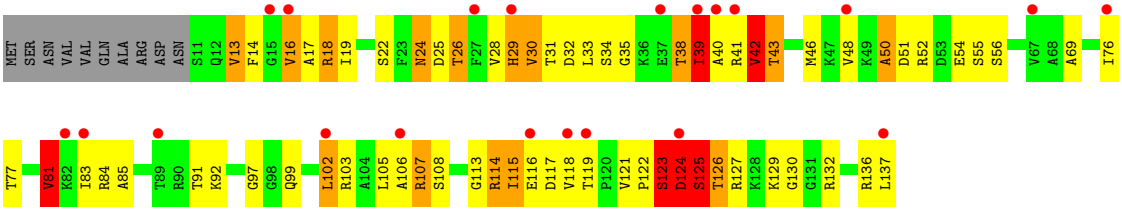
Chain CN:



• Molecule 16: 40S ribosomal protein S14-A

Chain AO:

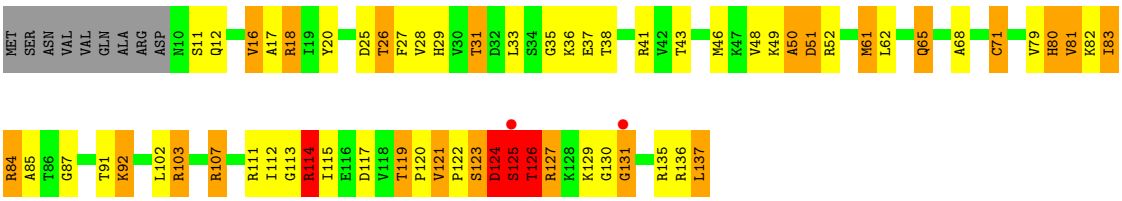




• Molecule 16: 40S ribosomal protein S14-A

Chain CO:

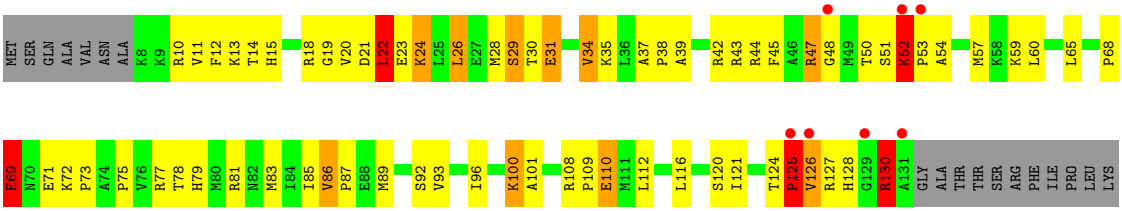




• Molecule 17: 40S ribosomal protein S15

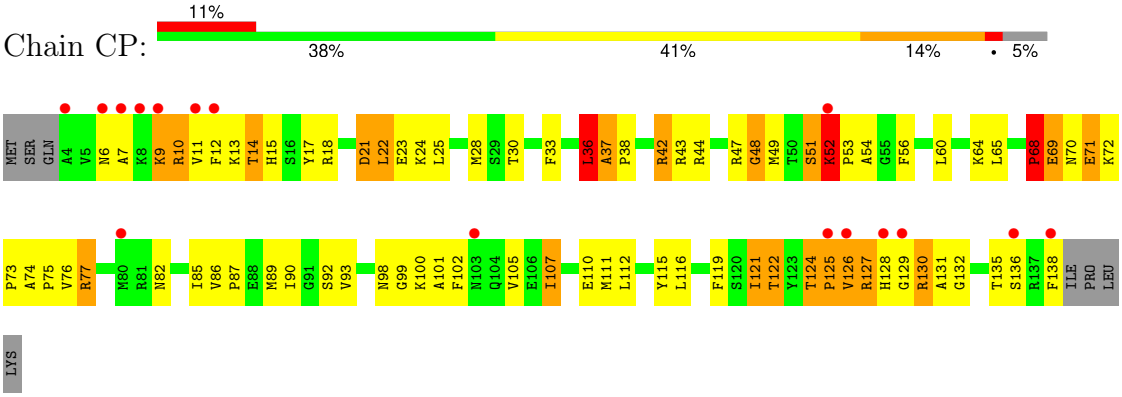
Chain AP:





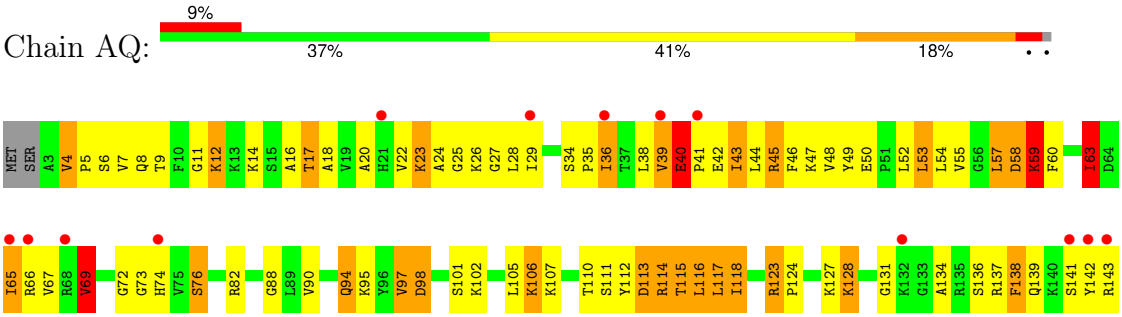
• Molecule 17: 40S ribosomal protein S15

Chain CP:



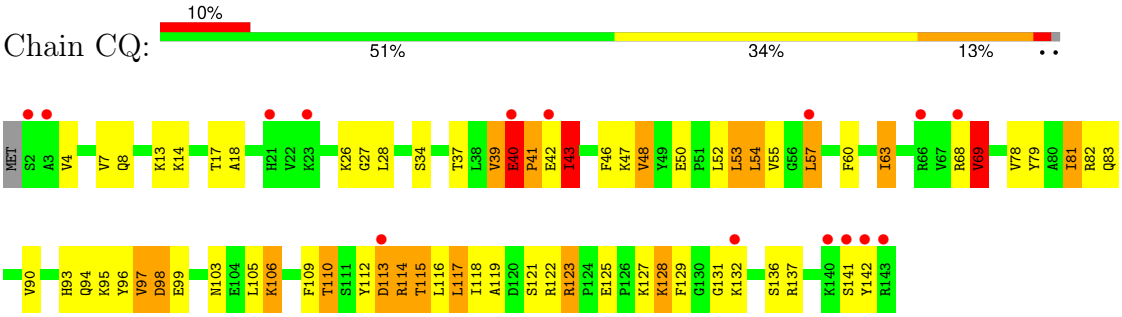
• Molecule 18: 40S ribosomal protein S16-A

Chain AQ:



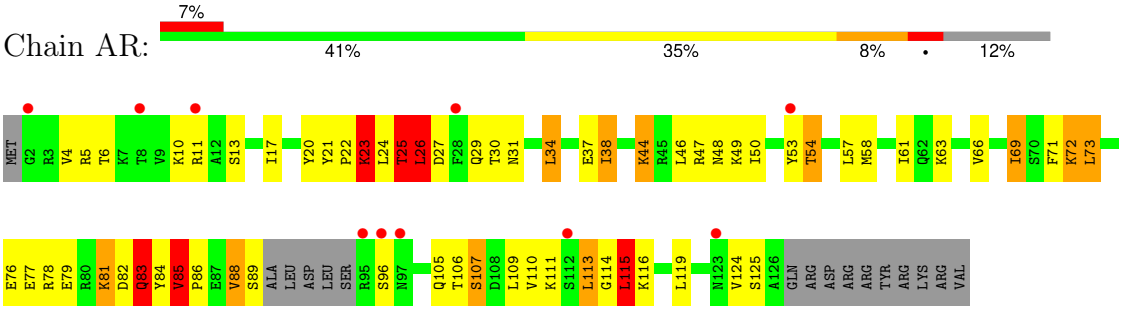
• Molecule 18: 40S ribosomal protein S16-A

Chain CQ:



• Molecule 19: 40S ribosomal protein S17-A

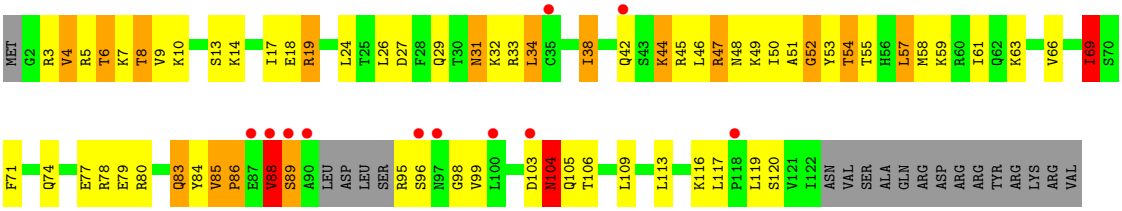
Chain AR:



• Molecule 19: 40S ribosomal protein S17-A

Chain CR:

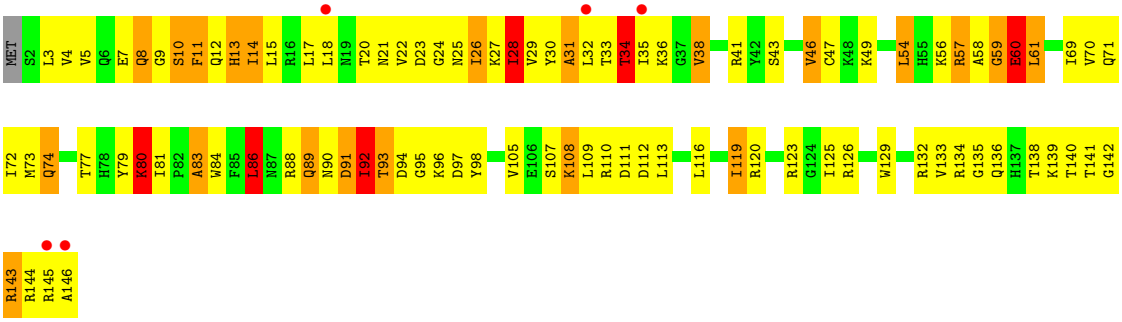




• Molecule 20: 40S ribosomal protein S18-A

Chain AS:

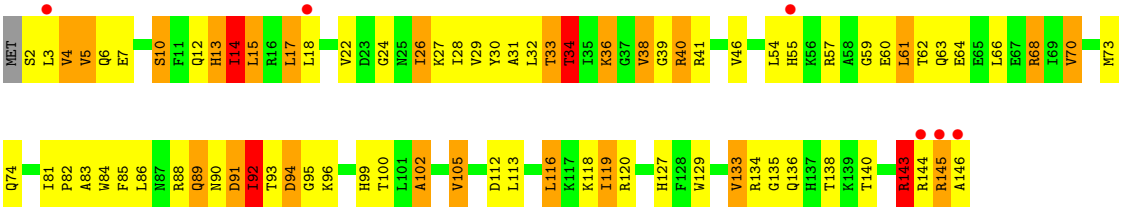




• Molecule 20: 40S ribosomal protein S18-A

Chain CS:

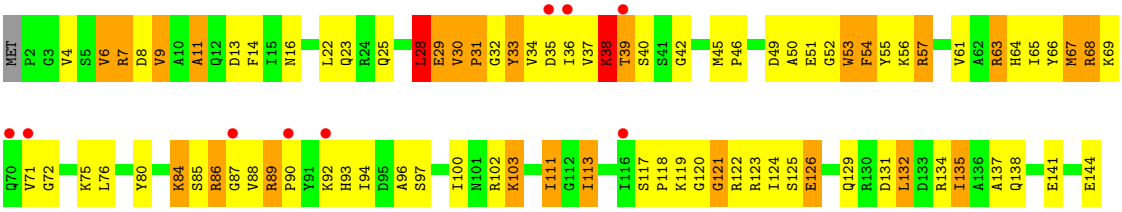




• Molecule 21: 40S ribosomal protein S19-A

Chain AT:

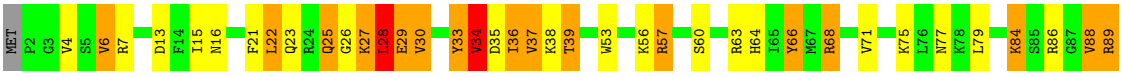


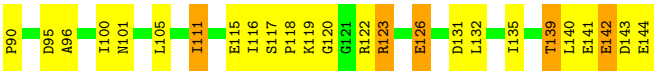


• Molecule 21: 40S ribosomal protein S19-A

Chain CT:

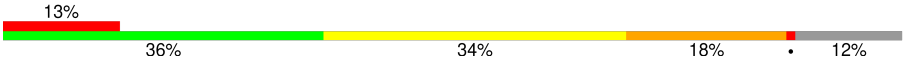


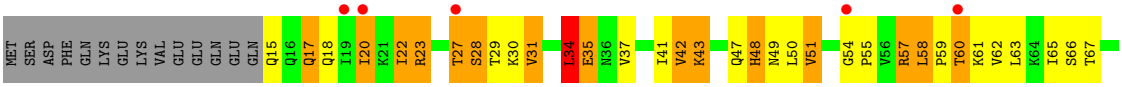


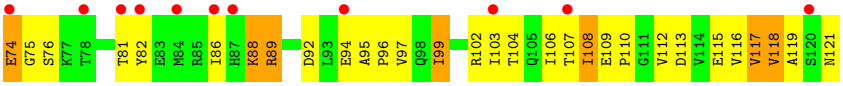


• Molecule 22: 40S ribosomal protein S20

Chain AU:



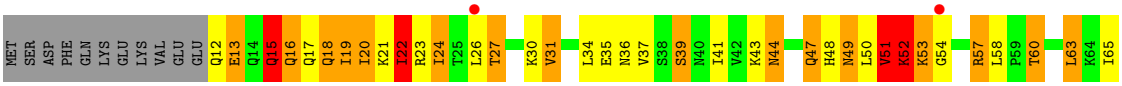




• Molecule 22: 40S ribosomal protein S20

Chain CU:



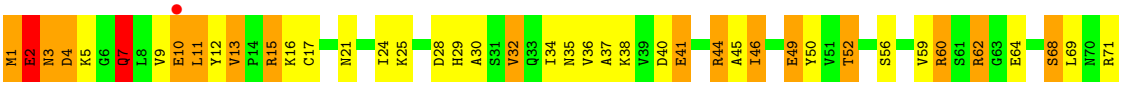


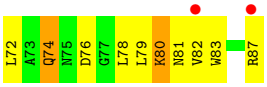


• Molecule 23: 40S ribosomal protein S21-A

Chain AV:



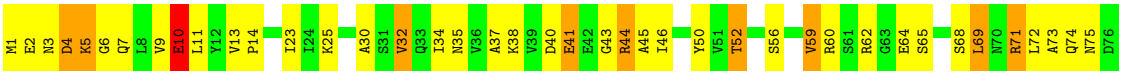


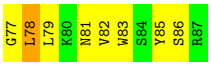


• Molecule 23: 40S ribosomal protein S21-A

Chain CV:



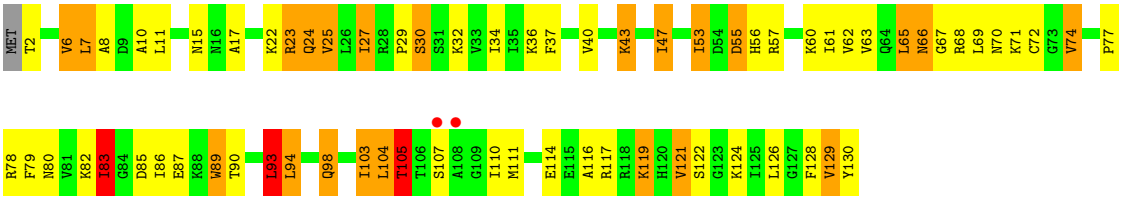




• Molecule 24: 40S ribosomal protein S22-A

Chain AW:



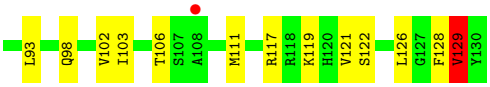


• Molecule 24: 40S ribosomal protein S22-A

Chain CW:



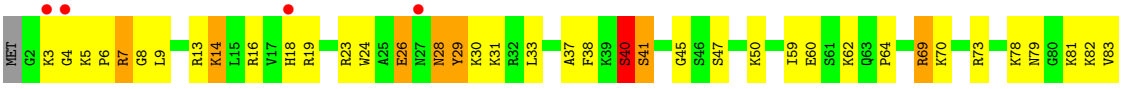


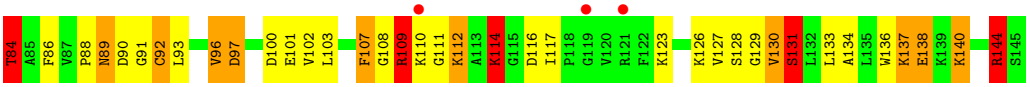


• Molecule 25: 40S ribosomal protein S23-A

Chain AX:



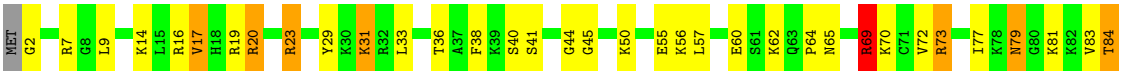




• Molecule 25: 40S ribosomal protein S23-A

Chain CX:

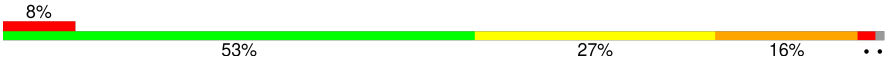


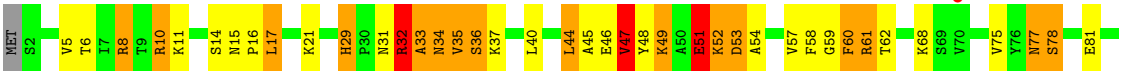


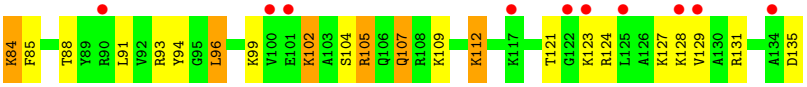


• Molecule 26: 40S ribosomal protein S24-A

Chain AY:

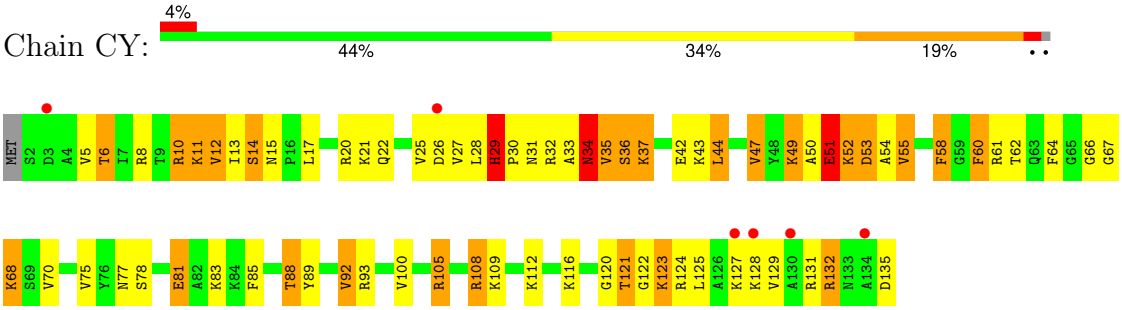






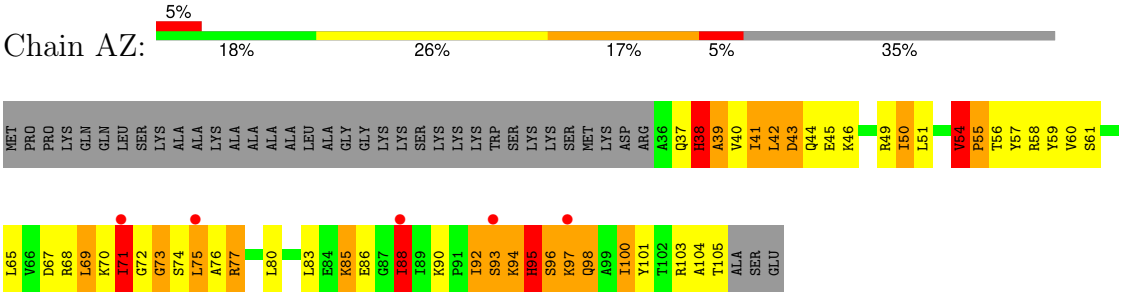
• Molecule 26: 40S ribosomal protein S24-A

Chain CY:



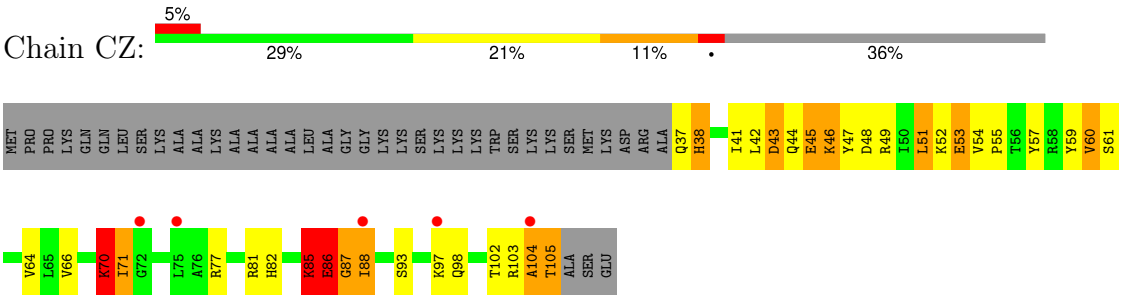
• Molecule 27: 40S ribosomal protein S25-A

Chain AZ:



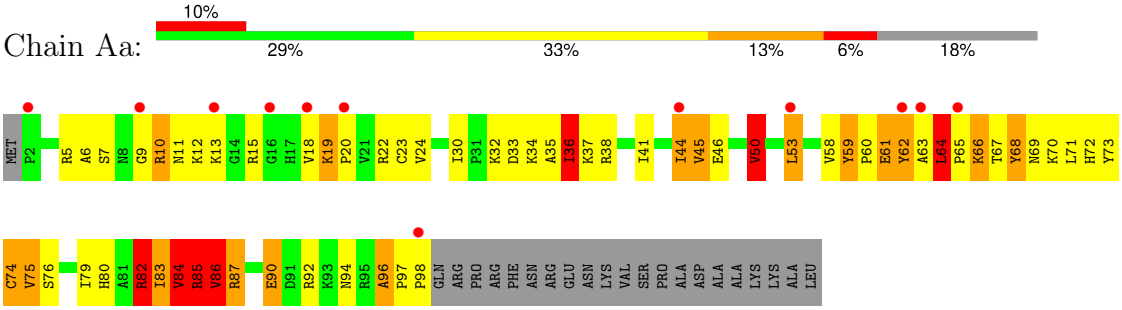
• Molecule 27: 40S ribosomal protein S25-A

Chain CZ:



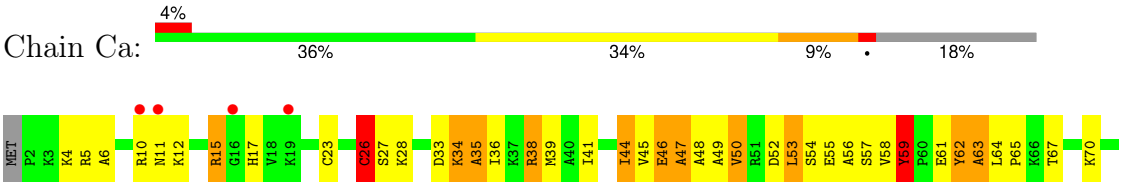
• Molecule 28: 40S ribosomal protein S26-A

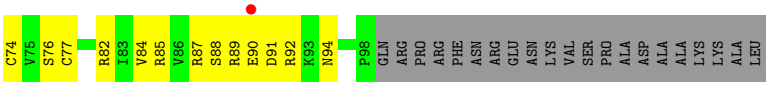
Chain Aa:



• Molecule 28: 40S ribosomal protein S26-A

Chain Ca:

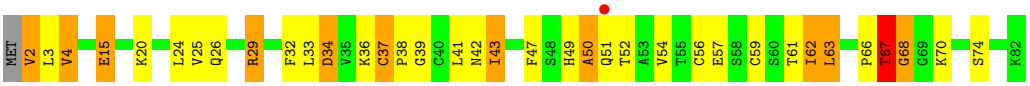




• Molecule 29: 40S ribosomal protein S27-A

Chain Ab:

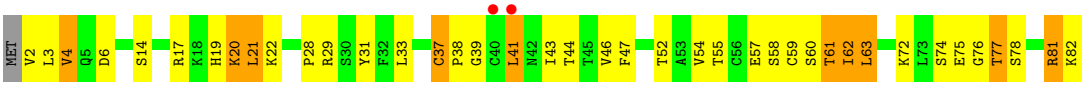




• Molecule 29: 40S ribosomal protein S27-A

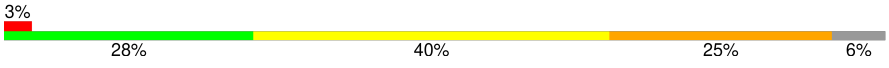
Chain Cb:

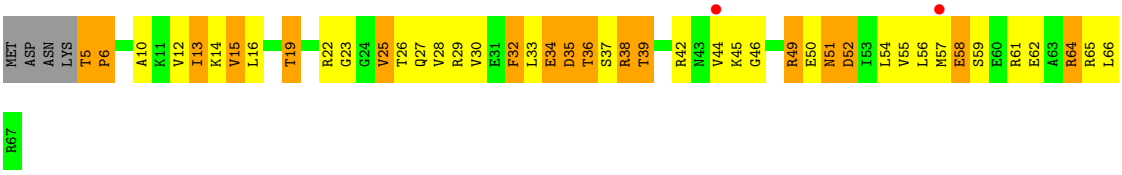




• Molecule 30: 40S ribosomal protein S28-A

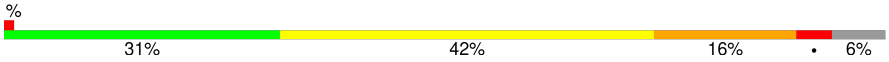
Chain Ac:





• Molecule 30: 40S ribosomal protein S28-A

Chain Cc:

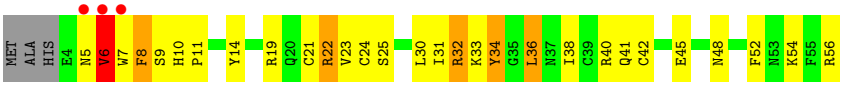




• Molecule 31: 40S ribosomal protein S29-A

Chain Ad:

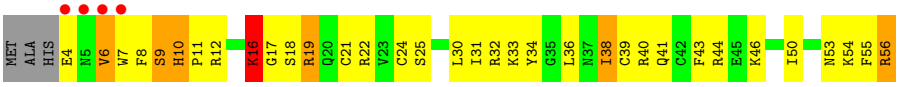




• Molecule 31: 40S ribosomal protein S29-A

Chain Cd:

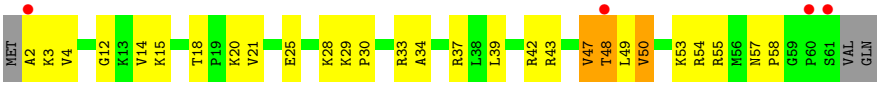




• Molecule 32: 40S ribosomal protein S30-A

Chain Ae:

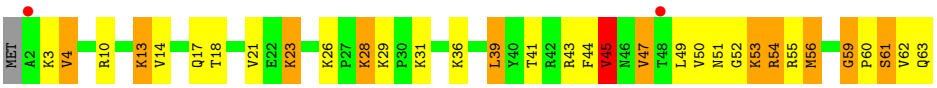




• Molecule 32: 40S ribosomal protein S30-A

Chain Ce:

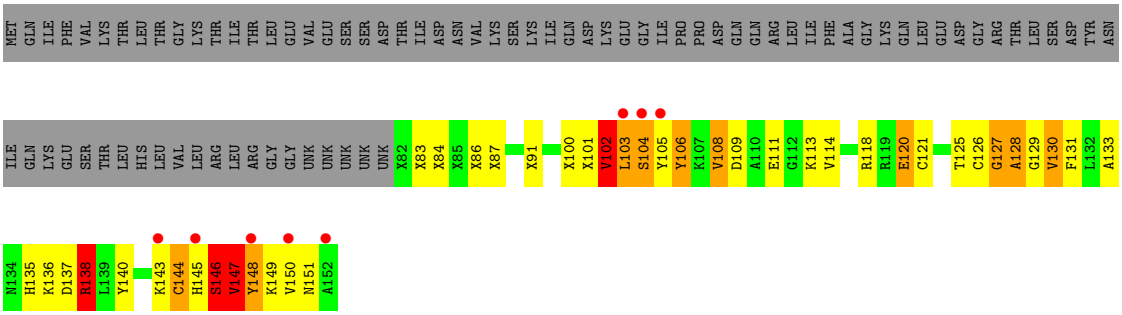




• Molecule 33: 40S ribosomal protein S31

Chain Af:

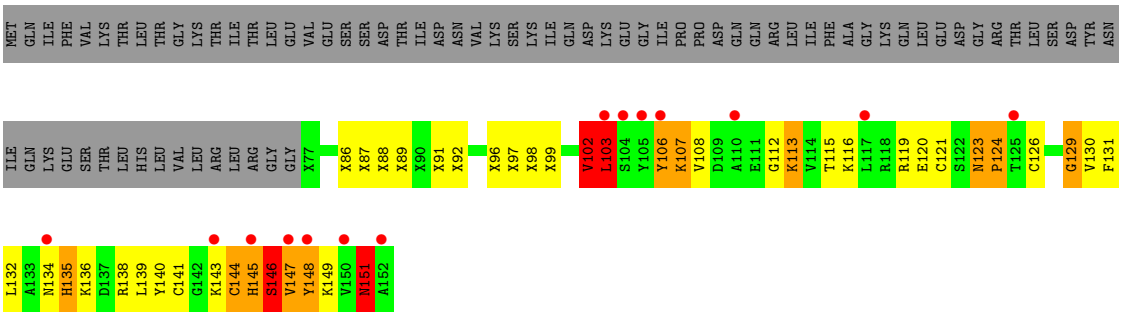




• Molecule 33: 40S ribosomal protein S31

Chain Cf:

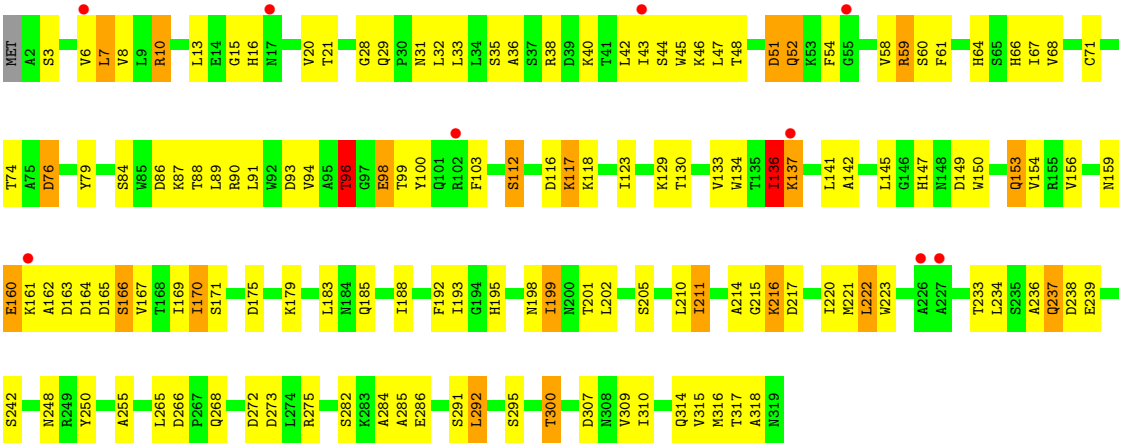




• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)

Chain Ag:

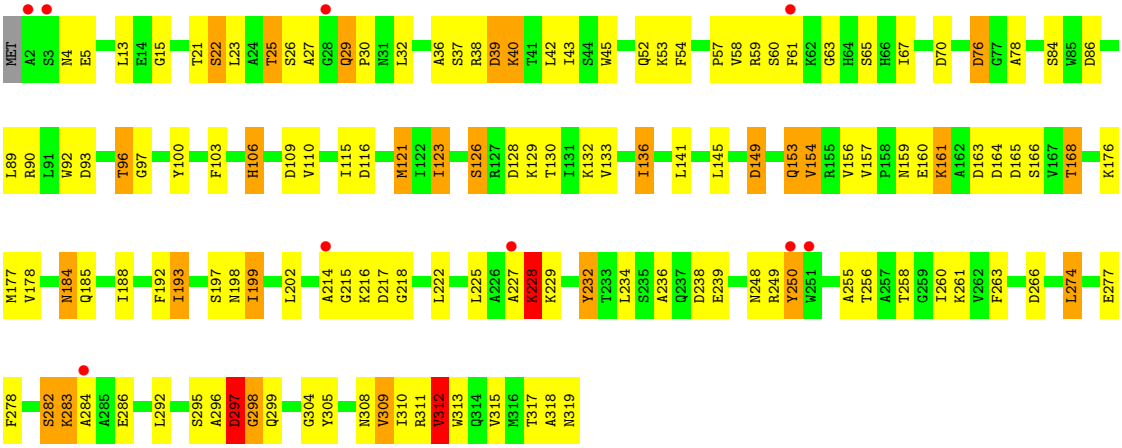




• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein (ASC1, RACK1)

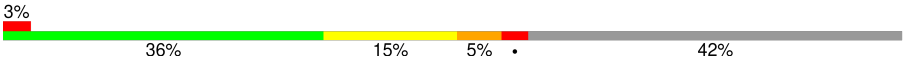
Chain Cg:

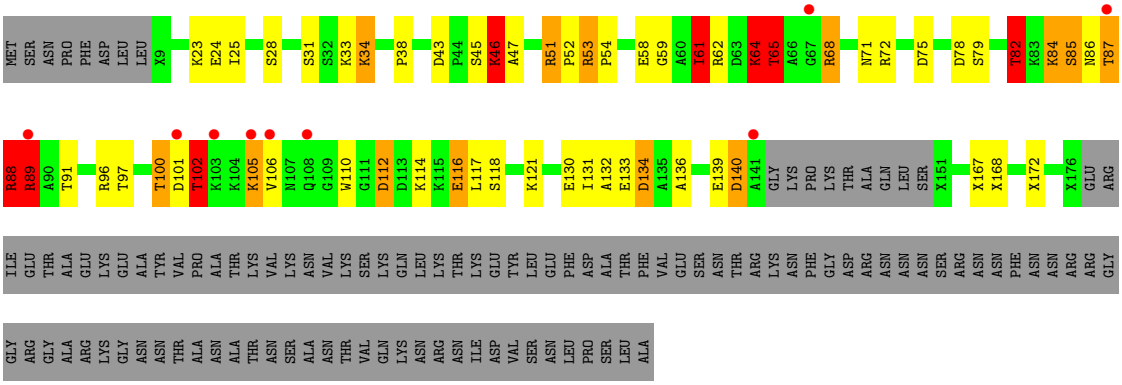




• Molecule 35: Suppressor protein STM1

Chain Ah:

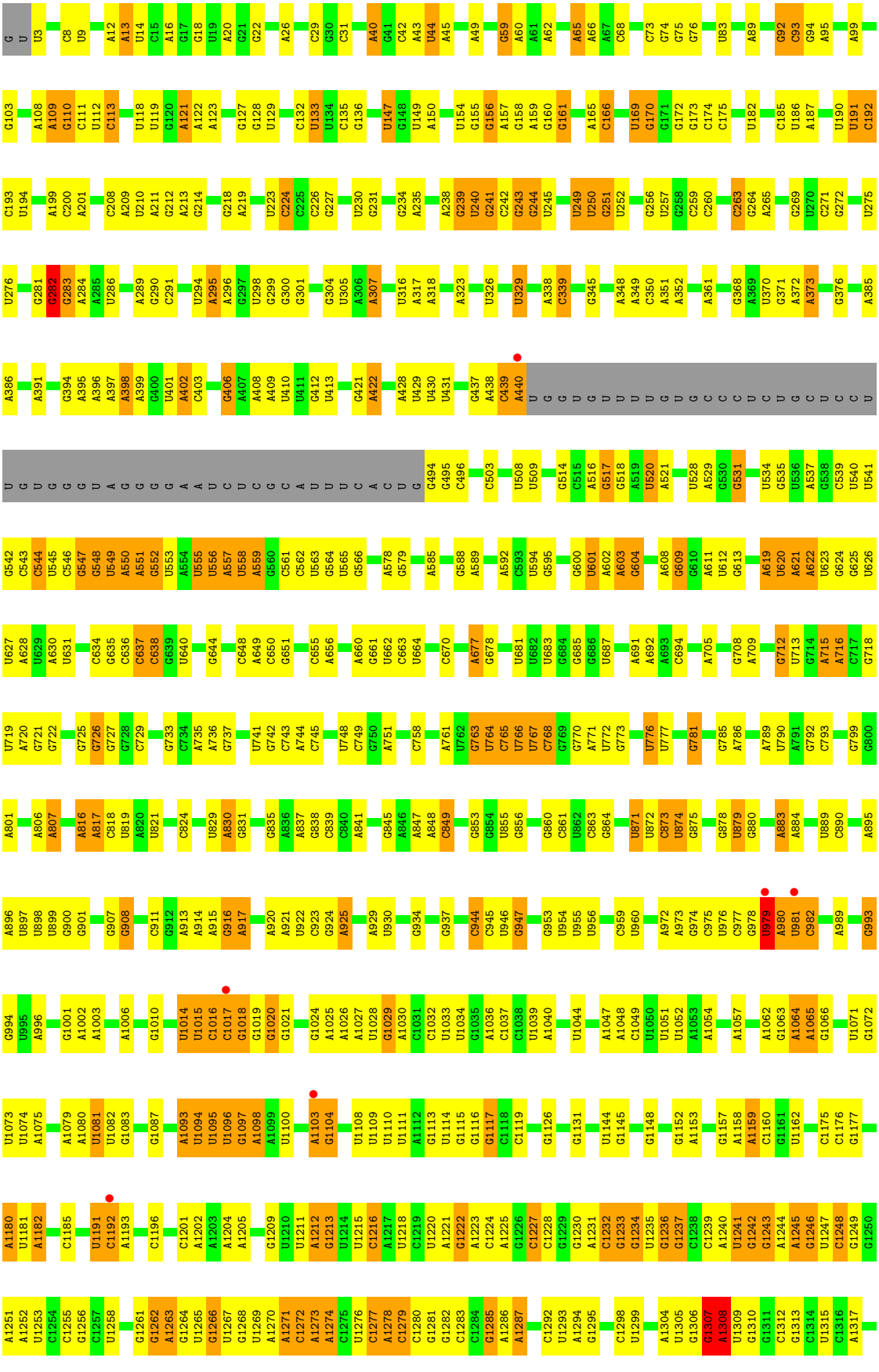


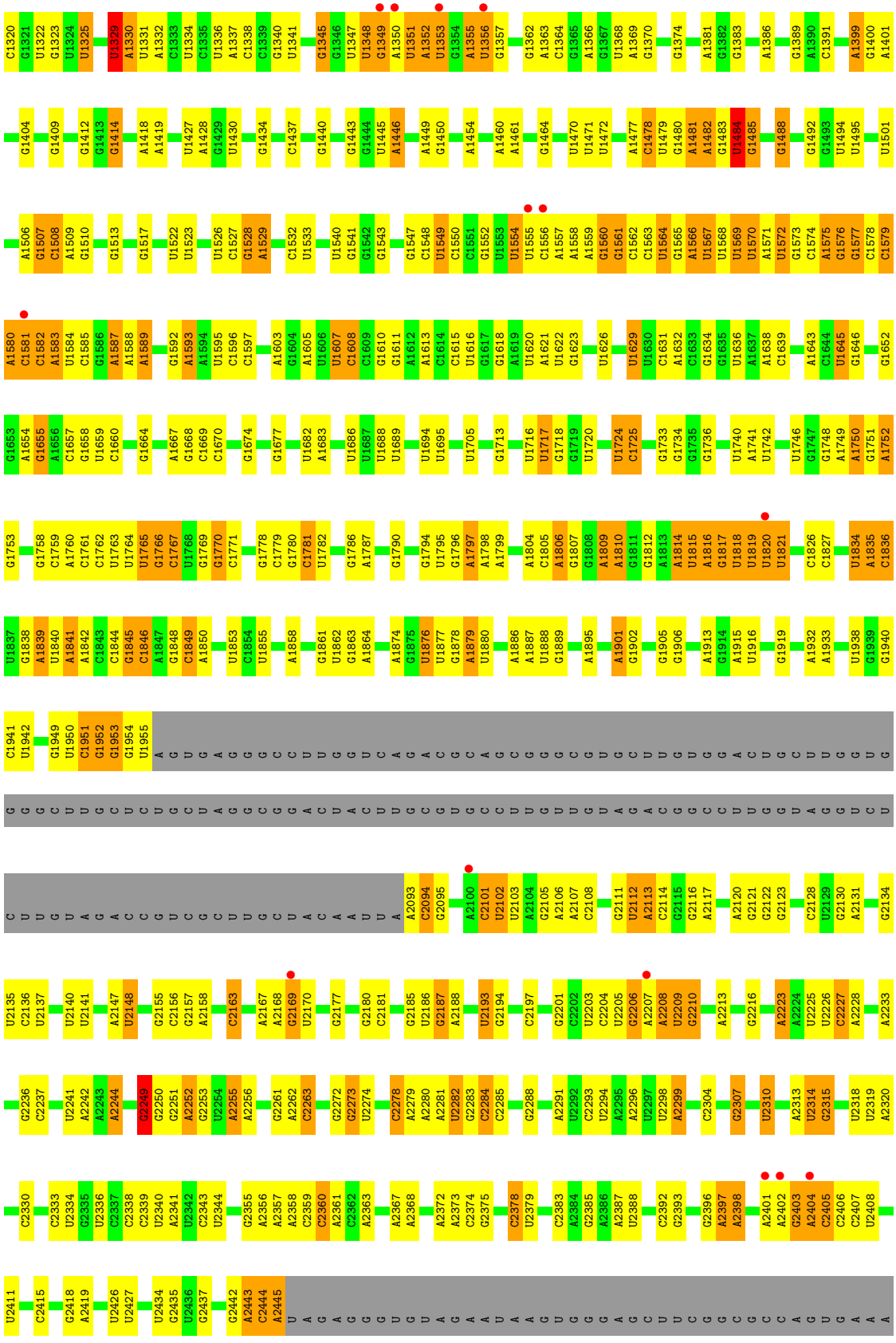


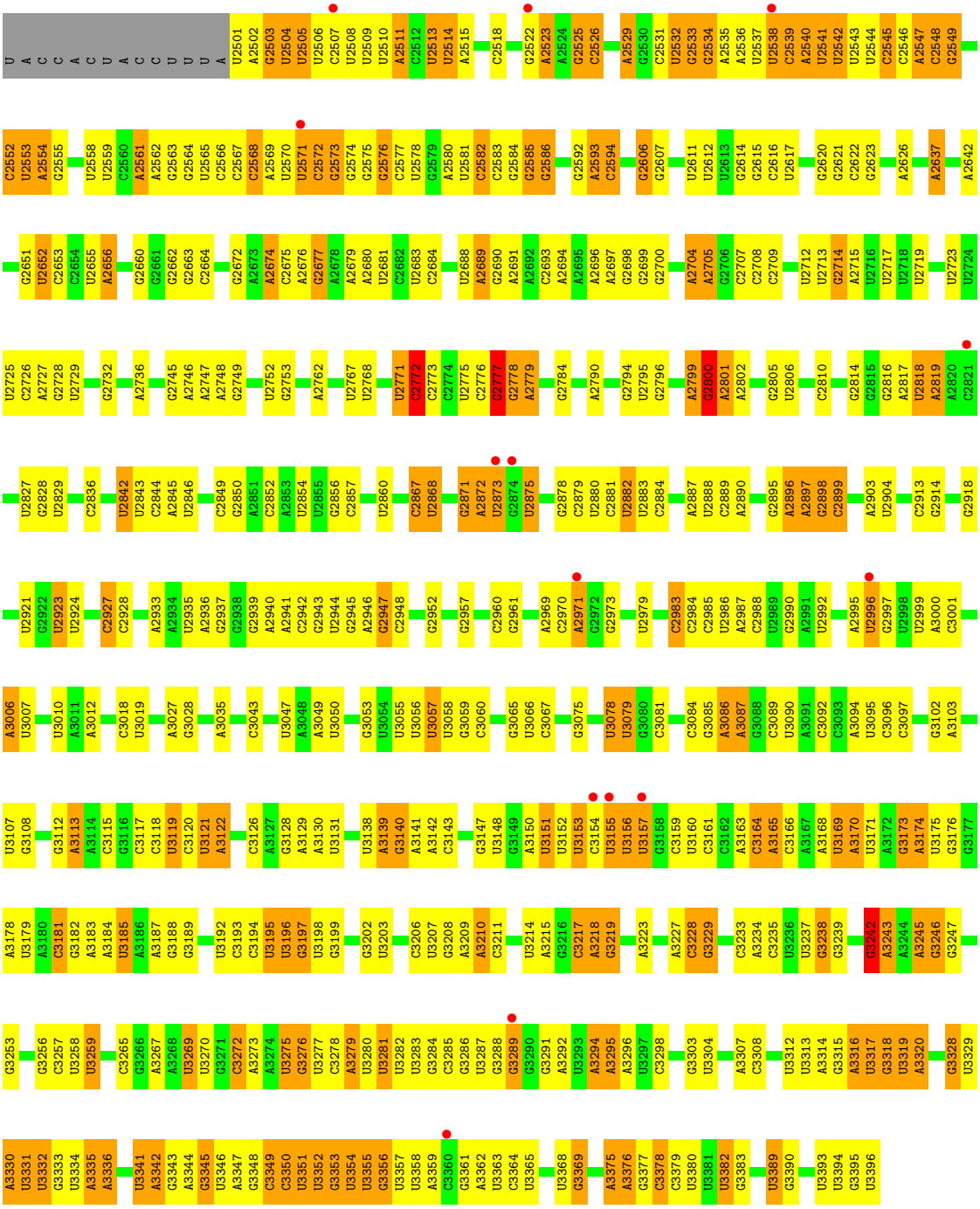
• Molecule 36: 25S rRNA

Chain A1:





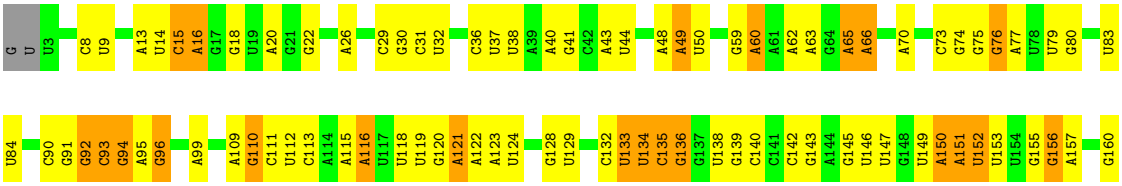


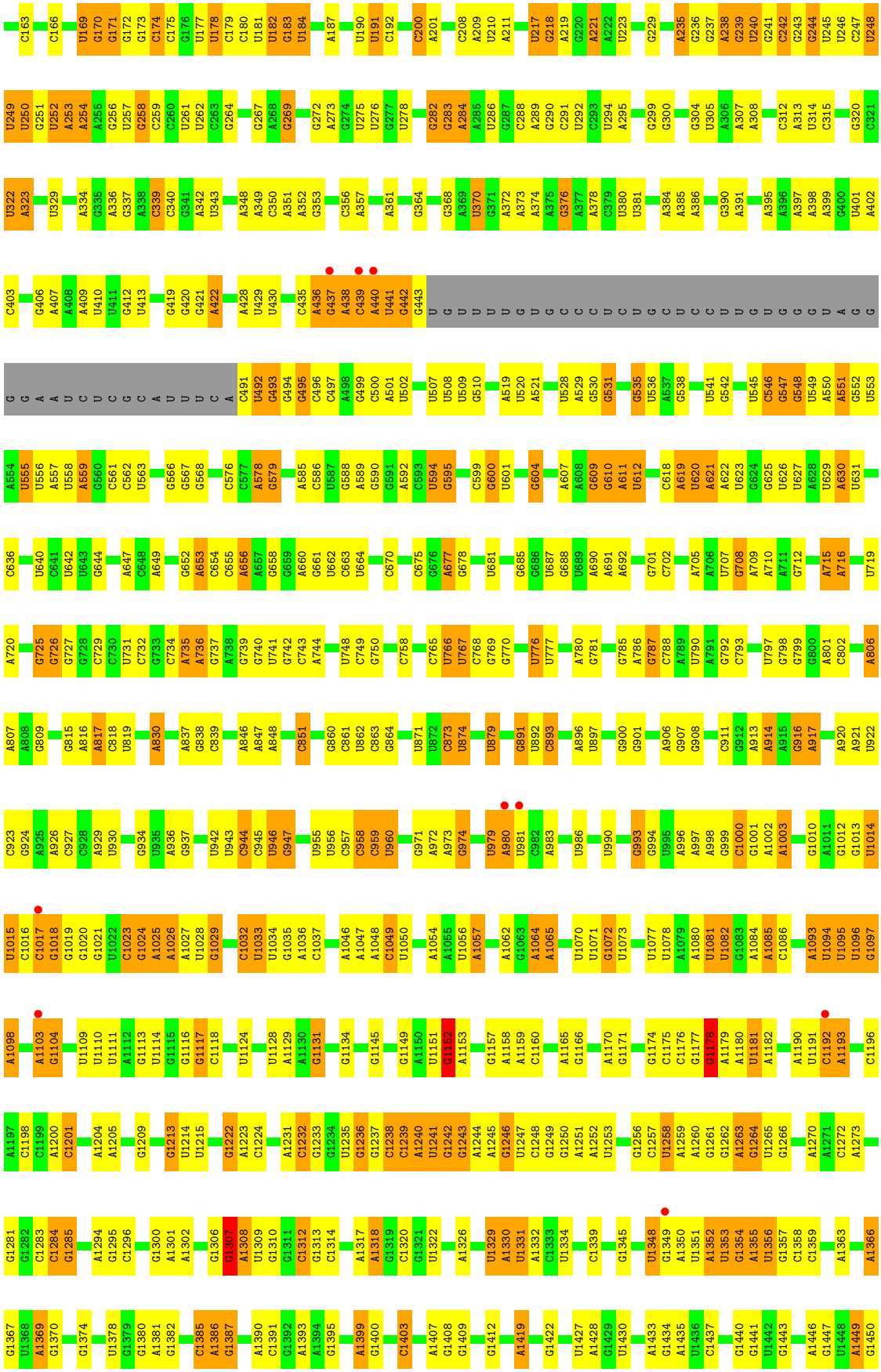


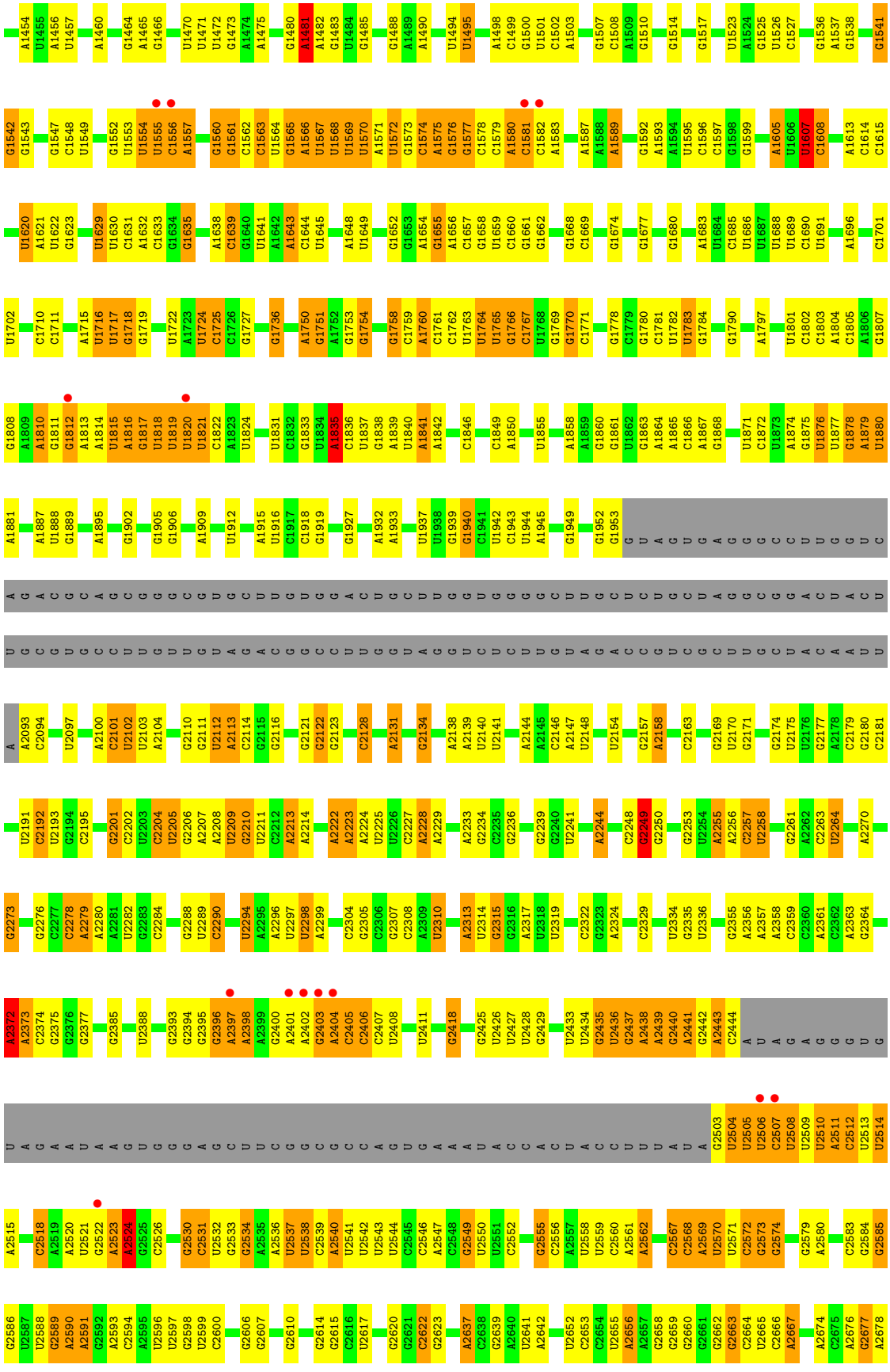
• Molecule 36: 25S rRNA

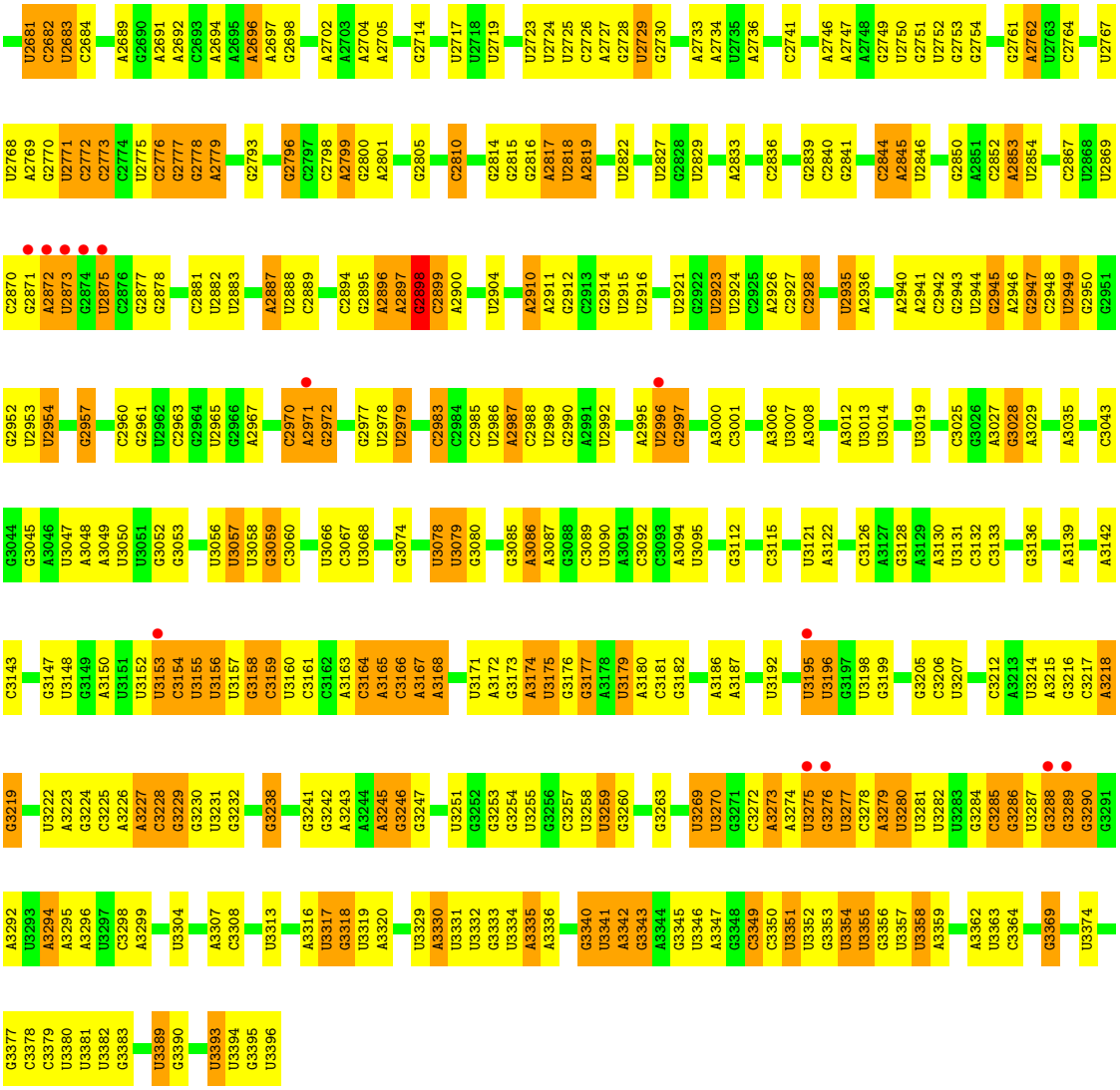
Chain A5:







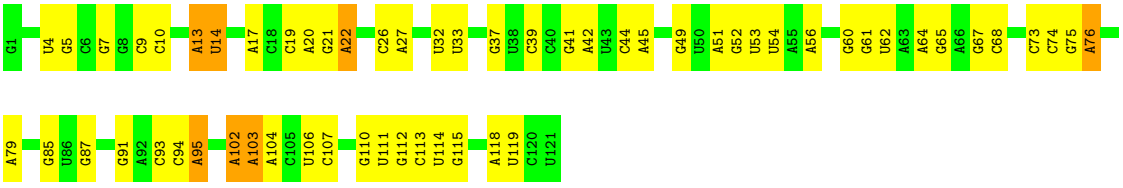




• Molecule 37: 5S rRNA

Chain A3:

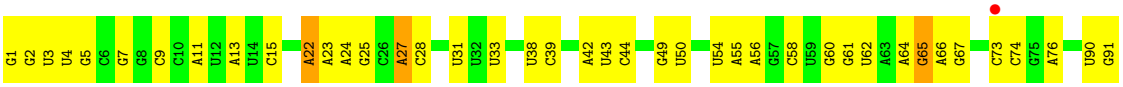




• Molecule 37: 5S rRNA

Chain A7:



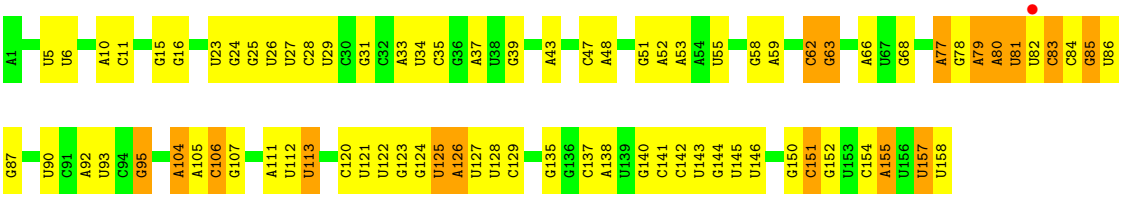




• Molecule 38: 5.8S rRNA

Chain A4:

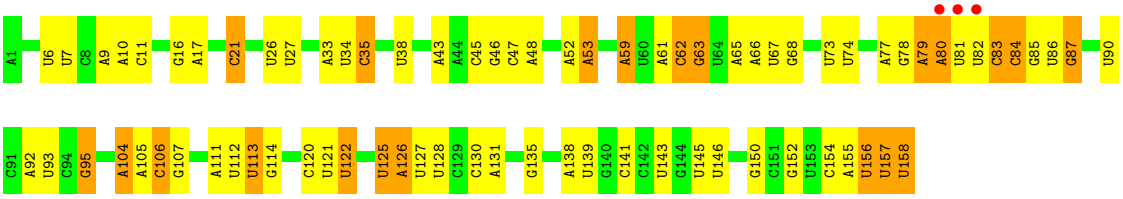




• Molecule 38: 5.8S rRNA

Chain A8:

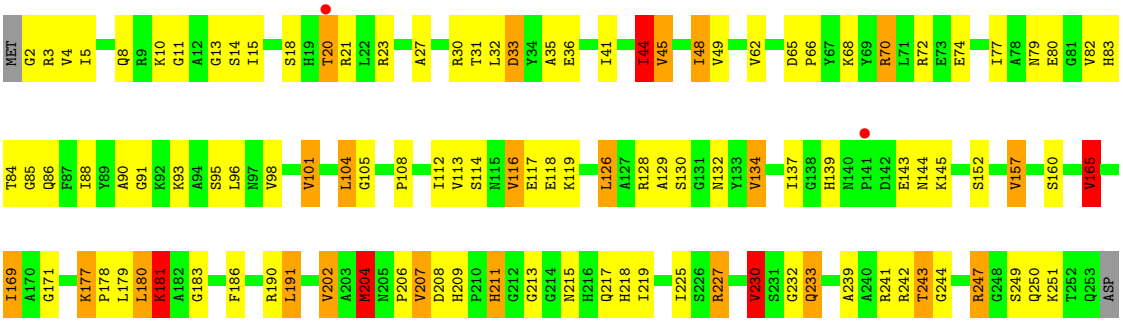




• Molecule 39: 60S ribosomal protein L2-A

Chain BA:

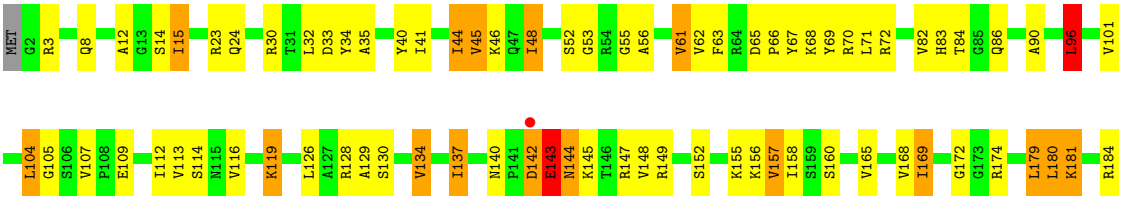


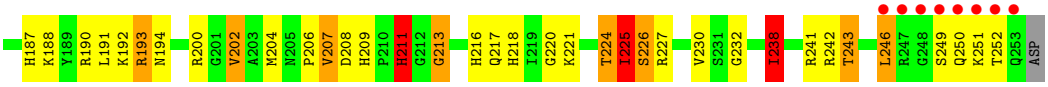


• Molecule 39: 60S ribosomal protein L2-A

Chain DA:

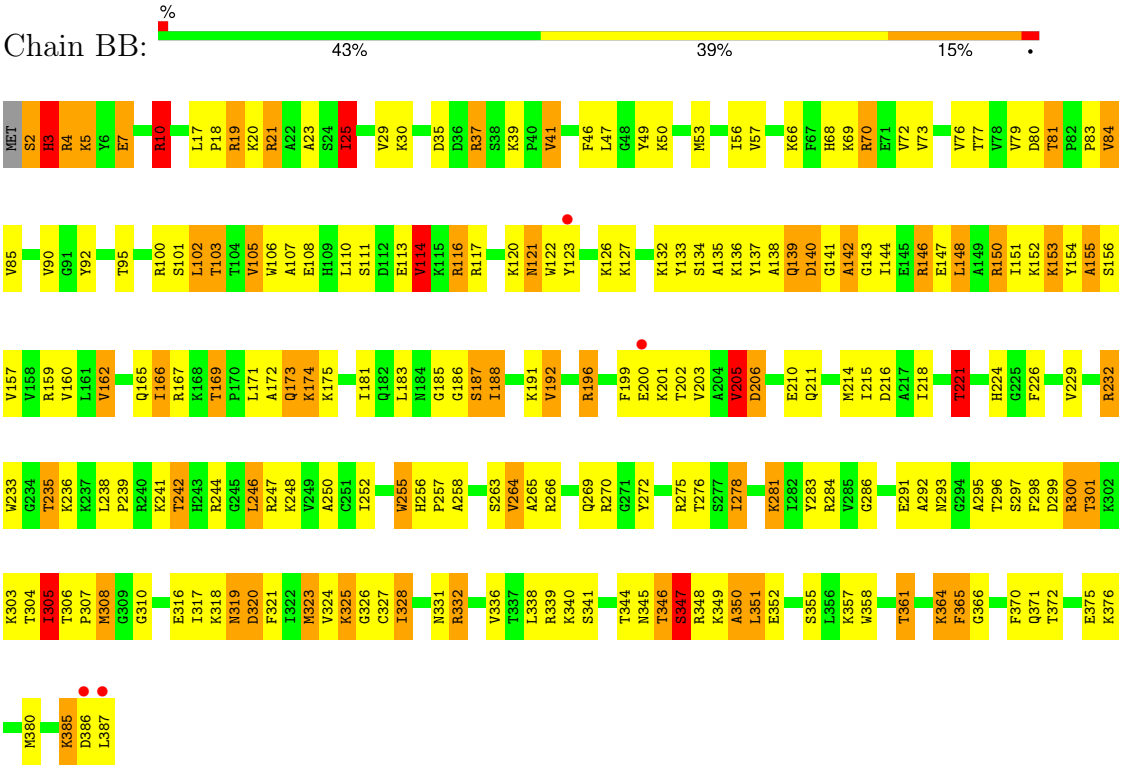






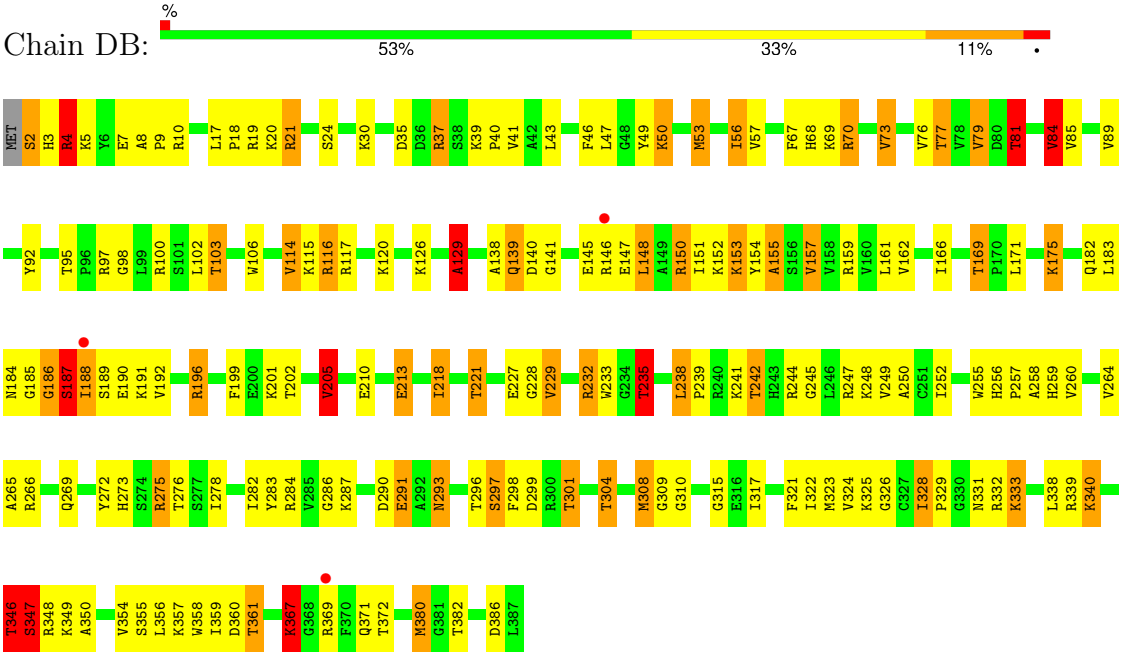
• Molecule 40: 60S ribosomal protein L3

Chain BB:



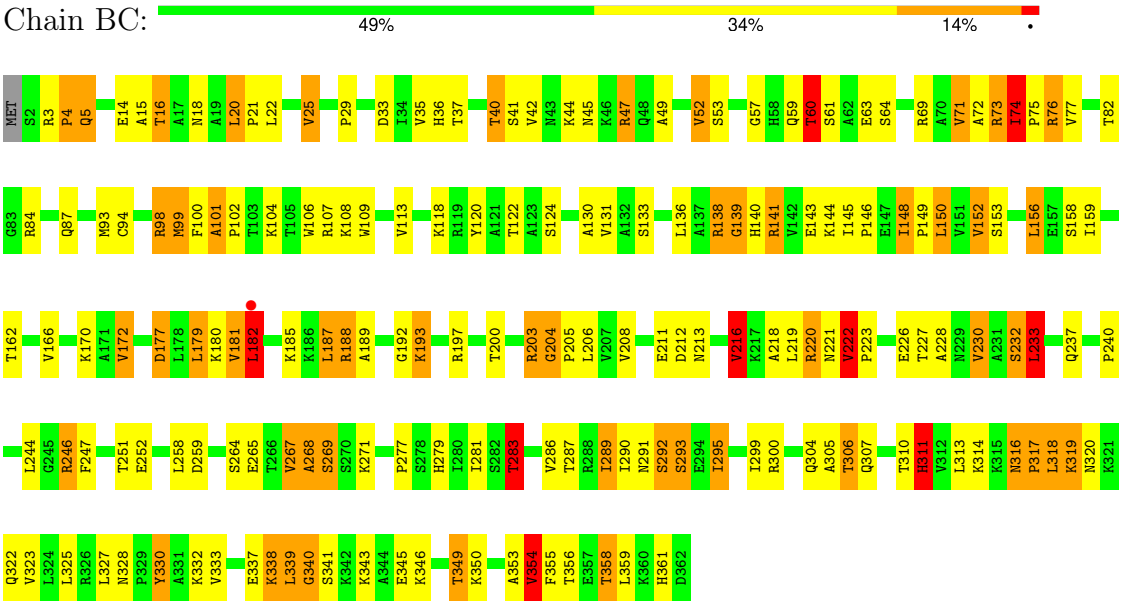
• Molecule 40: 60S ribosomal protein L3

Chain DB:



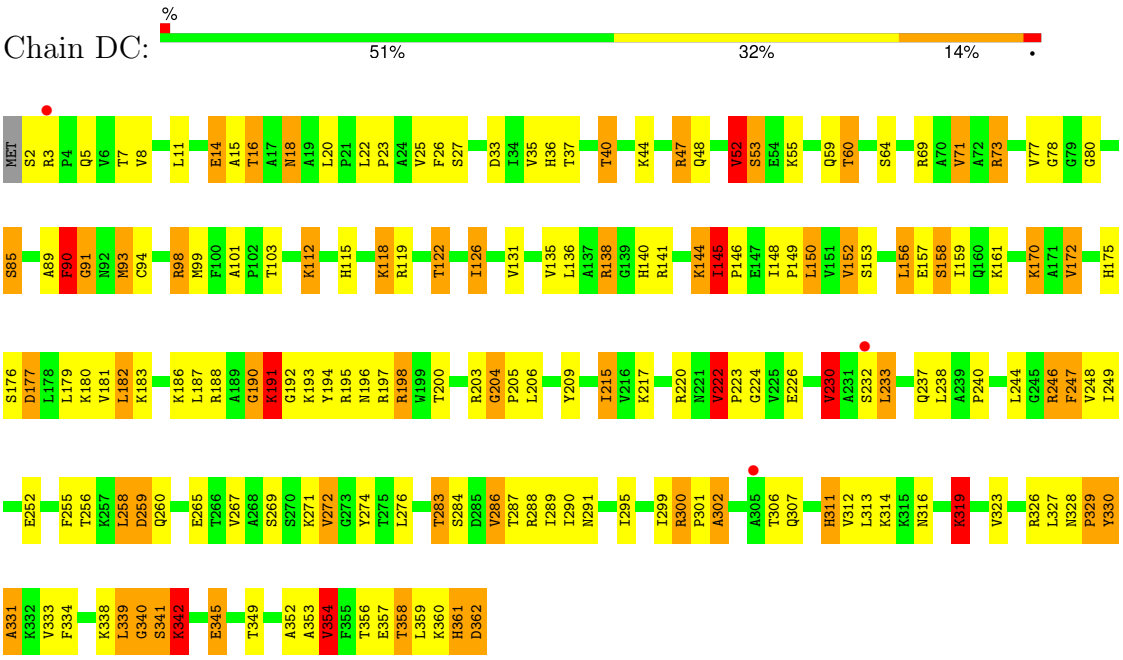
• Molecule 41: 60S ribosomal protein L4-A

Chain BC:



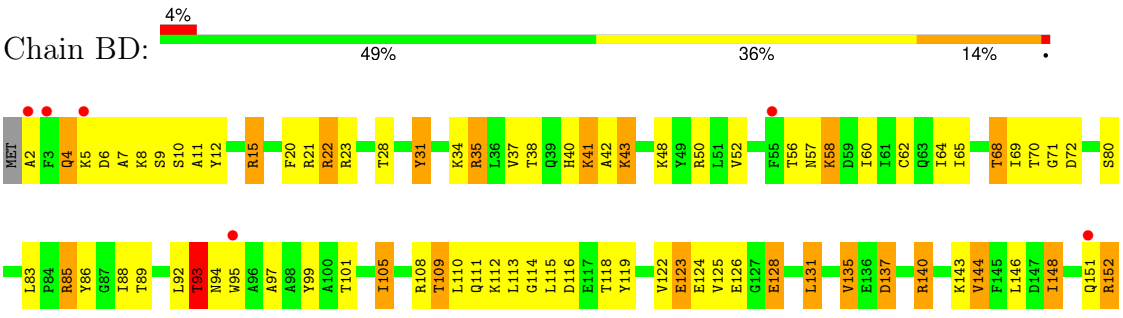
• Molecule 41: 60S ribosomal protein L4-A

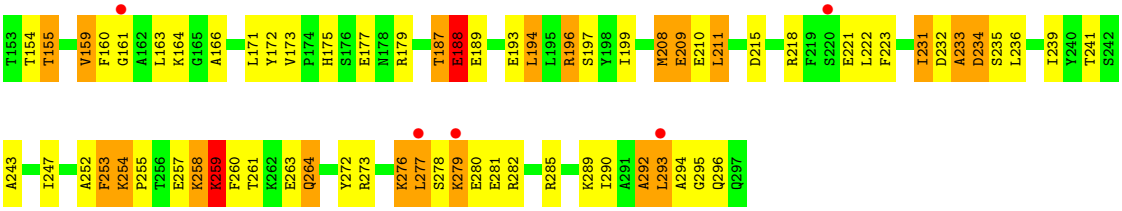
Chain DC:



• Molecule 42: 60S ribosomal protein L5

Chain BD:

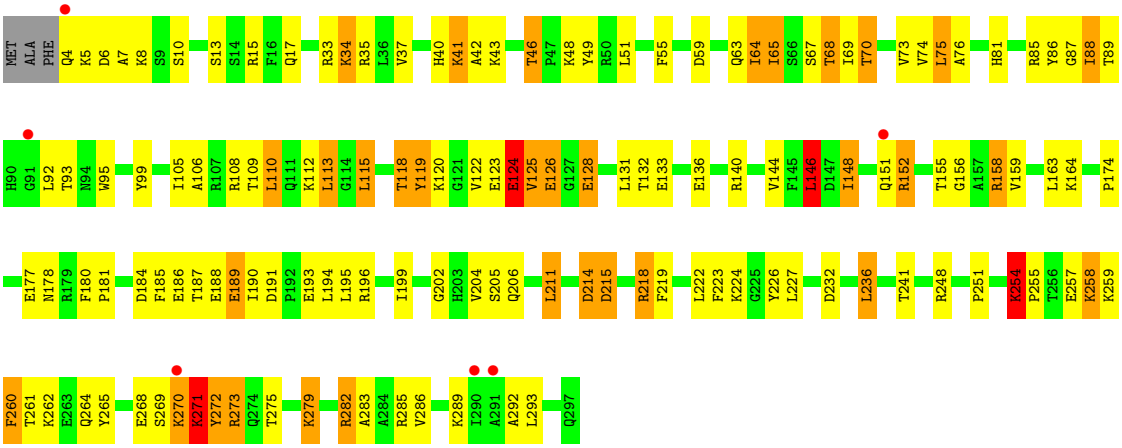




• Molecule 42: 60S ribosomal protein L5

Chain DD:

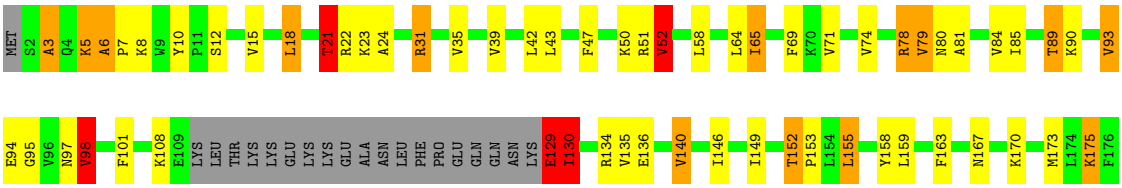




• Molecule 43: 60S ribosomal protein L6-A

Chain BE:

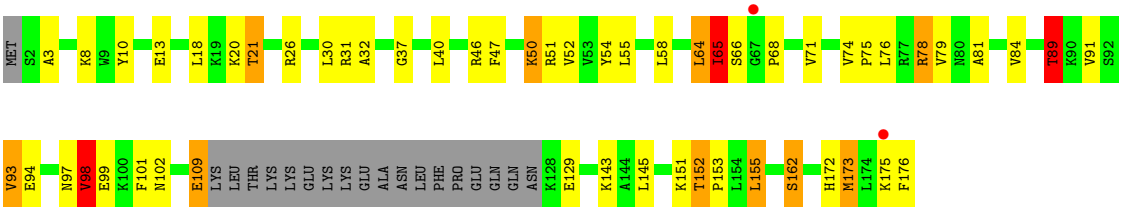




• Molecule 43: 60S ribosomal protein L6-A

Chain DE:

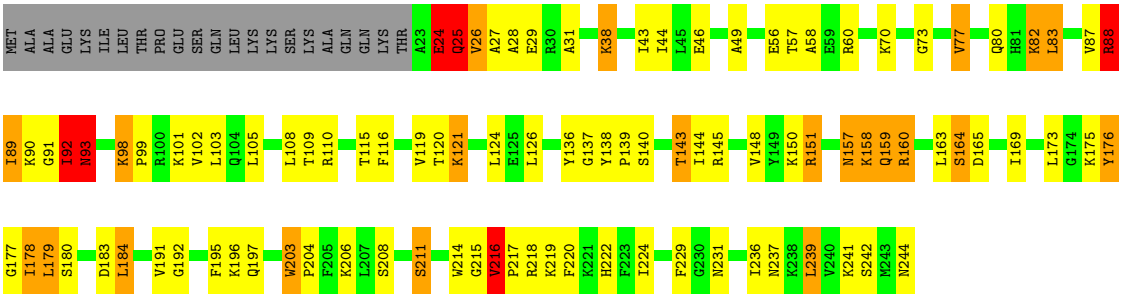




• Molecule 44: 60S ribosomal protein L7-A

Chain BF:

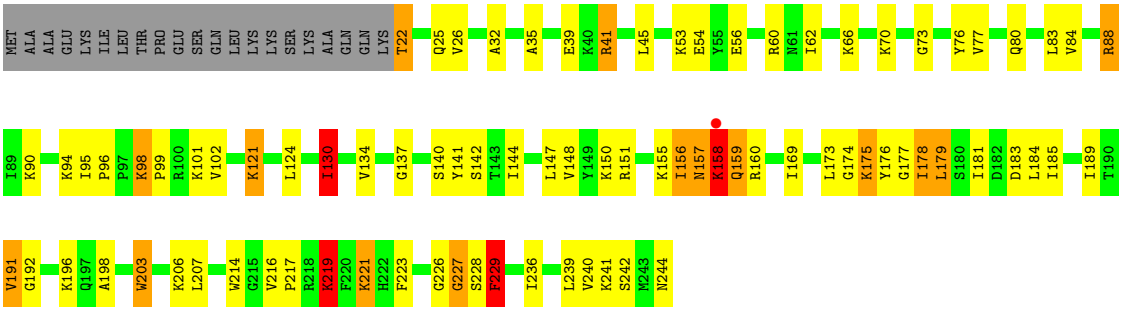




• Molecule 44: 60S ribosomal protein L7-A

Chain DF:

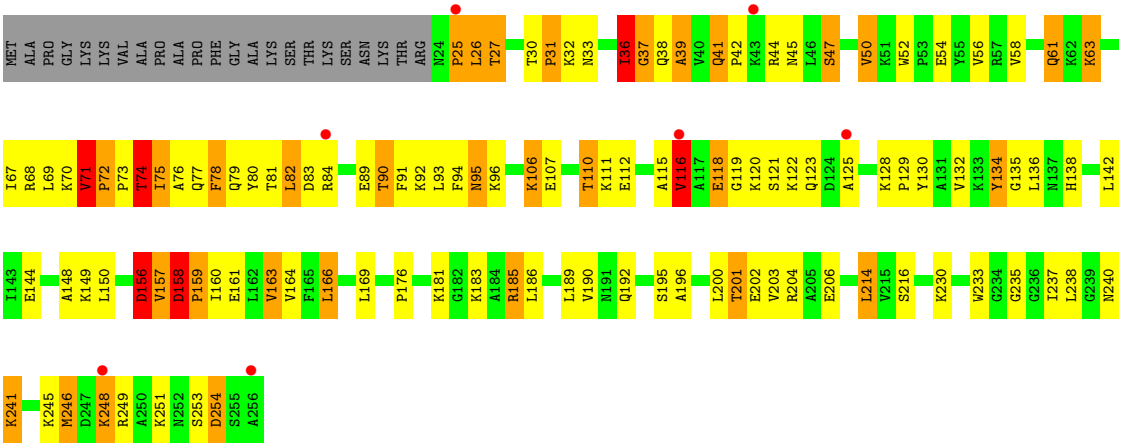




• Molecule 45: 60S ribosomal protein L8-A

Chain BG:

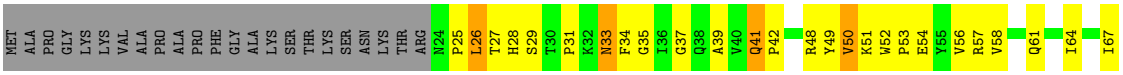


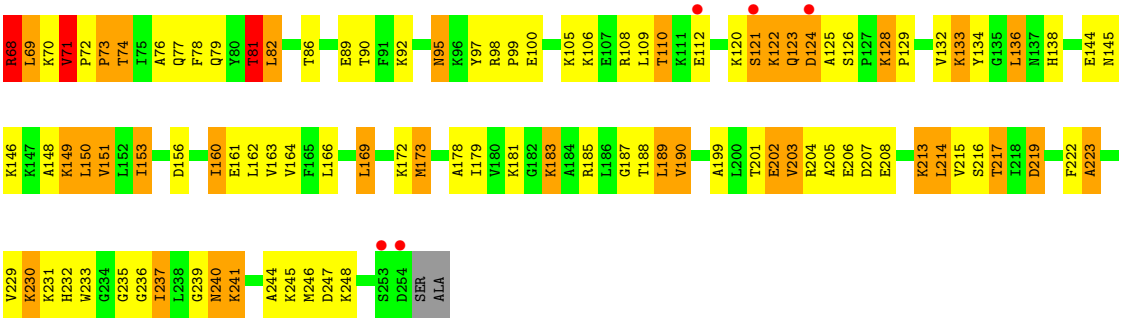


• Molecule 45: 60S ribosomal protein L8-A

Chain DG:



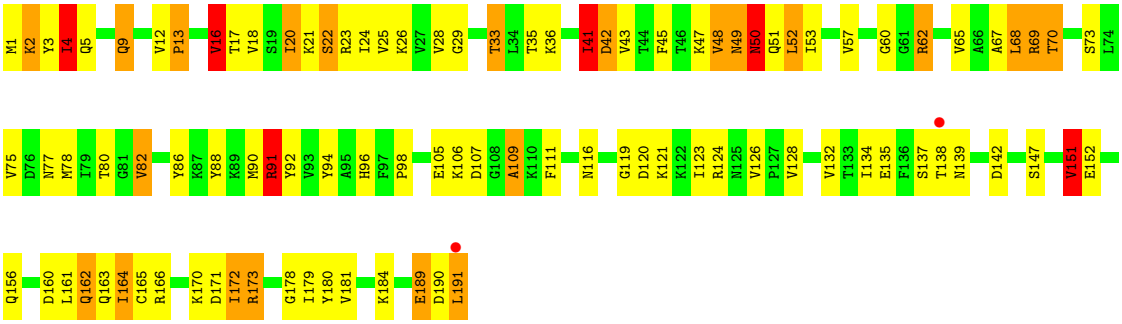




• Molecule 46: 60S ribosomal protein L9-A

Chain BH:

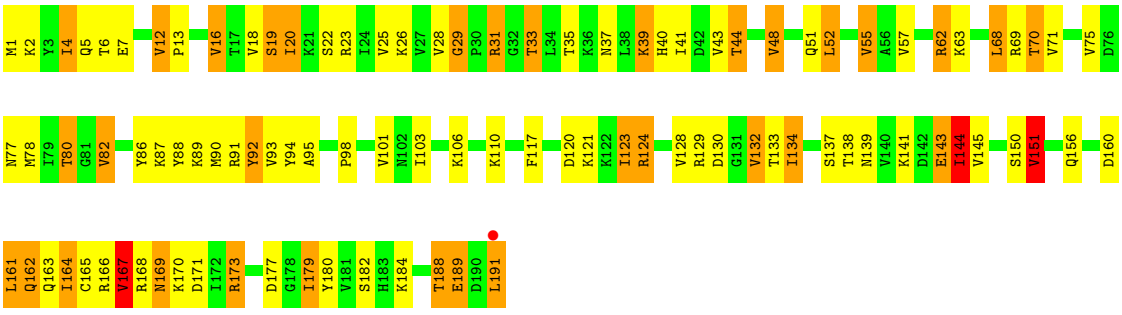




• Molecule 46: 60S ribosomal protein L9-A

Chain DH:

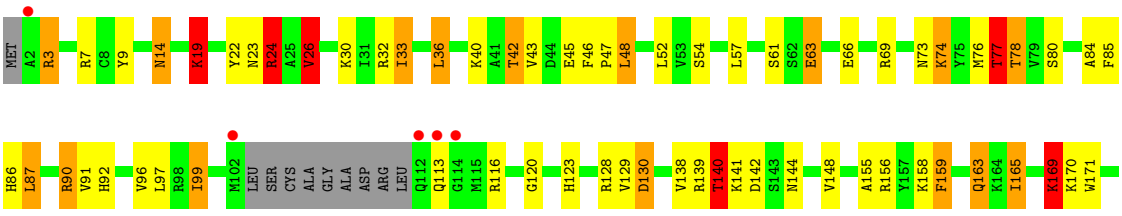


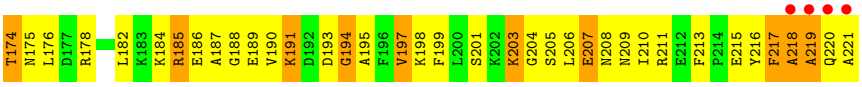


• Molecule 47: 60S ribosomal protein L10

Chain BI:



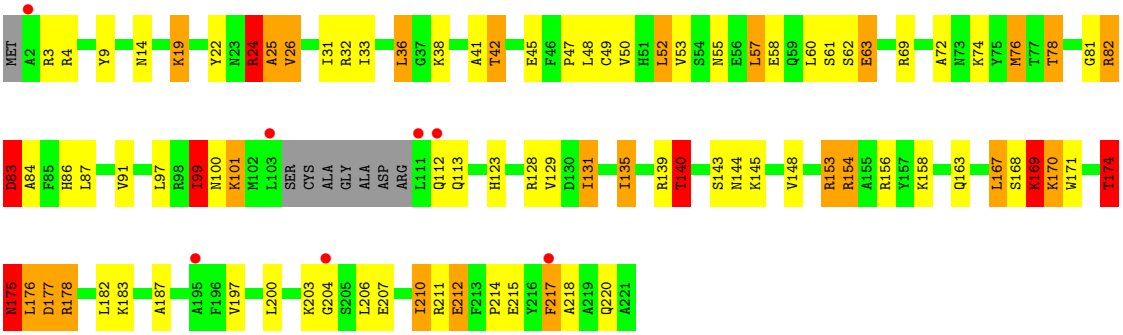




• Molecule 47: 60S ribosomal protein L10

Chain DI:

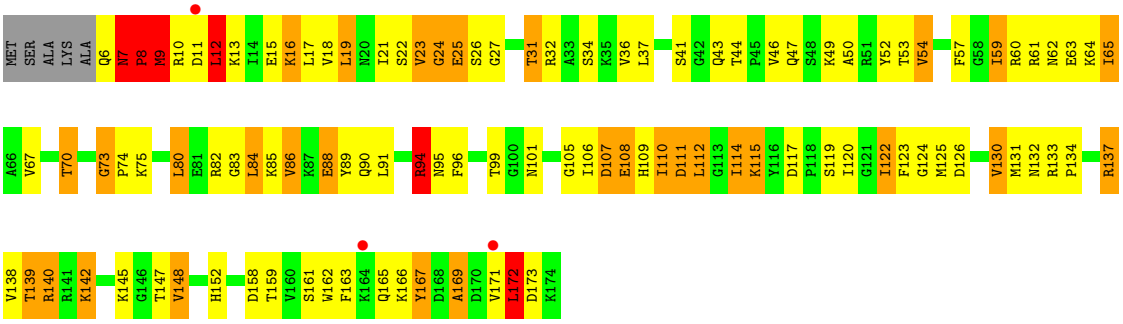




• Molecule 48: 60S ribosomal protein L11-A

Chain BJ:

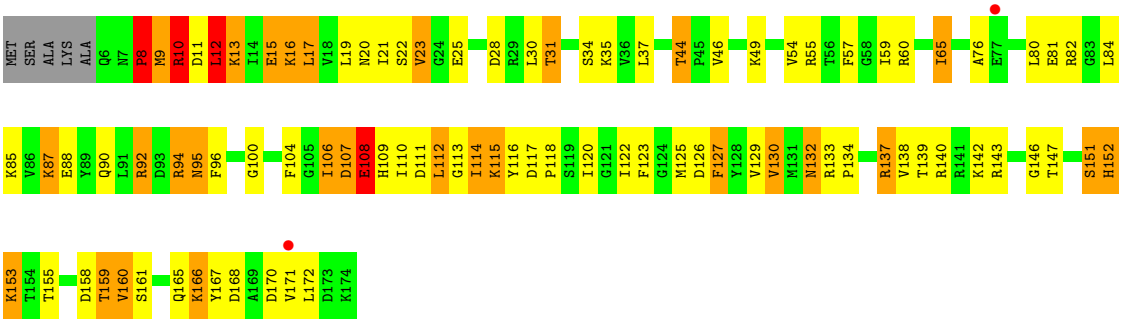




• Molecule 48: 60S ribosomal protein L11-A

Chain DJ:

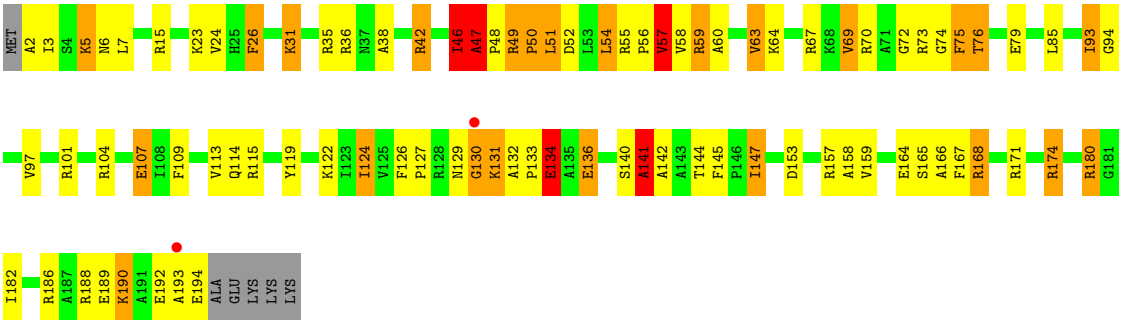




• Molecule 49: 60S ribosomal protein L13-A

Chain BL:

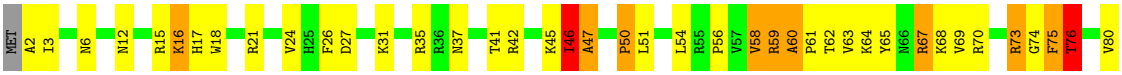


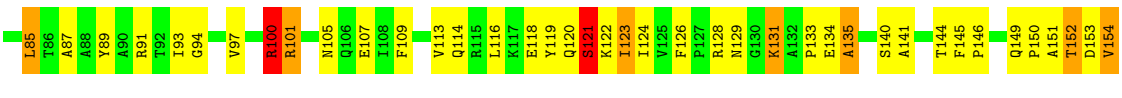


• Molecule 49: 60S ribosomal protein L13-A

Chain DL:





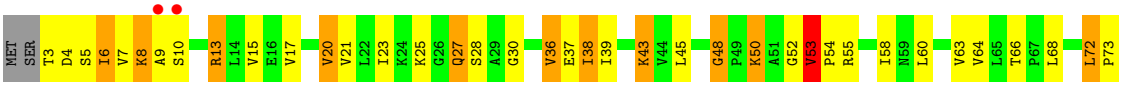




• Molecule 50: 60S ribosomal protein L14-A

Chain BM:



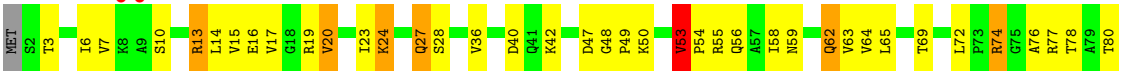




• Molecule 50: 60S ribosomal protein L14-A

Chain DM:



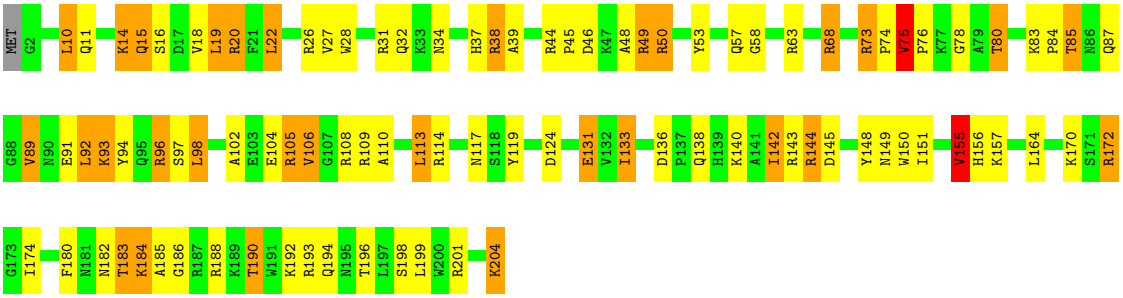




• Molecule 51: 60S ribosomal protein L15-A

Chain BN:

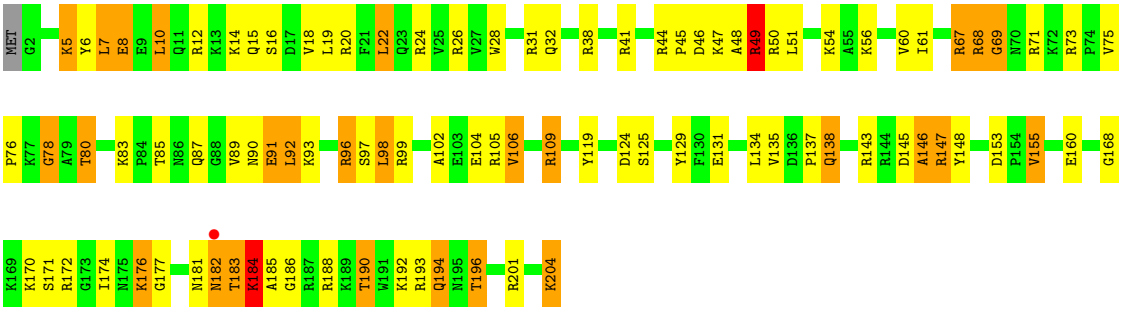




• Molecule 51: 60S ribosomal protein L15-A

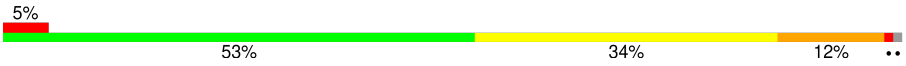
Chain DN:

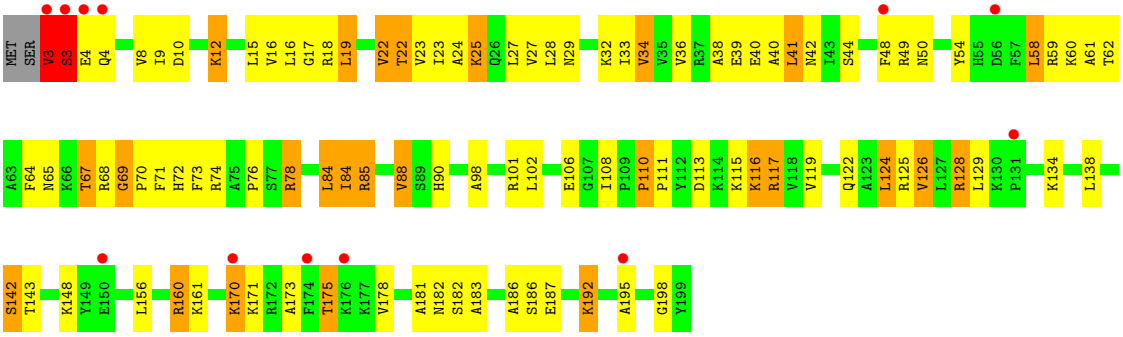




• Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain BO:

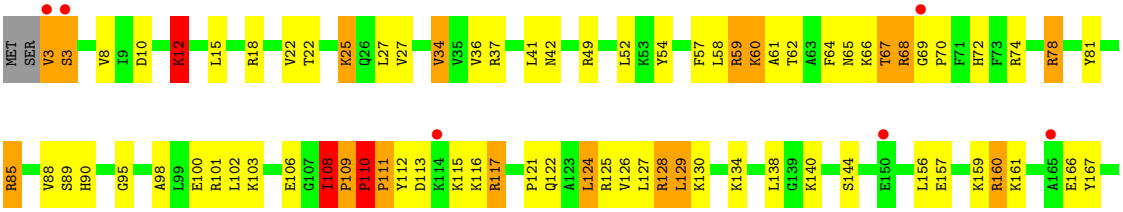


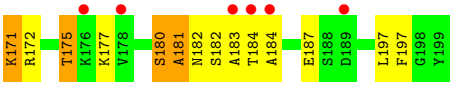


• Molecule 52: 60S ribosomal protein L16-A, 60S ribosomal protein L16-B

Chain DO:

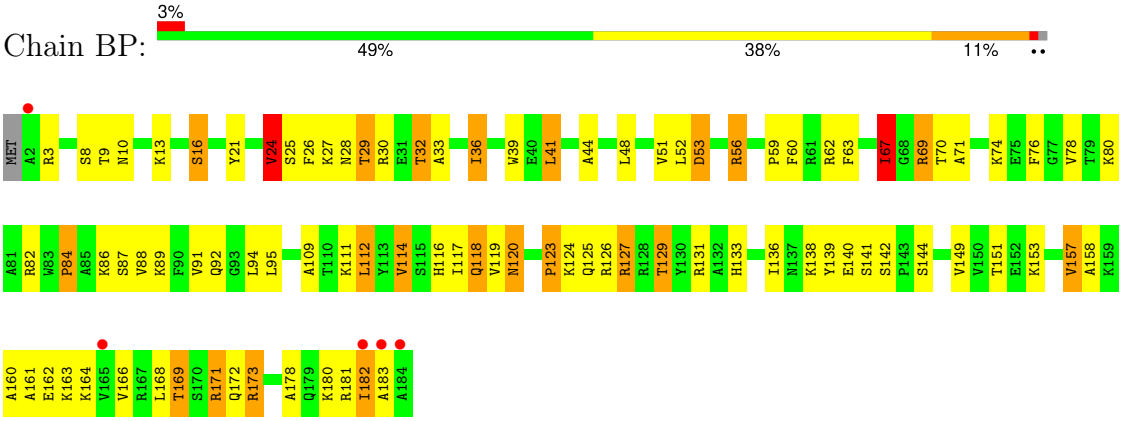






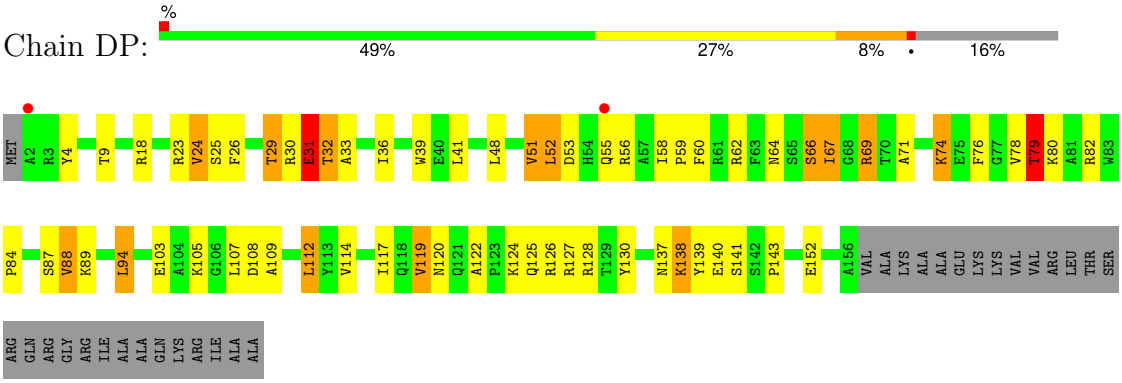
• Molecule 53: 60S ribosomal protein L17-A

Chain BP:



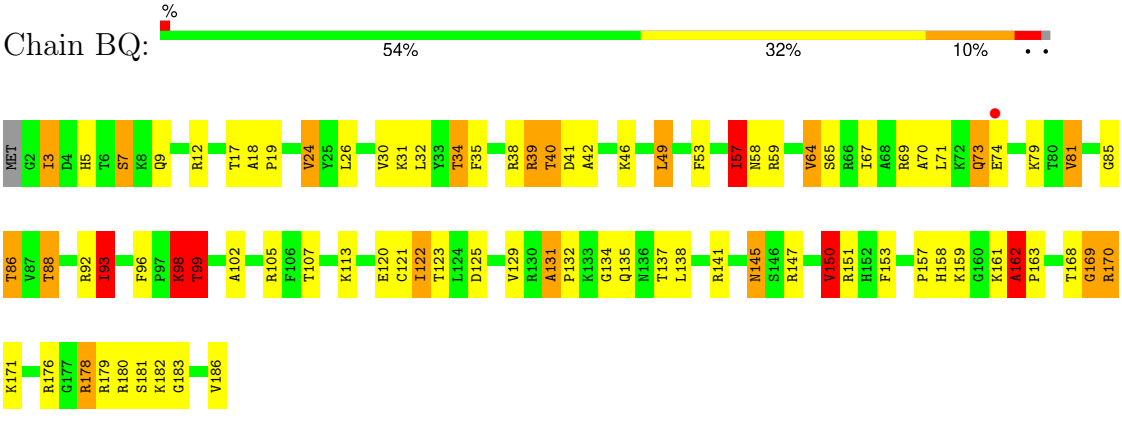
• Molecule 53: 60S ribosomal protein L17-A

Chain DP:



• Molecule 54: 60S ribosomal protein L18-A

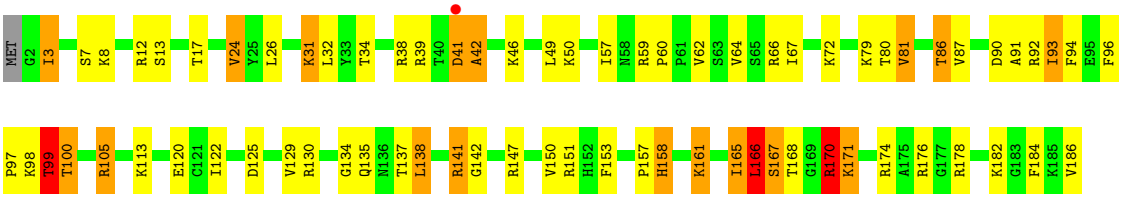
Chain BQ:



• Molecule 54: 60S ribosomal protein L18-A

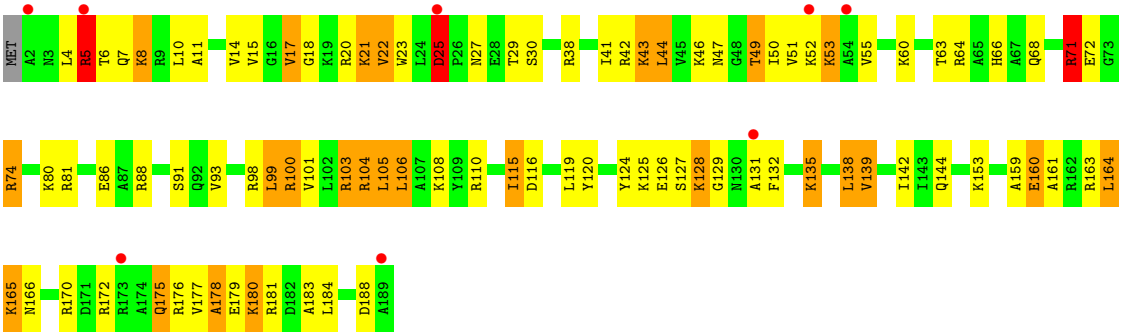
Chain DQ:





• Molecule 55: 60S ribosomal protein L19-A





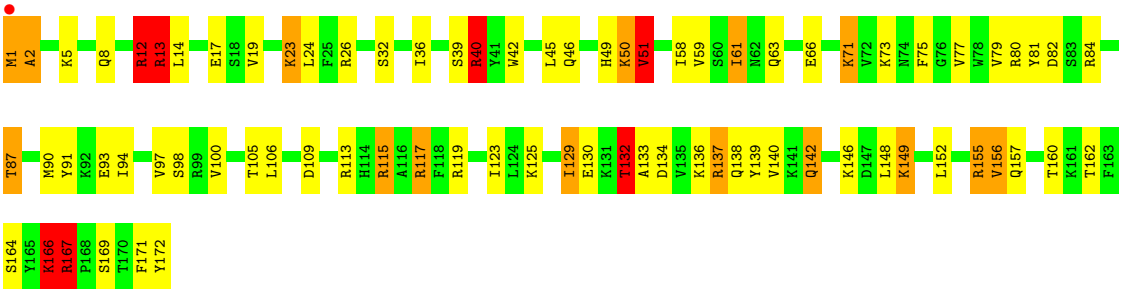
• Molecule 55: 60S ribosomal protein L19-A





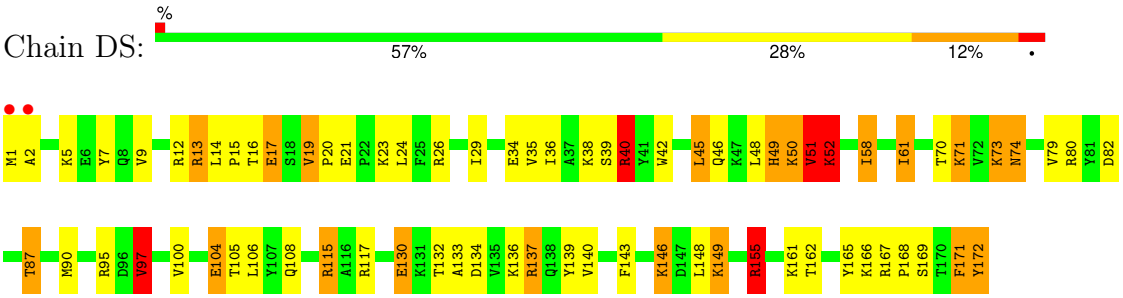
• Molecule 56: 60S ribosomal protein L20-A





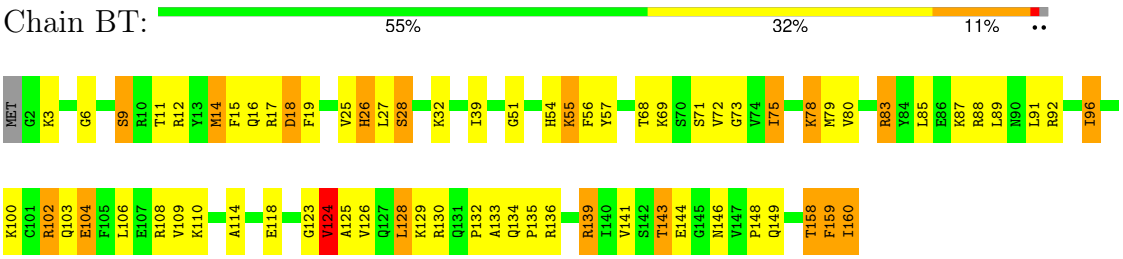
• Molecule 56: 60S ribosomal protein L20-A

Chain DS:



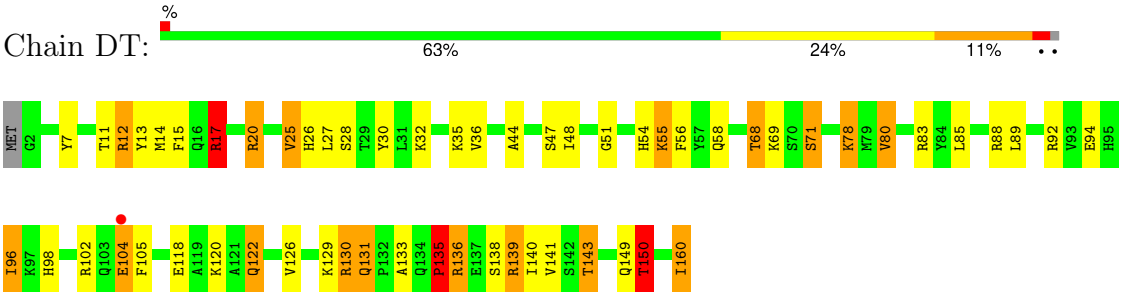
• Molecule 57: 60S ribosomal protein L21-A

Chain BT:



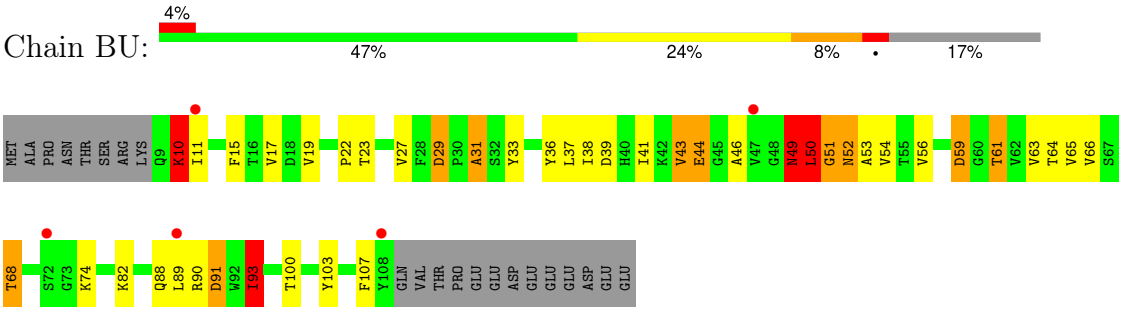
• Molecule 57: 60S ribosomal protein L21-A

Chain DT:



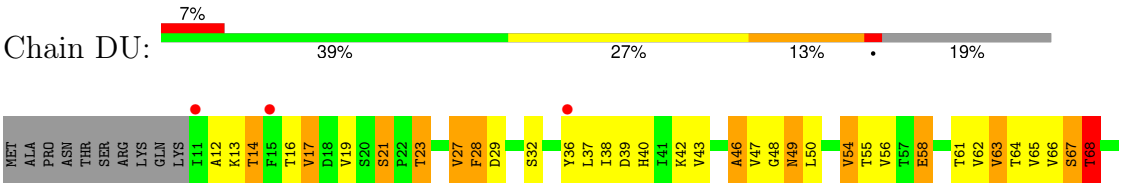
• Molecule 58: 60S ribosomal protein L22-A

Chain BU:



• Molecule 58: 60S ribosomal protein L22-A

Chain DU:

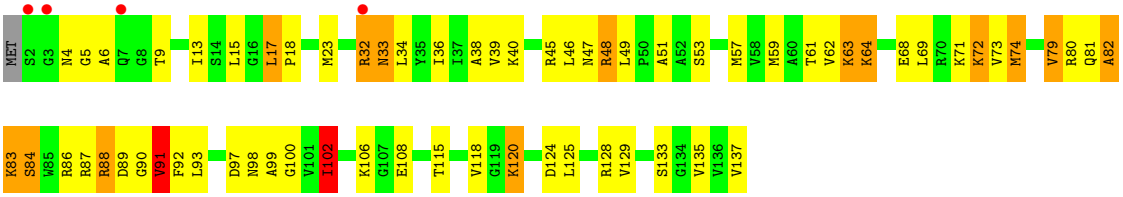




• Molecule 59: 60S ribosomal protein L23-A

Chain BV:

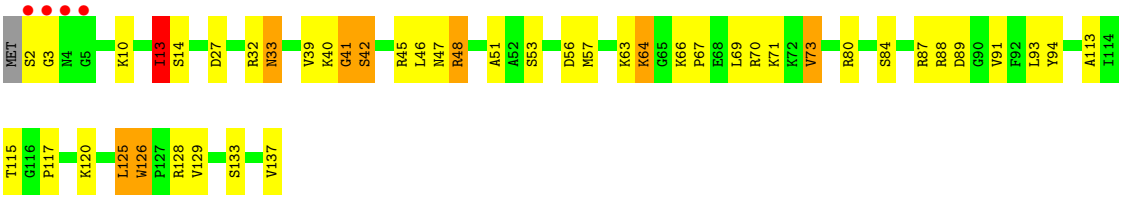




• Molecule 59: 60S ribosomal protein L23-A

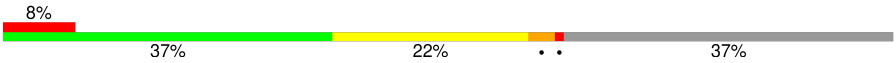
Chain DV:

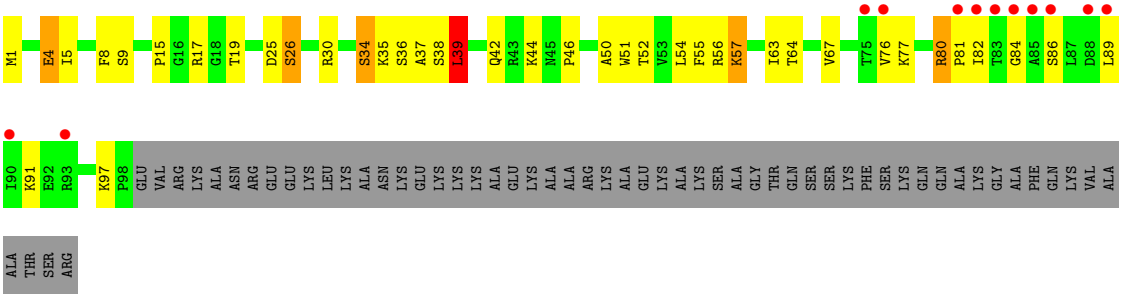




• Molecule 60: 60S ribosomal protein L24-A

Chain BW:

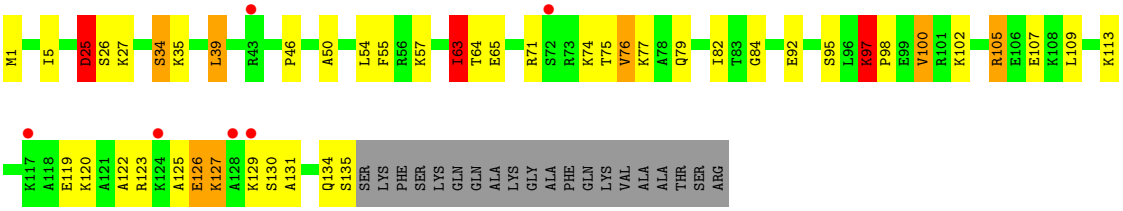




• Molecule 60: 60S ribosomal protein L24-A

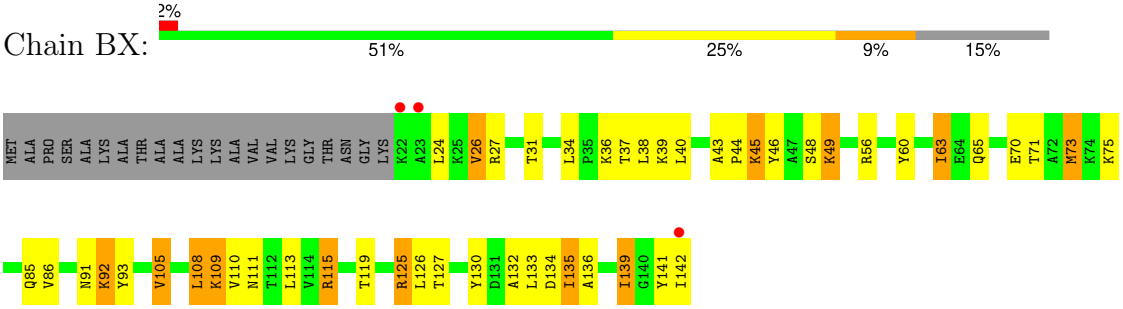
Chain DW:





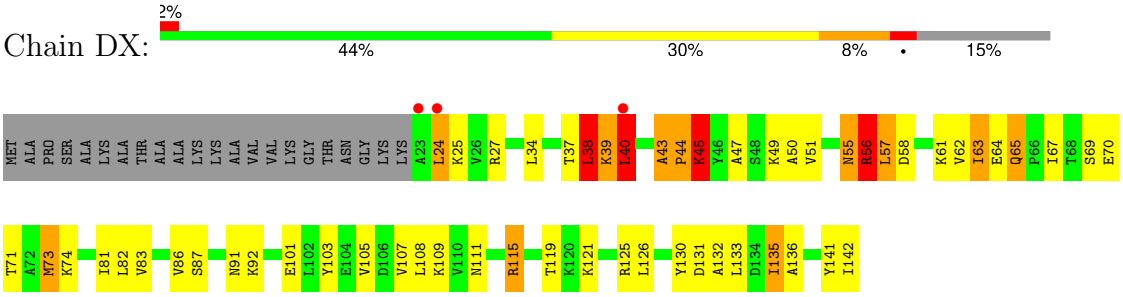
• Molecule 61: 60S ribosomal protein L25

Chain BX:



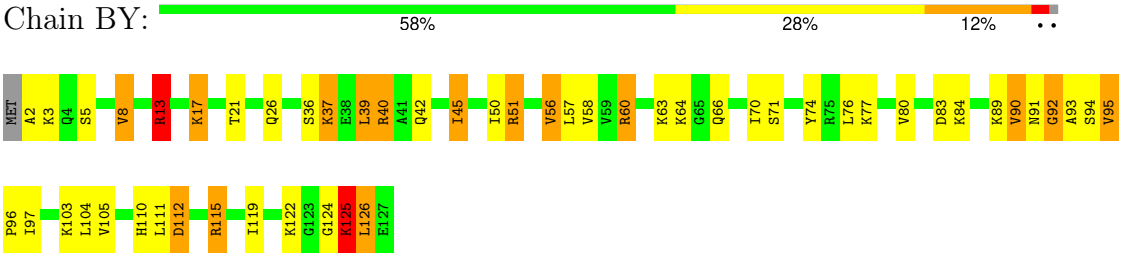
• Molecule 61: 60S ribosomal protein L25

Chain DX:



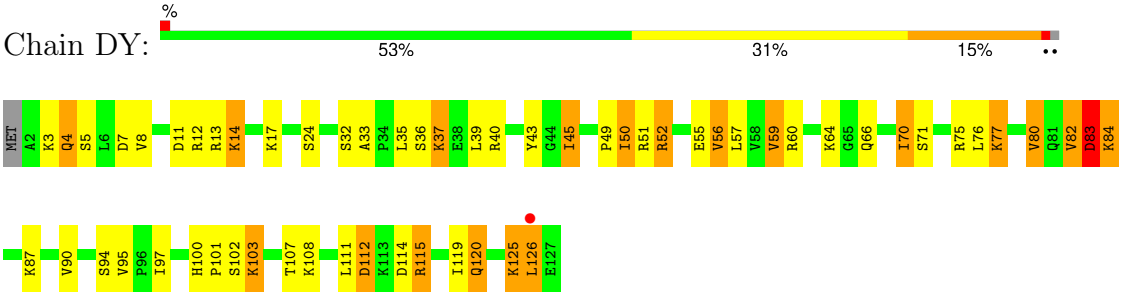
• Molecule 62: 60S ribosomal protein L26-A

Chain BY:



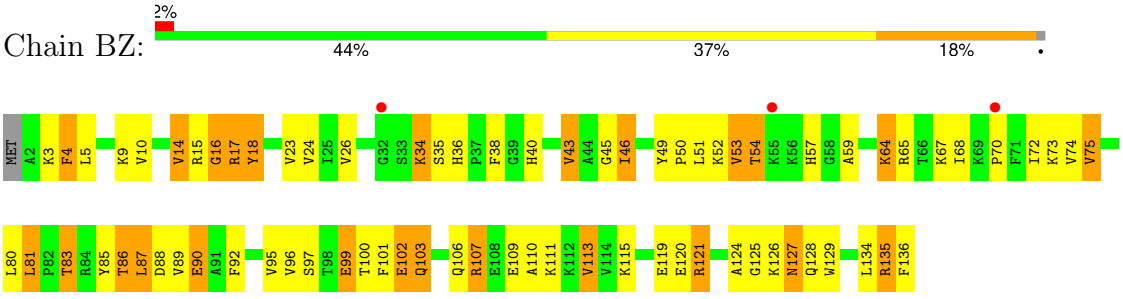
• Molecule 62: 60S ribosomal protein L26-A

Chain DY:



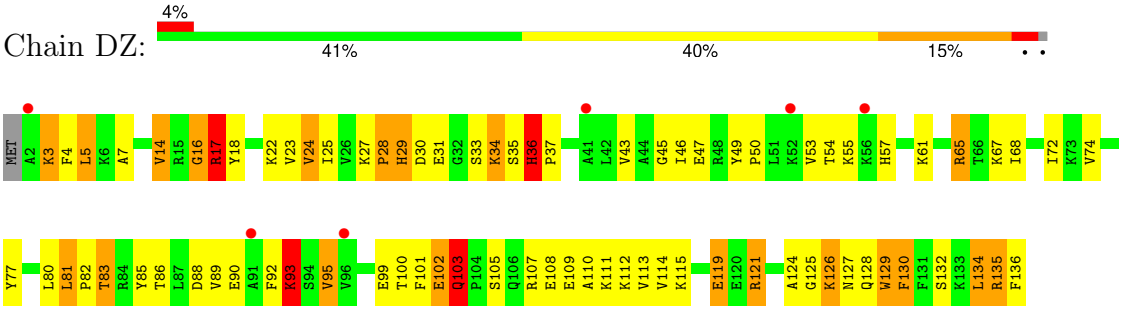
• Molecule 63: 60S ribosomal protein L27-A

Chain BZ:



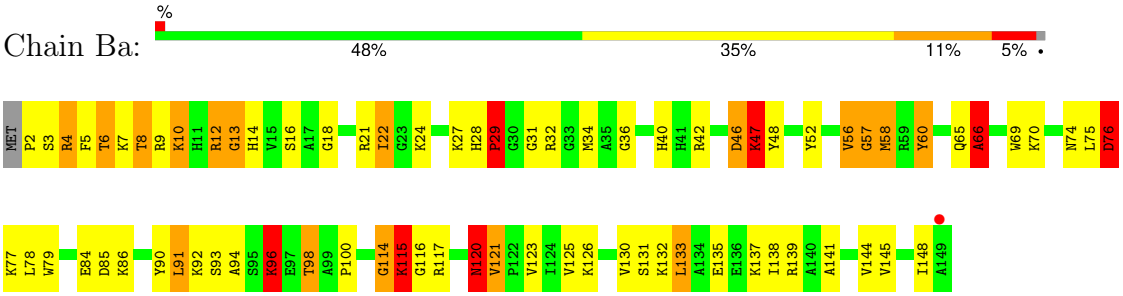
• Molecule 63: 60S ribosomal protein L27-A

Chain DZ:



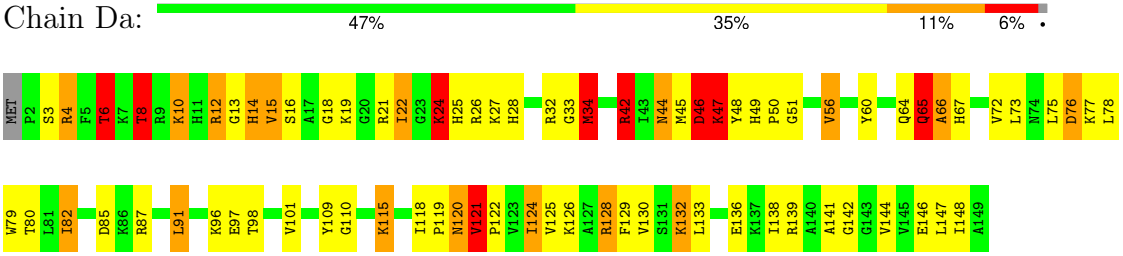
• Molecule 64: 60S ribosomal protein L28

Chain Ba:



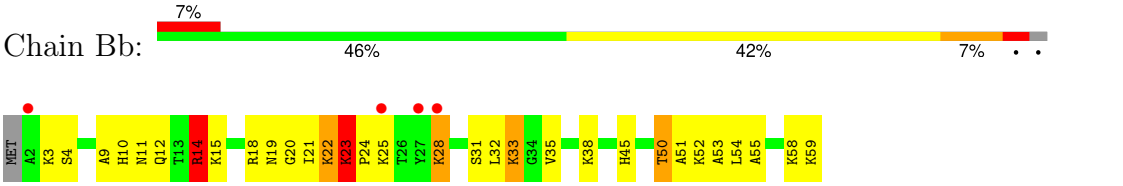
• Molecule 64: 60S ribosomal protein L28

Chain Da:



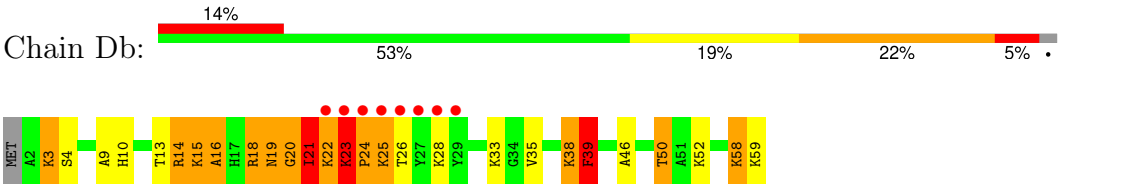
• Molecule 65: 60S ribosomal protein L29

Chain Bb:



• Molecule 65: 60S ribosomal protein L29

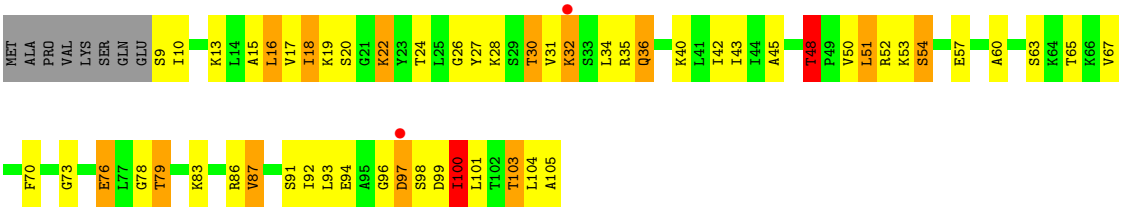
Chain Db:



• Molecule 66: 60S ribosomal protein L30

Chain Bc:

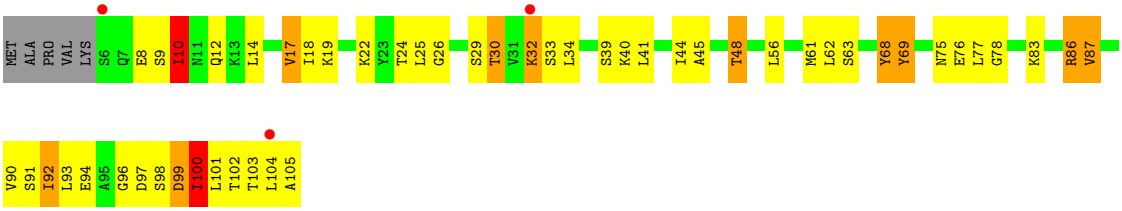




• Molecule 66: 60S ribosomal protein L30

Chain Dc:

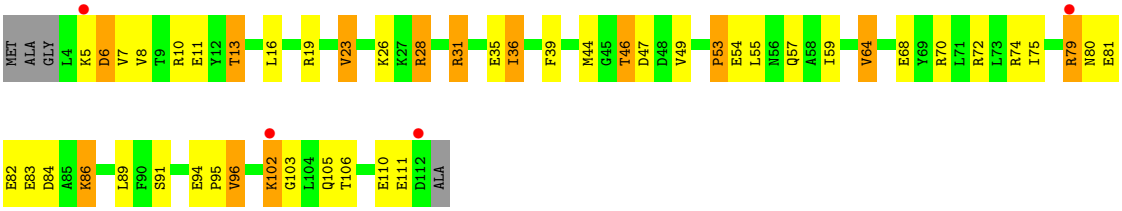




• Molecule 67: 60S ribosomal protein L31-A

Chain Bd:

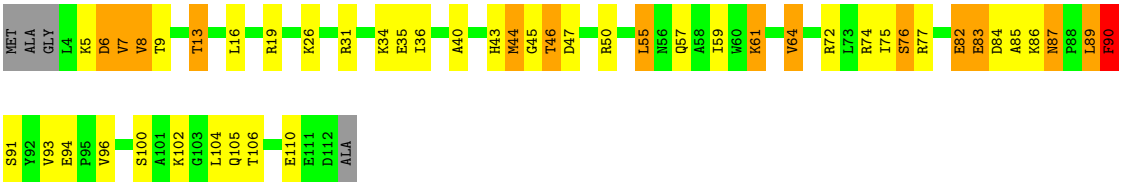




• Molecule 67: 60S ribosomal protein L31-A

Chain Dd:

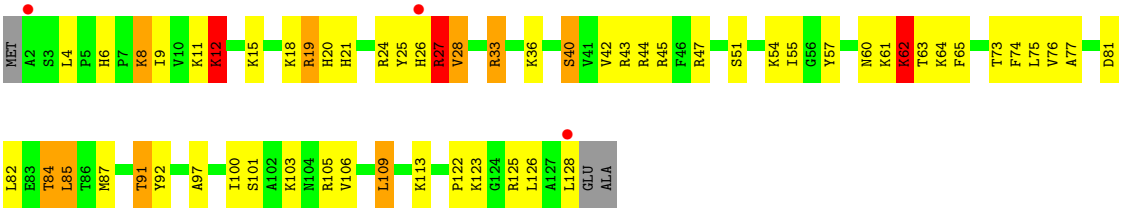




• Molecule 68: 60S ribosomal protein L32

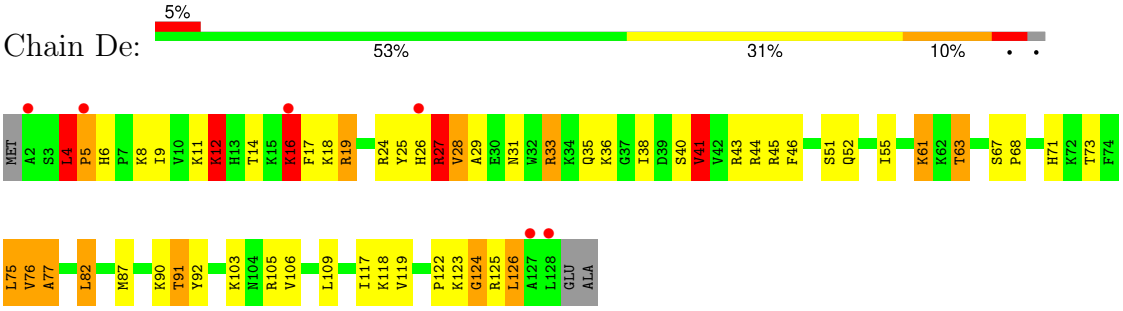
Chain Be:





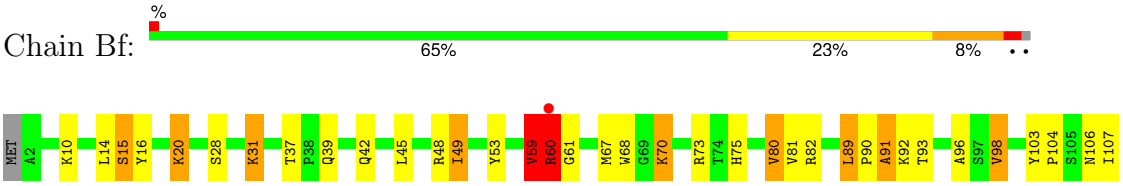
• Molecule 68: 60S ribosomal protein L32

Chain De:



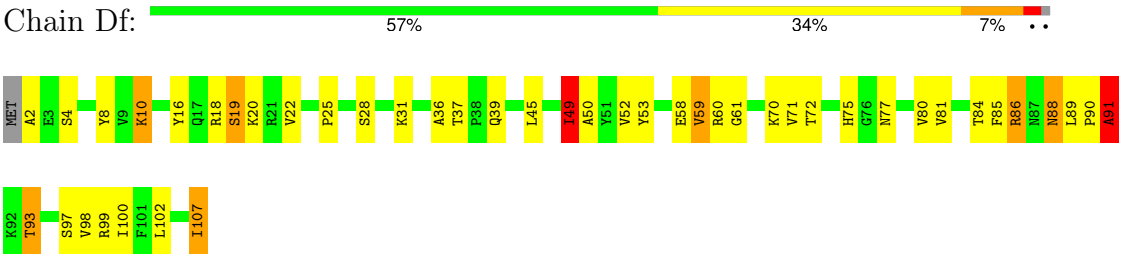
• Molecule 69: 60S ribosomal protein L33-A

Chain Bf:



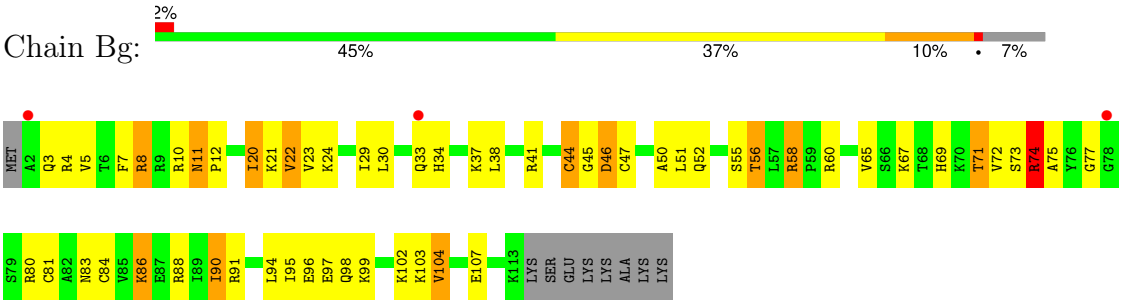
• Molecule 69: 60S ribosomal protein L33-A

Chain Df:



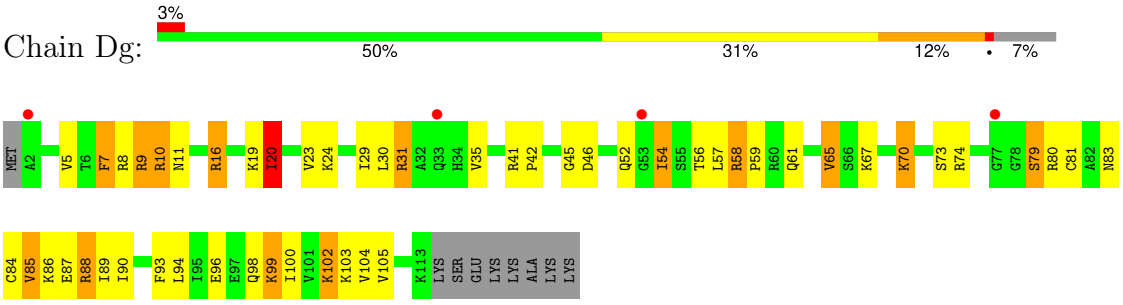
• Molecule 70: 60S ribosomal protein L34-A

Chain Bg:



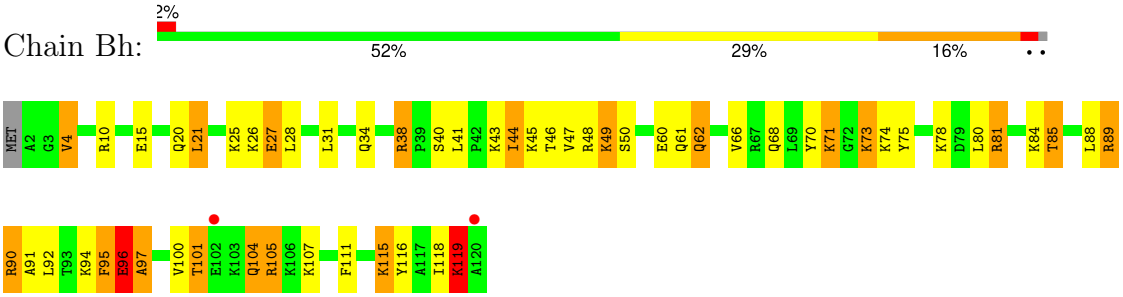
• Molecule 70: 60S ribosomal protein L34-A

Chain Dg:



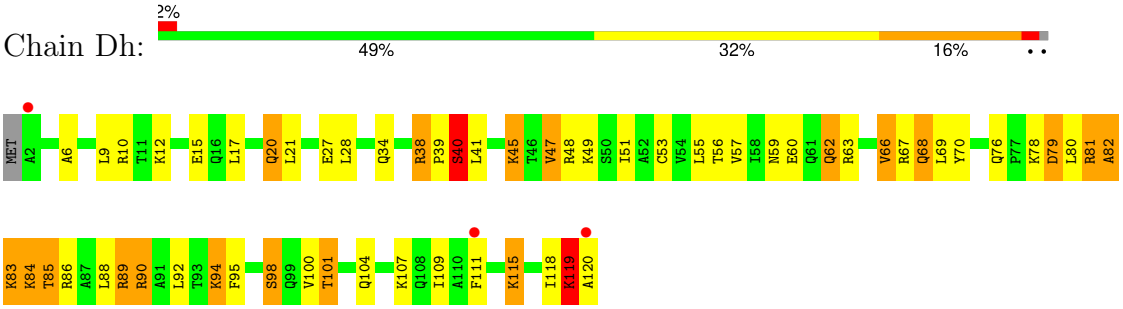
• Molecule 71: 60S ribosomal protein L35-A

Chain Bh:



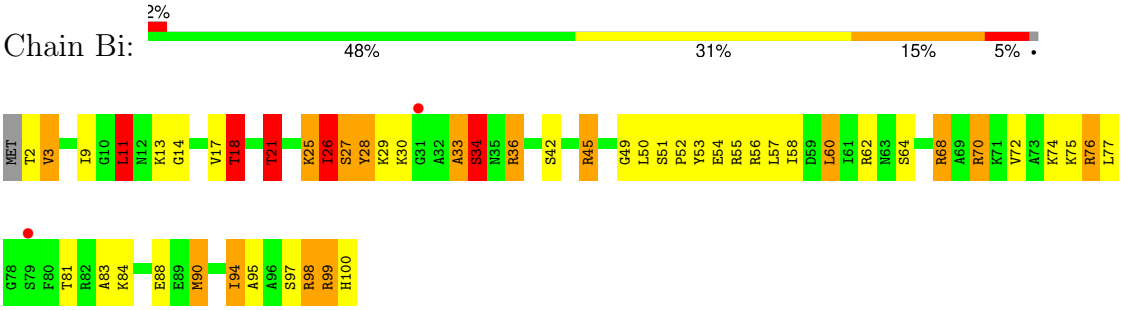
• Molecule 71: 60S ribosomal protein L35-A

Chain Dh:



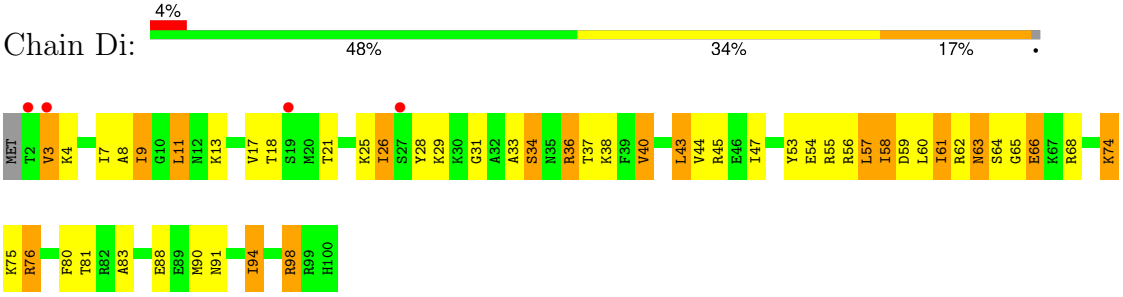
• Molecule 72: 60S ribosomal protein L36-A

Chain Bi:



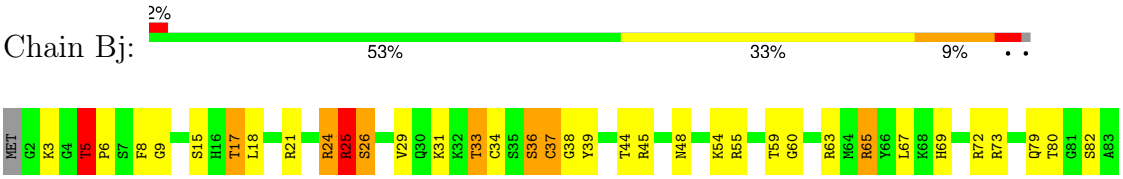
• Molecule 72: 60S ribosomal protein L36-A

Chain Di:



• Molecule 73: 60S ribosomal protein L37-A

Chain Bj:

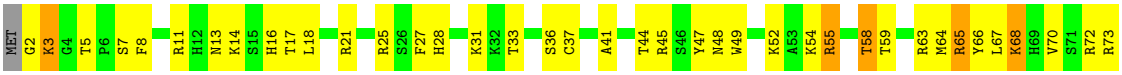


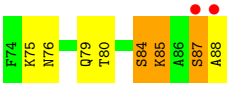


• Molecule 73: 60S ribosomal protein L37-A

Chain Dj:



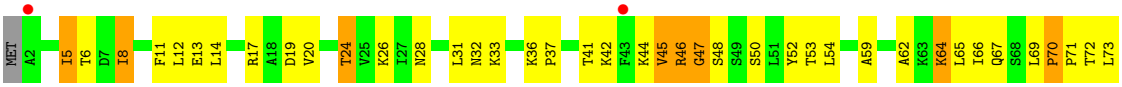




• Molecule 74: 60S ribosomal protein L38

Chain Bk:

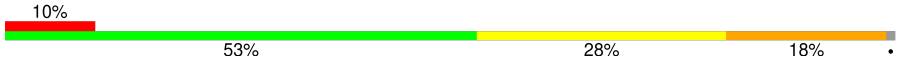


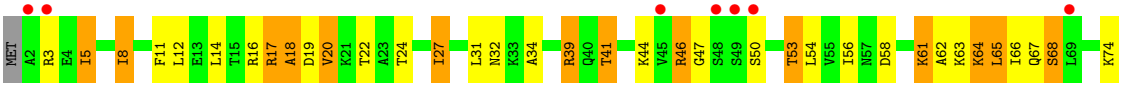




• Molecule 74: 60S ribosomal protein L38

Chain Dk:



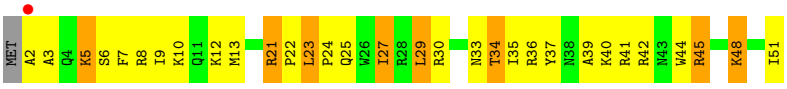




• Molecule 75: 60S ribosomal protein L39

Chain Bl:

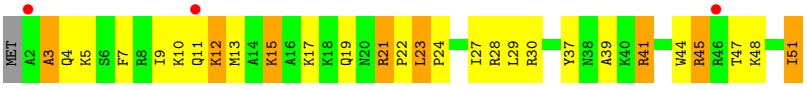




• Molecule 75: 60S ribosomal protein L39

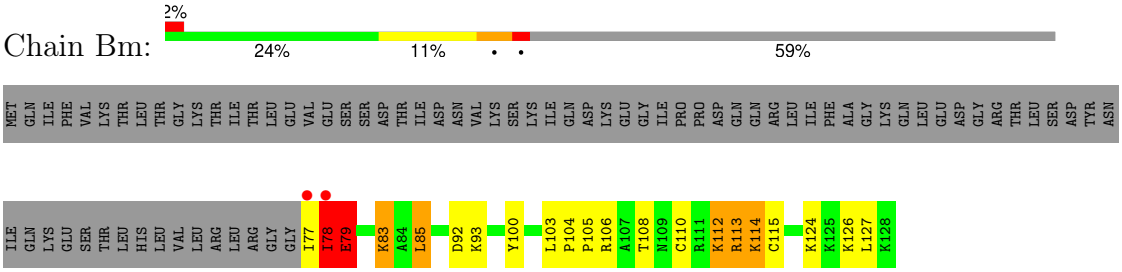
Chain Dl:





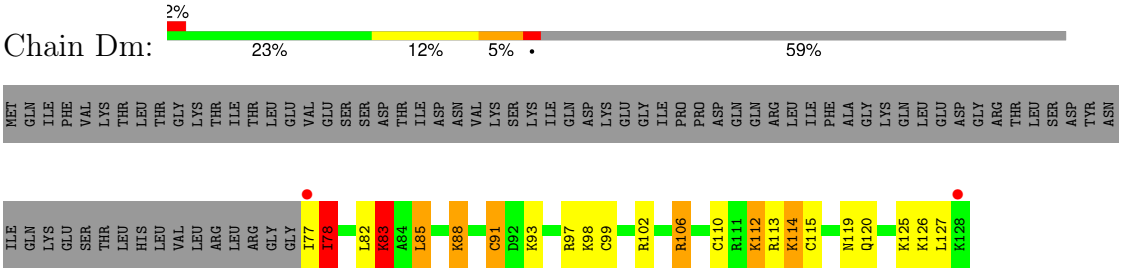
• Molecule 76: 60S ribosomal protein L40

Chain Bm:



• Molecule 76: 60S ribosomal protein L40

Chain Dm:



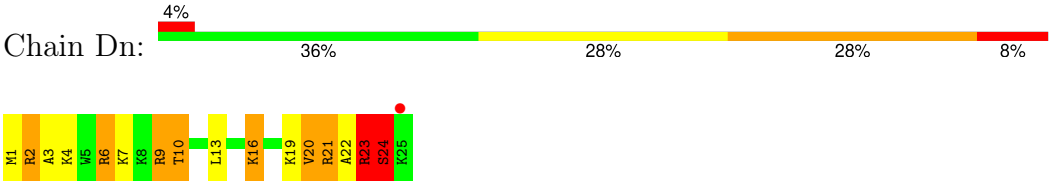
• Molecule 77: 60S ribosomal protein L41-A

Chain Bn:



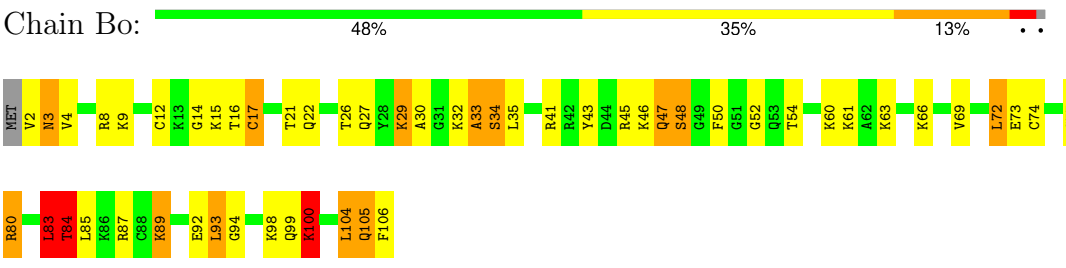
• Molecule 77: 60S ribosomal protein L41-A

Chain Dn:



• Molecule 78: 60S ribosomal protein L42-A

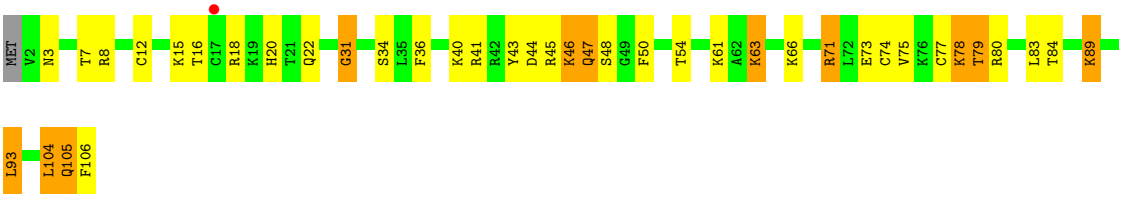
Chain Bo:



• Molecule 78: 60S ribosomal protein L42-A

Chain Do:

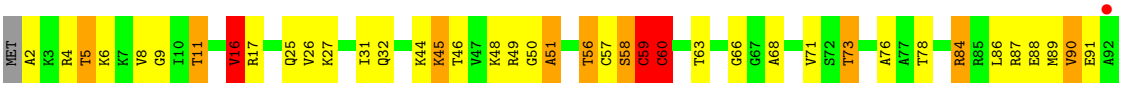




• Molecule 79: 60S ribosomal protein L43-A

Chain Bp:

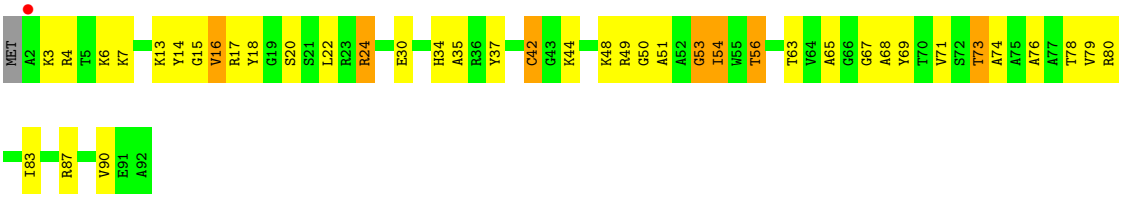




• Molecule 79: 60S ribosomal protein L43-A

Chain Dp:

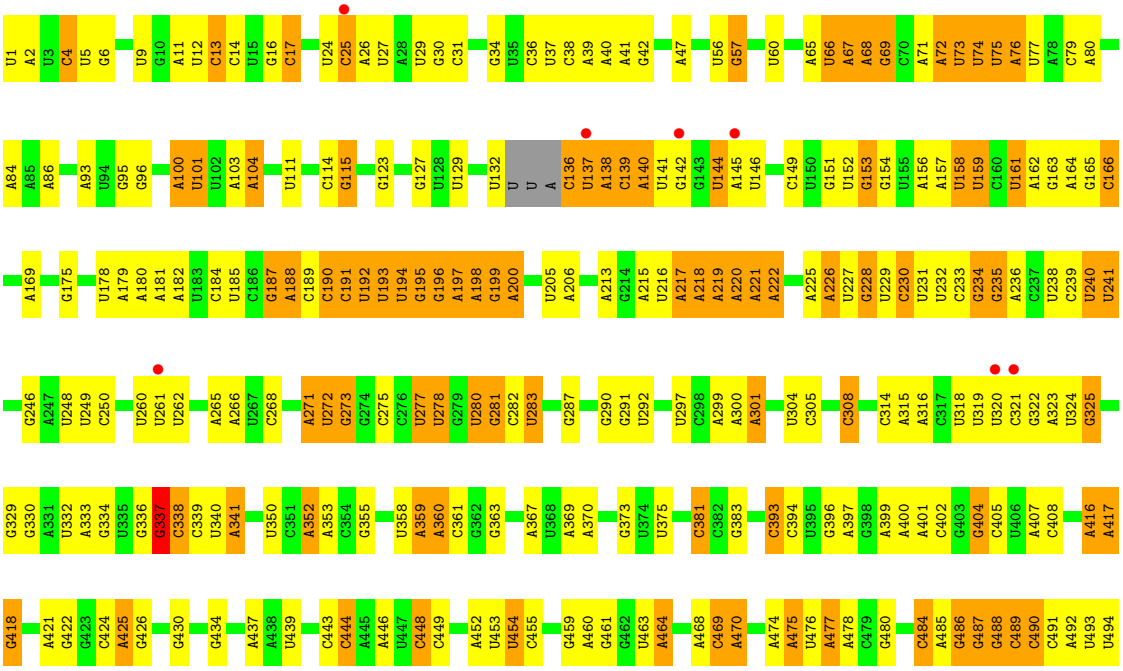


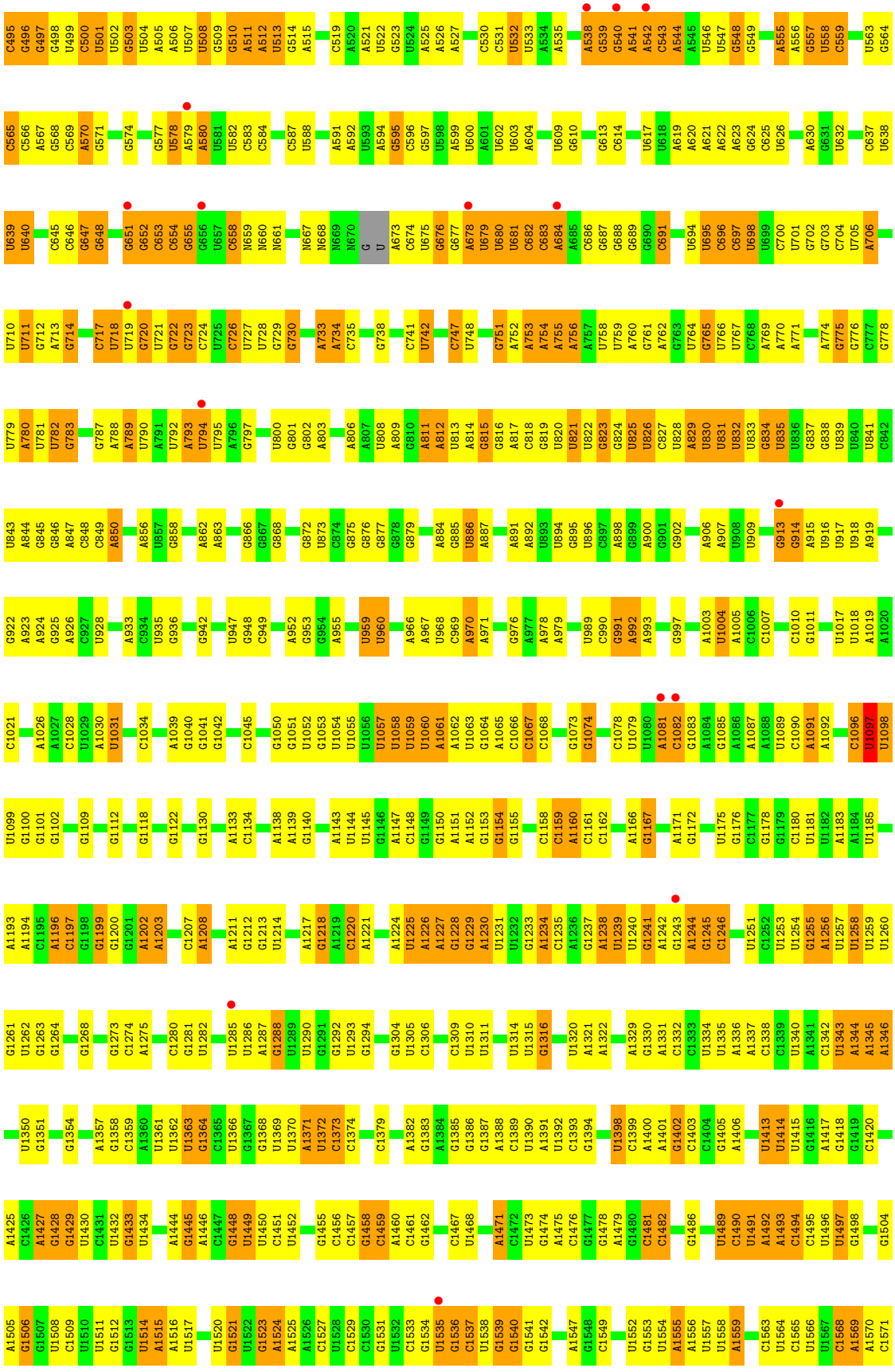


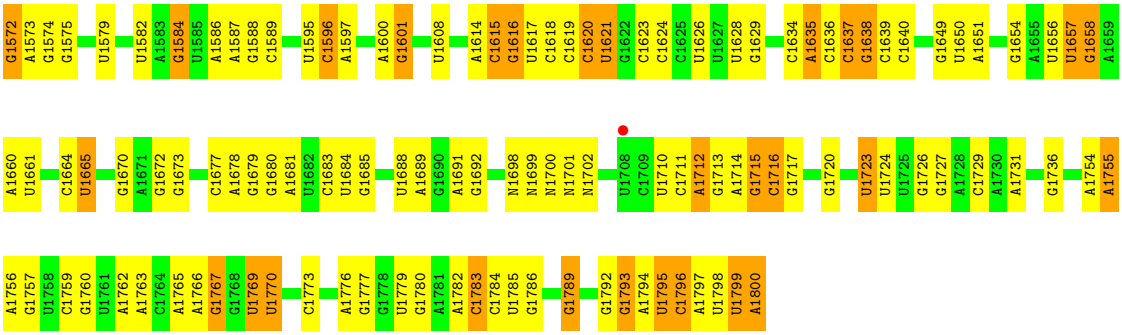
• Molecule 80: 18S rRNA

Chain A6:





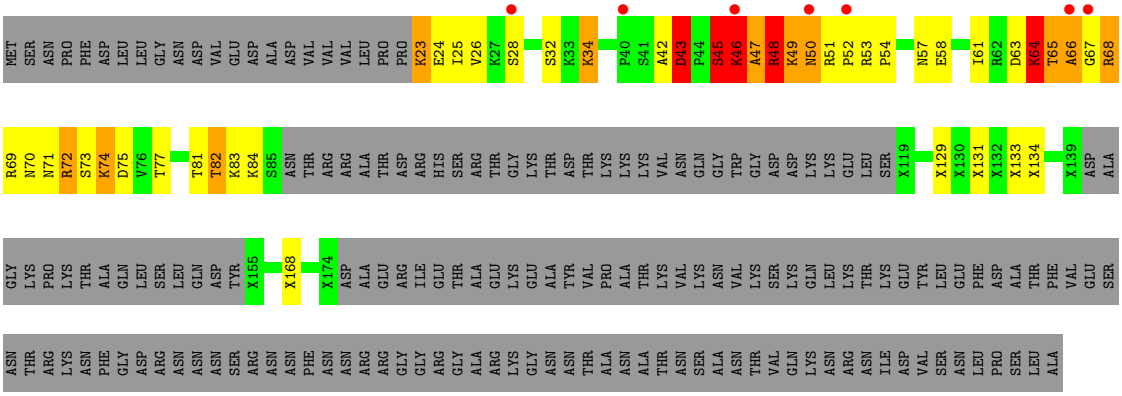




• Molecule 81: Suppressor protein STM1

Chain Ch:

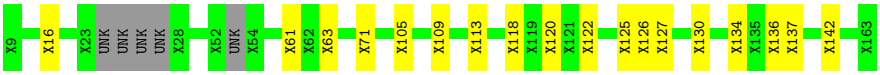




• Molecule 82: Ribosomal protein L12

Chain DK:

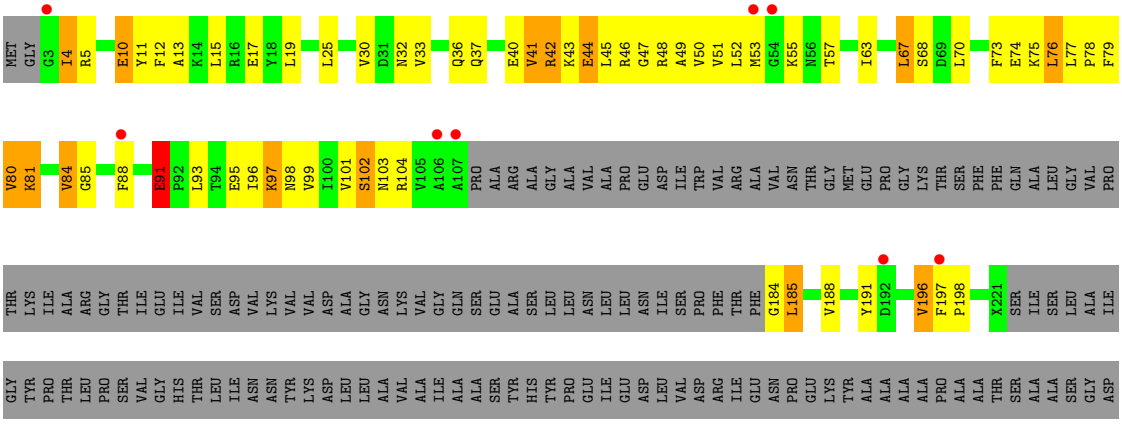




• Molecule 83: 60S acidic ribosomal protein P0

Chain Dq:



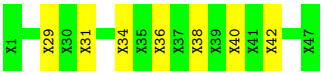




• Molecule 84: Ribosomal protein P1 alpha

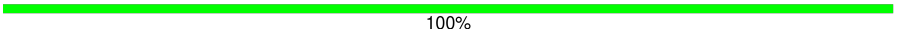
Chain Dr:





• Molecule 85: Ribosomal protein P2 beta

Chain Ds:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	436.43Å 288.22Å 305.08Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	300.00 – 3.00 300.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (300.00-3.00) 99.9 (300.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.229 0.189 , 0.228	Depositor DCC
R_{free} test set	32787 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 79.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	416785	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A2	0.53	1/42128 (0.0%)	0.58	0/65642
2	AA	0.71	1/1617 (0.1%)	1.22	18/2215 (0.8%)
2	CA	0.82	1/1623 (0.1%)	1.30	17/2222 (0.8%)
3	AB	0.62	0/1735	1.13	11/2335 (0.5%)
3	CB	0.76	1/1748 (0.1%)	1.12	9/2352 (0.4%)
4	AC	0.81	3/1665 (0.2%)	1.19	6/2263 (0.3%)
4	CC	0.94	1/1665 (0.1%)	1.27	16/2263 (0.7%)
5	AD	0.76	0/1759	1.15	11/2368 (0.5%)
5	CD	0.69	0/1759	1.15	11/2368 (0.5%)
6	AE	0.74	0/2109	1.20	17/2839 (0.6%)
6	CE	0.89	0/2109	1.27	19/2839 (0.7%)
7	AF	0.65	0/1629	1.11	7/2202 (0.3%)
7	CF	0.78	1/1629 (0.1%)	1.25	13/2202 (0.6%)
8	AG	0.70	0/1823	1.12	7/2439 (0.3%)
8	CG	0.82	0/1779	1.15	5/2379 (0.2%)
9	AH	0.68	0/1506	1.15	12/2028 (0.6%)
9	CH	0.76	1/1516 (0.1%)	1.22	13/2043 (0.6%)
10	AI	0.84	0/1514	1.18	7/2021 (0.3%)
10	CI	0.92	0/1514	1.29	7/2021 (0.3%)
11	AJ	0.73	0/1519	1.19	7/2035 (0.3%)
11	CJ	0.83	0/1519	1.25	9/2035 (0.4%)
12	AK	0.71	0/789	1.20	7/1067 (0.7%)
12	CK	0.67	0/776	1.18	4/1047 (0.4%)
13	AL	0.86	0/1239	1.17	6/1673 (0.4%)
13	CL	0.99	0/1194	1.36	9/1610 (0.6%)
14	AM	0.70	0/898	1.13	4/1220 (0.3%)
14	CM	0.63	0/898	1.09	3/1220 (0.2%)
15	AN	0.79	0/1215	1.17	7/1638 (0.4%)
15	CN	0.86	1/1215 (0.1%)	1.20	5/1638 (0.3%)
16	AO	0.69	0/901	1.25	7/1217 (0.6%)
16	CO	0.87	1/960 (0.1%)	1.31	11/1290 (0.9%)
17	AP	0.75	0/998	1.21	8/1341 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	CP	0.75	0/1060	1.30	13/1426 (0.9%)
18	AQ	0.70	0/1125	1.19	8/1510 (0.5%)
18	CQ	0.84	0/1131	1.27	8/1518 (0.5%)
19	AR	0.73	0/935	1.25	7/1254 (0.6%)
19	CR	0.78	0/914	1.33	13/1224 (1.1%)
20	AS	0.74	0/1211	1.13	5/1628 (0.3%)
20	CS	0.78	0/1211	1.21	6/1628 (0.4%)
21	AT	0.72	1/1130 (0.1%)	1.09	5/1517 (0.3%)
21	CT	0.78	0/1130	1.11	3/1517 (0.2%)
22	AU	0.71	0/865	1.18	8/1169 (0.7%)
22	CU	0.78	0/892	1.26	7/1205 (0.6%)
23	AV	0.68	1/693 (0.1%)	1.07	3/935 (0.3%)
23	CV	0.82	0/693	1.17	3/935 (0.3%)
24	AW	0.83	0/1038	1.23	8/1395 (0.6%)
24	CW	0.98	1/1038 (0.1%)	1.21	5/1395 (0.4%)
25	AX	0.91	1/1139 (0.1%)	1.25	6/1518 (0.4%)
25	CX	1.05	0/1139	1.33	9/1518 (0.6%)
26	AY	0.69	1/1087 (0.1%)	1.08	2/1449 (0.1%)
26	CY	0.78	0/1087	1.16	3/1449 (0.2%)
27	AZ	0.65	0/571	1.22	4/768 (0.5%)
27	CZ	0.66	0/566	1.14	5/761 (0.7%)
28	Aa	0.76	0/782	1.15	4/1047 (0.4%)
28	Ca	0.83	0/782	1.19	5/1047 (0.5%)
29	Ab	0.69	0/620	1.23	7/838 (0.8%)
29	Cb	0.71	0/620	1.23	3/838 (0.4%)
30	Ac	0.55	0/499	1.09	0/670
30	Cc	0.71	0/499	1.28	5/670 (0.7%)
31	Ad	0.85	1/452 (0.2%)	1.24	2/600 (0.3%)
31	Cd	0.90	0/452	1.32	5/600 (0.8%)
32	Ae	0.61	0/483	1.13	2/643 (0.3%)
32	Ce	0.74	0/499	1.29	4/665 (0.6%)
33	Af	0.72	0/404	1.37	5/542 (0.9%)
33	Cf	0.59	0/404	1.27	8/542 (1.5%)
34	Ag	0.63	0/2490	1.03	7/3389 (0.2%)
34	Cg	0.64	0/2495	1.01	7/3395 (0.2%)
35	Ah	1.09	3/925 (0.3%)	1.29	8/1240 (0.6%)
36	A1	0.79	11/75394 (0.0%)	0.67	14/117545 (0.0%)
36	A5	0.82	24/75414 (0.0%)	0.66	13/117575 (0.0%)
37	A3	0.67	0/2883	0.59	0/4491
37	A7	0.78	0/2883	0.63	0/4491
38	A4	0.77	0/3746	0.62	0/5832
38	A8	0.66	0/3746	0.61	0/5832
39	BA	1.04	3/1948 (0.2%)	1.38	16/2617 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	DA	1.11	4/1946 (0.2%)	1.43	18/2614 (0.7%)
40	BB	1.10	5/3146 (0.2%)	1.42	36/4228 (0.9%)
40	DB	1.23	4/3146 (0.1%)	1.44	26/4228 (0.6%)
41	BC	1.19	6/2800 (0.2%)	1.53	40/3790 (1.1%)
41	DC	1.12	6/2800 (0.2%)	1.43	34/3790 (0.9%)
42	BD	0.86	0/2425	1.19	10/3271 (0.3%)
42	DD	1.02	1/2408 (0.0%)	1.27	21/3248 (0.6%)
43	BE	1.10	0/1260	1.38	16/1694 (0.9%)
43	DE	1.07	0/1269	1.37	11/1705 (0.6%)
44	BF	1.21	2/1821 (0.1%)	1.45	24/2451 (1.0%)
44	DF	1.17	2/1828 (0.1%)	1.43	26/2461 (1.1%)
45	BG	0.79	0/1836	1.23	17/2481 (0.7%)
45	DG	0.78	0/1795	1.18	14/2429 (0.6%)
46	BH	0.96	1/1539 (0.1%)	1.27	10/2073 (0.5%)
46	DH	1.17	0/1539	1.45	13/2073 (0.6%)
47	BI	1.08	3/1741 (0.2%)	1.33	13/2335 (0.6%)
47	DI	1.11	0/1758	1.38	12/2358 (0.5%)
48	BJ	0.82	0/1374	1.24	7/1842 (0.4%)
48	DJ	0.99	1/1374 (0.1%)	1.36	17/1842 (0.9%)
49	BL	1.09	3/1568 (0.2%)	1.47	23/2106 (1.1%)
49	DL	1.06	3/1573 (0.2%)	1.40	19/2113 (0.9%)
50	BM	1.11	3/1068 (0.3%)	1.37	15/1438 (1.0%)
50	DM	1.18	0/1074	1.37	9/1446 (0.6%)
51	BN	1.05	1/1757 (0.1%)	1.37	14/2354 (0.6%)
51	DN	0.99	2/1757 (0.1%)	1.30	14/2354 (0.6%)
52	BO	0.59	1/3160 (0.0%)	0.83	6/4208 (0.1%)
52	DO	0.64	0/3159	0.95	14/4205 (0.3%)
53	BP	1.17	2/1443 (0.1%)	1.39	9/1944 (0.5%)
53	DP	1.34	4/1250 (0.3%)	1.41	6/1683 (0.4%)
54	BQ	1.21	3/1465 (0.2%)	1.57	25/1965 (1.3%)
54	DQ	1.08	1/1465 (0.1%)	1.43	10/1965 (0.5%)
55	BR	0.89	1/1538 (0.1%)	1.24	10/2050 (0.5%)
55	DR	0.94	0/1538	1.21	5/2050 (0.2%)
56	BS	1.12	3/1481 (0.2%)	1.40	13/1990 (0.7%)
56	DS	1.20	3/1481 (0.2%)	1.44	17/1990 (0.9%)
57	BT	1.09	1/1300 (0.1%)	1.31	9/1743 (0.5%)
57	DT	1.16	2/1300 (0.2%)	1.35	6/1743 (0.3%)
58	BU	0.64	0/812	1.04	4/1099 (0.4%)
58	DU	0.67	0/794	1.20	8/1076 (0.7%)
59	BV	1.09	1/1018 (0.1%)	1.37	11/1369 (0.8%)
59	DV	1.24	2/1018 (0.2%)	1.42	6/1369 (0.4%)
60	BW	0.83	0/712	1.45	4/958 (0.4%)
60	DW	0.99	0/1052	1.22	7/1398 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
61	BX	0.88	0/979	1.23	6/1321 (0.5%)
61	DX	0.87	0/974	1.24	7/1314 (0.5%)
62	BY	0.96	0/1004	1.35	7/1341 (0.5%)
62	DY	0.94	0/1004	1.30	6/1341 (0.4%)
63	BZ	0.68	0/1118	1.17	7/1497 (0.5%)
63	DZ	0.65	0/1118	1.19	9/1497 (0.6%)
64	Ba	1.20	4/1204 (0.3%)	1.51	16/1612 (1.0%)
64	Da	1.20	7/1204 (0.6%)	1.59	29/1612 (1.8%)
65	Bb	0.98	0/473	1.27	5/629 (0.8%)
65	Db	1.20	2/473 (0.4%)	1.61	10/629 (1.6%)
66	Bc	0.70	0/751	1.12	4/1008 (0.4%)
66	Dc	0.72	0/775	1.11	3/1040 (0.3%)
67	Bd	0.90	0/890	1.28	9/1196 (0.8%)
67	Dd	1.11	1/897 (0.1%)	1.32	8/1205 (0.7%)
68	Be	1.20	1/1041 (0.1%)	1.43	6/1394 (0.4%)
68	De	1.23	4/1041 (0.4%)	1.58	9/1394 (0.6%)
69	Bf	1.35	2/868 (0.2%)	1.48	10/1168 (0.9%)
69	Df	1.34	6/868 (0.7%)	1.40	6/1168 (0.5%)
70	Bg	0.90	1/890 (0.1%)	1.31	8/1189 (0.7%)
70	Dg	0.87	0/890	1.26	3/1189 (0.3%)
71	Bh	0.97	0/978	1.29	6/1301 (0.5%)
71	Dh	0.81	0/974	1.15	2/1297 (0.2%)
72	Bi	1.02	3/778 (0.4%)	1.37	7/1034 (0.7%)
72	Di	0.84	0/777	1.17	2/1033 (0.2%)
73	Bj	1.17	2/696 (0.3%)	1.52	8/923 (0.9%)
73	Dj	1.02	0/696	1.35	4/923 (0.4%)
74	Bk	0.71	0/618	1.18	5/826 (0.6%)
74	Dk	0.66	0/614	1.07	1/822 (0.1%)
75	Bl	1.02	0/443	1.39	5/588 (0.9%)
75	Dl	1.03	0/443	1.28	0/588
76	Bm	1.08	0/423	1.32	3/562 (0.5%)
76	Dm	1.29	0/423	1.42	5/562 (0.9%)
77	Bn	0.90	0/234	1.23	0/300
77	Dn	1.05	0/234	1.25	2/300 (0.7%)
78	Bo	0.95	0/860	1.26	5/1136 (0.4%)
78	Do	0.95	0/860	1.24	0/1136
79	Bp	0.98	0/701	1.36	5/934 (0.5%)
79	Dp	1.01	1/701 (0.1%)	1.38	8/934 (0.9%)
80	A6	0.63	4/42174 (0.0%)	0.60	2/65711 (0.0%)
81	Ch	0.84	0/480	1.26	3/642 (0.5%)
83	Dq	0.62	0/977	1.10	4/1313 (0.3%)
All	All	0.82	168/432157 (0.0%)	0.94	1413/634038 (0.2%)

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
2	CA	0	1
3	AB	0	1
5	CD	0	1
7	CF	0	2
9	AH	0	1
11	CJ	0	3
13	AL	0	1
16	AO	0	1
16	CO	0	1
17	CP	0	1
18	CQ	0	1
19	AR	0	2
22	CU	0	1
25	CX	0	1
27	AZ	0	3
27	CZ	0	2
29	Ab	0	1
33	Af	0	2
33	Cf	0	2
35	Ah	0	1
36	A1	0	3
36	A5	0	1
39	DA	0	2
40	BB	0	1
41	BC	0	1
41	DC	0	1
42	DD	0	1
43	BE	0	2
43	DE	0	1
44	BF	0	1
44	DF	0	2
45	BG	0	3
46	BH	0	1
48	BJ	0	1
52	BO	0	2
52	DO	0	2
56	DS	0	1
57	BT	0	1
59	DV	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
62	DY	0	1
63	DZ	0	1
64	Da	0	3
65	Bb	0	2
65	Db	0	1
67	Bd	0	1
78	Bo	0	1
All	All	0	67

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Ah	134	ASP	CG-OD1	16.84	1.57	1.25
35	Ah	134	ASP	CG-OD2	15.23	1.54	1.25
39	DA	211	HIS	C-O	12.14	1.38	1.24
36	A1	2777	G	C5-C6	-11.61	1.19	1.42
52	BO	3[B]	SER	C-N	10.53	1.47	1.33

The worst 5 of 1413 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	De	4	LEU	CA-C-N	-17.06	98.52	119.84
68	De	4	LEU	C-N-CA	-17.06	98.52	119.84
60	BW	80	ARG	CA-C-N	16.93	141.00	119.84
60	BW	80	ARG	C-N-CA	16.93	141.00	119.84
54	BQ	18	ALA	CA-C-N	-13.34	107.24	120.31

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AB	131	ASP	Peptide
9	AH	131	PHE	Peptide
13	AL	127	GLN	Peptide
16	AO	124	ASP	Peptide
19	AR	22	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37835	0	19062	1110	0
2	AA	1577	0	1567	102	0
2	CA	1583	0	1578	88	0
3	AB	1709	0	1784	128	0
3	CB	1722	0	1793	79	0
4	AC	1635	0	1723	58	0
4	CC	1635	0	1723	64	0
5	AD	1734	0	1817	70	0
5	CD	1734	0	1817	55	0
6	AE	2068	0	2154	71	0
6	CE	2068	0	2154	93	0
7	AF	1609	0	1675	76	0
7	CF	1609	0	1675	82	0
8	AG	1799	0	1879	93	0
8	CG	1755	0	1846	64	0
9	AH	1481	0	1572	83	0
9	CH	1491	0	1578	66	0
10	AI	1489	0	1525	67	0
10	CI	1489	0	1525	49	0
11	AJ	1494	0	1573	85	0
11	CJ	1494	0	1573	84	0
12	AK	772	0	727	45	0
12	CK	761	0	697	37	0
13	AL	1213	0	1257	51	0
13	CL	1168	0	1233	42	0
14	AM	890	0	887	55	0
14	CM	890	0	887	54	0
15	AN	1192	0	1255	49	0
15	CN	1192	0	1255	44	0
16	AO	891	0	883	63	0
16	CO	949	0	985	48	0
17	AP	977	0	1002	49	0
17	CP	1039	0	1050	77	0
18	AQ	1105	0	1166	70	0
18	CQ	1111	0	1171	52	0
19	AR	926	0	930	45	0
19	CR	906	0	909	41	0
20	AS	1192	0	1222	75	1
20	CS	1192	0	1222	65	0
21	AT	1112	0	1124	70	0
21	CT	1112	0	1124	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AU	855	0	917	41	0
22	CU	882	0	939	59	0
23	AV	684	0	672	44	0
23	CV	684	0	672	34	0
24	AW	1021	0	1060	57	0
24	CW	1021	0	1060	33	0
25	AX	1121	0	1196	54	0
25	CX	1121	0	1196	35	0
26	AY	1073	0	1132	41	0
26	CY	1073	0	1132	54	0
27	AZ	563	0	603	44	0
27	CZ	558	0	598	29	0
28	Aa	769	0	814	55	0
28	Ca	769	0	815	43	0
29	Ab	610	0	630	26	0
29	Cb	610	0	631	25	0
30	Ac	497	0	535	33	0
30	Cc	497	0	535	27	0
31	Ad	442	0	428	27	0
31	Cd	442	0	428	23	0
32	Ae	475	0	525	16	0
32	Ce	491	0	542	24	0
33	Af	516	0	517	42	0
33	Cf	544	0	546	30	0
34	Ag	2437	0	2386	77	0
34	Cg	2442	0	2392	84	0
35	Ah	1105	0	960	46	0
36	A1	67355	0	33821	1412	0
36	A5	67376	0	33831	1372	0
37	A3	2579	0	1304	38	0
37	A7	2579	0	1303	46	0
38	A4	3353	0	1691	58	0
38	A8	3353	0	1695	65	0
39	BA	1914	0	1981	68	0
39	DA	1912	0	1976	83	0
40	BB	3075	0	3142	159	0
40	DB	3075	0	3142	123	0
41	BC	2748	0	2859	104	0
41	DC	2748	0	2859	99	0
42	BD	2375	0	2325	105	0
42	DD	2359	0	2311	94	0
43	BE	1239	0	1326	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DE	1248	0	1339	39	0
44	BF	1784	0	1862	63	0
44	DF	1791	0	1869	47	0
45	BG	1804	0	1877	84	0
45	DG	1763	0	1819	78	0
46	BH	1518	0	1587	64	0
46	DH	1518	0	1587	69	0
47	BI	1705	0	1736	81	0
47	DI	1722	0	1755	54	1
48	BJ	1353	0	1383	66	0
48	DJ	1353	0	1383	55	0
49	BL	1543	0	1608	56	0
49	DL	1548	0	1613	61	0
50	BM	1053	0	1149	42	0
50	DM	1059	0	1154	39	0
51	BN	1720	0	1779	69	0
51	DN	1720	0	1779	72	0
52	BO	3119	0	3302	76	0
52	DO	3119	0	3302	90	0
53	BP	1420	0	1437	66	0
53	DP	1227	0	1236	35	0
54	BQ	1441	0	1543	59	0
54	DQ	1441	0	1543	50	0
55	BR	1521	0	1617	65	0
55	DR	1521	0	1617	38	0
56	BS	1445	0	1487	54	0
56	DS	1445	0	1487	52	0
57	BT	1276	0	1323	41	0
57	DT	1276	0	1323	55	0
58	BU	796	0	812	24	0
58	DU	778	0	791	26	0
59	BV	1003	0	1048	53	0
59	DV	1003	0	1048	31	0
60	BW	699	0	640	19	0
60	DW	1038	0	1071	23	0
61	BX	964	0	1025	25	0
61	DX	959	0	1023	29	0
62	BY	993	0	1081	31	0
62	DY	993	0	1081	30	0
63	BZ	1092	0	1155	49	0
63	DZ	1092	0	1155	62	0
64	Ba	1173	0	1215	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Da	1173	0	1215	58	0
65	Bb	462	0	491	18	0
65	Db	462	0	491	18	0
66	Bc	743	0	797	37	0
66	Dc	767	0	816	35	0
67	Bd	876	0	912	22	0
67	Dd	883	0	918	26	0
68	Be	1020	0	1090	32	0
68	De	1020	0	1090	39	0
69	Bf	850	0	880	35	0
69	Df	850	0	880	29	0
70	Bg	880	0	945	39	0
70	Dg	880	0	945	37	0
71	Bh	969	0	1078	38	0
71	Dh	965	0	1067	45	0
72	Bi	771	0	849	33	0
72	Di	770	0	846	26	0
73	Bj	681	0	683	25	0
73	Dj	681	0	683	30	0
74	Bk	612	0	682	21	0
74	Dk	608	0	671	22	0
75	Bl	436	0	475	25	0
75	Dl	436	0	475	21	0
76	Bm	417	0	456	15	0
76	Dm	417	0	455	16	0
77	Bn	233	0	284	16	0
77	Dn	233	0	284	14	0
78	Bo	847	0	916	38	0
78	Do	847	0	915	34	0
79	Bp	694	0	734	26	0
79	Dp	694	0	734	25	0
80	A6	38021	0	19178	939	0
81	Ch	680	0	542	44	0
82	DK	750	0	185	12	0
83	Dq	1077	0	1012	32	0
84	Dr	235	0	50	5	0
85	Ds	230	0	49	0	0
86	A1	2891	0	0	451	1
86	A2	1316	0	0	223	0
86	A3	91	0	0	7	0
86	A4	105	0	0	9	0
86	A5	2926	0	0	449	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	A6	1399	0	0	192	0
86	A7	91	0	0	12	0
86	A8	133	0	0	20	0
86	AC	7	0	0	5	0
86	AI	7	0	0	1	0
86	AL	7	0	0	1	0
86	AN	7	0	0	1	0
86	AP	7	0	0	5	0
86	Ad	7	0	0	4	0
86	Ag	7	0	0	0	0
86	BA	7	0	0	5	0
86	BB	14	0	0	2	0
86	BC	7	0	0	2	0
86	BD	7	0	0	1	0
86	BI	28	0	0	16	0
86	BN	7	0	0	0	0
86	BO	7	0	0	0	0
86	BP	14	0	0	2	0
86	BR	7	0	0	1	0
86	BT	7	0	0	0	0
86	Bb	7	0	0	0	0
86	Bf	7	0	0	0	0
86	Bj	21	0	0	6	0
86	Bo	7	0	0	3	0
86	CB	7	0	0	0	0
86	CG	14	0	0	4	1
86	CI	7	0	0	1	0
86	CJ	7	0	0	3	0
86	CL	7	0	0	5	0
86	CN	7	0	0	2	0
86	CP	14	0	0	7	0
86	CS	7	0	0	0	0
86	CY	14	0	0	0	0
86	Cd	7	0	0	4	0
86	Cg	7	0	0	0	0
86	DA	7	0	0	6	0
86	DB	14	0	0	1	0
86	DC	14	0	0	2	0
86	DD	7	0	0	1	0
86	DG	7	0	0	6	0
86	DH	7	0	0	0	0
86	DI	14	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	DJ	7	0	0	1	0
86	DM	7	0	0	0	0
86	DO	7	0	0	0	0
86	DP	7	0	0	1	0
86	DQ	7	0	0	0	0
86	DR	7	0	0	1	0
86	DV	7	0	0	1	0
86	Db	7	0	0	1	0
86	De	7	0	0	0	0
86	Df	7	0	0	0	0
86	Dg	7	0	0	0	0
86	Dh	7	0	0	0	0
86	Dj	7	0	0	0	0
86	Do	7	0	0	2	0
87	A1	695	0	0	0	0
87	A2	171	0	0	0	0
87	A3	19	0	0	0	0
87	A4	34	0	0	0	0
87	A5	763	0	0	0	0
87	A6	239	0	0	0	0
87	A7	26	0	0	0	0
87	A8	20	0	0	0	0
87	AB	2	0	0	0	0
87	AC	1	0	0	0	0
87	AE	1	0	0	0	0
87	AI	2	0	0	0	0
87	AJ	1	0	0	0	0
87	AL	2	0	0	0	0
87	AN	1	0	0	0	0
87	AP	1	0	0	0	0
87	AS	2	0	0	0	0
87	AX	1	0	0	0	0
87	Aa	1	0	0	0	0
87	Ad	3	0	0	0	0
87	Af	1	0	0	0	0
87	BA	5	0	0	0	0
87	BB	4	0	0	0	0
87	BC	6	0	0	0	0
87	BD	1	0	0	0	0
87	BE	1	0	0	0	0
87	BF	2	0	0	0	0
87	BG	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	BI	4	0	0	0	0
87	BJ	1	0	0	0	0
87	BL	5	0	0	0	0
87	BN	6	0	0	0	0
87	BO	8	0	0	0	0
87	BP	10	0	0	0	0
87	BQ	4	0	0	0	0
87	BR	4	0	0	0	0
87	BS	2	0	0	0	0
87	BT	1	0	0	0	0
87	BV	5	0	0	0	0
87	BY	2	0	0	0	0
87	Ba	8	0	0	0	0
87	Bd	1	0	0	0	0
87	Be	2	0	0	0	0
87	Bf	1	0	0	0	0
87	Bg	1	0	0	0	0
87	Bj	7	0	0	0	0
87	Bl	1	0	0	0	0
87	Bm	1	0	0	0	0
87	Bo	3	0	0	0	0
87	CB	1	0	0	0	0
87	CE	1	0	0	0	0
87	CF	2	0	0	0	0
87	CG	2	0	0	0	0
87	CI	2	0	0	0	0
87	CL	3	0	0	0	0
87	CP	1	0	0	0	0
87	CQ	2	0	0	0	0
87	CS	2	0	0	0	0
87	CX	2	0	0	0	0
87	CY	2	0	0	0	0
87	CZ	1	0	0	0	0
87	Ca	1	0	0	0	0
87	Cd	1	0	0	0	0
87	Ch	2	0	0	0	0
87	DA	4	0	0	0	0
87	DB	13	0	0	0	0
87	DC	5	0	0	0	0
87	DD	7	0	0	0	0
87	DF	4	0	0	0	0
87	DG	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	DH	2	0	0	0	0
87	DJ	2	0	0	0	0
87	DL	1	0	0	0	0
87	DM	2	0	0	0	0
87	DN	1	0	0	0	0
87	DO	8	0	0	0	0
87	DP	7	0	0	0	0
87	DQ	1	0	0	0	0
87	DR	1	0	0	0	0
87	DS	4	0	0	0	0
87	DT	3	0	0	0	0
87	DV	3	0	0	0	0
87	DW	1	0	0	0	0
87	DY	2	0	0	0	0
87	Da	4	0	0	0	0
87	Db	1	0	0	0	0
87	Dd	1	0	0	0	0
87	De	2	0	0	0	0
87	Df	4	0	0	0	0
87	Dg	2	0	0	0	0
87	Dj	3	0	0	0	0
87	Dl	1	0	0	0	0
87	Dm	1	0	0	0	0
87	Dn	1	0	0	0	0
87	Do	1	0	0	0	0
87	Dp	3	0	0	0	0
87	Dq	1	0	0	0	0
88	Aa	1	0	0	0	0
88	Ab	1	0	0	0	0
88	Ad	1	0	0	0	0
88	Af	1	0	0	0	0
88	Bj	1	0	0	0	0
88	Bm	1	0	0	0	0
88	Bo	1	0	0	2	0
88	Bp	1	0	0	0	0
88	Ca	1	0	0	0	0
88	Cb	1	0	0	0	0
88	Cd	1	0	0	0	0
88	Cf	1	0	0	0	0
88	Dj	1	0	0	0	0
88	Dm	1	0	0	0	0
88	Do	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Dp	1	0	0	0	0
89	CI	1	0	0	0	0
89	DB	1	0	0	0	0
All	All	416785	0	300420	11745	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 11745 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DQ:171:LYS:NZ	54:DQ:171:LYS:CE	1.67	1.52
48:DJ:8:PRO:CG	48:DJ:8:PRO:CB	1.75	1.50
1:A2:1686:C:H2'	1:A2:1687:U:H6	1.07	1.16
36:A1:1733:G:OP2	86:A1:3811:OHX:N6	1.84	1.10
80:A6:1636:C:H4'	80:A6:1637:C:H5'	1.34	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AS:97:ASP:OD2	86:A1:3788:OHX:N2[2_545]	2.06	0.14
47:DI:218:ALA:O	86:CG:301:OHX:N3[2_647]	2.16	0.04

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
2	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0 1
2	CA	204/252 (81%)	146 (72%)	33 (16%)	25 (12%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AB	212/255 (83%)	133 (63%)	41 (19%)	38 (18%)	0 0
3	CB	214/255 (84%)	174 (81%)	25 (12%)	15 (7%)	1 4
4	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	1 8
4	CC	215/254 (85%)	188 (87%)	14 (6%)	13 (6%)	1 7
5	AD	221/240 (92%)	180 (81%)	28 (13%)	13 (6%)	1 7
5	CD	221/240 (92%)	177 (80%)	23 (10%)	21 (10%)	0 2
6	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1 3
6	CE	258/261 (99%)	219 (85%)	19 (7%)	20 (8%)	1 4
7	AF	204/225 (91%)	154 (76%)	31 (15%)	19 (9%)	0 2
7	CF	204/225 (91%)	155 (76%)	32 (16%)	17 (8%)	0 3
8	AG	224/236 (95%)	190 (85%)	22 (10%)	12 (5%)	1 9
8	CG	216/236 (92%)	183 (85%)	21 (10%)	12 (6%)	1 8
9	AH	182/190 (96%)	127 (70%)	28 (15%)	27 (15%)	0 0
9	CH	184/190 (97%)	143 (78%)	23 (12%)	18 (10%)	0 2
10	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	0 3
10	CI	184/200 (92%)	160 (87%)	17 (9%)	7 (4%)	2 15
11	AJ	183/197 (93%)	152 (83%)	19 (10%)	12 (7%)	1 5
11	CJ	183/197 (93%)	152 (83%)	17 (9%)	14 (8%)	1 4
12	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0 2
12	CK	92/105 (88%)	59 (64%)	15 (16%)	18 (20%)	0 0
13	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1 7
13	CL	144/156 (92%)	118 (82%)	15 (10%)	11 (8%)	1 4
14	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0 0
14	CM	122/143 (85%)	60 (49%)	31 (25%)	31 (25%)	0 0
15	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	1 9
15	CN	148/151 (98%)	129 (87%)	10 (7%)	9 (6%)	1 7
16	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0 1
16	CO	126/137 (92%)	101 (80%)	20 (16%)	5 (4%)	2 14
17	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0 1
17	CP	133/142 (94%)	91 (68%)	20 (15%)	22 (16%)	0 0
18	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	CQ	140/143 (98%)	122 (87%)	10 (7%)	8 (6%)	1 8
19	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0 2
19	CR	113/136 (83%)	92 (81%)	12 (11%)	9 (8%)	1 3
20	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0 2
20	CS	143/146 (98%)	111 (78%)	25 (18%)	7 (5%)	1 10
21	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	0 3
21	CT	141/144 (98%)	125 (89%)	9 (6%)	7 (5%)	1 10
22	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2 11
22	CU	108/121 (89%)	81 (75%)	12 (11%)	15 (14%)	0 1
23	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0 1
23	CV	85/87 (98%)	71 (84%)	7 (8%)	7 (8%)	0 3
24	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	4 24
24	CW	127/130 (98%)	115 (91%)	12 (9%)	0	100 100
25	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0 1
25	CX	142/145 (98%)	127 (89%)	13 (9%)	2 (1%)	9 36
26	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0 2
26	CY	132/135 (98%)	100 (76%)	17 (13%)	15 (11%)	0 1
27	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0 0
27	CZ	67/108 (62%)	50 (75%)	10 (15%)	7 (10%)	0 2
28	Aa	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0 0
28	Ca	95/119 (80%)	67 (70%)	20 (21%)	8 (8%)	0 3
29	Ab	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	1 10
29	Cb	79/82 (96%)	62 (78%)	9 (11%)	8 (10%)	0 2
30	Ac	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	0 3
30	Cc	61/67 (91%)	41 (67%)	17 (28%)	3 (5%)	1 10
31	Ad	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	2 14
31	Cd	51/56 (91%)	45 (88%)	2 (4%)	4 (8%)	1 4
32	Ae	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3 17
32	Ce	60/63 (95%)	45 (75%)	9 (15%)	6 (10%)	0 2
33	Af	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0 0
33	Cf	50/152 (33%)	26 (52%)	13 (26%)	11 (22%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	Ag	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	2 13
34	Cg	316/319 (99%)	262 (83%)	38 (12%)	16 (5%)	1 10
35	Ah	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	0 2
39	BA	250/254 (98%)	230 (92%)	14 (6%)	6 (2%)	4 24
39	DA	250/254 (98%)	213 (85%)	30 (12%)	7 (3%)	4 21
40	BB	384/387 (99%)	333 (87%)	37 (10%)	14 (4%)	2 16
40	DB	384/387 (99%)	341 (89%)	34 (9%)	9 (2%)	5 25
41	BC	359/362 (99%)	304 (85%)	34 (10%)	21 (6%)	1 8
41	DC	359/362 (99%)	306 (85%)	32 (9%)	21 (6%)	1 8
42	BD	294/297 (99%)	242 (82%)	31 (10%)	21 (7%)	1 4
42	DD	292/297 (98%)	267 (91%)	19 (6%)	6 (2%)	5 27
43	BE	152/176 (86%)	137 (90%)	11 (7%)	4 (3%)	4 23
43	DE	153/176 (87%)	134 (88%)	15 (10%)	4 (3%)	4 23
44	BF	220/244 (90%)	200 (91%)	11 (5%)	9 (4%)	2 13
44	DF	221/244 (91%)	201 (91%)	15 (7%)	5 (2%)	5 25
45	BG	231/256 (90%)	186 (80%)	26 (11%)	19 (8%)	0 3
45	DG	229/256 (90%)	180 (79%)	28 (12%)	21 (9%)	0 2
46	BH	189/191 (99%)	166 (88%)	17 (9%)	6 (3%)	3 18
46	DH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	5 27
47	BI	207/221 (94%)	181 (87%)	19 (9%)	7 (3%)	3 17
47	DI	209/221 (95%)	175 (84%)	22 (10%)	12 (6%)	1 8
48	BJ	167/174 (96%)	120 (72%)	26 (16%)	21 (13%)	0 1
48	DJ	167/174 (96%)	135 (81%)	19 (11%)	13 (8%)	1 4
49	BL	191/199 (96%)	161 (84%)	18 (9%)	12 (6%)	1 6
49	DL	192/199 (96%)	161 (84%)	20 (10%)	11 (6%)	1 8
50	BM	134/138 (97%)	117 (87%)	8 (6%)	9 (7%)	1 5
50	DM	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18 53
51	BN	201/204 (98%)	184 (92%)	10 (5%)	7 (4%)	3 16
51	DN	201/204 (98%)	182 (90%)	13 (6%)	6 (3%)	3 19
52	BO	353/219 (161%)	332 (94%)	14 (4%)	7 (2%)	6 28
52	DO	352/219 (161%)	324 (92%)	18 (5%)	10 (3%)	4 21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	BP	181/184 (98%)	155 (86%)	17 (9%)	9 (5%)	1 10
53	DP	153/184 (83%)	142 (93%)	9 (6%)	2 (1%)	9 38
54	BQ	183/186 (98%)	162 (88%)	17 (9%)	4 (2%)	5 26
54	DQ	183/186 (98%)	168 (92%)	9 (5%)	6 (3%)	3 17
55	BR	186/189 (98%)	170 (91%)	12 (6%)	4 (2%)	5 26
55	DR	186/189 (98%)	167 (90%)	16 (9%)	3 (2%)	7 34
56	BS	170/172 (99%)	154 (91%)	12 (7%)	4 (2%)	4 24
56	DS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	21 56
57	BT	157/160 (98%)	140 (89%)	10 (6%)	7 (4%)	2 12
57	DT	157/160 (98%)	146 (93%)	9 (6%)	2 (1%)	9 38
58	BU	98/121 (81%)	75 (76%)	14 (14%)	9 (9%)	0 2
58	DU	96/121 (79%)	80 (83%)	13 (14%)	3 (3%)	3 19
59	BV	134/137 (98%)	124 (92%)	9 (7%)	1 (1%)	18 53
59	DV	134/137 (98%)	124 (92%)	8 (6%)	2 (2%)	8 35
60	BW	96/155 (62%)	69 (72%)	16 (17%)	11 (12%)	0 1
60	DW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1 7
61	BX	119/142 (84%)	106 (89%)	11 (9%)	2 (2%)	7 32
61	DX	118/142 (83%)	103 (87%)	7 (6%)	8 (7%)	1 5
62	BY	124/127 (98%)	107 (86%)	15 (12%)	2 (2%)	7 34
62	DY	124/127 (98%)	107 (86%)	12 (10%)	5 (4%)	2 14
63	BZ	133/136 (98%)	114 (86%)	9 (7%)	10 (8%)	1 4
63	DZ	133/136 (98%)	107 (80%)	13 (10%)	13 (10%)	0 2
64	Ba	146/149 (98%)	120 (82%)	15 (10%)	11 (8%)	1 4
64	Da	146/149 (98%)	123 (84%)	18 (12%)	5 (3%)	3 17
65	Bb	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	1 9
65	Db	56/59 (95%)	44 (79%)	7 (12%)	5 (9%)	0 3
66	Bc	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	11 43
66	Dc	98/105 (93%)	87 (89%)	8 (8%)	3 (3%)	3 19
67	Bd	107/113 (95%)	94 (88%)	8 (8%)	5 (5%)	2 11
67	Dd	107/113 (95%)	88 (82%)	13 (12%)	6 (6%)	1 8
68	Be	125/130 (96%)	111 (89%)	10 (8%)	4 (3%)	3 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
68	De	125/130 (96%)	110 (88%)	9 (7%)	6 (5%)	2 11
69	Bf	104/107 (97%)	100 (96%)	2 (2%)	2 (2%)	6 30
69	Df	104/107 (97%)	96 (92%)	5 (5%)	3 (3%)	3 20
70	Bg	110/121 (91%)	97 (88%)	9 (8%)	4 (4%)	2 16
70	Dg	110/121 (91%)	93 (84%)	13 (12%)	4 (4%)	2 16
71	Bh	117/120 (98%)	99 (85%)	10 (8%)	8 (7%)	1 5
71	Dh	117/120 (98%)	99 (85%)	14 (12%)	4 (3%)	3 17
72	Bi	97/100 (97%)	75 (77%)	11 (11%)	11 (11%)	0 1
72	Di	97/100 (97%)	77 (79%)	13 (13%)	7 (7%)	1 4
73	Bj	85/88 (97%)	70 (82%)	12 (14%)	3 (4%)	3 16
73	Dj	85/88 (97%)	75 (88%)	8 (9%)	2 (2%)	4 24
74	Bk	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	9 38
74	Dk	75/78 (96%)	61 (81%)	10 (13%)	4 (5%)	1 9
75	Bl	48/51 (94%)	44 (92%)	4 (8%)	0	100 100
75	Dl	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	5 27
76	Bm	50/128 (39%)	45 (90%)	3 (6%)	2 (4%)	2 14
76	Dm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6 28
77	Bn	23/25 (92%)	20 (87%)	3 (13%)	0	100 100
77	Dn	23/25 (92%)	22 (96%)	0	1 (4%)	2 12
78	Bo	103/106 (97%)	86 (84%)	13 (13%)	4 (4%)	2 14
78	Do	103/106 (97%)	90 (87%)	11 (11%)	2 (2%)	6 30
79	Bp	89/92 (97%)	77 (86%)	9 (10%)	3 (3%)	3 17
79	Dp	89/92 (97%)	81 (91%)	8 (9%)	0	100 100
81	Ch	61/273 (22%)	38 (62%)	9 (15%)	14 (23%)	0 0
83	Dq	117/312 (38%)	93 (80%)	18 (15%)	6 (5%)	1 10
All	All	22511/24658 (91%)	18787 (84%)	2329 (10%)	1395 (6%)	1 6

5 of 1395 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	4	PRO
2	AA	29	VAL
2	AA	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AA	39	ASN
2	AA	66	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	164/210 (78%)	114 (70%)	50 (30%)	0	1
2	CA	165/210 (79%)	126 (76%)	39 (24%)	1	4
3	AB	191/224 (85%)	137 (72%)	54 (28%)	0	2
3	CB	192/224 (86%)	141 (73%)	51 (27%)	0	3
4	AC	176/205 (86%)	124 (70%)	52 (30%)	0	2
4	CC	176/205 (86%)	131 (74%)	45 (26%)	0	3
5	AD	182/195 (93%)	133 (73%)	49 (27%)	0	2
5	CD	182/195 (93%)	139 (76%)	43 (24%)	1	4
6	AE	221/222 (100%)	160 (72%)	61 (28%)	0	2
6	CE	221/222 (100%)	165 (75%)	56 (25%)	0	3
7	AF	173/191 (91%)	139 (80%)	34 (20%)	1	8
7	CF	173/191 (91%)	128 (74%)	45 (26%)	0	3
8	AG	188/201 (94%)	145 (77%)	43 (23%)	1	5
8	CG	187/201 (93%)	136 (73%)	51 (27%)	0	2
9	AH	165/170 (97%)	116 (70%)	49 (30%)	0	2
9	CH	165/170 (97%)	126 (76%)	39 (24%)	1	4
10	AI	150/161 (93%)	114 (76%)	36 (24%)	1	4
10	CI	150/161 (93%)	118 (79%)	32 (21%)	1	6
11	AJ	158/166 (95%)	121 (77%)	37 (23%)	1	4
11	CJ	158/166 (95%)	124 (78%)	34 (22%)	1	6
12	AK	77/98 (79%)	57 (74%)	20 (26%)	0	3
12	CK	73/98 (74%)	56 (77%)	17 (23%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	AL	129/137 (94%)	102 (79%)	27 (21%)	1 7
13	CL	129/137 (94%)	99 (77%)	30 (23%)	1 4
14	AM	88/119 (74%)	53 (60%)	35 (40%)	0 1
14	CM	88/119 (74%)	53 (60%)	35 (40%)	0 1
15	AN	127/128 (99%)	86 (68%)	41 (32%)	0 1
15	CN	127/128 (99%)	97 (76%)	30 (24%)	1 4
16	AO	81/105 (77%)	57 (70%)	24 (30%)	0 2
16	CO	97/105 (92%)	70 (72%)	27 (28%)	0 2
17	AP	101/118 (86%)	81 (80%)	20 (20%)	1 8
17	CP	103/118 (87%)	84 (82%)	19 (18%)	1 9
18	AQ	117/119 (98%)	82 (70%)	35 (30%)	0 2
18	CQ	118/119 (99%)	90 (76%)	28 (24%)	1 4
19	AR	94/124 (76%)	72 (77%)	22 (23%)	1 4
19	CR	92/124 (74%)	67 (73%)	25 (27%)	0 2
20	AS	128/129 (99%)	87 (68%)	41 (32%)	0 1
20	CS	128/129 (99%)	92 (72%)	36 (28%)	0 2
21	AT	115/116 (99%)	84 (73%)	31 (27%)	0 2
21	CT	115/116 (99%)	86 (75%)	29 (25%)	0 3
22	AU	100/114 (88%)	69 (69%)	31 (31%)	0 1
22	CU	103/114 (90%)	65 (63%)	38 (37%)	0 1
23	AV	74/74 (100%)	54 (73%)	20 (27%)	0 2
23	CV	74/74 (100%)	57 (77%)	17 (23%)	1 5
24	AW	110/111 (99%)	82 (74%)	28 (26%)	0 3
24	CW	110/111 (99%)	94 (86%)	16 (14%)	3 15
25	AX	119/120 (99%)	93 (78%)	26 (22%)	1 6
25	CX	119/120 (99%)	96 (81%)	23 (19%)	1 8
26	AY	112/113 (99%)	81 (72%)	31 (28%)	0 2
26	CY	112/113 (99%)	82 (73%)	30 (27%)	0 2
27	AZ	61/89 (68%)	42 (69%)	19 (31%)	0 1
27	CZ	61/89 (68%)	44 (72%)	17 (28%)	0 2
28	Aa	83/101 (82%)	60 (72%)	23 (28%)	0 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	Ca	83/101 (82%)	68 (82%)	15 (18%)	2 9
29	Ab	70/71 (99%)	60 (86%)	10 (14%)	3 16
29	Cb	70/71 (99%)	57 (81%)	13 (19%)	1 9
30	Ac	56/60 (93%)	36 (64%)	20 (36%)	0 1
30	Cc	56/60 (93%)	35 (62%)	21 (38%)	0 1
31	Ad	47/49 (96%)	40 (85%)	7 (15%)	3 15
31	Cd	47/49 (96%)	35 (74%)	12 (26%)	0 3
32	Ae	51/54 (94%)	41 (80%)	10 (20%)	1 8
32	Ce	53/54 (98%)	37 (70%)	16 (30%)	0 1
33	Af	43/112 (38%)	31 (72%)	12 (28%)	0 2
33	Cf	43/112 (38%)	29 (67%)	14 (33%)	0 1
34	Ag	259/262 (99%)	215 (83%)	44 (17%)	2 11
34	Cg	260/262 (99%)	222 (85%)	38 (15%)	3 15
35	Ah	97/195 (50%)	71 (73%)	26 (27%)	0 2
39	BA	193/196 (98%)	153 (79%)	40 (21%)	1 7
39	DA	192/196 (98%)	149 (78%)	43 (22%)	1 5
40	BB	321/323 (99%)	231 (72%)	90 (28%)	0 2
40	DB	321/323 (99%)	242 (75%)	79 (25%)	1 4
41	BC	288/289 (100%)	221 (77%)	67 (23%)	1 4
41	DC	288/289 (100%)	213 (74%)	75 (26%)	0 3
42	BD	244/245 (100%)	183 (75%)	61 (25%)	0 3
42	DD	243/245 (99%)	185 (76%)	58 (24%)	1 4
43	BE	134/153 (88%)	110 (82%)	24 (18%)	2 10
43	DE	135/153 (88%)	113 (84%)	22 (16%)	2 12
44	BF	186/205 (91%)	162 (87%)	24 (13%)	4 19
44	DF	187/205 (91%)	158 (84%)	29 (16%)	2 13
45	BG	187/208 (90%)	146 (78%)	41 (22%)	1 5
45	DG	177/208 (85%)	136 (77%)	41 (23%)	1 4
46	BH	171/171 (100%)	127 (74%)	44 (26%)	0 3
46	DH	171/171 (100%)	128 (75%)	43 (25%)	0 3
47	BI	177/187 (95%)	140 (79%)	37 (21%)	1 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	DI	179/187 (96%)	134 (75%)	45 (25%)	0 3
48	BJ	147/150 (98%)	104 (71%)	43 (29%)	0 2
48	DJ	147/150 (98%)	113 (77%)	34 (23%)	1 5
49	BL	154/159 (97%)	121 (79%)	33 (21%)	1 6
49	DL	154/159 (97%)	126 (82%)	28 (18%)	2 9
50	BM	107/109 (98%)	81 (76%)	26 (24%)	1 4
50	DM	108/109 (99%)	80 (74%)	28 (26%)	0 3
51	BN	175/176 (99%)	137 (78%)	38 (22%)	1 6
51	DN	175/176 (99%)	139 (79%)	36 (21%)	1 7
52	BO	323/179 (180%)	260 (80%)	63 (20%)	1 8
52	DO	323/179 (180%)	254 (79%)	69 (21%)	1 6
53	BP	140/146 (96%)	104 (74%)	36 (26%)	0 3
53	DP	125/146 (86%)	98 (78%)	27 (22%)	1 6
54	BQ	150/151 (99%)	122 (81%)	28 (19%)	1 9
54	DQ	150/151 (99%)	121 (81%)	29 (19%)	1 8
55	BR	153/154 (99%)	109 (71%)	44 (29%)	0 2
55	DR	153/154 (99%)	113 (74%)	40 (26%)	0 3
56	BS	156/156 (100%)	119 (76%)	37 (24%)	1 4
56	DS	156/156 (100%)	119 (76%)	37 (24%)	1 4
57	BT	136/137 (99%)	104 (76%)	32 (24%)	1 4
57	DT	136/137 (99%)	107 (79%)	29 (21%)	1 6
58	BU	87/107 (81%)	72 (83%)	15 (17%)	2 11
58	DU	85/107 (79%)	60 (71%)	25 (29%)	0 2
59	BV	104/105 (99%)	84 (81%)	20 (19%)	1 8
59	DV	104/105 (99%)	93 (89%)	11 (11%)	6 27
60	BW	57/129 (44%)	48 (84%)	9 (16%)	2 13
60	DW	100/129 (78%)	83 (83%)	17 (17%)	2 11
61	BX	104/118 (88%)	75 (72%)	29 (28%)	0 2
61	DX	104/118 (88%)	77 (74%)	27 (26%)	0 3
62	BY	109/110 (99%)	83 (76%)	26 (24%)	1 4
62	DY	109/110 (99%)	81 (74%)	28 (26%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
63	BZ	115/116 (99%)	84 (73%)	31 (27%)	0 2
63	DZ	115/116 (99%)	87 (76%)	28 (24%)	1 4
64	Ba	118/119 (99%)	95 (80%)	23 (20%)	1 8
64	Da	118/119 (99%)	90 (76%)	28 (24%)	1 4
65	Bb	46/47 (98%)	36 (78%)	10 (22%)	1 6
65	Db	46/47 (98%)	32 (70%)	14 (30%)	0 1
66	Bc	81/88 (92%)	61 (75%)	20 (25%)	1 4
66	Dc	84/88 (96%)	65 (77%)	19 (23%)	1 5
67	Bd	92/97 (95%)	69 (75%)	23 (25%)	0 3
67	Dd	94/97 (97%)	72 (77%)	22 (23%)	1 4
68	Be	109/111 (98%)	84 (77%)	25 (23%)	1 5
68	De	109/111 (98%)	85 (78%)	24 (22%)	1 5
69	Bf	90/91 (99%)	76 (84%)	14 (16%)	2 13
69	Df	90/91 (99%)	80 (89%)	10 (11%)	6 25
70	Bg	95/103 (92%)	71 (75%)	24 (25%)	0 3
70	Dg	95/103 (92%)	70 (74%)	25 (26%)	0 3
71	Bh	104/105 (99%)	74 (71%)	30 (29%)	0 2
71	Dh	103/105 (98%)	75 (73%)	28 (27%)	0 2
72	Bi	81/82 (99%)	57 (70%)	24 (30%)	0 2
72	Di	80/82 (98%)	51 (64%)	29 (36%)	0 1
73	Bj	70/71 (99%)	55 (79%)	15 (21%)	1 6
73	Dj	70/71 (99%)	55 (79%)	15 (21%)	1 6
74	Bk	68/69 (99%)	49 (72%)	19 (28%)	0 2
74	Dk	67/69 (97%)	50 (75%)	17 (25%)	0 3
75	Bl	45/46 (98%)	32 (71%)	13 (29%)	0 2
75	Dl	45/46 (98%)	30 (67%)	15 (33%)	0 1
76	Bm	47/116 (40%)	36 (77%)	11 (23%)	1 4
76	Dm	47/116 (40%)	35 (74%)	12 (26%)	0 3
77	Bn	23/23 (100%)	15 (65%)	8 (35%)	0 1
77	Dn	23/23 (100%)	13 (56%)	10 (44%)	0 0
78	Bo	90/91 (99%)	64 (71%)	26 (29%)	0 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
78	Do	90/91 (99%)	72 (80%)	18 (20%)	1 7
79	Bp	71/72 (99%)	53 (75%)	18 (25%)	0 3
79	Dp	71/72 (99%)	59 (83%)	12 (17%)	2 11
81	Ch	54/199 (27%)	38 (70%)	16 (30%)	0 2
83	Dq	105/233 (45%)	74 (70%)	31 (30%)	0 2
All	All	19013/20583 (92%)	14450 (76%)	4563 (24%)	1 4

5 of 4563 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	DI	52	LEU
50	DM	63	VAL
47	DI	33	ILE
61	DX	57	LEU
49	BL	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 239 such sidechains are listed below:

Mol	Chain	Res	Type
63	BZ	57	HIS
60	DW	59	HIS
6	CE	157	ASN
59	DV	33	ASN
75	Dl	33	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1763/1800 (97%)	548 (31%)	86 (4%)
36	A1	3146/3396 (92%)	758 (24%)	127 (4%)
36	A5	3145/3396 (92%)	747 (23%)	129 (4%)
37	A3	120/121 (99%)	22 (18%)	3 (2%)
37	A7	120/121 (99%)	18 (15%)	0
38	A4	157/158 (99%)	39 (24%)	5 (3%)
38	A8	157/158 (99%)	33 (21%)	3 (1%)
80	A6	1765/1800 (98%)	506 (28%)	60 (3%)
All	All	10373/10950 (94%)	2671 (25%)	413 (3%)

5 of 2671 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	4	C
1	A2	8	U
1	A2	16	G
1	A2	20	G

5 of 413 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
80	A6	187	G
36	A5	183	G
36	A5	3218	A
80	A6	400	A
80	A6	1058	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3566 ligands modelled in this entry, 2221 are monoatomic - leaving 1345 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3724	-	0,6,6	-	-	-		
86	OHX	A5	3802	-	0,6,6	-	-	-		
86	OHX	A6	2069	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A2	1940	-	0,6,6	-	-	-		
86	OHX	A5	3763	87	0,6,6	-	-	-		
86	OHX	A2	1993	-	0,6,6	-	-	-		
86	OHX	A2	1921	87	0,6,6	-	-	-		
86	OHX	A5	3622	-	0,6,6	-	-	-		
86	OHX	A5	3742	-	0,6,6	-	-	-		
86	OHX	A2	2002	-	0,6,6	-	-	-		
86	OHX	A1	3441	-	0,6,6	-	-	-		
86	OHX	A1	3704	-	0,6,6	-	-	-		
86	OHX	A1	3420	-	0,6,6	-	-	-		
86	OHX	A6	2042	-	0,6,6	-	-	-		
86	OHX	A5	3700	87	0,6,6	-	-	-		
86	OHX	A6	2001	-	0,6,6	-	-	-		
86	OHX	A1	3515	-	0,6,6	-	-	-		
86	OHX	A5	3597	-	0,6,6	-	-	-		
86	OHX	A2	2066	-	0,6,6	-	-	-		
86	OHX	A1	3559	-	0,6,6	-	-	-		
86	OHX	A6	1920	-	0,6,6	-	-	-		
86	OHX	A2	1919	-	0,6,6	-	-	-		
86	OHX	A1	3665	-	0,6,6	-	-	-		
86	OHX	A2	2051	-	0,6,6	-	-	-		
86	OHX	A2	2063	-	0,6,6	-	-	-		
86	OHX	A1	3518	-	0,6,6	-	-	-		
86	OHX	A1	3621	-	0,6,6	-	-	-		
86	OHX	A1	3632	-	0,6,6	-	-	-		
86	OHX	A5	3436	-	0,6,6	-	-	-		
86	OHX	A1	3611	-	0,6,6	-	-	-		
86	OHX	A1	3414	-	0,6,6	-	-	-		
86	OHX	A2	2084	-	0,6,6	-	-	-		
86	OHX	A4	214	87	0,6,6	-	-	-		
86	OHX	A6	1942	-	0,6,6	-	-	-		
86	OHX	A5	3554	-	0,6,6	-	-	-		
86	OHX	A6	2085	-	0,6,6	-	-	-		
86	OHX	A2	1963	-	0,6,6	-	-	-		
86	OHX	A2	2001	-	0,6,6	-	-	-		
86	OHX	A5	3815	-	0,6,6	-	-	-		
86	OHX	A2	2067	87,86	0,6,6	-	-	-		
86	OHX	A5	3800	-	0,6,6	-	-	-		
86	OHX	A2	1909	86	0,6,6	-	-	-		
86	OHX	A1	3607	-	0,6,6	-	-	-		
86	OHX	A5	3416	87	0,6,6	-	-	-		
86	OHX	A1	3493	-	0,6,6	-	-	-		
86	OHX	A1	3442	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	Db	101	-	0,6,6	-	-	-		
86	OHX	A5	3770	-	0,6,6	-	-	-		
86	OHX	A1	3669	87	0,6,6	-	-	-		
86	OHX	A1	3587	-	0,6,6	-	-	-		
86	OHX	A6	1940	-	0,6,6	-	-	-		
86	OHX	A5	3788	-	0,6,6	-	-	-		
86	OHX	A1	3580	-	0,6,6	-	-	-		
86	OHX	A6	2014	-	0,6,6	-	-	-		
86	OHX	A5	3635	-	0,6,6	-	-	-		
86	OHX	A1	3469	-	0,6,6	-	-	-		
86	OHX	A1	3754	-	0,6,6	-	-	-		
86	OHX	A5	3486	-	0,6,6	-	-	-		
86	OHX	A5	3488	-	0,6,6	-	-	-		
86	OHX	A1	3663	87	0,6,6	-	-	-		
86	OHX	A2	1901	-	0,6,6	-	-	-		
86	OHX	A5	3623	-	0,6,6	-	-	-		
86	OHX	DM	201	-	0,6,6	-	-	-		
86	OHX	A1	3638	-	0,6,6	-	-	-		
86	OHX	A1	3792	-	0,6,6	-	-	-		
86	OHX	A1	3742	-	0,6,6	-	-	-		
86	OHX	A1	3670	-	0,6,6	-	-	-		
86	OHX	A5	3645	-	0,6,6	-	-	-		
86	OHX	A5	3413	-	0,6,6	-	-	-		
86	OHX	A6	1961	-	0,6,6	-	-	-		
86	OHX	A6	2093	-	0,6,6	-	-	-		
86	OHX	A6	2080	-	0,6,6	-	-	-		
86	OHX	A5	3696	-	0,6,6	-	-	-		
86	OHX	CL	201	-	0,6,6	-	-	-		
86	OHX	A5	3713	87	0,6,6	-	-	-		
86	OHX	A1	3720	-	0,6,6	-	-	-		
86	OHX	A2	2055	87	0,6,6	-	-	-		
86	OHX	A6	2082	-	0,6,6	-	-	-		
86	OHX	A1	3519	87	0,6,6	-	-	-		
86	OHX	A1	3641	87	0,6,6	-	-	-		
86	OHX	A6	1963	-	0,6,6	-	-	-		
86	OHX	A5	3447	-	0,6,6	-	-	-		
86	OHX	A2	1932	-	0,6,6	-	-	-		
86	OHX	A6	1947	87	0,6,6	-	-	-		
86	OHX	A8	204	-	0,6,6	-	-	-		
86	OHX	A2	1985	-	0,6,6	-	-	-		
86	OHX	A5	3474	87	0,6,6	-	-	-		
86	OHX	A5	3519	-	0,6,6	-	-	-		
86	OHX	A1	3672	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A3	213	-	0,6,6	-	-	-		
86	OHX	A5	3602	87	0,6,6	-	-	-		
86	OHX	A2	2005	-	0,6,6	-	-	-		
86	OHX	A5	3465	-	0,6,6	-	-	-		
86	OHX	A1	3489	-	0,6,6	-	-	-		
86	OHX	A2	1943	-	0,6,6	-	-	-		
86	OHX	A1	3771	-	0,6,6	-	-	-		
86	OHX	A6	1972	87	0,6,6	-	-	-		
86	OHX	A1	3680	-	0,6,6	-	-	-		
86	OHX	A2	2057	-	0,6,6	-	-	-		
86	OHX	A1	3688	-	0,6,6	-	-	-		
86	OHX	A1	3520	87	0,6,6	-	-	-		
86	OHX	A2	2035	87	0,6,6	-	-	-		
86	OHX	A6	2065	-	0,6,6	-	-	-		
86	OHX	A6	2092	-	0,6,6	-	-	-		
86	OHX	A1	3535	-	0,6,6	-	-	-		
86	OHX	A1	3635	-	0,6,6	-	-	-		
86	OHX	A5	3487	-	0,6,6	-	-	-		
86	OHX	A2	2024	-	0,6,6	-	-	-		
86	OHX	A2	1971	-	0,6,6	-	-	-		
86	OHX	A2	2040	-	0,6,6	-	-	-		
86	OHX	A6	1999	-	0,6,6	-	-	-		
86	OHX	Bj	103	-	0,6,6	-	-	-		
86	OHX	A1	3481	-	0,6,6	-	-	-		
86	OHX	A5	3403	-	0,6,6	-	-	-		
86	OHX	A1	3726	-	0,6,6	-	-	-		
86	OHX	A1	3756	-	0,6,6	-	-	-		
86	OHX	A1	3623	-	0,6,6	-	-	-		
86	OHX	A1	3736	-	0,6,6	-	-	-		
86	OHX	A1	3498	87	0,6,6	-	-	-		
86	OHX	A6	1907	-	0,6,6	-	-	-		
86	OHX	A5	3481	-	0,6,6	-	-	-		
86	OHX	A1	3512	-	0,6,6	-	-	-		
86	OHX	A5	3444	87	0,6,6	-	-	-		
86	OHX	A6	2034	-	0,6,6	-	-	-		
86	OHX	A6	2006	87	0,6,6	-	-	-		
86	OHX	A5	3807	86	0,6,6	-	-	-		
86	OHX	A5	3801	-	0,6,6	-	-	-		
86	OHX	A1	3568	-	0,6,6	-	-	-		
86	OHX	A5	3699	-	0,6,6	-	-	-		
86	OHX	A6	1985	-	0,6,6	-	-	-		
86	OHX	A6	2066	-	0,6,6	-	-	-		
86	OHX	A2	1903	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3443	-	0,6,6	-	-	-		
86	OHX	A5	3540	87	0,6,6	-	-	-		
86	OHX	A1	3778	-	0,6,6	-	-	-		
86	OHX	A2	1936	87	0,6,6	-	-	-		
86	OHX	A2	2020	-	0,6,6	-	-	-		
86	OHX	A6	1945	-	0,6,6	-	-	-		
86	OHX	BB	401	-	0,6,6	-	-	-		
86	OHX	A5	3735	87	0,6,6	-	-	-		
86	OHX	A1	3407	-	0,6,6	-	-	-		
86	OHX	A1	3463	87	0,6,6	-	-	-		
86	OHX	DC	401	-	0,6,6	-	-	-		
86	OHX	A5	3504	87	0,6,6	-	-	-		
86	OHX	A1	3575	-	0,6,6	-	-	-		
86	OHX	A6	2040	87	0,6,6	-	-	-		
86	OHX	A5	3667	-	0,6,6	-	-	-		
86	OHX	A5	3424	-	0,6,6	-	-	-		
86	OHX	A2	1976	-	0,6,6	-	-	-		
86	OHX	A1	3698	-	0,6,6	-	-	-		
86	OHX	A5	3538	-	0,6,6	-	-	-		
86	OHX	A5	3805	-	0,6,6	-	-	-		
86	OHX	A1	3563	-	0,6,6	-	-	-		
86	OHX	A6	1902	-	0,6,6	-	-	-		
86	OHX	A5	3698	-	0,6,6	-	-	-		
86	OHX	A2	2073	-	0,6,6	-	-	-		
86	OHX	A5	3556	-	0,6,6	-	-	-		
86	OHX	A7	205	-	0,6,6	-	-	-		
86	OHX	A8	217	-	0,6,6	-	-	-		
86	OHX	A5	3808	87	0,6,6	-	-	-		
86	OHX	BN	301	-	0,6,6	-	-	-		
86	OHX	DI	302	-	0,6,6	-	-	-		
86	OHX	A2	2028	-	0,6,6	-	-	-		
86	OHX	A5	3640	-	0,6,6	-	-	-		
86	OHX	A1	3534	-	0,6,6	-	-	-		
86	OHX	A2	2039	-	0,6,6	-	-	-		
86	OHX	A5	3462	-	0,6,6	-	-	-		
86	OHX	A5	3634	-	0,6,6	-	-	-		
86	OHX	A5	3451	87	0,6,6	-	-	-		
86	OHX	A5	3604	-	0,6,6	-	-	-		
86	OHX	A5	3767	-	0,6,6	-	-	-		
86	OHX	A5	3686	-	0,6,6	-	-	-		
86	OHX	A2	1945	-	0,6,6	-	-	-		
86	OHX	A5	3757	-	0,6,6	-	-	-		
86	OHX	A5	3401	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	DQ	201	-	0,6,6	-	-	-		
86	OHX	A6	1982	-	0,6,6	-	-	-		
86	OHX	A6	1915	-	0,6,6	-	-	-		
86	OHX	A5	3684	87	0,6,6	-	-	-		
86	OHX	Dh	201	-	0,6,6	-	-	-		
86	OHX	A5	3708	-	0,6,6	-	-	-		
86	OHX	A4	209	87	0,6,6	-	-	-		
86	OHX	A5	3773	-	0,6,6	-	-	-		
86	OHX	A6	1980	87	0,6,6	-	-	-		
86	OHX	A2	1947	87	0,6,6	-	-	-		
86	OHX	A6	2073	-	0,6,6	-	-	-		
86	OHX	A1	3492	-	0,6,6	-	-	-		
86	OHX	A1	3766	-	0,6,6	-	-	-		
86	OHX	A2	2078	-	0,6,6	-	-	-		
86	OHX	A5	3655	-	0,6,6	-	-	-		
86	OHX	A5	3455	-	0,6,6	-	-	-		
86	OHX	A3	202	87	0,6,6	-	-	-		
86	OHX	A5	3404	87	0,6,6	-	-	-		
86	OHX	A6	2081	87	0,6,6	-	-	-		
86	OHX	A5	3626	87	0,6,6	-	-	-		
86	OHX	A1	3703	87	0,6,6	-	-	-		
86	OHX	A5	3530	-	0,6,6	-	-	-		
86	OHX	A1	3552	-	0,6,6	-	-	-		
86	OHX	A1	3805	-	0,6,6	-	-	-		
86	OHX	A6	2028	-	0,6,6	-	-	-		
86	OHX	A6	2007	-	0,6,6	-	-	-		
86	OHX	A3	208	-	0,6,6	-	-	-		
86	OHX	A6	1996	-	0,6,6	-	-	-		
86	OHX	A2	2004	-	0,6,6	-	-	-		
86	OHX	A5	3500	-	0,6,6	-	-	-		
86	OHX	A2	2013	-	0,6,6	-	-	-		
86	OHX	A1	3808	87	0,6,6	-	-	-		
86	OHX	A1	3636	87	0,6,6	-	-	-		
86	OHX	A1	3598	-	0,6,6	-	-	-		
86	OHX	A6	1916	87	0,6,6	-	-	-		
86	OHX	A1	3762	87	0,6,6	-	-	-		
86	OHX	A2	2062	-	0,6,6	-	-	-		
86	OHX	BI	304	47	0,6,6	-	-	-		
86	OHX	A5	3636	87	0,6,6	-	-	-		
86	OHX	A2	2003	-	0,6,6	-	-	-		
86	OHX	A7	211	87	0,6,6	-	-	-		
86	OHX	A1	3415	87	0,6,6	-	-	-		
86	OHX	A5	3733	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3645	87	0,6,6	-	-	-		
86	OHX	A5	3477	-	0,6,6	-	-	-		
86	OHX	A5	3581	-	0,6,6	-	-	-		
86	OHX	A1	3478	-	0,6,6	-	-	-		
86	OHX	DI	301	-	0,6,6	-	-	-		
86	OHX	A5	3485	-	0,6,6	-	-	-		
86	OHX	A1	3765	-	0,6,6	-	-	-		
86	OHX	A2	1916	-	0,6,6	-	-	-		
86	OHX	A5	3669	87	0,6,6	-	-	-		
86	OHX	A2	2022	-	0,6,6	-	-	-		
86	OHX	A1	3423	87	0,6,6	-	-	-		
86	OHX	A1	3480	87	0,6,6	-	-	-		
86	OHX	A5	3513	-	0,6,6	-	-	-		
86	OHX	A1	3751	-	0,6,6	-	-	-		
86	OHX	A5	3595	-	0,6,6	-	-	-		
86	OHX	BI	301	-	0,6,6	-	-	-		
86	OHX	A2	2023	87	0,6,6	-	-	-		
86	OHX	A1	3648	87	0,6,6	-	-	-		
86	OHX	A2	2027	-	0,6,6	-	-	-		
86	OHX	A1	3504	-	0,6,6	-	-	-		
86	OHX	A6	2004	-	0,6,6	-	-	-		
86	OHX	A2	2060	-	0,6,6	-	-	-		
86	OHX	A5	3816	-	0,6,6	-	-	-		
86	OHX	A5	3650	-	0,6,6	-	-	-		
86	OHX	A6	1992	-	0,6,6	-	-	-		
86	OHX	A5	3557	-	0,6,6	-	-	-		
86	OHX	A1	3566	87	0,6,6	-	-	-		
86	OHX	A5	3747	-	0,6,6	-	-	-		
86	OHX	A6	1934	87	0,6,6	-	-	-		
86	OHX	A1	3687	-	0,6,6	-	-	-		
86	OHX	A1	3475	-	0,6,6	-	-	-		
86	OHX	A2	2014	-	0,6,6	-	-	-		
86	OHX	A1	3605	-	0,6,6	-	-	-		
86	OHX	A1	3615	-	0,6,6	-	-	-		
86	OHX	A1	3588	-	0,6,6	-	-	-		
86	OHX	A5	3564	87	0,6,6	-	-	-		
86	OHX	A6	2087	-	0,6,6	-	-	-		
86	OHX	A5	3786	-	0,6,6	-	-	-		
86	OHX	A5	3555	-	0,6,6	-	-	-		
86	OHX	A5	3648	-	0,6,6	-	-	-		
86	OHX	A5	3774	87	0,6,6	-	-	-		
86	OHX	A6	1952	87	0,6,6	-	-	-		
86	OHX	A6	1922	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3565	-	0,6,6	-	-	-		
86	OHX	A1	3620	87	0,6,6	-	-	-		
86	OHX	CG	301	-	0,6,6	-	-	-		
86	OHX	A1	3803	87	0,6,6	-	-	-		
86	OHX	A1	3547	-	0,6,6	-	-	-		
86	OHX	A2	1984	87	0,6,6	-	-	-		
86	OHX	A2	2036	-	0,6,6	-	-	-		
86	OHX	A1	3536	-	0,6,6	-	-	-		
86	OHX	A1	3760	87	0,6,6	-	-	-		
86	OHX	A1	3702	-	0,6,6	-	-	-		
86	OHX	A5	3647	87	0,6,6	-	-	-		
86	OHX	A5	3479	87	0,6,6	-	-	-		
86	OHX	A1	3693	-	0,6,6	-	-	-		
86	OHX	A1	3773	-	0,6,6	-	-	-		
86	OHX	A1	3550	-	0,6,6	-	-	-		
86	OHX	A5	3758	87	0,6,6	-	-	-		
86	OHX	A1	3650	-	0,6,6	-	-	-		
86	OHX	BI	302	-	0,6,6	-	-	-		
86	OHX	A6	1913	-	0,6,6	-	-	-		
86	OHX	CJ	201	-	0,6,6	-	-	-		
86	OHX	A6	2013	87	0,6,6	-	-	-		
86	OHX	A6	2031	-	0,5,6	-	-	-		
86	OHX	A6	1993	87	0,6,6	-	-	-		
86	OHX	A6	1921	-	0,6,6	-	-	-		
86	OHX	A6	2050	-	0,6,6	-	-	-		
86	OHX	A2	1961	-	0,6,6	-	-	-		
86	OHX	A3	209	-	0,6,6	-	-	-		
86	OHX	A5	3625	-	0,6,6	-	-	-		
86	OHX	A6	1926	87	0,6,6	-	-	-		
86	OHX	A5	3723	87	0,6,6	-	-	-		
86	OHX	A2	2047	-	0,6,6	-	-	-		
86	OHX	DD	301	-	0,6,6	-	-	-		
86	OHX	A1	3802	36,86	0,6,6	-	-	-		
86	OHX	A5	3785	-	0,6,6	-	-	-		
86	OHX	A7	203	87	0,6,6	-	-	-		
86	OHX	A2	1926	-	0,6,6	-	-	-		
86	OHX	A6	1910	87	0,6,6	-	-	-		
86	OHX	A1	3450	-	0,6,6	-	-	-		
86	OHX	A1	3506	-	0,6,6	-	-	-		
86	OHX	CY	201	-	0,6,6	-	-	-		
86	OHX	A5	3675	-	0,6,6	-	-	-		
86	OHX	A1	3743	-	0,6,6	-	-	-		
86	OHX	A6	2051	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	A2	2074	1	0,6,6	-	-	-		
86	OHX	A5	3676	87	0,6,6	-	-	-		
86	OHX	A1	3700	-	0,6,6	-	-	-		
86	OHX	AL	201	-	0,6,6	-	-	-		
86	OHX	A6	2060	-	0,6,6	-	-	-		
86	OHX	A6	2084	-	0,6,6	-	-	-		
86	OHX	A2	2044	-	0,6,6	-	-	-		
86	OHX	A1	3597	-	0,6,6	-	-	-		
86	OHX	A5	3662	-	0,6,6	-	-	-		
86	OHX	A6	1923	-	0,6,6	-	-	-		
86	OHX	A6	2064	-	0,6,6	-	-	-		
86	OHX	A7	213	-	0,6,6	-	-	-		
86	OHX	A6	2035	-	0,6,6	-	-	-		
86	OHX	A5	3633	-	0,6,6	-	-	-		
86	OHX	A5	3629	-	0,6,6	-	-	-		
86	OHX	A1	3436	-	0,6,6	-	-	-		
86	OHX	A5	3611	-	0,6,6	-	-	-		
86	OHX	A1	3652	-	0,6,6	-	-	-		
86	OHX	A2	1950	-	0,6,6	-	-	-		
86	OHX	A1	3800	-	0,6,6	-	-	-		
86	OHX	A8	205	-	0,6,6	-	-	-		
86	OHX	A5	3406	-	0,6,6	-	-	-		
86	OHX	A5	3505	-	0,6,6	-	-	-		
86	OHX	A1	3783	-	0,6,6	-	-	-		
86	OHX	A6	2047	-	0,6,6	-	-	-		
86	OHX	A6	1901	-	0,6,6	-	-	-		
86	OHX	A1	3770	-	0,6,6	-	-	-		
86	OHX	A5	3642	87	0,6,6	-	-	-		
86	OHX	A5	3563	87	0,6,6	-	-	-		
86	OHX	A1	3435	-	0,6,6	-	-	-		
86	OHX	A5	3749	-	0,6,6	-	-	-		
86	OHX	A5	3600	87	0,6,6	-	-	-		
86	OHX	A1	3789	-	0,6,6	-	-	-		
86	OHX	A6	1983	-	0,6,6	-	-	-		
86	OHX	A5	3582	-	0,6,6	-	-	-		
86	OHX	A6	1954	-	0,6,6	-	-	-		
86	OHX	A1	3510	-	0,6,6	-	-	-		
86	OHX	A1	3577	-	0,6,6	-	-	-		
86	OHX	A5	3417	-	0,6,6	-	-	-		
86	OHX	A6	2044	-	0,6,6	-	-	-		
86	OHX	A6	1939	-	0,6,6	-	-	-		
86	OHX	A2	1965	-	0,6,6	-	-	-		
86	OHX	A1	3657	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A5	3624	-	0,6,6	-	-	-		
86	OHX	A6	1978	87	0,6,6	-	-	-		
86	OHX	A1	3696	-	0,6,6	-	-	-		
86	OHX	A1	3713	-	0,6,6	-	-	-		
86	OHX	A6	1970	87	0,6,6	-	-	-		
86	OHX	A2	2021	-	0,6,6	-	-	-		
86	OHX	A6	2090	-	0,6,6	-	-	-		
86	OHX	A5	3719	-	0,6,6	-	-	-		
86	OHX	A2	1983	-	0,6,6	-	-	-		
86	OHX	A2	1906	87	0,6,6	-	-	-		
86	OHX	A6	2075	-	0,6,6	-	-	-		
86	OHX	A1	3524	-	0,6,6	-	-	-		
86	OHX	A1	3809	-	0,6,6	-	-	-		
86	OHX	A1	3465	-	0,6,6	-	-	-		
86	OHX	A1	3579	-	0,6,6	-	-	-		
86	OHX	A5	3456	87	0,6,6	-	-	-		
86	OHX	A5	3780	-	0,6,6	-	-	-		
86	OHX	A5	3794	-	0,6,6	-	-	-		
86	OHX	A5	3514	87	0,6,6	-	-	-		
86	OHX	A6	2010	-	0,6,6	-	-	-		
86	OHX	A1	3487	-	0,6,6	-	-	-		
86	OHX	A1	3681	87	0,6,6	-	-	-		
86	OHX	A5	3452	-	0,6,6	-	-	-		
86	OHX	A6	1965	-	0,6,6	-	-	-		
86	OHX	A2	2038	-	0,6,6	-	-	-		
86	OHX	CP	201	-	0,6,6	-	-	-		
86	OHX	A5	3572	-	0,6,6	-	-	-		
86	OHX	A2	1987	-	0,6,6	-	-	-		
86	OHX	A7	210	-	0,6,6	-	-	-		
86	OHX	A5	3755	-	0,6,6	-	-	-		
86	OHX	A1	3444	87	0,6,6	-	-	-		
86	OHX	A2	1951	-	0,6,6	-	-	-		
86	OHX	A2	1982	-	0,6,6	-	-	-		
86	OHX	A5	3439	-	0,6,6	-	-	-		
86	OHX	A1	3746	-	0,6,6	-	-	-		
86	OHX	A5	3522	-	0,6,6	-	-	-		
86	OHX	A1	3801	87,86	0,6,6	-	-	-		
86	OHX	A6	2096	-	0,6,6	-	-	-		
86	OHX	AP	201	-	0,6,6	-	-	-		
86	OHX	A1	3699	-	0,6,6	-	-	-		
86	OHX	A1	3529	87	0,6,6	-	-	-		
86	OHX	A5	3445	-	0,6,6	-	-	-		
86	OHX	A1	3716	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3722	-	0,6,6	-	-	-		
86	OHX	A1	3775	86	0,6,6	-	-	-		
86	OHX	A6	2089	-	0,6,6	-	-	-		
86	OHX	A8	202	-	0,6,6	-	-	-		
86	OHX	A1	3447	87	0,6,6	-	-	-		
86	OHX	A5	3608	87	0,6,6	-	-	-		
86	OHX	A5	3813	-	0,6,6	-	-	-		
86	OHX	A1	3639	-	0,6,6	-	-	-		
86	OHX	A1	3602	-	0,6,6	-	-	-		
86	OHX	A6	2043	-	0,6,6	-	-	-		
86	OHX	A5	3603	-	0,6,6	-	-	-		
86	OHX	A1	3538	-	0,6,6	-	-	-		
86	OHX	A1	3539	-	0,6,6	-	-	-		
86	OHX	A6	1987	87	0,6,6	-	-	-		
86	OHX	A5	3748	-	0,6,6	-	-	-		
86	OHX	A2	2068	-	0,6,6	-	-	-		
86	OHX	A2	1937	-	0,6,6	-	-	-		
86	OHX	A5	3533	-	0,6,6	-	-	-		
86	OHX	A1	3723	-	0,6,6	-	-	-		
86	OHX	A5	3590	-	0,6,6	-	-	-		
86	OHX	A2	2033	86	0,6,6	-	-	-		
86	OHX	A6	2046	-	0,6,6	-	-	-		
86	OHX	A1	3589	87	0,6,6	-	-	-		
86	OHX	A6	1968	-	0,6,6	-	-	-		
86	OHX	A2	2016	-	0,6,6	-	-	-		
86	OHX	A5	3542	-	0,6,6	-	-	-		
86	OHX	A3	201	-	0,6,6	-	-	-		
86	OHX	A1	3461	87	0,6,6	-	-	-		
86	OHX	A1	3741	87	0,6,6	-	-	-		
86	OHX	A5	3799	-	0,6,6	-	-	-		
86	OHX	A1	3451	87	0,6,6	-	-	-		
86	OHX	A6	2021	87	0,6,6	-	-	-		
86	OHX	A1	3767	-	0,6,6	-	-	-		
86	OHX	A1	3686	-	0,6,6	-	-	-		
86	OHX	A5	3430	87	0,6,6	-	-	-		
86	OHX	A6	1911	87	0,6,6	-	-	-		
86	OHX	A1	3454	-	0,6,6	-	-	-		
86	OHX	A1	3521	86	0,6,6	-	-	-		
86	OHX	A1	3401	-	0,6,6	-	-	-		
86	OHX	A5	3759	87	0,6,6	-	-	-		
86	OHX	A5	3766	-	0,6,6	-	-	-		
86	OHX	A1	3753	-	0,6,6	-	-	-		
86	OHX	A1	3662	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	A1	3684	87	0,6,6	-	-	-		
86	OHX	A5	3442	-	0,6,6	-	-	-		
86	OHX	A5	3818	-	0,6,6	-	-	-		
86	OHX	A1	3708	-	0,6,6	-	-	-		
86	OHX	A4	215	-	0,6,6	-	-	-		
86	OHX	A1	3471	-	0,6,6	-	-	-		
86	OHX	A2	1920	-	0,6,6	-	-	-		
86	OHX	A2	1911	87	0,6,6	-	-	-		
86	OHX	A2	2025	-	0,6,6	-	-	-		
86	OHX	A6	1962	-	0,6,6	-	-	-		
86	OHX	A6	1928	-	0,6,6	-	-	-		
86	OHX	A1	3725	-	0,6,6	-	-	-		
86	OHX	A1	3811	36	0,6,6	-	-	-		
86	OHX	A6	2000	87	0,6,6	-	-	-		
86	OHX	A5	3587	-	0,6,6	-	-	-		
86	OHX	A5	3697	-	0,6,6	-	-	-		
86	OHX	A6	2041	-	0,6,6	-	-	-		
86	OHX	A3	211	87	0,6,6	-	-	-		
86	OHX	A1	3500	87	0,6,6	-	-	-		
86	OHX	A5	3643	-	0,6,6	-	-	-		
86	OHX	A2	2079	-	0,6,6	-	-	-		
86	OHX	DA	302	-	0,6,6	-	-	-		
86	OHX	A2	1918	86	0,6,6	-	-	-		
86	OHX	A1	3545	87	0,6,6	-	-	-		
86	OHX	A6	1904	87	0,6,6	-	-	-		
86	OHX	A6	2048	-	0,6,6	-	-	-		
86	OHX	A1	3509	-	0,6,6	-	-	-		
86	OHX	A5	3559	-	0,6,6	-	-	-		
86	OHX	CI	301	-	0,6,6	-	-	-		
86	OHX	A5	3630	-	0,6,6	-	-	-		
86	OHX	BA	301	-	0,6,6	-	-	-		
86	OHX	A1	3733	-	0,6,6	-	-	-		
86	OHX	A1	3494	-	0,6,6	-	-	-		
86	OHX	A5	3720	87	0,6,6	-	-	-		
86	OHX	A6	1957	-	0,6,6	-	-	-		
86	OHX	A2	2041	-	0,6,6	-	-	-		
86	OHX	A1	3477	-	0,6,6	-	-	-		
86	OHX	A1	3573	87	0,6,6	-	-	-		
86	OHX	A5	3541	87	0,6,6	-	-	-		
86	OHX	A5	3562	-	0,6,6	-	-	-		
86	OHX	A6	2025	-	0,6,6	-	-	-		
86	OHX	A6	1995	-	0,6,6	-	-	-		
86	OHX	A2	1969	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3485	-	0,6,6	-	-	-		
86	OHX	A6	1938	-	0,6,6	-	-	-		
86	OHX	A1	3472	-	0,6,6	-	-	-		
86	OHX	A5	3822	-	0,6,6	-	-	-		
86	OHX	A5	3585	-	0,6,6	-	-	-		
86	OHX	A1	3673	87	0,6,6	-	-	-		
86	OHX	A1	3595	-	0,6,6	-	-	-		
86	OHX	A5	3644	-	0,6,6	-	-	-		
86	OHX	A1	3503	87	0,6,6	-	-	-		
86	OHX	A3	203	87	0,6,6	-	-	-		
86	OHX	A6	1960	-	0,6,6	-	-	-		
86	OHX	A5	3726	-	0,6,6	-	-	-		
86	OHX	A2	2071	-	0,6,6	-	-	-		
86	OHX	A4	213	-	0,6,6	-	-	-		
86	OHX	A5	3618	-	0,6,6	-	-	-		
86	OHX	A5	3491	-	0,6,6	-	-	-		
86	OHX	A2	1938	-	0,6,6	-	-	-		
86	OHX	A1	3816	-	0,6,6	-	-	-		
86	OHX	A5	3806	-	0,6,6	-	-	-		
86	OHX	A5	3431	87	0,6,6	-	-	-		
86	OHX	A5	3512	-	0,6,6	-	-	-		
86	OHX	A1	3557	-	0,6,6	-	-	-		
86	OHX	A5	3678	87	0,6,6	-	-	-		
86	OHX	A2	2069	-	0,6,6	-	-	-		
86	OHX	A6	1937	-	0,6,6	-	-	-		
86	OHX	A8	210	-	0,6,6	-	-	-		
86	OHX	A5	3571	-	0,6,6	-	-	-		
86	OHX	A1	3799	-	0,6,6	-	-	-		
86	OHX	A2	2065	-	0,6,6	-	-	-		
86	OHX	A1	3537	87	0,6,6	-	-	-		
86	OHX	A6	2077	-	0,6,6	-	-	-		
86	OHX	A5	3577	-	0,6,6	-	-	-		
86	OHX	A2	2258	-	0,6,6	-	-	-		
86	OHX	A1	3784	-	0,6,6	-	-	-		
86	OHX	A2	1960	-	0,6,6	-	-	-		
86	OHX	A5	3779	-	0,6,6	-	-	-		
86	OHX	A1	3564	-	0,6,6	-	-	-		
86	OHX	A1	3572	-	0,6,6	-	-	-		
86	OHX	A5	3657	87	0,6,6	-	-	-		
86	OHX	A1	3555	-	0,6,6	-	-	-		
86	OHX	A5	3761	-	0,6,6	-	-	-		
86	OHX	A5	3744	-	0,6,6	-	-	-		
86	OHX	A1	3738	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3774	-	0,6,6	-	-	-		
86	OHX	A5	3526	87	0,6,6	-	-	-		
86	OHX	A2	2077	-	0,6,6	-	-	-		
86	OHX	A2	1912	-	0,6,6	-	-	-		
86	OHX	BP	201	87	0,6,6	-	-	-		
86	OHX	A5	3737	87,86	0,6,6	-	-	-		
86	OHX	A1	3656	-	0,6,6	-	-	-		
86	OHX	A1	3782	87	0,6,6	-	-	-		
86	OHX	A1	3424	-	0,6,6	-	-	-		
86	OHX	A2	2085	-	0,6,6	-	-	-		
86	OHX	A8	212	-	0,6,6	-	-	-		
86	OHX	A2	2008	87	0,6,6	-	-	-		
86	OHX	A5	3596	87	0,6,6	-	-	-		
86	OHX	DO	201	87	0,6,6	-	-	-		
86	OHX	A1	3409	-	0,6,6	-	-	-		
86	OHX	A2	1952	-	0,6,6	-	-	-		
86	OHX	A1	3479	-	0,6,6	-	-	-		
86	OHX	A6	1974	-	0,6,6	-	-	-		
86	OHX	BT	201	-	0,6,6	-	-	-		
86	OHX	A6	1944	-	0,6,6	-	-	-		
86	OHX	A2	2030	87	0,6,6	-	-	-		
86	OHX	A6	2088	-	0,6,6	-	-	-		
86	OHX	A2	1931	-	0,6,6	-	-	-		
86	OHX	A5	3507	87	0,6,6	-	-	-		
86	OHX	A5	3520	-	0,6,6	-	-	-		
86	OHX	A1	3571	87	0,6,6	-	-	-		
86	OHX	A2	2012	-	0,6,6	-	-	-		
86	OHX	A2	1994	-	0,6,6	-	-	-		
86	OHX	A2	1974	-	0,6,6	-	-	-		
86	OHX	A1	3411	-	0,6,6	-	-	-		
86	OHX	A1	3625	-	0,6,6	-	-	-		
86	OHX	A5	3666	-	0,6,6	-	-	-		
86	OHX	A2	2052	87	0,6,6	-	-	-		
86	OHX	A1	3412	-	0,6,6	-	-	-		
86	OHX	A1	3785	-	0,6,6	-	-	-		
86	OHX	A6	2074	-	0,6,6	-	-	-		
86	OHX	A6	2020	87	0,6,6	-	-	-		
86	OHX	A2	2045	-	0,6,6	-	-	-		
86	OHX	DV	201	87	0,6,6	-	-	-		
86	OHX	A3	204	-	0,6,6	-	-	-		
86	OHX	A5	3506	-	0,6,6	-	-	-		
86	OHX	AN	201	-	0,6,6	-	-	-		
86	OHX	A6	1929	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	AC	301	-	0,6,6	-	-	-		
86	OHX	A1	3651	-	0,6,6	-	-	-		
86	OHX	A1	3797	-	0,6,6	-	-	-		
86	OHX	A2	1939	-	0,6,6	-	-	-		
86	OHX	A6	1979	-	0,6,6	-	-	-		
86	OHX	A2	2058	-	0,6,6	-	-	-		
86	OHX	A2	1958	87	0,6,6	-	-	-		
86	OHX	A1	3628	-	0,6,6	-	-	-		
86	OHX	A5	3775	-	0,6,6	-	-	-		
86	OHX	A2	1991	-	0,6,6	-	-	-		
86	OHX	A1	3647	87	0,6,6	-	-	-		
86	OHX	A1	3558	-	0,6,6	-	-	-		
86	OHX	A6	1909	87	0,6,6	-	-	-		
86	OHX	A6	2003	-	0,6,6	-	-	-		
86	OHX	A5	3610	-	0,6,6	-	-	-		
86	OHX	A1	3677	-	0,6,6	-	-	-		
86	OHX	A1	3554	-	0,6,6	-	-	-		
86	OHX	A1	3781	-	0,6,6	-	-	-		
86	OHX	A5	3558	87	0,6,6	-	-	-		
86	OHX	A5	3639	-	0,6,6	-	-	-		
86	OHX	A5	3498	-	0,6,6	-	-	-		
86	OHX	A2	2083	-	0,6,6	-	-	-		
86	OHX	A2	1917	-	0,6,6	-	-	-		
86	OHX	A5	3703	-	0,6,6	-	-	-		
86	OHX	A1	3705	-	0,6,6	-	-	-		
86	OHX	A6	2017	-	0,6,6	-	-	-		
86	OHX	A5	3695	36	0,6,6	-	-	-		
86	OHX	A1	3600	87	0,6,6	-	-	-		
86	OHX	A6	2022	-	0,6,6	-	-	-		
86	OHX	A4	212	-	0,6,6	-	-	-		
86	OHX	A5	3419	-	0,6,6	-	-	-		
86	OHX	A1	3646	87	0,6,6	-	-	-		
86	OHX	A2	1933	-	0,6,6	-	-	-		
86	OHX	A5	3584	87	0,6,6	-	-	-		
86	OHX	A1	3417	-	0,6,6	-	-	-		
86	OHX	A5	3484	-	0,6,6	-	-	-		
86	OHX	A6	1935	87	0,6,6	-	-	-		
86	OHX	A1	3476	-	0,6,6	-	-	-		
86	OHX	A5	3709	-	0,6,6	-	-	-		
86	OHX	A1	3719	-	0,6,6	-	-	-		
86	OHX	A2	1990	-	0,6,6	-	-	-		
86	OHX	A6	2100	-	0,6,6	-	-	-		
86	OHX	A6	2049	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A6	2098	-	0,6,6	-	-	-		
86	OHX	A5	3771	-	0,6,6	-	-	-		
86	OHX	A1	3511	-	0,6,6	-	-	-		
86	OHX	A6	2026	-	0,6,6	-	-	-		
86	OHX	A1	3474	87	0,6,6	-	-	-		
86	OHX	A1	3676	87	0,6,6	-	-	-		
86	OHX	A5	3532	-	0,6,6	-	-	-		
86	OHX	A2	1959	-	0,6,6	-	-	-		
86	OHX	A5	3701	-	0,6,6	-	-	-		
86	OHX	A2	1966	87	0,6,6	-	-	-		
86	OHX	A6	2037	87	0,6,6	-	-	-		
86	OHX	A2	1975	-	0,6,6	-	-	-		
86	OHX	A6	2078	-	0,6,6	-	-	-		
86	OHX	A6	2070	-	0,6,6	-	-	-		
86	OHX	A2	1953	87	0,6,6	-	-	-		
86	OHX	A5	3468	-	0,6,6	-	-	-		
86	OHX	A5	3583	87	0,6,6	-	-	-		
86	OHX	A6	1914	-	0,6,6	-	-	-		
86	OHX	A6	1955	-	0,6,6	-	-	-		
86	OHX	A8	206	-	0,6,6	-	-	-		
86	OHX	A7	207	-	0,6,6	-	-	-		
86	OHX	A1	3815	-	0,6,6	-	-	-		
86	OHX	A5	3817	-	0,6,6	-	-	-		
86	OHX	A1	3514	-	0,6,6	-	-	-		
86	OHX	A5	3588	87	0,6,6	-	-	-		
86	OHX	A1	3661	87	0,6,6	-	-	-		
86	OHX	A1	3464	-	0,6,6	-	-	-		
86	OHX	A6	2009	-	0,6,6	-	-	-		
86	OHX	A5	3681	-	0,6,6	-	-	-		
86	OHX	A2	2032	-	0,6,6	-	-	-		
86	OHX	A1	3488	-	0,6,6	-	-	-		
86	OHX	A5	3764	87	0,6,6	-	-	-		
86	OHX	A6	1903	-	0,6,6	-	-	-		
86	OHX	DB	402	-	0,6,6	-	-	-		
86	OHX	A5	3547	87	0,6,6	-	-	-		
86	OHX	A1	3807	87	0,6,6	-	-	-		
86	OHX	A5	3466	-	0,6,6	-	-	-		
86	OHX	A1	3755	-	0,6,6	-	-	-		
86	OHX	A2	1915	-	0,6,6	-	-	-		
86	OHX	A5	3631	87	0,6,6	-	-	-		
86	OHX	A1	3522	-	0,6,6	-	-	-		
86	OHX	A5	3492	86	0,6,6	-	-	-		
86	OHX	A2	1980	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A2	1964	-	0,6,6	-	-	-		
86	OHX	A5	3727	87	0,6,6	-	-	-		
86	OHX	A1	3540	-	0,6,6	-	-	-		
86	OHX	A2	1924	87	0,6,6	-	-	-		
86	OHX	A2	1925	-	0,6,6	-	-	-		
86	OHX	A1	3734	87	0,6,6	-	-	-		
86	OHX	A5	3685	-	0,6,6	-	-	-		
86	OHX	A1	3701	87	0,6,6	-	-	-		
86	OHX	A5	3796	-	0,6,6	-	-	-		
86	OHX	A3	206	-	0,6,6	-	-	-		
86	OHX	A6	2056	87	0,6,6	-	-	-		
86	OHX	A5	3638	-	0,6,6	-	-	-		
86	OHX	A5	3535	-	0,6,6	-	-	-		
86	OHX	A6	2027	-	0,6,6	-	-	-		
86	OHX	A6	2002	87	0,6,6	-	-	-		
86	OHX	A5	3728	-	0,6,6	-	-	-		
86	OHX	A5	3756	-	0,6,6	-	-	-		
86	OHX	A1	3429	87	0,6,6	-	-	-		
86	OHX	A1	3813	-	0,6,6	-	-	-		
86	OHX	A1	3576	-	0,6,6	-	-	-		
86	OHX	A1	3603	-	0,6,6	-	-	-		
86	OHX	A2	2018	87	0,6,6	-	-	-		
86	OHX	A5	3548	-	0,6,6	-	-	-		
86	OHX	A6	2039	-	0,6,6	-	-	-		
86	OHX	A5	3450	-	0,6,6	-	-	-		
86	OHX	A6	2063	-	0,6,6	-	-	-		
86	OHX	A1	3556	-	0,6,6	-	-	-		
86	OHX	A5	3502	-	0,6,6	-	-	-		
86	OHX	A5	3569	-	0,6,6	-	-	-		
86	OHX	A5	3593	-	0,6,6	-	-	-		
86	OHX	A5	3798	-	0,6,6	-	-	-		
86	OHX	A1	3525	87	0,6,6	-	-	-		
86	OHX	A5	3679	-	0,6,6	-	-	-		
86	OHX	A2	1913	87	0,6,6	-	-	-		
86	OHX	A5	3674	87	0,6,6	-	-	-		
86	OHX	A1	3640	-	0,6,6	-	-	-		
86	OHX	A2	2042	87	0,6,6	-	-	-		
86	OHX	A6	2067	87	0,6,6	-	-	-		
86	OHX	A5	3525	-	0,6,6	-	-	-		
86	OHX	A1	3462	-	0,6,6	-	-	-		
86	OHX	A5	3637	87	0,6,6	-	-	-		
86	OHX	A2	1908	-	0,6,6	-	-	-		
86	OHX	A1	3634	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3452	87	0,6,6	-	-	-		
86	OHX	A2	1946	-	0,6,6	-	-	-		
86	OHX	A1	3410	-	0,6,6	-	-	-		
86	OHX	A5	3494	-	0,6,6	-	-	-		
86	OHX	A6	1988	-	0,6,6	-	-	-		
86	OHX	A5	3426	-	0,6,6	-	-	-		
86	OHX	A1	3446	87	0,6,6	-	-	-		
86	OHX	A2	1934	-	0,6,6	-	-	-		
86	OHX	A5	3531	-	0,6,6	-	-	-		
86	OHX	A5	3490	-	0,6,6	-	-	-		
86	OHX	A5	3497	-	0,6,6	-	-	-		
86	OHX	A5	3467	-	0,6,6	-	-	-		
86	OHX	A5	3627	87	0,6,6	-	-	-		
86	OHX	A5	3543	87	0,6,6	-	-	-		
86	OHX	A1	3757	-	0,6,6	-	-	-		
86	OHX	A5	3652	87	0,6,6	-	-	-		
86	OHX	A5	3495	-	0,6,6	-	-	-		
86	OHX	A5	3707	87	0,6,6	-	-	-		
86	OHX	A5	3574	-	0,6,6	-	-	-		
86	OHX	A1	3759	87	0,6,6	-	-	-		
86	OHX	A5	3710	-	0,6,6	-	-	-		
86	OHX	A1	3516	-	0,6,6	-	-	-		
86	OHX	A5	3435	-	0,6,6	-	-	-		
86	OHX	A8	220	87	0,6,6	-	-	-		
86	OHX	A5	3551	-	0,6,6	-	-	-		
86	OHX	A2	1962	-	0,6,6	-	-	-		
86	OHX	A1	3561	-	0,6,6	-	-	-		
86	OHX	A1	3626	-	0,6,6	-	-	-		
86	OHX	A6	2054	87	0,6,6	-	-	-		
86	OHX	A5	3745	-	0,6,6	-	-	-		
86	OHX	A6	2062	-	0,6,6	-	-	-		
86	OHX	A5	3721	-	0,6,6	-	-	-		
86	OHX	A2	1902	-	0,6,6	-	-	-		
86	OHX	A1	3460	-	0,6,6	-	-	-		
86	OHX	A6	1932	-	0,6,6	-	-	-		
86	OHX	A2	2072	-	0,6,6	-	-	-		
86	OHX	A1	3593	-	0,6,6	-	-	-		
86	OHX	A5	3614	87	0,6,6	-	-	-		
86	OHX	A1	3643	87	0,6,6	-	-	-		
86	OHX	A6	1986	-	0,6,6	-	-	-		
86	OHX	A1	3599	87	0,6,6	-	-	-		
86	OHX	A5	3567	87	0,6,6	-	-	-		
86	OHX	A5	3791	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	Cd	101	-	0,6,6	-	-	-		
86	OHX	A1	3796	-	0,6,6	-	-	-		
86	OHX	A2	2017	-	0,6,6	-	-	-		
86	OHX	A6	2011	87	0,6,6	-	-	-		
86	OHX	A6	2059	-	0,6,6	-	-	-		
86	OHX	A5	3717	-	0,6,6	-	-	-		
86	OHX	A6	1927	-	0,6,6	-	-	-		
86	OHX	Bj	102	-	0,6,6	-	-	-		
86	OHX	A1	3709	87	0,6,6	-	-	-		
86	OHX	A1	3541	87	0,6,6	-	-	-		
86	OHX	A5	3546	-	0,6,6	-	-	-		
86	OHX	A2	1978	-	0,6,6	-	-	-		
86	OHX	A5	3658	-	0,6,6	-	-	-		
86	OHX	A1	3586	-	0,6,6	-	-	-		
86	OHX	A6	2071	-	0,6,6	-	-	-		
86	OHX	A1	3780	-	0,6,6	-	-	-		
86	OHX	A2	1992	87	0,6,6	-	-	-		
86	OHX	A1	3731	-	0,6,6	-	-	-		
86	OHX	A1	3644	-	0,6,6	-	-	-		
86	OHX	A5	3659	-	0,6,6	-	-	-		
86	OHX	A5	3694	-	0,6,6	-	-	-		
86	OHX	A2	2059	-	0,6,6	-	-	-		
86	OHX	A1	3422	-	0,6,6	-	-	-		
86	OHX	A2	2053	87	0,6,6	-	-	-		
86	OHX	A1	3618	87	0,6,6	-	-	-		
86	OHX	A1	3729	87	0,6,6	-	-	-		
86	OHX	A1	3806	-	0,6,6	-	-	-		
86	OHX	A5	3711	-	0,6,6	-	-	-		
86	OHX	A1	3678	87	0,6,6	-	-	-		
86	OHX	A5	3692	-	0,6,6	-	-	-		
86	OHX	A1	3649	87	0,6,6	-	-	-		
86	OHX	A4	208	-	0,6,6	-	-	-		
86	OHX	A1	3445	87	0,6,6	-	-	-		
86	OHX	A2	2080	-	0,6,6	-	-	-		
86	OHX	A1	3617	-	0,6,6	-	-	-		
86	OHX	A6	2076	86	0,6,6	-	-	-		
86	OHX	A8	215	-	0,6,6	-	-	-		
86	OHX	A1	3744	-	0,6,6	-	-	-		
86	OHX	A1	3427	87	0,6,6	-	-	-		
86	OHX	A5	3689	-	0,6,6	-	-	-		
86	OHX	A5	3511	-	0,6,6	-	-	-		
86	OHX	A1	3581	87	0,6,6	-	-	-		
86	OHX	A6	1969	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	AI	301	-	0,6,6	-	-	-		
86	OHX	A1	3585	-	0,6,6	-	-	-		
86	OHX	Bf	201	-	0,6,6	-	-	-		
86	OHX	A5	3527	-	0,6,6	-	-	-		
86	OHX	A1	3737	-	0,6,6	-	-	-		
86	OHX	A6	2095	-	0,6,6	-	-	-		
86	OHX	A5	3440	-	0,6,6	-	-	-		
86	OHX	A6	2030	-	0,6,6	-	-	-		
86	OHX	A5	3819	87	0,6,6	-	-	-		
86	OHX	A5	3705	-	0,6,6	-	-	-		
86	OHX	A5	3539	-	0,6,6	-	-	-		
86	OHX	A5	3804	-	0,6,6	-	-	-		
86	OHX	A5	3509	-	0,6,6	-	-	-		
86	OHX	A8	218	-	0,6,6	-	-	-		
86	OHX	CG	302	-	0,6,6	-	-	-		
86	OHX	A5	3612	87	0,6,6	-	-	-		
86	OHX	A6	2012	-	0,6,6	-	-	-		
86	OHX	A1	3788	-	0,6,6	-	-	-		
86	OHX	A5	3576	87	0,6,6	-	-	-		
86	OHX	DG	301	-	0,6,6	-	-	-		
86	OHX	A5	3457	86	0,6,6	-	-	-		
86	OHX	A4	205	-	0,6,6	-	-	-		
86	OHX	A5	3664	87	0,6,6	-	-	-		
86	OHX	A2	1999	-	0,6,6	-	-	-		
86	OHX	A5	3769	-	0,6,6	-	-	-		
86	OHX	A6	2055	-	0,6,6	-	-	-		
86	OHX	A1	3768	87	0,6,6	-	-	-		
86	OHX	A1	3666	-	0,6,6	-	-	-		
86	OHX	A5	3443	87	0,6,6	-	-	-		
86	OHX	A5	3499	87	0,6,6	-	-	-		
86	OHX	A6	1973	87	0,6,6	-	-	-		
86	OHX	A1	3787	-	0,6,6	-	-	-		
86	OHX	A2	1922	87	0,6,6	-	-	-		
86	OHX	A1	3786	-	0,6,6	-	-	-		
86	OHX	A6	1991	-	0,6,6	-	-	-		
86	OHX	A7	202	-	0,6,6	-	-	-		
86	OHX	A6	2036	-	0,6,6	-	-	-		
86	OHX	A5	3787	-	0,6,6	-	-	-		
86	OHX	Dj	104	-	0,6,6	-	-	-		
86	OHX	A5	3690	-	0,6,6	-	-	-		
86	OHX	A5	3734	87	0,6,6	-	-	-		
86	OHX	A5	3628	-	0,6,6	-	-	-		
86	OHX	A5	3592	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3629	87	0,6,6	-	-	-		
86	OHX	A2	1973	-	0,6,6	-	-	-		
86	OHX	A1	3810	-	0,6,6	-	-	-		
86	OHX	A5	3553	-	0,6,6	-	-	-		
86	OHX	A6	2083	-	0,6,6	-	-	-		
86	OHX	A1	3739	-	0,6,6	-	-	-		
86	OHX	A1	3610	-	0,6,6	-	-	-		
86	OHX	A5	3725	-	0,6,6	-	-	-		
86	OHX	A5	3654	-	0,6,6	-	-	-		
86	OHX	A5	3682	-	0,6,6	-	-	-		
86	OHX	A5	3510	-	0,6,6	-	-	-		
86	OHX	A1	3486	-	0,6,6	-	-	-		
86	OHX	A2	1955	-	0,6,6	-	-	-		
86	OHX	A6	1981	-	0,6,6	-	-	-		
86	OHX	A1	3752	-	0,6,6	-	-	-		
86	OHX	A3	210	-	0,6,6	-	-	-		
86	OHX	A8	211	-	0,6,6	-	-	-		
86	OHX	A1	3473	87	0,6,6	-	-	-		
86	OHX	A1	3612	-	0,6,6	-	-	-		
86	OHX	A1	3419	-	0,6,6	-	-	-		
86	OHX	A6	2032	-	0,6,6	-	-	-		
86	OHX	A1	3582	87	0,6,6	-	-	-		
86	OHX	A1	3619	-	0,6,6	-	-	-		
86	OHX	A5	3646	-	0,6,6	-	-	-		
86	OHX	A2	2070	-	0,6,6	-	-	-		
86	OHX	A1	3642	-	0,6,6	-	-	-		
86	OHX	A6	2015	-	0,6,6	-	-	-		
86	OHX	A5	3418	87	0,6,6	-	-	-		
86	OHX	A5	3632	-	0,6,6	-	-	-		
86	OHX	A5	3508	-	0,6,6	-	-	-		
86	OHX	A8	219	-	0,6,6	-	-	-		
86	OHX	A6	2023	-	0,6,6	-	-	-		
86	OHX	A5	3716	-	0,6,6	-	-	-		
86	OHX	A2	2009	-	0,6,6	-	-	-		
86	OHX	A4	211	-	0,6,6	-	-	-		
86	OHX	A1	3624	-	0,6,6	-	-	-		
86	OHX	A2	2056	-	0,6,6	-	-	-		
86	OHX	A1	3484	-	0,6,6	-	-	-		
86	OHX	A5	3752	-	0,6,6	-	-	-		
86	OHX	A6	1966	87	0,6,6	-	-	-		
86	OHX	A1	3456	87	0,6,6	-	-	-		
86	OHX	A5	3601	-	0,6,6	-	-	-		
86	OHX	A2	1977	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3491	-	0,6,6	-	-	-		
86	OHX	A5	3718	-	0,6,6	-	-	-		
86	OHX	A6	1953	-	0,6,6	-	-	-		
86	OHX	A5	3516	-	0,6,6	-	-	-		
86	OHX	A1	3591	-	0,6,6	-	-	-		
86	OHX	A5	3482	87	0,6,6	-	-	-		
86	OHX	A1	3706	-	0,6,6	-	-	-		
86	OHX	A5	3552	87	0,6,6	-	-	-		
86	OHX	A5	3453	-	0,6,6	-	-	-		
86	OHX	A1	3433	87	0,6,6	-	-	-		
86	OHX	A2	1935	-	0,6,6	-	-	-		
86	OHX	A2	2019	-	0,6,6	-	-	-		
86	OHX	A5	3754	-	0,6,6	-	-	-		
86	OHX	A6	1949	87	0,6,6	-	-	-		
86	OHX	A5	3641	-	0,6,6	-	-	-		
86	OHX	A5	3715	-	0,6,6	-	-	-		
86	OHX	A4	202	-	0,6,6	-	-	-		
86	OHX	A1	3468	87	0,6,6	-	-	-		
86	OHX	A1	3583	87	0,6,6	-	-	-		
86	OHX	A2	2086	-	0,6,6	-	-	-		
86	OHX	A1	3659	87	0,6,6	-	-	-		
86	OHX	A5	3784	-	0,6,6	-	-	-		
86	OHX	A5	3793	87	0,6,6	-	-	-		
86	OHX	A6	1930	-	0,6,6	-	-	-		
86	OHX	A5	3762	-	0,6,6	-	-	-		
86	OHX	A2	1996	-	0,6,6	-	-	-		
86	OHX	A6	1998	-	0,6,6	-	-	-		
86	OHX	A6	1936	-	0,6,6	-	-	-		
86	OHX	A5	3458	-	0,6,6	-	-	-		
86	OHX	A4	203	-	0,6,6	-	-	-		
86	OHX	DP	201	-	0,6,6	-	-	-		
86	OHX	A1	3448	-	0,6,6	-	-	-		
86	OHX	A2	2029	-	0,6,6	-	-	-		
86	OHX	A5	3480	-	0,6,6	-	-	-		
86	OHX	A5	3459	-	0,6,6	-	-	-		
86	OHX	A5	3599	-	0,6,6	-	-	-		
86	OHX	A5	3680	-	0,6,6	-	-	-		
86	OHX	A5	3790	-	0,6,6	-	-	-		
86	OHX	A6	2005	-	0,6,6	-	-	-		
86	OHX	A2	1930	-	0,6,6	-	-	-		
86	OHX	A6	1925	87	0,6,6	-	-	-		
86	OHX	A5	3653	-	0,6,6	-	-	-		
86	OHX	A1	3631	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A3	205	-	0,6,6	-	-	-		
86	OHX	A6	2024	-	0,6,6	-	-	-		
86	OHX	A5	3809	86	0,6,6	-	-	-		
86	OHX	A5	3402	-	0,6,6	-	-	-		
86	OHX	A5	3579	87	0,6,6	-	-	-		
86	OHX	A6	2097	-	0,6,6	-	-	-		
86	OHX	A1	3660	87	0,6,6	-	-	-		
86	OHX	A1	3685	-	0,6,6	-	-	-		
86	OHX	A1	3482	-	0,6,6	-	-	-		
86	OHX	A5	3656	-	0,6,6	-	-	-		
86	OHX	A1	3683	-	0,6,6	-	-	-		
86	OHX	A1	3440	-	0,6,6	-	-	-		
86	OHX	A1	3758	87	0,6,6	-	-	-		
86	OHX	A1	3533	-	0,6,6	-	-	-		
86	OHX	A1	3728	-	0,6,6	-	-	-		
86	OHX	A2	1907	-	0,6,6	-	-	-		
86	OHX	A2	1956	-	0,6,6	-	-	-		
86	OHX	A2	1997	-	0,6,6	-	-	-		
86	OHX	A2	1995	-	0,6,6	-	-	-		
86	OHX	A5	3429	-	0,6,6	-	-	-		
86	OHX	A2	2006	-	0,6,6	-	-	-		
86	OHX	A1	3735	-	0,6,6	-	-	-		
86	OHX	A5	3501	-	0,6,6	-	-	-		
86	OHX	A1	3548	-	0,6,6	-	-	-		
86	OHX	A1	3604	-	0,6,6	-	-	-		
86	OHX	CB	301	-	0,6,6	-	-	-		
86	OHX	A1	3664	-	0,6,6	-	-	-		
86	OHX	A5	3589	-	0,6,6	-	-	-		
86	OHX	A5	3566	87	0,6,6	-	-	-		
86	OHX	A1	3502	-	0,6,6	-	-	-		
86	OHX	A1	3569	-	0,6,6	-	-	-		
86	OHX	A1	3764	87	0,6,6	-	-	-		
86	OHX	A5	3714	87	0,6,6	-	-	-		
86	OHX	A2	2034	-	0,6,6	-	-	-		
86	OHX	A1	3776	-	0,6,6	-	-	-		
86	OHX	A5	3820	87	0,6,6	-	-	-		
86	OHX	A1	3790	-	0,6,6	-	-	-		
86	OHX	A5	3575	87	0,6,6	-	-	-		
86	OHX	A1	3674	-	0,6,6	-	-	-		
86	OHX	A5	3421	-	0,6,6	-	-	-		
86	OHX	A6	1950	-	0,6,6	-	-	-		
86	OHX	A5	3620	-	0,6,6	-	-	-		
86	OHX	A1	3613	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	CY	202	-	0,6,6	-	-	-		
86	OHX	A1	3633	-	0,6,6	-	-	-		
86	OHX	A1	3653	87	0,6,6	-	-	-		
86	OHX	BI	303	-	0,6,6	-	-	-		
86	OHX	A1	3426	-	0,6,6	-	-	-		
86	OHX	A2	1942	87	0,6,6	-	-	-		
86	OHX	A1	3483	-	0,6,6	-	-	-		
86	OHX	DR	201	-	0,6,6	-	-	-		
86	OHX	A2	1923	-	0,6,6	-	-	-		
86	OHX	A1	3531	87	0,6,6	-	-	-		
86	OHX	A5	3677	-	0,6,6	-	-	-		
86	OHX	A1	3497	-	0,6,6	-	-	-		
86	OHX	A5	3446	-	0,6,6	-	-	-		
86	OHX	A5	3598	-	0,6,6	-	-	-		
86	OHX	A5	3425	87	0,6,6	-	-	-		
86	OHX	A1	3455	-	0,6,6	-	-	-		
86	OHX	A1	3528	87	0,6,6	-	-	-		
86	OHX	BR	201	-	0,6,6	-	-	-		
86	OHX	A4	204	-	0,6,6	-	-	-		
86	OHX	A2	2061	-	0,6,6	-	-	-		
86	OHX	A1	3495	-	0,6,6	-	-	-		
86	OHX	A1	3574	-	0,6,6	-	-	-		
86	OHX	A6	2019	87	0,6,6	-	-	-		
86	OHX	A5	3464	-	0,6,6	-	-	-		
86	OHX	A5	3528	-	0,6,6	-	-	-		
86	OHX	A6	1971	-	0,6,6	-	-	-		
86	OHX	A6	1919	86	0,6,6	-	-	-		
86	OHX	A1	3578	-	0,6,6	-	-	-		
86	OHX	A5	3570	-	0,6,6	-	-	-		
86	OHX	A1	3551	-	0,6,6	-	-	-		
86	OHX	A1	3745	-	0,6,6	-	-	-		
86	OHX	A5	3438	-	0,6,6	-	-	-		
86	OHX	A5	3594	-	0,6,6	-	-	-		
86	OHX	A5	3561	-	0,6,6	-	-	-		
86	OHX	A1	3721	-	0,6,6	-	-	-		
86	OHX	A1	3630	87	0,6,6	-	-	-		
86	OHX	A6	2091	-	0,6,6	-	-	-		
86	OHX	A1	3584	-	0,6,6	-	-	-		
86	OHX	CP	202	17	0,6,6	-	-	-		
86	OHX	A5	3460	87	0,6,6	-	-	-		
86	OHX	A5	3795	86	0,6,6	-	-	-		
86	OHX	A1	3614	-	0,6,6	-	-	-		
86	OHX	A5	3768	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	A4	210	87	0,6,6	-	-	-		
86	OHX	A2	1910	-	0,6,6	-	-	-		
86	OHX	A5	3671	-	0,6,6	-	-	-		
86	OHX	A6	1975	-	0,6,6	-	-	-		
86	OHX	A5	3476	87	0,6,6	-	-	-		
86	OHX	A1	3567	87	0,6,6	-	-	-		
86	OHX	A1	3791	87	0,6,6	-	-	-		
86	OHX	A1	3542	-	0,6,6	-	-	-		
86	OHX	A6	2018	-	0,6,6	-	-	-		
86	OHX	Ag	401	-	0,6,6	-	-	-		
86	OHX	A5	3673	-	0,6,6	-	-	-		
86	OHX	A5	3668	87	0,6,6	-	-	-		
86	OHX	A2	1944	87	0,6,6	-	-	-		
86	OHX	A1	3562	-	0,6,6	-	-	-		
86	OHX	A1	3717	-	0,6,6	-	-	-		
86	OHX	A2	2064	-	0,6,6	-	-	-		
86	OHX	A5	3750	87	0,6,6	-	-	-		
86	OHX	A7	212	87	0,6,6	-	-	-		
86	OHX	A1	3794	-	0,6,6	-	-	-		
86	OHX	A5	3432	-	0,6,6	-	-	-		
86	OHX	Cg	401	-	0,6,6	-	-	-		
86	OHX	A6	2052	-	0,6,6	-	-	-		
86	OHX	A5	3517	-	0,6,6	-	-	-		
86	OHX	A1	3658	87	0,6,6	-	-	-		
86	OHX	A6	2038	87	0,6,6	-	-	-		
86	OHX	A6	2053	-	0,6,6	-	-	-		
86	OHX	A5	3609	-	0,6,6	-	-	-		
86	OHX	A6	1989	-	0,6,6	-	-	-		
86	OHX	A2	2011	-	0,6,6	-	-	-		
86	OHX	A6	1948	-	0,6,6	-	-	-		
86	OHX	A1	3694	-	0,6,6	-	-	-		
86	OHX	A2	2010	87	0,6,6	-	-	-		
86	OHX	A1	3457	-	0,6,6	-	-	-		
86	OHX	A6	2099	87	0,6,6	-	-	-		
86	OHX	A7	209	87	0,6,6	-	-	-		
86	OHX	A5	3454	-	0,6,6	-	-	-		
86	OHX	A6	1924	-	0,6,6	-	-	-		
86	OHX	A2	2007	-	0,6,6	-	-	-		
86	OHX	A5	3823	-	0,6,6	-	-	-		
86	OHX	A6	2057	-	0,6,6	-	-	-		
86	OHX	Bj	101	87	0,6,6	-	-	-		
86	OHX	A5	3765	-	0,6,6	-	-	-		
86	OHX	A5	3661	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A5	3772	87	0,6,6	-	-	-		
86	OHX	A8	209	-	0,6,6	-	-	-		
86	OHX	A1	3711	87	0,6,6	-	-	-		
86	OHX	Bo	201	87	0,6,6	-	-	-		
86	OHX	A2	1989	-	0,6,6	-	-	-		
86	OHX	A1	3795	-	0,6,6	-	-	-		
86	OHX	A2	1929	87	0,6,6	-	-	-		
86	OHX	A2	1954	-	0,6,6	-	-	-		
86	OHX	A5	3550	-	0,6,6	-	-	-		
86	OHX	A5	3811	-	0,6,6	-	-	-		
86	OHX	A2	1948	87	0,6,6	-	-	-		
86	OHX	A8	213	-	0,6,6	-	-	-		
86	OHX	A5	3812	-	0,6,6	-	-	-		
86	OHX	A2	1904	-	0,6,6	-	-	-		
86	OHX	A1	3692	-	0,6,6	-	-	-		
86	OHX	DB	401	-	0,6,6	-	-	-		
86	OHX	A1	3438	86	0,6,6	-	-	-		
86	OHX	A5	3810	-	0,6,6	-	-	-		
86	OHX	A2	1979	-	0,6,6	-	-	-		
86	OHX	A5	3423	87	0,6,6	-	-	-		
86	OHX	A1	3470	-	0,6,6	-	-	-		
86	OHX	A8	207	-	0,6,6	-	-	-		
86	OHX	A1	3526	87	0,6,6	-	-	-		
86	OHX	A6	2068	-	0,6,6	-	-	-		
86	OHX	DH	201	-	0,6,6	-	-	-		
86	OHX	A2	1928	-	0,6,6	-	-	-		
86	OHX	A1	3689	-	0,6,6	-	-	-		
86	OHX	A2	2075	-	0,6,6	-	-	-		
86	OHX	A2	2031	-	0,6,6	-	-	-		
86	OHX	A7	206	-	0,6,6	-	-	-		
86	OHX	A5	3473	-	0,6,6	-	-	-		
86	OHX	A1	3527	-	0,6,6	-	-	-		
86	OHX	A1	3403	-	0,6,6	-	-	-		
86	OHX	A1	3747	87	0,6,6	-	-	-		
86	OHX	A5	3814	-	0,6,6	-	-	-		
86	OHX	A2	2015	-	0,6,6	-	-	-		
86	OHX	A5	3472	87	0,6,6	-	-	-		
86	OHX	A2	1970	-	0,6,6	-	-	-		
86	OHX	A7	208	87	0,6,6	-	-	-		
86	OHX	A5	3615	-	0,6,6	-	-	-		
86	OHX	A4	206	-	0,6,6	-	-	-		
86	OHX	A5	3712	-	0,6,6	-	-	-		
86	OHX	A5	3560	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	A8	208	87	0,6,6	-	-	-		
86	OHX	A5	3496	-	0,6,6	-	-	-		
86	OHX	A5	3437	-	0,6,6	-	-	-		
86	OHX	A1	3675	-	0,6,6	-	-	-		
86	OHX	A1	3430	-	0,6,6	-	-	-		
86	OHX	DJ	201	-	0,6,6	-	-	-		
86	OHX	A1	3769	-	0,6,6	-	-	-		
86	OHX	A6	2045	87	0,6,6	-	-	-		
86	OHX	A5	3449	-	0,6,6	-	-	-		
86	OHX	A5	3778	-	0,6,6	-	-	-		
86	OHX	A2	2049	-	0,6,6	-	-	-		
86	OHX	A1	3543	-	0,6,6	-	-	-		
86	OHX	A1	3544	-	0,6,6	-	-	-		
86	OHX	A1	3499	87	0,6,6	-	-	-		
86	OHX	A6	2079	-	0,6,6	-	-	-		
86	OHX	A5	3722	-	0,6,6	-	-	-		
86	OHX	A5	3428	87	0,6,6	-	-	-		
86	OHX	A5	3536	-	0,6,6	-	-	-		
86	OHX	A1	3616	-	0,6,6	-	-	-		
86	OHX	A1	3761	-	0,6,6	-	-	-		
86	OHX	BO	201	-	0,6,6	-	-	-		
86	OHX	A5	3724	-	0,6,6	-	-	-		
86	OHX	A1	3690	-	0,6,6	-	-	-		
86	OHX	A5	3660	-	0,6,6	-	-	-		
86	OHX	A1	3697	-	0,6,6	-	-	-		
86	OHX	A1	3434	87	0,6,6	-	-	-		
86	OHX	A1	3505	-	0,6,6	-	-	-		
86	OHX	A1	3592	-	0,6,6	-	-	-		
86	OHX	A1	3553	-	0,6,6	-	-	-		
86	OHX	A4	201	-	0,6,6	-	-	-		
86	OHX	A2	2050	-	0,6,6	-	-	-		
86	OHX	A5	3441	-	0,6,6	-	-	-		
86	OHX	A5	3730	87	0,6,6	-	-	-		
86	OHX	A5	3434	-	0,6,6	-	-	-		
86	OHX	A5	3420	-	0,6,6	-	-	-		
86	OHX	A1	3654	-	0,6,6	-	-	-		
86	OHX	A1	3682	-	0,6,6	-	-	-		
86	OHX	A6	1956	-	0,6,6	-	-	-		
86	OHX	A5	3515	87	0,6,6	-	-	-		
86	OHX	A1	3740	-	0,6,6	-	-	-		
86	OHX	A5	3665	-	0,6,6	-	-	-		
86	OHX	A5	3518	-	0,6,6	-	-	-		
86	OHX	A5	3621	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A5	3740	-	0,6,6	-	-	-		
86	OHX	A5	3523	-	0,6,6	-	-	-		
86	OHX	A1	3437	87	0,6,6	-	-	-		
86	OHX	A5	3414	-	0,6,6	-	-	-		
86	OHX	A1	3418	-	0,6,6	-	-	-		
86	OHX	A1	3507	-	0,6,6	-	-	-		
86	OHX	A1	3508	87	0,6,6	-	-	-		
86	OHX	A2	1972	-	0,6,6	-	-	-		
86	OHX	A2	1957	-	0,6,6	-	-	-		
86	OHX	A2	2046	-	0,6,6	-	-	-		
86	OHX	A5	3613	-	0,6,6	-	-	-		
86	OHX	A6	1905	-	0,6,6	-	-	-		
86	OHX	A5	3405	87	0,6,6	-	-	-		
86	OHX	DC	402	-	0,6,6	-	-	-		
86	OHX	BB	402	-	0,6,6	-	-	-		
86	OHX	A5	3753	-	0,6,6	-	-	-		
86	OHX	A5	3783	87	0,6,6	-	-	-		
86	OHX	A6	1977	-	0,6,6	-	-	-		
86	OHX	A5	3580	87	0,6,6	-	-	-		
86	OHX	A5	3469	-	0,6,6	-	-	-		
86	OHX	A5	3781	-	0,6,6	-	-	-		
86	OHX	A2	1986	-	0,6,6	-	-	-		
86	OHX	A5	3663	-	0,6,6	-	-	-		
86	OHX	A1	3655	87	0,6,6	-	-	-		
86	OHX	A1	3814	-	0,6,6	-	-	-		
86	OHX	A5	3792	-	0,6,6	-	-	-		
86	OHX	A2	1905	-	0,6,6	-	-	-		
86	OHX	A1	3718	-	0,6,6	-	-	-		
86	OHX	A5	3670	-	0,6,6	-	-	-		
86	OHX	A1	3413	-	0,6,6	-	-	-		
86	OHX	A6	1984	-	0,6,6	-	-	-		
86	OHX	A6	1912	-	0,6,6	-	-	-		
86	OHX	A5	3746	-	0,6,6	-	-	-		
86	OHX	A5	3821	-	0,6,6	-	-	-		
86	OHX	A5	3578	87	0,6,6	-	-	-		
86	OHX	A1	3453	-	0,6,6	-	-	-		
86	OHX	A5	3591	-	0,6,6	-	-	-		
86	OHX	A8	203	-	0,6,6	-	-	-		
86	OHX	A5	3789	-	0,6,6	-	-	-		
86	OHX	BD	301	-	0,6,6	-	-	-		
86	OHX	A6	1951	87	0,6,6	-	-	-		
86	OHX	A1	3609	-	0,6,6	-	-	-		
86	OHX	A1	3715	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3749	-	0,6,6	-	-	-		
86	OHX	A5	3549	-	0,6,6	-	-	-		
86	OHX	A6	1906	-	0,6,6	-	-	-		
86	OHX	A6	2029	87	0,6,6	-	-	-		
86	OHX	A8	216	-	0,6,6	-	-	-		
86	OHX	A5	3544	-	0,6,6	-	-	-		
86	OHX	A1	3793	-	0,6,6	-	-	-		
86	OHX	A5	3729	-	0,6,6	-	-	-		
86	OHX	A5	3672	-	0,6,6	-	-	-		
86	OHX	A5	3545	-	0,6,6	-	-	-		
86	OHX	A2	2082	-	0,6,6	-	-	-		
86	OHX	A2	1988	-	0,6,6	-	-	-		
86	OHX	A5	3489	-	0,6,6	-	-	-		
86	OHX	A6	1908	-	0,6,6	-	-	-		
86	OHX	A1	3458	-	0,6,6	-	-	-		
86	OHX	A2	1967	-	0,6,6	-	-	-		
86	OHX	A1	3459	87	0,6,6	-	-	-		
86	OHX	A5	3688	-	0,6,6	-	-	-		
86	OHX	A1	3732	-	0,6,6	-	-	-		
86	OHX	A2	2048	-	0,6,6	-	-	-		
86	OHX	A2	2000	-	0,6,6	-	-	-		
86	OHX	BP	202	-	0,6,6	-	-	-		
86	OHX	A5	3573	-	0,6,6	-	-	-		
86	OHX	A1	3513	-	0,6,6	-	-	-		
86	OHX	A6	1931	87	0,6,6	-	-	-		
86	OHX	A5	3524	87	0,6,6	-	-	-		
86	OHX	A5	3493	-	0,6,6	-	-	-		
86	OHX	A5	3732	36	0,6,6	-	-	-		
86	OHX	A1	3727	87	0,6,6	-	-	-		
86	OHX	A1	3402	-	0,6,6	-	-	-		
86	OHX	A5	3736	87	0,6,6	-	-	-		
86	OHX	A5	3475	-	0,6,6	-	-	-		
86	OHX	A5	3503	87	0,6,6	-	-	-		
86	OHX	A1	3804	-	0,6,6	-	-	-		
86	OHX	A6	1994	-	0,6,6	-	-	-		
86	OHX	A2	2076	-	0,6,6	-	-	-		
86	OHX	A1	3763	-	0,6,6	-	-	-		
86	OHX	A1	3622	87	0,6,6	-	-	-		
86	OHX	A5	3568	-	0,6,6	-	-	-		
86	OHX	A1	3748	-	0,6,6	-	-	-		
86	OHX	A1	3431	87	0,6,6	-	-	-		
86	OHX	A6	2016	-	0,6,6	-	-	-		
86	OHX	A5	3683	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A1	3679	-	0,6,6	-	-	-		
86	OHX	A5	3529	87	0,6,6	-	-	-		
86	OHX	A6	2058	-	0,6,6	-	-	-		
86	OHX	A6	1967	87	0,6,6	-	-	-		
86	OHX	A5	3422	87	0,6,6	-	-	-		
86	OHX	A6	1943	-	0,6,6	-	-	-		
86	OHX	A1	3501	87	0,6,6	-	-	-		
86	OHX	A2	2037	-	0,6,6	-	-	-		
86	OHX	A5	3407	-	0,6,6	-	-	-		
86	OHX	A5	3777	-	0,6,6	-	-	-		
86	OHX	A1	3627	-	0,6,6	-	-	-		
86	OHX	A1	3408	-	0,6,6	-	-	-		
86	OHX	A1	3667	-	0,6,6	-	-	-		
86	OHX	A1	3523	-	0,6,6	-	-	-		
86	OHX	A1	3714	-	0,6,6	-	-	-		
86	OHX	A3	212	-	0,6,6	-	-	-		
86	OHX	A5	3776	87	0,6,6	-	-	-		
86	OHX	A1	3421	-	0,6,6	-	-	-		
86	OHX	A1	3546	-	0,6,6	-	-	-		
86	OHX	A1	3416	-	0,6,6	-	-	-		
86	OHX	A5	3586	-	0,6,6	-	-	-		
86	OHX	A1	3466	-	0,6,6	-	-	-		
86	OHX	A1	3490	87	0,6,6	-	-	-		
86	OHX	A1	3668	-	0,6,6	-	-	-		
86	OHX	A5	3739	-	0,6,6	-	-	-		
86	OHX	A1	3596	87	0,6,6	-	-	-		
86	OHX	A1	3750	87	0,6,6	-	-	-		
86	OHX	A2	2043	-	0,6,6	-	-	-		
86	OHX	A1	3425	-	0,6,6	-	-	-		
86	OHX	A1	3707	-	0,6,6	-	-	-		
86	OHX	A5	3534	-	0,6,6	-	-	-		
86	OHX	A1	3695	-	0,6,6	-	-	-		
86	OHX	A1	3570	87	0,6,6	-	-	-		
86	OHX	A1	3730	87	0,6,6	-	-	-		
86	OHX	A6	1958	-	0,6,6	-	-	-		
86	OHX	A1	3772	-	0,6,6	-	-	-		
86	OHX	A5	3617	87	0,6,6	-	-	-		
86	OHX	A6	1990	87	0,6,6	-	-	-		
86	OHX	A1	3594	-	0,6,6	-	-	-		
86	OHX	A5	3741	-	0,6,6	-	-	-		
86	OHX	A1	3777	-	0,6,6	-	-	-		
86	OHX	A2	1981	-	0,6,6	-	-	-		
86	OHX	CN	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A5	3743	-	0,6,6	-	-	-		
86	OHX	A5	3461	87	0,6,6	-	-	-		
86	OHX	Df	201	-	0,6,6	-	-	-		
86	OHX	A5	3651	-	0,6,6	-	-	-		
86	OHX	A5	3463	-	0,6,6	-	-	-		
86	OHX	A5	3521	86	0,6,6	-	-	-		
86	OHX	A5	3607	-	0,6,6	-	-	-		
86	OHX	A7	204	87	0,6,6	-	-	-		
86	OHX	A1	3671	87	0,6,6	-	-	-		
86	OHX	A1	3532	-	0,6,6	-	-	-		
86	OHX	Ad	101	-	0,6,6	-	-	-		
86	OHX	A6	1976	-	0,6,6	-	-	-		
86	OHX	A1	3637	-	0,6,6	-	-	-		
86	OHX	A5	3471	-	0,6,6	-	-	-		
86	OHX	BC	401	-	0,6,6	-	-	-		
86	OHX	A5	3706	-	0,6,6	-	-	-		
86	OHX	A1	3779	-	0,6,6	-	-	-		
86	OHX	A6	1917	-	0,6,6	-	-	-		
86	OHX	Dg	201	-	0,6,6	-	-	-		
86	OHX	A1	3530	-	0,6,6	-	-	-		
86	OHX	A2	2081	-	0,6,6	-	-	-		
86	OHX	A1	3467	-	0,6,6	-	-	-		
86	OHX	A6	2061	-	0,6,6	-	-	-		
86	OHX	A1	3432	-	0,6,6	-	-	-		
86	OHX	A5	3415	-	0,6,6	-	-	-		
86	OHX	A1	3517	87	0,6,6	-	-	-		
86	OHX	A5	3433	87	0,6,6	-	-	-		
86	OHX	A1	3691	-	0,6,6	-	-	-		
86	OHX	A6	1918	-	0,6,6	-	-	-		
86	OHX	CS	201	-	0,6,6	-	-	-		
86	OHX	A5	3478	-	0,6,6	-	-	-		
86	OHX	A6	2033	-	0,6,6	-	-	-		
86	OHX	A5	3448	87	0,6,6	-	-	-		
86	OHX	A6	2072	-	0,6,6	-	-	-		
86	OHX	A4	207	-	0,6,6	-	-	-		
86	OHX	A1	3549	-	0,6,6	-	-	-		
86	OHX	A5	3691	-	0,6,6	-	-	-		
86	OHX	A2	1949	-	0,6,6	-	-	-		
86	OHX	A5	3704	87	0,6,6	-	-	-		
86	OHX	A5	3427	-	0,6,6	-	-	-		
86	OHX	A5	3751	-	0,6,6	-	-	-		
86	OHX	A1	3812	87	0,6,6	-	-	-		
86	OHX	A6	1959	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	A2	2054	-	0,6,6	-	-	-		
86	OHX	A5	3470	86	0,6,6	-	-	-		
86	OHX	A5	3619	-	0,6,6	-	-	-		
86	OHX	A1	3590	-	0,6,6	-	-	-		
86	OHX	A5	3687	87	0,6,6	-	-	-		
86	OHX	A2	1927	87	0,6,6	-	-	-		
86	OHX	A7	201	-	0,6,6	-	-	-		
86	OHX	A5	3731	-	0,6,6	-	-	-		
86	OHX	A6	1997	-	0,6,6	-	-	-		
86	OHX	De	201	-	0,6,6	-	-	-		
86	OHX	A2	2026	-	0,6,6	-	-	-		
86	OHX	A6	2086	-	0,6,6	-	-	-		
86	OHX	A5	3605	-	0,6,6	-	-	-		
86	OHX	A8	214	-	0,6,6	-	-	-		
86	OHX	A1	3601	-	0,6,6	-	-	-		
86	OHX	A1	3439	86	0,6,6	-	-	-		
86	OHX	A3	207	-	0,6,6	-	-	-		
86	OHX	A5	3797	87	0,6,6	-	-	-		
86	OHX	A2	1968	-	0,6,6	-	-	-		
86	OHX	A1	3798	-	0,6,6	-	-	-		
86	OHX	A6	1946	-	0,6,6	-	-	-		
86	OHX	A5	3537	-	0,6,6	-	-	-		
86	OHX	A2	1914	-	0,6,6	-	-	-		
86	OHX	A5	3565	-	0,6,6	-	-	-		
86	OHX	A2	2087	-	0,6,6	-	-	-		
86	OHX	A5	3803	87	0,6,6	-	-	-		
86	OHX	A6	1933	-	0,6,6	-	-	-		
86	OHX	A1	3712	-	0,6,6	-	-	-		
86	OHX	A5	3649	-	0,6,6	-	-	-		
86	OHX	A1	3560	-	0,6,6	-	-	-		
86	OHX	A5	3760	-	0,6,6	-	-	-		
86	OHX	A6	1941	-	0,6,6	-	-	-		
86	OHX	A1	3496	-	0,6,6	-	-	-		
86	OHX	A6	1964	-	0,6,6	-	-	-		
86	OHX	A5	3702	-	0,6,6	-	-	-		
86	OHX	A5	3738	-	0,6,6	-	-	-		
86	OHX	A6	2008	-	0,6,6	-	-	-		
86	OHX	A1	3606	-	0,6,6	-	-	-		
86	OHX	A5	3693	87	0,6,6	-	-	-		
86	OHX	A5	3483	-	0,6,6	-	-	-		
86	OHX	A1	3449	87	0,6,6	-	-	-		
86	OHX	Bb	101	-	0,6,6	-	-	-		
86	OHX	A5	3606	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	Do	201	87	0,6,6	-	-	-		
86	OHX	A5	3782	-	0,6,6	-	-	-		
86	OHX	A1	3710	87	0,6,6	-	-	-		
86	OHX	A2	1941	-	0,6,6	-	-	-		
86	OHX	A1	3428	-	0,6,6	-	-	-		
86	OHX	A6	2094	87	0,6,6	-	-	-		
86	OHX	A2	1998	-	0,6,6	-	-	-		
86	OHX	A1	3608	-	0,6,6	-	-	-		
86	OHX	A5	3616	-	0,6,6	-	-	-		

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.

660 monomers are involved in 1432 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A6	2069	OHX	2	0
86	A2	1940	OHX	5	0
86	A5	3763	OHX	4	0
86	A2	1921	OHX	6	0
86	A5	3622	OHX	1	0
86	A2	2002	OHX	3	0
86	A1	3704	OHX	2	0
86	A5	3700	OHX	2	0
86	A6	2001	OHX	1	0
86	A1	3559	OHX	1	0
86	A2	1919	OHX	1	0
86	A2	2051	OHX	2	0
86	A2	2063	OHX	1	0
86	A1	3621	OHX	1	0
86	A1	3632	OHX	2	0
86	A5	3436	OHX	1	0
86	A1	3414	OHX	5	0
86	A6	1942	OHX	1	0
86	A6	2085	OHX	1	0
86	A2	1963	OHX	1	0
86	A5	3815	OHX	5	0
86	A2	2067	OHX	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3800	OHX	1	0
86	A2	1909	OHX	2	0
86	A1	3607	OHX	6	0
86	A1	3442	OHX	2	0
86	Db	101	OHX	1	0
86	A1	3587	OHX	2	0
86	A6	1940	OHX	8	0
86	A1	3754	OHX	1	0
86	A5	3486	OHX	2	0
86	A5	3488	OHX	1	0
86	A2	1901	OHX	1	0
86	A5	3623	OHX	2	0
86	A1	3792	OHX	5	0
86	A1	3742	OHX	7	0
86	A1	3670	OHX	1	0
86	A5	3645	OHX	1	0
86	A5	3413	OHX	1	0
86	A6	1961	OHX	5	0
86	A6	2093	OHX	2	0
86	A6	2080	OHX	1	0
86	CL	201	OHX	5	0
86	A5	3713	OHX	1	0
86	A2	2055	OHX	1	0
86	A1	3519	OHX	1	0
86	A5	3474	OHX	7	0
86	A3	213	OHX	1	0
86	A2	2005	OHX	1	0
86	A5	3465	OHX	5	0
86	A1	3680	OHX	6	0
86	A1	3520	OHX	5	0
86	A6	2092	OHX	8	0
86	A1	3535	OHX	1	0
86	A5	3487	OHX	5	0
86	A2	2024	OHX	3	0
86	A2	1971	OHX	1	0
86	A2	2040	OHX	1	0
86	A6	1999	OHX	1	0
86	A1	3481	OHX	6	0
86	A1	3726	OHX	3	0
86	A1	3756	OHX	1	0
86	A1	3498	OHX	1	0
86	A1	3512	OHX	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3444	OHX	3	0
86	A6	2006	OHX	1	0
86	A5	3807	OHX	7	0
86	A5	3801	OHX	7	0
86	A5	3699	OHX	7	0
86	A6	1985	OHX	2	0
86	BB	401	OHX	2	0
86	A1	3463	OHX	4	0
86	DC	401	OHX	2	0
86	A5	3504	OHX	1	0
86	A6	2040	OHX	1	0
86	A5	3667	OHX	4	0
86	A2	1976	OHX	3	0
86	A1	3698	OHX	4	0
86	A5	3538	OHX	4	0
86	A5	3805	OHX	1	0
86	A1	3563	OHX	1	0
86	A2	2073	OHX	1	0
86	A5	3808	OHX	7	0
86	A2	2028	OHX	2	0
86	A5	3640	OHX	4	0
86	A1	3534	OHX	1	0
86	A5	3634	OHX	1	0
86	A5	3604	OHX	3	0
86	A5	3686	OHX	1	0
86	A2	1945	OHX	1	0
86	A6	1915	OHX	6	0
86	A5	3684	OHX	1	0
86	A5	3708	OHX	1	0
86	A1	3492	OHX	2	0
86	A1	3766	OHX	1	0
86	A2	2078	OHX	1	0
86	A3	202	OHX	1	0
86	A1	3703	OHX	1	0
86	A5	3530	OHX	1	0
86	A1	3805	OHX	6	0
86	A3	208	OHX	2	0
86	A5	3500	OHX	1	0
86	A2	2013	OHX	1	0
86	A1	3808	OHX	1	0
86	A1	3598	OHX	6	0
86	A1	3762	OHX	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A2	2062	OHX	1	0
86	BI	304	OHX	7	0
86	A7	211	OHX	6	0
86	A1	3645	OHX	1	0
86	A5	3477	OHX	6	0
86	A5	3581	OHX	4	0
86	A1	3478	OHX	4	0
86	DI	301	OHX	1	0
86	A2	1916	OHX	1	0
86	A5	3669	OHX	1	0
86	A1	3423	OHX	1	0
86	A5	3513	OHX	6	0
86	A1	3751	OHX	14	0
86	A5	3595	OHX	6	0
86	A2	2027	OHX	2	0
86	A6	2004	OHX	1	0
86	A2	2060	OHX	1	0
86	A5	3816	OHX	1	0
86	A5	3650	OHX	1	0
86	A1	3687	OHX	7	0
86	A2	2014	OHX	8	0
86	A5	3564	OHX	1	0
86	A6	2087	OHX	2	0
86	A5	3786	OHX	2	0
86	A5	3555	OHX	1	0
86	A6	1922	OHX	8	0
86	A1	3565	OHX	7	0
86	CG	301	OHX	4	1
86	A1	3547	OHX	1	0
86	A2	2036	OHX	1	0
86	A1	3536	OHX	1	0
86	A1	3760	OHX	1	0
86	A5	3647	OHX	1	0
86	A1	3693	OHX	11	0
86	A1	3550	OHX	2	0
86	A5	3758	OHX	1	0
86	A1	3650	OHX	9	0
86	CJ	201	OHX	3	0
86	A6	1993	OHX	2	0
86	A6	1921	OHX	2	0
86	A6	2050	OHX	2	0
86	A2	1961	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3625	OHX	1	0
86	A5	3723	OHX	7	0
86	A2	2047	OHX	1	0
86	DD	301	OHX	1	0
86	A1	3802	OHX	11	0
86	A5	3785	OHX	1	0
86	A7	203	OHX	6	0
86	A2	1926	OHX	1	0
86	A1	3506	OHX	6	0
86	A6	2051	OHX	1	0
86	A2	2074	OHX	17	0
86	AL	201	OHX	1	0
86	A6	2060	OHX	1	0
86	A2	2044	OHX	1	0
86	A5	3662	OHX	7	0
86	A6	1923	OHX	4	0
86	A5	3633	OHX	2	0
86	A2	1950	OHX	2	0
86	A1	3800	OHX	5	0
86	A1	3783	OHX	1	0
86	A5	3642	OHX	1	0
86	A1	3789	OHX	6	0
86	A6	1983	OHX	5	0
86	A5	3582	OHX	1	0
86	A2	1965	OHX	6	0
86	A1	3657	OHX	2	0
86	A6	1978	OHX	1	0
86	A6	2090	OHX	5	0
86	A2	1983	OHX	5	0
86	A2	1906	OHX	3	0
86	A6	2075	OHX	2	0
86	A1	3524	OHX	1	0
86	A1	3465	OHX	1	0
86	A1	3579	OHX	1	0
86	A5	3780	OHX	3	0
86	A5	3794	OHX	1	0
86	A5	3514	OHX	5	0
86	A6	2010	OHX	3	0
86	A1	3487	OHX	1	0
86	A1	3681	OHX	1	0
86	CP	201	OHX	3	0
86	A2	1987	OHX	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3439	OHX	3	0
86	A1	3746	OHX	8	0
86	A1	3801	OHX	1	0
86	A6	2096	OHX	1	0
86	AP	201	OHX	5	0
86	A1	3722	OHX	6	0
86	A1	3775	OHX	1	0
86	A8	202	OHX	1	0
86	A5	3813	OHX	8	0
86	A1	3602	OHX	4	0
86	A6	2043	OHX	1	0
86	A5	3603	OHX	7	0
86	A1	3538	OHX	3	0
86	A1	3539	OHX	3	0
86	A2	2068	OHX	2	0
86	A2	1937	OHX	1	0
86	A5	3533	OHX	7	0
86	A5	3590	OHX	1	0
86	A2	2033	OHX	1	0
86	A6	2046	OHX	2	0
86	A1	3589	OHX	1	0
86	A6	1968	OHX	1	0
86	A2	2016	OHX	1	0
86	A5	3542	OHX	7	0
86	A3	201	OHX	2	0
86	A5	3759	OHX	3	0
86	A5	3766	OHX	1	0
86	A1	3753	OHX	2	0
86	A1	3708	OHX	2	0
86	A4	215	OHX	1	0
86	A1	3471	OHX	14	0
86	A6	1928	OHX	1	0
86	A1	3725	OHX	4	0
86	A1	3811	OHX	13	0
86	A3	211	OHX	1	0
86	A5	3643	OHX	1	0
86	A2	2079	OHX	1	0
86	DA	302	OHX	6	0
86	A2	1918	OHX	8	0
86	A1	3509	OHX	6	0
86	CI	301	OHX	1	0
86	BA	301	OHX	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3720	OHX	5	0
86	A6	1957	OHX	3	0
86	A2	2041	OHX	1	0
86	A1	3477	OHX	1	0
86	A1	3573	OHX	1	0
86	A5	3541	OHX	1	0
86	A2	1969	OHX	6	0
86	A1	3485	OHX	1	0
86	A5	3822	OHX	3	0
86	A1	3673	OHX	2	0
86	A5	3644	OHX	7	0
86	A1	3503	OHX	5	0
86	A5	3726	OHX	1	0
86	A2	2071	OHX	6	0
86	A5	3618	OHX	1	0
86	A5	3491	OHX	4	0
86	A2	1938	OHX	1	0
86	A1	3816	OHX	8	0
86	A5	3806	OHX	1	0
86	A5	3431	OHX	2	0
86	A2	2065	OHX	1	0
86	A5	3577	OHX	6	0
86	A5	3779	OHX	6	0
86	A5	3657	OHX	1	0
86	A5	3761	OHX	1	0
86	A1	3738	OHX	8	0
86	A1	3774	OHX	1	0
86	A5	3526	OHX	5	0
86	BP	201	OHX	1	0
86	A5	3737	OHX	7	0
86	A1	3424	OHX	1	0
86	A8	212	OHX	1	0
86	A2	1952	OHX	2	0
86	A1	3479	OHX	7	0
86	A5	3507	OHX	1	0
86	A2	2012	OHX	2	0
86	A2	1974	OHX	1	0
86	A5	3666	OHX	7	0
86	A2	2052	OHX	6	0
86	A1	3412	OHX	2	0
86	A1	3785	OHX	7	0
86	A6	2020	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A2	2045	OHX	1	0
86	DV	201	OHX	1	0
86	AN	201	OHX	1	0
86	AC	301	OHX	5	0
86	A6	1979	OHX	1	0
86	A5	3775	OHX	2	0
86	A2	1991	OHX	1	0
86	A6	1909	OHX	4	0
86	A5	3610	OHX	10	0
86	A1	3677	OHX	1	0
86	A1	3554	OHX	1	0
86	A5	3639	OHX	1	0
86	A2	2083	OHX	1	0
86	A2	1917	OHX	2	0
86	A6	2017	OHX	1	0
86	A5	3695	OHX	6	0
86	A6	2022	OHX	2	0
86	A4	212	OHX	1	0
86	A5	3484	OHX	1	0
86	A5	3709	OHX	1	0
86	A1	3719	OHX	2	0
86	A2	1990	OHX	1	0
86	A6	2100	OHX	12	0
86	A6	2098	OHX	2	0
86	A1	3676	OHX	1	0
86	A5	3532	OHX	5	0
86	A2	1966	OHX	2	0
86	A2	1975	OHX	7	0
86	A6	2070	OHX	1	0
86	A2	1953	OHX	2	0
86	A6	1914	OHX	1	0
86	A6	1955	OHX	1	0
86	A8	206	OHX	1	0
86	A5	3588	OHX	3	0
86	A6	2009	OHX	6	0
86	A5	3681	OHX	9	0
86	A2	2032	OHX	1	0
86	A1	3807	OHX	1	0
86	A1	3755	OHX	1	0
86	A2	1915	OHX	6	0
86	A1	3522	OHX	1	0
86	A5	3492	OHX	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A2	1980	OHX	1	0
86	A2	1964	OHX	4	0
86	A2	1924	OHX	1	0
86	A2	1925	OHX	1	0
86	A1	3701	OHX	1	0
86	A5	3796	OHX	1	0
86	A6	2056	OHX	1	0
86	A6	2027	OHX	1	0
86	A6	2002	OHX	7	0
86	A5	3728	OHX	2	0
86	A1	3813	OHX	2	0
86	A1	3576	OHX	3	0
86	A1	3603	OHX	6	0
86	A5	3548	OHX	6	0
86	A6	2039	OHX	1	0
86	A1	3556	OHX	1	0
86	A5	3569	OHX	6	0
86	A5	3593	OHX	1	0
86	A1	3525	OHX	1	0
86	A5	3674	OHX	2	0
86	A2	2042	OHX	1	0
86	A6	2067	OHX	1	0
86	A1	3634	OHX	1	0
86	A1	3452	OHX	5	0
86	A2	1946	OHX	1	0
86	A1	3410	OHX	1	0
86	A5	3494	OHX	2	0
86	A5	3497	OHX	2	0
86	A5	3467	OHX	2	0
86	A5	3543	OHX	1	0
86	A1	3757	OHX	5	0
86	A1	3516	OHX	8	0
86	A2	1962	OHX	4	0
86	A6	2054	OHX	3	0
86	A6	2062	OHX	7	0
86	A2	2072	OHX	2	0
86	A1	3593	OHX	3	0
86	A6	1986	OHX	1	0
86	A5	3567	OHX	1	0
86	Cd	101	OHX	4	0
86	A2	2017	OHX	8	0
86	A5	3717	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A6	1927	OHX	1	0
86	Bj	102	OHX	1	0
86	A1	3541	OHX	1	0
86	A5	3546	OHX	2	0
86	A2	1978	OHX	7	0
86	A1	3586	OHX	1	0
86	A6	2071	OHX	8	0
86	A2	1992	OHX	3	0
86	A1	3731	OHX	1	0
86	A1	3729	OHX	1	0
86	A1	3806	OHX	7	0
86	A5	3692	OHX	1	0
86	A2	2080	OHX	2	0
86	A6	2076	OHX	2	0
86	A8	215	OHX	2	0
86	A1	3744	OHX	6	0
86	A5	3511	OHX	1	0
86	A1	3581	OHX	1	0
86	A6	1969	OHX	1	0
86	AI	301	OHX	1	0
86	A1	3585	OHX	1	0
86	A1	3737	OHX	1	0
86	A5	3819	OHX	2	0
86	A5	3509	OHX	7	0
86	A8	218	OHX	4	0
86	CG	302	OHX	4	0
86	A6	2012	OHX	1	0
86	A1	3788	OHX	5	1
86	A5	3576	OHX	1	0
86	DG	301	OHX	6	0
86	A5	3457	OHX	7	0
86	A4	205	OHX	2	0
86	A5	3499	OHX	1	0
86	A2	1922	OHX	7	0
86	A1	3786	OHX	2	0
86	A6	1991	OHX	1	0
86	A7	202	OHX	1	0
86	A5	3690	OHX	1	0
86	A5	3734	OHX	4	0
86	A5	3628	OHX	1	0
86	A2	1973	OHX	3	0
86	A5	3553	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A6	2083	OHX	1	0
86	A1	3739	OHX	3	0
86	A5	3725	OHX	1	0
86	A5	3654	OHX	2	0
86	A5	3510	OHX	1	0
86	A2	1955	OHX	1	0
86	A6	1981	OHX	2	0
86	A8	211	OHX	8	0
86	A6	2032	OHX	1	0
86	A1	3582	OHX	1	0
86	A1	3619	OHX	1	0
86	A5	3646	OHX	2	0
86	A1	3642	OHX	1	0
86	A6	2015	OHX	2	0
86	A5	3632	OHX	2	0
86	A5	3716	OHX	1	0
86	A2	2009	OHX	1	0
86	A4	211	OHX	3	0
86	A1	3456	OHX	1	0
86	A5	3601	OHX	1	0
86	A1	3491	OHX	6	0
86	A6	1953	OHX	2	0
86	A5	3516	OHX	6	0
86	A1	3591	OHX	7	0
86	A1	3706	OHX	6	0
86	A1	3433	OHX	2	0
86	A2	2019	OHX	1	0
86	A6	1949	OHX	1	0
86	A2	2086	OHX	11	0
86	A1	3659	OHX	4	0
86	A6	1930	OHX	2	0
86	A5	3762	OHX	7	0
86	A5	3458	OHX	6	0
86	DP	201	OHX	1	0
86	A2	2029	OHX	7	0
86	A5	3480	OHX	4	0
86	A5	3680	OHX	7	0
86	A5	3790	OHX	2	0
86	A6	2005	OHX	5	0
86	A6	1925	OHX	1	0
86	A5	3653	OHX	1	0
86	A1	3631	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3809	OHX	4	0
86	A5	3579	OHX	3	0
86	A1	3482	OHX	2	0
86	A5	3656	OHX	2	0
86	A1	3758	OHX	2	0
86	A2	1907	OHX	6	0
86	A2	1997	OHX	1	0
86	A1	3735	OHX	6	0
86	A1	3604	OHX	5	0
86	A1	3664	OHX	1	0
86	A5	3566	OHX	2	0
86	A1	3502	OHX	2	0
86	A1	3569	OHX	1	0
86	A5	3714	OHX	1	0
86	A1	3776	OHX	1	0
86	A5	3820	OHX	11	0
86	A1	3790	OHX	1	0
86	A6	1950	OHX	1	0
86	A5	3620	OHX	1	0
86	A1	3613	OHX	1	0
86	BI	303	OHX	9	0
86	A1	3426	OHX	1	0
86	A2	1942	OHX	1	0
86	A1	3483	OHX	7	0
86	DR	201	OHX	1	0
86	A2	1923	OHX	1	0
86	A1	3497	OHX	6	0
86	A5	3598	OHX	7	0
86	A1	3455	OHX	1	0
86	BR	201	OHX	1	0
86	A4	204	OHX	1	0
86	A2	2061	OHX	2	0
86	A1	3495	OHX	3	0
86	A1	3574	OHX	6	0
86	A6	2019	OHX	1	0
86	A5	3464	OHX	6	0
86	A5	3528	OHX	2	0
86	A6	1971	OHX	2	0
86	A6	1919	OHX	2	0
86	A1	3578	OHX	6	0
86	A1	3584	OHX	4	0
86	CP	202	OHX	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3795	OHX	6	0
86	A5	3768	OHX	3	0
86	A5	3476	OHX	3	0
86	A1	3567	OHX	1	0
86	A1	3542	OHX	6	0
86	A1	3562	OHX	6	0
86	A1	3717	OHX	5	0
86	A5	3750	OHX	1	0
86	A7	212	OHX	1	0
86	A5	3517	OHX	4	0
86	A6	2053	OHX	1	0
86	A5	3609	OHX	1	0
86	A2	2010	OHX	2	0
86	A1	3457	OHX	6	0
86	A6	2099	OHX	4	0
86	A7	209	OHX	4	0
86	A6	2057	OHX	2	0
86	Bj	101	OHX	5	0
86	A5	3661	OHX	1	0
86	A5	3772	OHX	4	0
86	Bo	201	OHX	3	0
86	A2	1989	OHX	8	0
86	A1	3795	OHX	6	0
86	A2	1929	OHX	1	0
86	A2	1954	OHX	6	0
86	A5	3550	OHX	6	0
86	A5	3811	OHX	6	0
86	A2	1948	OHX	1	0
86	A5	3812	OHX	8	0
86	A1	3692	OHX	1	0
86	DB	401	OHX	1	0
86	A5	3810	OHX	6	0
86	A8	207	OHX	3	0
86	A6	2068	OHX	6	0
86	A2	1928	OHX	1	0
86	A2	2031	OHX	1	0
86	A5	3473	OHX	7	0
86	A1	3527	OHX	1	0
86	A5	3814	OHX	6	0
86	A2	2015	OHX	1	0
86	A2	1970	OHX	8	0
86	A4	206	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3712	OHX	1	0
86	A5	3437	OHX	1	0
86	DJ	201	OHX	1	0
86	A5	3778	OHX	1	0
86	A2	2049	OHX	1	0
86	A1	3543	OHX	1	0
86	A1	3544	OHX	3	0
86	A5	3722	OHX	4	0
86	A1	3690	OHX	2	0
86	A5	3660	OHX	5	0
86	A1	3697	OHX	3	0
86	A1	3434	OHX	1	0
86	A1	3505	OHX	2	0
86	A2	2050	OHX	1	0
86	A1	3654	OHX	3	0
86	A6	1956	OHX	4	0
86	A5	3515	OHX	6	0
86	A5	3518	OHX	7	0
86	A5	3740	OHX	6	0
86	A5	3414	OHX	1	0
86	A1	3508	OHX	1	0
86	A2	1957	OHX	1	0
86	A5	3613	OHX	1	0
86	A5	3405	OHX	1	0
86	A5	3753	OHX	3	0
86	A6	1977	OHX	1	0
86	A5	3580	OHX	6	0
86	A5	3469	OHX	2	0
86	A5	3781	OHX	2	0
86	A1	3655	OHX	1	0
86	A1	3814	OHX	2	0
86	A1	3718	OHX	7	0
86	A6	1984	OHX	1	0
86	A5	3821	OHX	6	0
86	A5	3591	OHX	6	0
86	A8	203	OHX	8	0
86	BD	301	OHX	1	0
86	A6	1951	OHX	2	0
86	A5	3549	OHX	2	0
86	A1	3793	OHX	3	0
86	A5	3729	OHX	6	0
86	A2	2082	OHX	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A2	1988	OHX	2	0
86	A5	3489	OHX	7	0
86	A1	3458	OHX	5	0
86	A1	3732	OHX	2	0
86	A2	2048	OHX	6	0
86	BP	202	OHX	1	0
86	A5	3573	OHX	1	0
86	A1	3513	OHX	1	0
86	A6	1931	OHX	3	0
86	A5	3524	OHX	1	0
86	A5	3493	OHX	1	0
86	A5	3732	OHX	10	0
86	A5	3736	OHX	1	0
86	A1	3804	OHX	1	0
86	A2	2076	OHX	6	0
86	A1	3763	OHX	1	0
86	A1	3622	OHX	2	0
86	A5	3568	OHX	3	0
86	A1	3748	OHX	6	0
86	A6	2016	OHX	8	0
86	A5	3683	OHX	1	0
86	A1	3679	OHX	1	0
86	A6	2058	OHX	4	0
86	A1	3501	OHX	1	0
86	A2	2037	OHX	3	0
86	A1	3627	OHX	1	0
86	A1	3667	OHX	6	0
86	A1	3523	OHX	1	0
86	A5	3586	OHX	1	0
86	A1	3466	OHX	4	0
86	A5	3739	OHX	6	0
86	A1	3750	OHX	5	0
86	A1	3707	OHX	1	0
86	A1	3570	OHX	1	0
86	A1	3730	OHX	2	0
86	A5	3617	OHX	5	0
86	A6	1990	OHX	1	0
86	A5	3741	OHX	4	0
86	A1	3777	OHX	7	0
86	CN	201	OHX	2	0
86	A5	3743	OHX	5	0
86	A5	3461	OHX	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A5	3463	OHX	1	0
86	A5	3521	OHX	8	0
86	A5	3607	OHX	6	0
86	A1	3671	OHX	11	0
86	A1	3532	OHX	1	0
86	Ad	101	OHX	4	0
86	A6	1976	OHX	1	0
86	A1	3637	OHX	1	0
86	BC	401	OHX	2	0
86	A5	3706	OHX	1	0
86	A1	3779	OHX	1	0
86	A6	1917	OHX	1	0
86	A2	2081	OHX	1	0
86	A1	3467	OHX	6	0
86	A1	3432	OHX	5	0
86	A1	3517	OHX	1	0
86	A1	3691	OHX	3	0
86	A6	2033	OHX	2	0
86	A1	3549	OHX	6	0
86	A2	1949	OHX	1	0
86	A5	3427	OHX	1	0
86	A1	3812	OHX	7	0
86	A5	3470	OHX	6	0
86	A5	3619	OHX	1	0
86	A1	3590	OHX	2	0
86	A5	3731	OHX	1	0
86	A2	2026	OHX	1	0
86	A6	2086	OHX	6	0
86	A1	3601	OHX	4	0
86	A1	3439	OHX	7	0
86	A1	3798	OHX	11	0
86	A6	1946	OHX	1	0
86	A2	1914	OHX	4	0
86	A5	3565	OHX	1	0
86	A2	2087	OHX	1	0
86	A5	3803	OHX	7	0
86	A6	1933	OHX	12	0
86	A1	3712	OHX	5	0
86	A6	1941	OHX	8	0
86	A1	3496	OHX	11	0
86	A6	1964	OHX	3	0
86	A5	3738	OHX	7	0

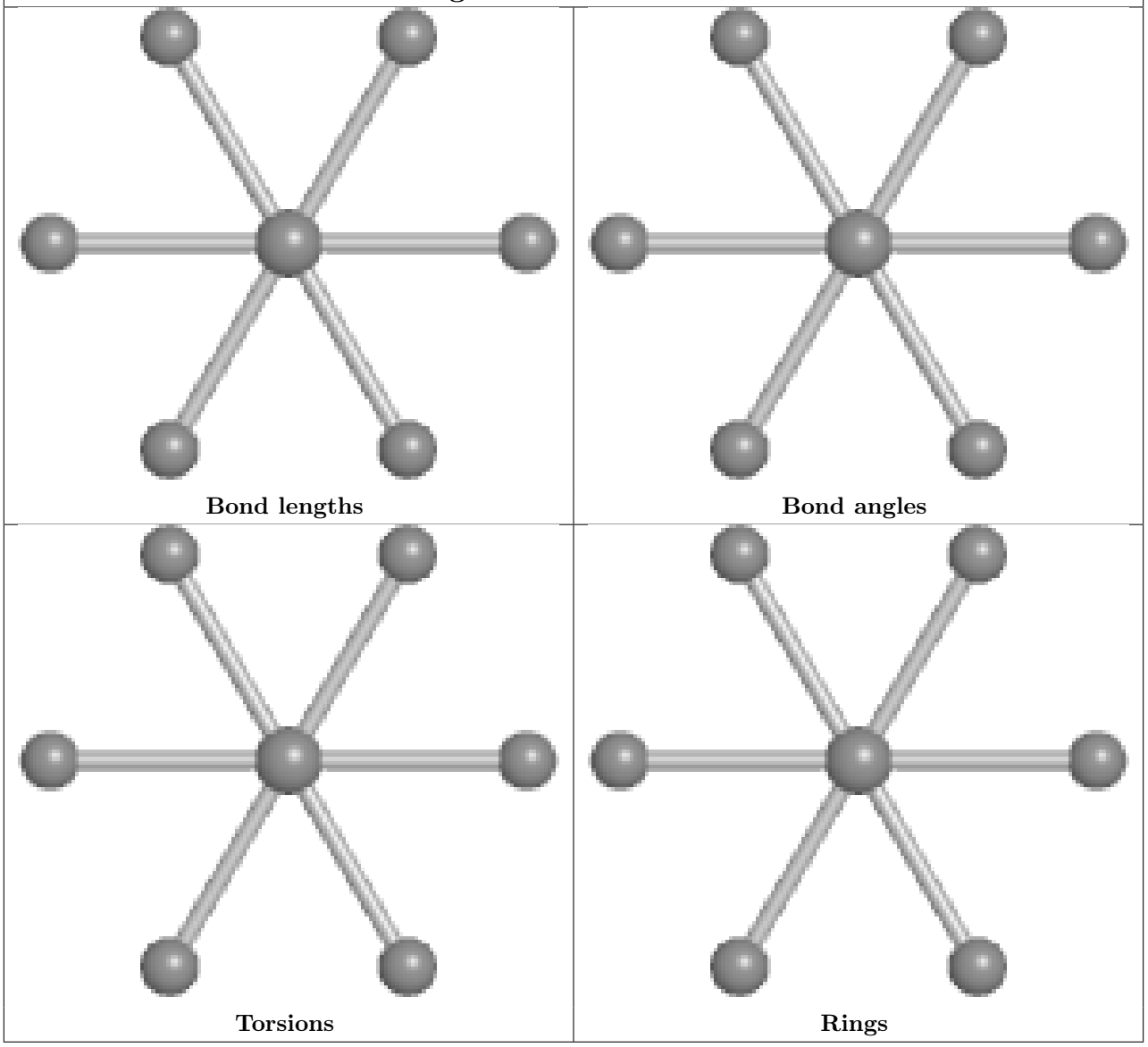
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A1	3449	OHX	1	0
86	A5	3606	OHX	6	0
86	Do	201	OHX	2	0
86	A5	3782	OHX	1	0
86	A1	3710	OHX	1	0
86	A6	2094	OHX	1	0
86	A1	3608	OHX	3	0
86	A5	3616	OHX	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OHX A5 3792



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, 95^{th} 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	A2	1767/1800 (98%)	-0.07	29 (1%) 70 47	40, 88, 220, 373	1 (0%)
2	AA	206/252 (81%)	0.80	17 (8%) 17 9	71, 111, 170, 202	0
2	CA	206/252 (81%)	0.80	12 (5%) 29 15	60, 90, 133, 228	0
3	AB	214/255 (83%)	1.06	25 (11%) 9 5	79, 144, 219, 256	0
3	CB	216/255 (84%)	0.26	2 (0%) 81 61	59, 85, 127, 171	0
4	AC	217/254 (85%)	0.57	7 (3%) 50 29	60, 91, 130, 170	0
4	CC	217/254 (85%)	0.27	8 (3%) 45 25	50, 75, 127, 193	0
5	AD	223/240 (92%)	0.57	5 (2%) 62 39	69, 97, 154, 222	0
5	CD	223/240 (92%)	0.25	3 (1%) 75 53	56, 91, 144, 182	0
6	AE	260/261 (99%)	0.48	7 (2%) 56 33	60, 89, 131, 187	0
6	CE	260/261 (99%)	0.24	4 (1%) 72 49	48, 74, 112, 237	0
7	AF	206/225 (91%)	0.41	5 (2%) 59 36	72, 116, 160, 231	0
7	CF	206/225 (91%)	0.60	8 (3%) 43 24	53, 87, 143, 207	0
8	AG	226/236 (95%)	0.86	20 (8%) 15 8	58, 102, 153, 209	0
8	CG	218/236 (92%)	0.39	8 (3%) 45 25	49, 83, 140, 239	0
9	AH	184/190 (96%)	0.92	15 (8%) 17 9	75, 121, 178, 259	0
9	CH	186/190 (97%)	0.57	8 (4%) 40 21	64, 102, 162, 222	0
10	AI	188/200 (94%)	0.30	4 (2%) 63 40	48, 76, 132, 165	0
10	CI	188/200 (94%)	0.39	2 (1%) 78 57	41, 68, 116, 154	0
11	AJ	185/197 (93%)	0.71	7 (3%) 44 24	70, 101, 163, 231	0
11	CJ	185/197 (93%)	0.51	3 (1%) 70 47	55, 78, 138, 196	0
12	AK	96/105 (91%)	0.36	3 (3%) 51 30	71, 101, 164, 198	0
12	CK	96/105 (91%)	0.61	8 (8%) 17 9	77, 116, 163, 222	0
13	AL	155/156 (99%)	0.35	5 (3%) 50 29	48, 71, 176, 236	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	CL	146/156 (93%)	0.46	12 (8%) 17 9	41, 63, 134, 219	0
14	AM	124/143 (86%)	0.75	9 (7%) 21 11	97, 148, 209, 234	0
14	CM	124/143 (86%)	0.98	11 (8%) 15 8	121, 191, 250, 311	0
15	AN	150/151 (99%)	0.40	4 (2%) 56 33	57, 89, 127, 183	0
15	CN	150/151 (99%)	0.06	2 (1%) 75 53	49, 73, 109, 130	0
16	AO	127/137 (92%)	1.23	21 (16%) 4 3	61, 134, 179, 240	0
16	CO	128/137 (93%)	0.28	2 (1%) 70 47	50, 84, 118, 140	0
17	AP	124/142 (87%)	0.79	7 (5%) 30 15	68, 93, 167, 197	0
17	CP	135/142 (95%)	0.67	16 (11%) 9 5	61, 93, 166, 196	0
18	AQ	141/143 (98%)	0.86	13 (9%) 14 8	72, 100, 138, 155	0
18	CQ	142/143 (99%)	0.65	15 (10%) 11 6	53, 79, 121, 171	0
19	AR	120/136 (88%)	0.85	10 (8%) 17 9	66, 112, 180, 214	0
19	CR	117/136 (86%)	0.58	11 (9%) 14 7	58, 88, 142, 199	0
20	AS	145/146 (99%)	0.56	5 (3%) 48 27	57, 104, 156, 182	0
20	CS	145/146 (99%)	0.48	6 (4%) 41 23	56, 79, 138, 165	0
21	AT	143/144 (99%)	0.80	9 (6%) 26 13	73, 102, 147, 180	0
21	CT	143/144 (99%)	0.33	0 100 100	48, 74, 114, 181	0
22	AU	107/121 (88%)	1.14	16 (14%) 5 3	64, 102, 189, 226	0
22	CU	110/121 (90%)	0.46	4 (3%) 46 26	56, 93, 183, 243	0
23	AV	87/87 (100%)	0.60	3 (3%) 48 27	75, 102, 151, 169	0
23	CV	87/87 (100%)	0.27	0 100 100	54, 79, 118, 185	0
24	AW	129/130 (99%)	0.54	2 (1%) 70 47	58, 82, 103, 121	0
24	CW	129/130 (99%)	0.18	1 (0%) 82 64	40, 62, 77, 98	0
25	AX	144/145 (99%)	0.25	7 (4%) 35 18	48, 68, 98, 150	0
25	CX	144/145 (99%)	-0.13	1 (0%) 84 66	37, 53, 80, 139	0
26	AY	134/135 (99%)	0.94	11 (8%) 17 9	70, 106, 166, 216	0
26	CY	134/135 (99%)	0.54	6 (4%) 38 20	57, 84, 143, 191	0
27	AZ	70/108 (64%)	0.58	5 (7%) 22 11	88, 132, 172, 235	0
27	CZ	69/108 (63%)	0.71	5 (7%) 21 11	68, 103, 151, 196	0
28	Aa	97/119 (81%)	1.09	12 (12%) 8 5	69, 113, 206, 223	0
28	Ca	97/119 (81%)	0.58	5 (5%) 33 17	54, 79, 129, 165	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	Ab	81/82 (98%)	0.53	1 (1%) 76 55	68, 102, 188, 225	0
29	Cb	81/82 (98%)	0.35	2 (2%) 58 35	51, 85, 170, 203	0
30	Ac	63/67 (94%)	0.77	2 (3%) 50 29	86, 130, 182, 204	0
30	Cc	63/67 (94%)	0.87	1 (1%) 70 47	74, 107, 155, 180	0
31	Ad	53/56 (94%)	0.73	3 (5%) 29 15	64, 76, 106, 155	0
31	Cd	53/56 (94%)	0.31	4 (7%) 20 10	51, 69, 108, 168	0
32	Ae	60/63 (95%)	0.54	4 (6%) 24 12	56, 103, 179, 270	0
32	Ce	62/63 (98%)	0.28	2 (3%) 50 29	47, 84, 184, 218	0
33	Af	51/152 (33%)	1.17	8 (15%) 5 3	92, 138, 186, 202	0
33	Cf	51/152 (33%)	1.44	14 (27%) 1 1	113, 172, 222, 254	0
34	Ag	318/319 (99%)	0.64	9 (2%) 55 32	74, 113, 171, 237	0
34	Cg	318/319 (99%)	0.64	9 (2%) 55 32	73, 105, 158, 232	0
35	Ah	121/273 (44%)	0.68	9 (7%) 20 10	54, 99, 162, 212	0
36	A1	3149/3396 (92%)	-0.30	34 (1%) 78 57	29, 54, 168, 351	0
36	A5	3150/3396 (92%)	-0.33	36 (1%) 78 57	28, 52, 157, 346	0
37	A3	121/121 (100%)	-0.05	0 100 100	34, 72, 92, 118	0
37	A7	121/121 (100%)	-0.21	1 (0%) 82 64	31, 57, 74, 144	0
38	A4	158/158 (100%)	-0.22	1 (0%) 85 69	37, 58, 112, 223	0
38	A8	158/158 (100%)	-0.12	3 (1%) 66 43	39, 65, 128, 263	0
39	BA	252/254 (99%)	-0.02	2 (0%) 82 64	27, 53, 78, 150	0
39	DA	252/254 (99%)	0.09	9 (3%) 46 26	29, 55, 83, 177	0
40	BB	386/387 (99%)	0.01	4 (1%) 79 59	26, 58, 86, 187	0
40	DB	386/387 (99%)	-0.34	3 (0%) 82 64	20, 44, 69, 188	0
41	BC	361/362 (99%)	-0.25	1 (0%) 90 79	26, 50, 86, 132	0
41	DC	361/362 (99%)	0.02	3 (0%) 82 64	30, 56, 90, 136	0
42	BD	296/297 (99%)	0.47	11 (3%) 45 25	47, 81, 132, 223	0
42	DD	294/297 (98%)	0.21	6 (2%) 65 41	38, 58, 110, 205	0
43	BE	156/176 (88%)	-0.28	0 100 100	34, 52, 89, 152	0
43	DE	157/176 (89%)	-0.14	2 (1%) 75 53	37, 54, 97, 160	0
44	BF	222/244 (90%)	-0.44	0 100 100	31, 46, 87, 247	0
44	DF	223/244 (91%)	-0.33	1 (0%) 88 76	26, 44, 99, 196	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	BG	233/256 (91%)	0.53	7 (3%) 52 30	52, 79, 148, 255	0
45	DG	231/256 (90%)	0.48	5 (2%) 62 39	63, 88, 132, 196	0
46	BH	191/191 (100%)	0.33	2 (1%) 79 59	44, 65, 99, 197	0
46	DH	191/191 (100%)	-0.40	1 (0%) 87 72	30, 47, 83, 206	0
47	BI	211/221 (95%)	0.13	9 (4%) 40 21	37, 60, 121, 229	0
47	DI	213/221 (96%)	0.37	7 (3%) 49 28	34, 60, 106, 207	0
48	BJ	169/174 (97%)	0.62	3 (1%) 67 44	50, 84, 123, 151	0
48	DJ	169/174 (97%)	0.12	2 (1%) 76 55	40, 64, 98, 123	0
49	BL	193/199 (96%)	-0.04	2 (1%) 79 59	30, 57, 126, 216	0
49	DL	194/199 (97%)	0.29	1 (0%) 87 72	38, 69, 134, 174	0
50	BM	136/138 (98%)	-0.01	3 (2%) 62 39	37, 55, 92, 132	0
50	DM	137/138 (99%)	-0.28	3 (2%) 62 39	30, 47, 83, 153	0
51	BN	203/204 (99%)	-0.08	0 100 100	32, 52, 68, 92	0
51	DN	203/204 (99%)	0.15	1 (0%) 87 72	37, 60, 82, 104	0
52	BO	177/219 (80%)	0.05	8 (4%) 38 20	13, 26, 44, 57	177 (100%)
52	DO	177/219 (80%)	-0.12	8 (4%) 38 20	11, 20, 43, 57	177 (100%)
53	BP	183/184 (99%)	-0.04	5 (2%) 56 33	30, 49, 149, 224	0
53	DP	155/184 (84%)	-0.33	2 (1%) 75 53	30, 44, 72, 161	0
54	BQ	185/186 (99%)	-0.35	1 (0%) 87 72	33, 48, 68, 107	0
54	DQ	185/186 (99%)	-0.06	1 (0%) 87 72	35, 54, 73, 125	0
55	BR	188/189 (99%)	0.35	8 (4%) 40 21	45, 71, 170, 201	0
55	DR	188/189 (99%)	0.25	4 (2%) 63 40	36, 64, 142, 199	0
56	BS	172/172 (100%)	-0.25	1 (0%) 85 69	36, 51, 85, 123	0
56	DS	172/172 (100%)	-0.40	2 (1%) 76 55	26, 44, 72, 141	0
57	BT	159/160 (99%)	-0.16	0 100 100	33, 52, 111, 149	0
57	DT	159/160 (99%)	-0.18	1 (0%) 85 69	30, 46, 97, 120	0
58	BU	100/121 (82%)	0.78	5 (5%) 34 18	79, 108, 150, 180	0
58	DU	98/121 (80%)	0.89	9 (9%) 14 8	67, 97, 128, 168	0
59	BV	136/137 (99%)	0.02	4 (2%) 53 31	35, 57, 95, 182	0
59	DV	136/137 (99%)	-0.37	4 (2%) 53 31	26, 42, 78, 210	0
60	BW	98/155 (63%)	0.69	12 (12%) 8 5	47, 77, 244, 306	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	DW	135/155 (87%)	0.51	6 (4%) 39 21	36, 94, 192, 249	0
61	BX	121/142 (85%)	0.22	3 (2%) 58 35	41, 68, 99, 152	0
61	DX	120/142 (84%)	0.33	3 (2%) 58 35	46, 71, 108, 135	0
62	BY	126/127 (99%)	-0.02	0 100 100	38, 59, 91, 150	0
62	DY	126/127 (99%)	0.29	1 (0%) 82 64	39, 66, 102, 168	0
63	BZ	135/136 (99%)	0.58	3 (2%) 62 39	68, 94, 138, 162	0
63	DZ	135/136 (99%)	0.74	6 (4%) 39 21	68, 103, 142, 170	0
64	Ba	148/149 (99%)	-0.29	1 (0%) 84 66	26, 50, 89, 116	0
64	Da	148/149 (99%)	0.09	0 100 100	28, 55, 93, 142	0
65	Bb	58/59 (98%)	0.28	4 (6%) 23 12	33, 58, 119, 142	0
65	Db	58/59 (98%)	0.45	8 (13%) 6 4	35, 59, 123, 160	0
66	Bc	97/105 (92%)	0.35	2 (2%) 63 40	63, 88, 129, 171	0
66	Dc	100/105 (95%)	0.43	3 (3%) 52 30	59, 86, 154, 173	0
67	Bd	109/113 (96%)	0.29	4 (3%) 45 25	40, 66, 132, 202	0
67	Dd	109/113 (96%)	-0.03	0 100 100	34, 57, 126, 199	0
68	Be	127/130 (97%)	-0.32	3 (2%) 59 36	22, 42, 65, 149	0
68	De	127/130 (97%)	-0.11	6 (4%) 36 19	25, 47, 77, 136	0
69	Bf	106/107 (99%)	-0.31	1 (0%) 81 61	30, 41, 73, 139	0
69	Df	106/107 (99%)	-0.35	0 100 100	27, 40, 75, 119	0
70	Bg	112/121 (92%)	0.57	3 (2%) 56 33	44, 71, 134, 197	0
70	Dg	112/121 (92%)	0.49	4 (3%) 46 26	41, 72, 139, 191	0
71	Bh	119/120 (99%)	0.26	2 (1%) 69 45	42, 68, 104, 119	0
71	Dh	119/120 (99%)	0.38	3 (2%) 58 35	51, 75, 109, 149	0
72	Bi	99/100 (99%)	0.35	2 (2%) 65 41	45, 69, 111, 172	0
72	Di	99/100 (99%)	0.37	4 (4%) 42 23	57, 75, 116, 171	0
73	Bj	87/88 (98%)	-0.10	2 (2%) 61 38	35, 45, 74, 216	0
73	Dj	87/88 (98%)	0.05	2 (2%) 61 38	30, 50, 91, 241	0
74	Bk	77/78 (98%)	0.59	3 (3%) 43 24	65, 95, 146, 168	0
74	Dk	77/78 (98%)	0.79	8 (10%) 11 6	64, 98, 138, 153	0
75	Bl	50/51 (98%)	0.10	1 (2%) 65 41	37, 59, 80, 95	0
75	Dl	50/51 (98%)	0.22	3 (6%) 27 14	44, 59, 82, 102	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
76	Bm	52/128 (40%)	0.04	2 (3%) 44 24	42, 55, 82, 139	0
76	Dm	52/128 (40%)	-0.21	2 (3%) 44 24	30, 39, 68, 106	0
77	Bn	25/25 (100%)	0.19	0 100 100	49, 62, 79, 94	0
77	Dn	25/25 (100%)	0.20	1 (4%) 42 23	37, 55, 72, 99	0
78	Bo	105/106 (99%)	-0.03	0 100 100	35, 60, 97, 219	0
78	Do	105/106 (99%)	-0.04	1 (0%) 79 59	37, 59, 101, 157	0
79	Bp	91/92 (98%)	0.19	1 (1%) 78 57	40, 61, 104, 126	0
79	Dp	91/92 (98%)	-0.10	1 (1%) 78 57	29, 60, 96, 111	0
80	A6	1769/1800 (98%)	-0.01	24 (1%) 73 51	34, 72, 189, 360	1 (0%)
81	Ch	63/273 (23%)	0.91	7 (11%) 10 6	50, 99, 156, 183	0
82	DK	0/155	-	-	-	-
83	Dq	120/312 (38%)	0.76	8 (6%) 24 12	70, 109, 166, 232	0
84	Dr	0/47	-	-	-	-
85	Ds	0/46	-	-	-	-
All	All	32867/35856 (91%)	0.13	890 (2%) 56 33	11, 71, 157, 373	356 (1%)

The worst 5 of 890 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	DA	248	GLY	8.9
36	A5	2873	U	7.0
56	DS	1	MET	6.4
39	DA	253	GLN	6.3
28	Ca	16	GLY	5.9

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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, 95^{th} 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
87	MG	A5	4320	1/1	0.09	0.27	117,117,117,117	0
87	MG	A5	4515	1/1	0.10	0.23	109,109,109,109	0
87	MG	A5	4004	1/1	0.12	0.34	55,55,55,55	0
87	MG	A1	4291	1/1	0.17	0.27	112,112,112,112	0
87	MG	A2	2194	1/1	0.19	0.32	113,113,113,113	0
87	MG	A1	4481	1/1	0.24	0.35	97,97,97,97	0
87	MG	A5	4131	1/1	0.32	0.27	85,85,85,85	0
87	MG	A2	2209	1/1	0.33	0.46	96,96,96,96	0
87	MG	A1	3906	1/1	0.36	0.27	91,91,91,91	0
87	MG	A1	4232	1/1	0.37	0.40	75,75,75,75	0
87	MG	A5	3897	1/1	0.37	0.49	100,100,100,100	0
87	MG	A6	2312	1/1	0.38	0.29	85,85,85,85	0
87	MG	A1	4301	1/1	0.38	0.12	118,118,118,118	0
87	MG	A2	2227	1/1	0.38	0.22	106,106,106,106	0
87	MG	DB	413	1/1	0.38	0.51	101,101,101,101	0
87	MG	A1	3863	1/1	0.43	0.40	125,125,125,125	0
87	MG	A5	4518	1/1	0.45	0.30	144,144,144,144	0
87	MG	A5	4254	1/1	0.45	0.72	103,103,103,103	0
87	MG	A2	2182	1/1	0.46	0.35	78,78,78,78	0
87	MG	A2	2219	1/1	0.46	0.25	93,93,93,93	0
87	MG	A1	4313	1/1	0.46	0.26	105,105,105,105	0
87	MG	A2	2159	1/1	0.46	0.44	88,88,88,88	0
87	MG	A5	4207	1/1	0.46	0.41	102,102,102,102	0
87	MG	A2	2251	1/1	0.47	0.36	77,77,77,77	0
87	MG	A1	4089	1/1	0.48	0.22	89,89,89,89	0
87	MG	A1	4501	1/1	0.48	0.38	103,103,103,103	0
87	MG	CQ	202	1/1	0.49	0.36	85,85,85,85	0
87	MG	A6	2337	1/1	0.50	0.24	127,127,127,127	0
87	MG	A6	2128	1/1	0.50	0.50	81,81,81,81	0
87	MG	A5	4492	1/1	0.50	0.49	73,73,73,73	0
87	MG	A1	4135	1/1	0.51	0.15	96,96,96,96	0
87	MG	A1	4370	1/1	0.51	0.27	104,104,104,104	0
87	MG	A2	2166	1/1	0.52	0.22	90,90,90,90	0
87	MG	A5	4371	1/1	0.52	0.43	90,90,90,90	0
87	MG	A1	4182	1/1	0.52	0.32	81,81,81,81	0
87	MG	A6	2316	1/1	0.53	0.27	112,112,112,112	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2149	1/1	0.53	0.29	83,83,83,83	0
87	MG	A1	4255	1/1	0.54	0.41	87,87,87,87	0
87	MG	A3	230	1/1	0.54	0.29	85,85,85,85	0
87	MG	AB	301	1/1	0.54	0.23	98,98,98,98	0
87	MG	A1	4190	1/1	0.55	0.46	98,98,98,98	0
87	MG	A5	4372	1/1	0.55	0.41	74,74,74,74	0
87	MG	A1	4364	1/1	0.56	0.19	92,92,92,92	0
87	MG	A5	4490	1/1	0.56	0.19	90,90,90,90	0
87	MG	A6	2287	1/1	0.57	0.30	96,96,96,96	0
87	MG	A1	4435	1/1	0.57	0.29	105,105,105,105	0
87	MG	A5	3906	1/1	0.57	0.28	56,56,56,56	0
87	MG	A1	4457	1/1	0.57	0.25	97,97,97,97	0
87	MG	A2	2123	1/1	0.57	0.41	81,81,81,81	0
87	MG	Dq	401	1/1	0.57	0.29	81,81,81,81	0
87	MG	A6	2253	1/1	0.58	0.39	85,85,85,85	0
87	MG	A2	2137	1/1	0.58	0.28	97,97,97,97	0
87	MG	A2	2147	1/1	0.58	0.28	93,93,93,93	0
87	MG	A1	4150	1/1	0.58	0.22	95,95,95,95	0
87	MG	A2	2094	1/1	0.58	0.45	68,68,68,68	0
87	MG	A5	4381	1/1	0.58	0.25	96,96,96,96	0
87	MG	A1	4502	1/1	0.58	0.15	93,93,93,93	0
87	MG	A3	220	1/1	0.58	0.43	83,83,83,83	0
87	MG	A2	2156	1/1	0.58	0.32	70,70,70,70	0
86	OHX	A5	3786	7/7	0.58	0.21	238,238,238,238	7
87	MG	A6	2195	1/1	0.58	0.39	93,93,93,93	0
87	MG	A5	4146	1/1	0.58	0.39	80,80,80,80	0
88	ZN	Cb	101	1/1	0.58	0.20	305,305,305,305	0
87	MG	A2	2208	1/1	0.59	0.32	109,109,109,109	0
87	MG	A5	4334	1/1	0.59	0.12	109,109,109,109	0
87	MG	CS	202	1/1	0.59	0.11	63,63,63,63	0
87	MG	A6	2182	1/1	0.59	0.17	63,63,63,63	0
87	MG	A6	2250	1/1	0.60	0.26	96,96,96,96	0
87	MG	A1	4495	1/1	0.60	0.31	109,109,109,109	0
87	MG	Ad	102	1/1	0.60	0.38	89,89,89,89	0
87	MG	A1	3870	1/1	0.61	0.35	57,57,57,57	0
87	MG	A1	4344	1/1	0.61	0.19	88,88,88,88	0
87	MG	A5	4527	1/1	0.61	0.23	78,78,78,78	0
87	MG	A5	4571	1/1	0.61	0.11	84,84,84,84	0
87	MG	A4	228	1/1	0.61	0.28	70,70,70,70	0
87	MG	A6	2116	1/1	0.61	0.47	80,80,80,80	0
87	MG	A5	4336	1/1	0.61	0.44	77,77,77,77	0
87	MG	A5	3847	1/1	0.62	0.35	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2097	1/1	0.62	0.40	78,78,78,78	0
87	MG	A5	4183	1/1	0.62	0.37	76,76,76,76	0
86	OHX	A5	3817	7/7	0.62	0.14	205,205,205,205	7
86	OHX	A5	3777	7/7	0.62	0.25	187,187,187,187	7
87	MG	A1	3920	1/1	0.63	0.30	53,53,53,53	0
87	MG	A1	4236	1/1	0.63	0.25	73,73,73,73	0
87	MG	A5	4137	1/1	0.63	0.23	104,104,104,104	0
87	MG	A2	2213	1/1	0.63	0.63	107,107,107,107	0
87	MG	A1	3841	1/1	0.63	0.22	47,47,47,47	0
87	MG	A2	2253	1/1	0.63	0.32	89,89,89,89	0
87	MG	A2	2242	1/1	0.63	0.41	105,105,105,105	0
87	MG	A6	2189	1/1	0.63	0.24	42,42,42,42	0
87	MG	A1	4327	1/1	0.63	0.22	108,108,108,108	0
87	MG	A6	2237	1/1	0.63	0.30	96,96,96,96	0
87	MG	AN	202	1/1	0.63	0.13	63,63,63,63	0
87	MG	A1	3922	1/1	0.64	0.47	107,107,107,107	0
87	MG	A1	4153	1/1	0.64	0.21	96,96,96,96	0
87	MG	A1	4256	1/1	0.64	0.21	86,86,86,86	0
87	MG	A1	4087	1/1	0.64	0.24	67,67,67,67	0
87	MG	A6	2191	1/1	0.64	0.30	84,84,84,84	0
87	MG	A1	4420	1/1	0.64	0.26	73,73,73,73	0
87	MG	Cd	102	1/1	0.64	0.26	75,75,75,75	0
87	MG	A2	2193	1/1	0.64	0.32	79,79,79,79	0
87	MG	A7	234	1/1	0.64	0.38	90,90,90,90	0
86	OHX	A6	2087	7/7	0.64	0.18	205,205,205,205	7
87	MG	A6	2104	1/1	0.64	0.38	68,68,68,68	0
87	MG	A5	3911	1/1	0.64	0.34	82,82,82,82	0
87	MG	BA	302	1/1	0.65	0.12	63,63,63,63	0
87	MG	A1	4109	1/1	0.65	0.20	80,80,80,80	0
86	OHX	A2	2082	7/7	0.65	0.17	225,225,225,225	7
87	MG	A5	4318	1/1	0.65	0.17	83,83,83,83	0
87	MG	A6	2249	1/1	0.65	0.26	71,71,71,71	0
87	MG	A5	4087	1/1	0.65	0.36	86,86,86,86	0
87	MG	A5	4100	1/1	0.65	0.33	86,86,86,86	0
87	MG	DB	404	1/1	0.65	0.49	68,68,68,68	0
87	MG	A1	4477	1/1	0.65	0.24	108,108,108,108	0
87	MG	A2	2236	1/1	0.65	0.19	100,100,100,100	0
87	MG	A1	4230	1/1	0.65	0.35	91,91,91,91	0
87	MG	A5	3995	1/1	0.66	0.37	53,53,53,53	0
87	MG	A1	3829	1/1	0.66	0.41	55,55,55,55	0
87	MG	A2	2231	1/1	0.66	0.24	75,75,75,75	0
87	MG	A6	2194	1/1	0.66	0.20	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	3968	1/1	0.66	0.30	68,68,68,68	0
87	MG	A2	2091	1/1	0.66	0.37	81,81,81,81	0
87	MG	A2	2226	1/1	0.66	0.32	87,87,87,87	0
87	MG	A2	2214	1/1	0.66	0.40	75,75,75,75	0
87	MG	A5	4186	1/1	0.66	0.34	84,84,84,84	0
87	MG	A1	4119	1/1	0.66	0.35	78,78,78,78	0
87	MG	A1	3909	1/1	0.66	0.40	67,67,67,67	0
87	MG	A8	229	1/1	0.66	0.41	95,95,95,95	0
87	MG	A6	2306	1/1	0.66	0.21	103,103,103,103	0
87	MG	A5	3921	1/1	0.66	0.53	82,82,82,82	0
87	MG	A5	4329	1/1	0.66	0.32	86,86,86,86	0
87	MG	A5	3988	1/1	0.66	0.38	51,51,51,51	0
87	MG	A6	2121	1/1	0.67	0.29	64,64,64,64	0
87	MG	A1	4059	1/1	0.67	0.25	84,84,84,84	0
87	MG	A6	2302	1/1	0.67	0.39	108,108,108,108	0
87	MG	A1	4261	1/1	0.67	0.31	79,79,79,79	0
87	MG	A1	4288	1/1	0.67	0.21	81,81,81,81	0
87	MG	A5	4524	1/1	0.67	0.16	85,85,85,85	0
86	OHX	A6	2095	7/7	0.67	0.25	213,213,213,213	7
87	MG	A5	4565	1/1	0.67	0.19	87,87,87,87	0
87	MG	A2	2212	1/1	0.67	0.34	100,100,100,100	0
87	MG	A5	4043	1/1	0.67	0.30	35,35,35,35	0
87	MG	A1	3994	1/1	0.67	0.33	64,64,64,64	0
87	MG	A5	4335	1/1	0.67	0.31	94,94,94,94	0
87	MG	A1	4473	1/1	0.67	0.17	111,111,111,111	0
87	MG	A1	4323	1/1	0.67	0.20	92,92,92,92	0
87	MG	A1	4117	1/1	0.67	0.37	80,80,80,80	0
86	OHX	A2	2077	7/7	0.68	0.21	206,206,206,206	7
87	MG	A2	2150	1/1	0.68	0.41	102,102,102,102	0
87	MG	A1	4108	1/1	0.68	0.25	60,60,60,60	0
87	MG	A5	4451	1/1	0.68	0.39	80,80,80,80	0
87	MG	A5	4479	1/1	0.68	0.22	64,64,64,64	0
86	OHX	A1	3772	7/7	0.68	0.26	171,171,171,171	7
87	MG	A4	229	1/1	0.68	0.10	54,54,54,54	0
87	MG	A1	4465	1/1	0.68	0.53	92,92,92,92	0
87	MG	A1	4114	1/1	0.68	0.17	71,71,71,71	0
87	MG	A5	4220	1/1	0.68	0.32	82,82,82,82	0
87	MG	A5	4251	1/1	0.68	0.20	85,85,85,85	0
87	MG	A2	2158	1/1	0.68	0.43	71,71,71,71	0
87	MG	A1	3888	1/1	0.68	0.48	67,67,67,67	0
87	MG	A1	4487	1/1	0.68	0.18	80,80,80,80	0
87	MG	A5	4323	1/1	0.68	0.25	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2117	1/1	0.68	0.40	80,80,80,80	0
87	MG	A1	4147	1/1	0.68	0.24	73,73,73,73	0
87	MG	A6	2323	1/1	0.68	0.23	77,77,77,77	0
87	MG	A6	2324	1/1	0.68	0.13	74,74,74,74	0
87	MG	A1	4480	1/1	0.69	0.18	91,91,91,91	0
87	MG	A5	3927	1/1	0.69	0.14	49,49,49,49	0
87	MG	A5	3929	1/1	0.69	0.41	80,80,80,80	0
87	MG	A1	4048	1/1	0.69	0.19	67,67,67,67	0
87	MG	A5	4270	1/1	0.69	0.21	57,57,57,57	0
87	MG	BV	201	1/1	0.69	0.35	95,95,95,95	0
87	MG	A6	2246	1/1	0.69	0.17	78,78,78,78	0
87	MG	A1	4219	1/1	0.69	0.35	85,85,85,85	0
87	MG	A1	4227	1/1	0.69	0.21	52,52,52,52	0
87	MG	CY	203	1/1	0.69	0.40	109,109,109,109	0
86	OHX	A5	3818	7/7	0.69	0.20	226,226,226,226	7
87	MG	A1	4078	1/1	0.69	0.33	80,80,80,80	0
87	MG	A2	2128	1/1	0.69	0.46	62,62,62,62	0
87	MG	A1	4175	1/1	0.69	0.14	69,69,69,69	0
87	MG	A2	2234	1/1	0.69	0.23	94,94,94,94	0
87	MG	A5	4420	1/1	0.69	0.16	93,93,93,93	0
87	MG	A6	2196	1/1	0.70	0.38	83,83,83,83	0
87	MG	A6	2200	1/1	0.70	0.29	82,82,82,82	0
87	MG	A1	4220	1/1	0.70	0.41	103,103,103,103	0
87	MG	A1	4221	1/1	0.70	0.17	92,92,92,92	0
87	MG	A3	229	1/1	0.70	0.36	99,99,99,99	0
86	OHX	A3	213	7/7	0.70	0.15	195,195,195,195	7
87	MG	A5	3933	1/1	0.70	0.35	74,74,74,74	0
87	MG	A1	3848	1/1	0.70	0.55	75,75,75,75	0
87	MG	A6	2259	1/1	0.70	0.29	119,119,119,119	0
87	MG	A1	4047	1/1	0.70	0.34	98,98,98,98	0
87	MG	A5	4412	1/1	0.70	0.49	104,104,104,104	0
87	MG	A2	2175	1/1	0.70	0.28	68,68,68,68	0
87	MG	A5	4056	1/1	0.70	0.42	78,78,78,78	0
86	OHX	CP	202	7/7	0.70	0.22	221,221,221,221	7
87	MG	A5	4099	1/1	0.70	0.40	93,93,93,93	0
87	MG	A2	2187	1/1	0.70	0.33	90,90,90,90	0
87	MG	A5	4499	1/1	0.70	0.43	76,76,76,76	0
87	MG	A5	4124	1/1	0.70	0.30	78,78,78,78	0
87	MG	A2	2126	1/1	0.70	0.43	54,54,54,54	0
87	MG	A1	4155	1/1	0.70	0.29	88,88,88,88	0
87	MG	A5	4138	1/1	0.70	0.38	77,77,77,77	0
86	OHX	A8	218	7/7	0.70	0.20	221,221,221,221	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A6	2168	1/1	0.70	0.49	77,77,77,77	0
87	MG	A5	4580	1/1	0.70	0.25	82,82,82,82	0
87	MG	A1	4299	1/1	0.70	0.18	84,84,84,84	0
87	MG	A8	228	1/1	0.70	0.18	86,86,86,86	0
87	MG	A1	4104	1/1	0.70	0.23	65,65,65,65	0
87	MG	A1	4489	1/1	0.70	0.23	94,94,94,94	0
87	MG	A2	2098	1/1	0.70	0.40	62,62,62,62	0
87	MG	DJ	202	1/1	0.70	0.28	81,81,81,81	0
87	MG	A2	2146	1/1	0.70	0.29	71,71,71,71	0
87	MG	A5	3871	1/1	0.70	0.28	56,56,56,56	0
87	MG	Bm	201	1/1	0.71	0.26	68,68,68,68	0
87	MG	A1	4359	1/1	0.71	0.28	70,70,70,70	0
87	MG	A5	4177	1/1	0.71	0.24	65,65,65,65	0
87	MG	A2	2144	1/1	0.71	0.27	57,57,57,57	0
87	MG	A1	4368	1/1	0.71	0.35	80,80,80,80	0
87	MG	A6	2288	1/1	0.71	0.24	106,106,106,106	0
87	MG	A2	2168	1/1	0.71	0.20	78,78,78,78	0
87	MG	A6	2141	1/1	0.71	0.42	78,78,78,78	0
87	MG	A1	4396	1/1	0.71	0.27	74,74,74,74	0
87	MG	A1	3851	1/1	0.71	0.22	53,53,53,53	0
87	MG	A5	4295	1/1	0.71	0.20	61,61,61,61	0
87	MG	A1	4425	1/1	0.71	0.30	106,106,106,106	0
87	MG	A5	4023	1/1	0.71	0.37	44,44,44,44	0
87	MG	AE	301	1/1	0.71	0.28	88,88,88,88	0
87	MG	A1	4311	1/1	0.71	0.26	92,92,92,92	0
87	MG	A4	226	1/1	0.71	0.41	70,70,70,70	0
86	OHX	A2	2051	7/7	0.71	0.26	209,209,209,209	7
87	MG	A2	2119	1/1	0.71	0.31	67,67,67,67	0
86	OHX	A6	2052	7/7	0.71	0.18	211,211,211,211	7
87	MG	A1	4281	1/1	0.71	0.32	74,74,74,74	0
87	MG	Bj	106	1/1	0.71	0.35	75,75,75,75	0
87	MG	A5	4390	1/1	0.71	0.37	70,70,70,70	0
87	MG	A1	4492	1/1	0.72	0.19	100,100,100,100	0
87	MG	A1	4038	1/1	0.72	0.39	89,89,89,89	0
87	MG	A5	3935	1/1	0.72	0.36	51,51,51,51	0
87	MG	A6	2298	1/1	0.72	0.16	77,77,77,77	0
86	OHX	A1	3793	7/7	0.72	0.18	232,232,232,232	7
87	MG	A5	4341	1/1	0.72	0.61	96,96,96,96	0
87	MG	A5	4359	1/1	0.72	0.17	86,86,86,86	0
86	OHX	A2	2063	7/7	0.72	0.16	183,183,183,183	7
87	MG	A6	2157	1/1	0.72	0.44	70,70,70,70	0
87	MG	A1	4504	1/1	0.72	0.33	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	BI	303	7/7	0.72	0.26	215,215,215,215	7
87	MG	A5	4078	1/1	0.72	0.28	49,49,49,49	0
87	MG	A1	4453	1/1	0.72	0.25	114,114,114,114	0
87	MG	A6	2326	1/1	0.72	0.20	117,117,117,117	0
86	OHX	A2	2079	7/7	0.72	0.22	157,157,157,157	7
87	MG	A5	4486	1/1	0.72	0.23	94,94,94,94	0
87	MG	A2	2161	1/1	0.72	0.29	58,58,58,58	0
87	MG	A1	3933	1/1	0.72	0.40	53,53,53,53	0
87	MG	A1	3958	1/1	0.72	0.32	45,45,45,45	0
87	MG	A5	4502	1/1	0.72	0.30	84,84,84,84	0
87	MG	A1	4479	1/1	0.72	0.23	74,74,74,74	0
87	MG	BP	211	1/1	0.72	0.44	123,123,123,123	0
87	MG	A6	2238	1/1	0.72	0.23	73,73,73,73	0
87	MG	A5	3880	1/1	0.72	0.32	45,45,45,45	0
87	MG	A5	3888	1/1	0.72	0.28	64,64,64,64	0
87	MG	A5	4203	1/1	0.72	0.22	82,82,82,82	0
87	MG	A1	4260	1/1	0.72	0.24	75,75,75,75	0
87	MG	A5	3905	1/1	0.72	0.27	75,75,75,75	0
87	MG	A2	2111	1/1	0.72	0.21	69,69,69,69	0
87	MG	Bj	109	1/1	0.72	0.39	122,122,122,122	0
87	MG	A5	3912	1/1	0.72	0.38	77,77,77,77	0
87	MG	A5	3920	1/1	0.72	0.31	83,83,83,83	0
87	MG	A5	4297	1/1	0.72	0.21	56,56,56,56	0
87	MG	Dp	102	1/1	0.72	0.12	63,63,63,63	0
87	MG	A1	3977	1/1	0.72	0.41	76,76,76,76	0
87	MG	A1	3883	1/1	0.72	0.27	37,37,37,37	0
87	MG	A2	2129	1/1	0.73	0.29	59,59,59,59	0
87	MG	A5	4206	1/1	0.73	0.37	110,110,110,110	0
87	MG	A5	3941	1/1	0.73	0.37	51,51,51,51	0
87	MG	A5	4214	1/1	0.73	0.21	66,66,66,66	0
87	MG	A2	2255	1/1	0.73	0.08	107,107,107,107	0
87	MG	A5	4228	1/1	0.73	0.26	82,82,82,82	0
87	MG	A1	4194	1/1	0.73	0.46	96,96,96,96	0
87	MG	A1	4506	1/1	0.73	0.31	77,77,77,77	0
87	MG	A1	4341	1/1	0.73	0.31	118,118,118,118	0
87	MG	A1	3926	1/1	0.73	0.29	55,55,55,55	0
87	MG	A6	2146	1/1	0.73	0.28	49,49,49,49	0
87	MG	A1	4357	1/1	0.73	0.18	89,89,89,89	0
87	MG	A5	4081	1/1	0.73	0.30	79,79,79,79	0
86	OHX	A1	3808	7/7	0.73	0.19	194,194,194,194	7
87	MG	A6	2171	1/1	0.73	0.33	77,77,77,77	0
87	MG	A6	2175	1/1	0.73	0.29	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	4362	1/1	0.73	0.33	85,85,85,85	0
87	MG	A2	2124	1/1	0.73	0.26	79,79,79,79	0
86	OHX	BI	304	7/7	0.73	0.26	193,193,193,193	7
87	MG	A2	2185	1/1	0.73	0.14	72,72,72,72	0
87	MG	A5	3925	1/1	0.73	0.24	57,57,57,57	0
86	OHX	A1	3796	7/7	0.73	0.29	174,174,174,174	7
87	MG	A1	4404	1/1	0.73	0.27	80,80,80,80	0
87	MG	A5	4382	1/1	0.73	0.37	99,99,99,99	0
87	MG	A2	2148	1/1	0.73	0.22	89,89,89,89	0
87	MG	A1	3919	1/1	0.74	0.67	138,138,138,138	0
87	MG	A1	4137	1/1	0.74	0.36	84,84,84,84	0
87	MG	A2	2165	1/1	0.74	0.34	78,78,78,78	0
86	OHX	A1	3728	7/7	0.74	0.17	203,203,203,203	7
86	OHX	A1	3753	7/7	0.74	0.20	243,243,243,243	7
87	MG	A1	4247	1/1	0.74	0.13	74,74,74,74	0
87	MG	A5	4144	1/1	0.74	0.27	75,75,75,75	0
87	MG	A6	2131	1/1	0.74	0.25	46,46,46,46	0
87	MG	A5	4428	1/1	0.74	0.20	75,75,75,75	0
87	MG	A5	4431	1/1	0.74	0.21	118,118,118,118	0
87	MG	A6	2272	1/1	0.74	0.25	115,115,115,115	0
87	MG	A1	4337	1/1	0.74	0.27	108,108,108,108	0
87	MG	A1	3859	1/1	0.74	0.47	78,78,78,78	0
87	MG	A1	4470	1/1	0.74	0.27	97,97,97,97	0
86	OHX	A5	3781	7/7	0.74	0.16	199,199,199,199	7
86	OHX	A2	2028	7/7	0.74	0.20	180,180,180,180	7
87	MG	A5	3928	1/1	0.74	0.44	90,90,90,90	0
87	MG	A6	2308	1/1	0.74	0.34	81,81,81,81	0
87	MG	AJ	201	1/1	0.74	0.27	82,82,82,82	0
87	MG	A2	2210	1/1	0.74	0.22	81,81,81,81	0
87	MG	A5	4526	1/1	0.74	0.16	83,83,83,83	0
87	MG	A5	3937	1/1	0.74	0.36	69,69,69,69	0
87	MG	A5	4529	1/1	0.74	0.16	91,91,91,91	0
87	MG	BO	202	1/1	0.74	0.20	77,77,77,77	0
87	MG	A5	4279	1/1	0.74	0.37	63,63,63,63	0
87	MG	A2	2183	1/1	0.74	0.28	49,49,49,49	0
87	MG	A5	4581	1/1	0.74	0.40	97,97,97,97	0
87	MG	BP	212	1/1	0.74	0.33	93,93,93,93	0
87	MG	A8	201	1/1	0.74	0.18	92,92,92,92	0
86	OHX	A2	2054	7/7	0.74	0.12	227,227,227,227	7
87	MG	CL	204	1/1	0.74	0.28	83,83,83,83	0
87	MG	A5	4028	1/1	0.74	0.34	47,47,47,47	0
87	MG	A1	4296	1/1	0.74	0.37	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	Bj	107	1/1	0.74	0.38	101,101,101,101	0
87	MG	DJ	203	1/1	0.74	0.33	80,80,80,80	0
87	MG	A6	2210	1/1	0.74	0.24	72,72,72,72	0
87	MG	A6	2222	1/1	0.74	0.27	86,86,86,86	0
87	MG	A5	3408	1/1	0.74	0.20	63,63,63,63	0
87	MG	A1	4497	1/1	0.75	0.14	79,79,79,79	0
87	MG	A6	2291	1/1	0.75	0.19	100,100,100,100	0
87	MG	A5	4395	1/1	0.75	0.36	58,58,58,58	0
87	MG	A5	4139	1/1	0.75	0.20	99,99,99,99	0
87	MG	A2	2240	1/1	0.75	0.20	97,97,97,97	0
87	MG	A5	4423	1/1	0.75	0.36	82,82,82,82	0
87	MG	A2	2103	1/1	0.75	0.41	58,58,58,58	0
87	MG	A2	2247	1/1	0.75	0.27	86,86,86,86	0
87	MG	A1	4105	1/1	0.75	0.49	84,84,84,84	0
87	MG	A6	2310	1/1	0.75	0.33	89,89,89,89	0
87	MG	A1	4478	1/1	0.75	0.34	100,100,100,100	0
87	MG	A6	2315	1/1	0.75	0.32	84,84,84,84	0
87	MG	A6	2102	1/1	0.75	0.27	63,63,63,63	0
87	MG	A5	4211	1/1	0.75	0.27	77,77,77,77	0
87	MG	A6	2103	1/1	0.75	0.37	64,64,64,64	0
87	MG	A5	4217	1/1	0.75	0.34	83,83,83,83	0
87	MG	A1	4226	1/1	0.75	0.29	63,63,63,63	0
87	MG	A6	2111	1/1	0.75	0.18	51,51,51,51	0
87	MG	A6	2334	1/1	0.75	0.25	72,72,72,72	0
87	MG	A5	3992	1/1	0.75	0.30	57,57,57,57	0
87	MG	A2	2191	1/1	0.75	0.41	91,91,91,91	0
87	MG	A6	2228	1/1	0.75	0.41	89,89,89,89	0
86	OHX	A5	3811	7/7	0.75	0.27	214,214,214,214	7
87	MG	A1	4482	1/1	0.75	0.54	129,129,129,129	0
87	MG	A6	2239	1/1	0.75	0.16	82,82,82,82	0
87	MG	A5	4055	1/1	0.75	0.28	81,81,81,81	0
87	MG	A6	2242	1/1	0.75	0.35	87,87,87,87	0
86	OHX	A2	2087	7/7	0.75	0.16	196,196,196,196	7
87	MG	A6	2133	1/1	0.75	0.26	65,65,65,65	0
87	MG	A4	238	1/1	0.75	0.21	68,68,68,68	0
87	MG	A5	4095	1/1	0.75	0.23	79,79,79,79	0
87	MG	A5	4098	1/1	0.75	0.27	55,55,55,55	0
87	MG	A1	4451	1/1	0.75	0.35	75,75,75,75	0
87	MG	A6	2151	1/1	0.75	0.39	64,64,64,64	0
87	MG	A1	3937	1/1	0.75	0.35	40,40,40,40	0
87	MG	A2	2239	1/1	0.75	0.23	92,92,92,92	0
87	MG	A5	4338	1/1	0.76	0.37	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2114	1/1	0.76	0.37	84,84,84,84	0
87	MG	A5	4086	1/1	0.76	0.18	59,59,59,59	0
87	MG	A6	2206	1/1	0.76	0.15	63,63,63,63	0
87	MG	CS	203	1/1	0.76	0.20	71,71,71,71	0
87	MG	A2	2115	1/1	0.76	0.31	78,78,78,78	0
87	MG	A2	2172	1/1	0.76	0.15	69,69,69,69	0
86	OHX	A1	3788	7/7	0.76	0.17	232,232,232,232	7
87	MG	A1	4197	1/1	0.76	0.22	74,74,74,74	0
87	MG	A5	4397	1/1	0.76	0.14	101,101,101,101	0
87	MG	A2	2181	1/1	0.76	0.19	79,79,79,79	0
86	OHX	A5	3765	7/7	0.76	0.15	201,201,201,201	7
86	OHX	A1	3736	7/7	0.76	0.33	174,174,174,174	7
87	MG	A1	3924	1/1	0.76	0.31	57,57,57,57	0
86	OHX	A5	3780	7/7	0.76	0.18	211,211,211,211	7
86	OHX	A2	2075	7/7	0.76	0.16	204,204,204,204	7
87	MG	A5	4175	1/1	0.76	0.50	114,114,114,114	0
86	OHX	A1	3803	7/7	0.76	0.21	196,196,196,196	7
87	MG	A1	4363	1/1	0.76	0.27	46,46,46,46	0
87	MG	A5	3915	1/1	0.76	0.39	78,78,78,78	0
87	MG	A2	2192	1/1	0.76	0.31	66,66,66,66	0
87	MG	A1	4118	1/1	0.76	0.15	74,74,74,74	0
87	MG	A6	2139	1/1	0.76	0.36	72,72,72,72	0
86	OHX	A2	2050	7/7	0.76	0.18	181,181,181,181	7
87	MG	A6	2293	1/1	0.76	0.22	78,78,78,78	0
87	MG	A1	4507	1/1	0.76	0.34	90,90,90,90	0
87	MG	A1	3972	1/1	0.76	0.34	45,45,45,45	0
87	MG	A6	2154	1/1	0.76	0.34	56,56,56,56	0
86	OHX	A1	3814	7/7	0.76	0.34	221,221,221,221	7
87	MG	A2	2200	1/1	0.76	0.23	88,88,88,88	0
87	MG	A5	4260	1/1	0.76	0.37	80,80,80,80	0
87	MG	A1	4262	1/1	0.76	0.20	70,70,70,70	0
87	MG	A7	220	1/1	0.76	0.20	61,61,61,61	0
87	MG	A6	2173	1/1	0.76	0.23	71,71,71,71	0
87	MG	A5	4291	1/1	0.76	0.20	78,78,78,78	0
87	MG	A1	4275	1/1	0.76	0.13	74,74,74,74	0
87	MG	A1	4021	1/1	0.76	0.35	54,54,54,54	0
87	MG	A1	4284	1/1	0.76	0.41	87,87,87,87	0
87	MG	A1	4035	1/1	0.76	0.19	59,59,59,59	0
87	MG	DC	404	1/1	0.76	0.17	70,70,70,70	0
87	MG	DC	406	1/1	0.76	0.43	111,111,111,111	0
87	MG	DD	305	1/1	0.76	0.23	74,74,74,74	0
87	MG	A6	2328	1/1	0.76	0.37	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	BG	301	1/1	0.76	0.31	91,91,91,91	0
87	MG	A2	2141	1/1	0.76	0.24	68,68,68,68	0
87	MG	A5	4068	1/1	0.76	0.17	72,72,72,72	0
87	MG	A1	4159	1/1	0.76	0.63	84,84,84,84	0
87	MG	A5	4368	1/1	0.77	0.29	75,75,75,75	0
87	MG	A1	4391	1/1	0.77	0.40	89,89,89,89	0
86	OHX	DM	201	7/7	0.77	0.15	208,208,208,208	7
87	MG	A1	4186	1/1	0.77	0.32	75,75,75,75	0
87	MG	A1	4103	1/1	0.77	0.14	74,74,74,74	0
87	MG	A6	2244	1/1	0.77	0.16	97,97,97,97	0
87	MG	A2	2179	1/1	0.77	0.37	81,81,81,81	0
86	OHX	A5	3727	7/7	0.77	0.18	167,167,167,167	7
87	MG	A5	4400	1/1	0.77	0.27	86,86,86,86	0
87	MG	A3	224	1/1	0.77	0.21	62,62,62,62	0
87	MG	A5	4414	1/1	0.77	0.29	101,101,101,101	0
87	MG	A6	2135	1/1	0.77	0.16	58,58,58,58	0
87	MG	A5	4155	1/1	0.77	0.27	95,95,95,95	0
87	MG	A1	4444	1/1	0.77	0.32	81,81,81,81	0
87	MG	A5	4430	1/1	0.77	0.37	95,95,95,95	0
86	OHX	A2	2258	7/7	0.77	0.13	162,162,162,162	7
87	MG	A3	232	1/1	0.77	0.21	95,95,95,95	0
87	MG	A2	2095	1/1	0.77	0.21	63,63,63,63	0
87	MG	A5	4189	1/1	0.77	0.34	96,96,96,96	0
87	MG	A5	4192	1/1	0.77	0.33	95,95,95,95	0
87	MG	A6	2290	1/1	0.77	0.24	82,82,82,82	0
87	MG	A2	2145	1/1	0.77	0.29	71,71,71,71	0
87	MG	A6	2156	1/1	0.77	0.40	62,62,62,62	0
87	MG	A1	3991	1/1	0.77	0.28	52,52,52,52	0
87	MG	A4	231	1/1	0.77	0.17	45,45,45,45	0
87	MG	A6	2169	1/1	0.77	0.25	77,77,77,77	0
86	OHX	A1	3779	7/7	0.77	0.27	164,164,164,164	7
87	MG	A1	4001	1/1	0.77	0.35	50,50,50,50	0
87	MG	A5	3966	1/1	0.77	0.39	56,56,56,56	0
87	MG	A5	4562	1/1	0.77	0.30	69,69,69,69	0
87	MG	A2	2221	1/1	0.77	0.32	83,83,83,83	0
87	MG	A6	2176	1/1	0.77	0.31	67,67,67,67	0
86	OHX	CN	201	7/7	0.77	0.21	174,174,174,174	7
87	MG	BO	209	1/1	0.77	0.31	95,95,95,95	0
87	MG	A5	4007	1/1	0.77	0.35	47,47,47,47	0
87	MG	A7	221	1/1	0.77	0.34	82,82,82,82	0
87	MG	A1	4239	1/1	0.77	0.23	60,60,60,60	0
87	MG	A6	2192	1/1	0.77	0.38	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2167	1/1	0.77	0.47	72,72,72,72	0
87	MG	A1	4252	1/1	0.77	0.39	121,121,121,121	0
86	OHX	A6	2081	7/7	0.77	0.20	201,201,201,201	7
87	MG	CF	302	1/1	0.77	0.27	73,73,73,73	0
87	MG	A5	4333	1/1	0.77	0.20	75,75,75,75	0
87	MG	A2	2170	1/1	0.77	0.33	88,88,88,88	0
87	MG	A1	3817	1/1	0.77	0.21	63,63,63,63	0
86	OHX	DG	301	7/7	0.77	0.31	226,226,226,226	7
87	MG	A1	3831	1/1	0.77	0.27	56,56,56,56	0
87	MG	DV	204	1/1	0.77	0.35	83,83,83,83	0
87	MG	A1	4273	1/1	0.77	0.43	85,85,85,85	0
87	MG	A5	4346	1/1	0.77	0.12	89,89,89,89	0
87	MG	A6	2233	1/1	0.77	0.21	63,63,63,63	0
87	MG	A1	4286	1/1	0.78	0.28	57,57,57,57	0
86	OHX	A6	2074	7/7	0.78	0.32	176,176,176,176	7
87	MG	A5	4347	1/1	0.78	0.19	78,78,78,78	0
87	MG	A5	4351	1/1	0.78	0.28	85,85,85,85	0
87	MG	A6	2203	1/1	0.78	0.14	63,63,63,63	0
87	MG	A5	4361	1/1	0.78	0.37	92,92,92,92	0
87	MG	CP	203	1/1	0.78	0.17	63,63,63,63	0
86	OHX	A1	3741	7/7	0.78	0.23	151,151,151,151	7
86	OHX	A5	3819	7/7	0.78	0.23	238,238,238,238	7
87	MG	A1	4298	1/1	0.78	0.25	95,95,95,95	0
87	MG	A6	2223	1/1	0.78	0.31	75,75,75,75	0
87	MG	A2	2211	1/1	0.78	0.21	94,94,94,94	0
86	OHX	A5	3770	7/7	0.78	0.24	198,198,198,198	7
87	MG	A1	4217	1/1	0.78	0.13	57,57,57,57	0
87	MG	A5	3860	1/1	0.78	0.30	66,66,66,66	0
86	OHX	A5	3792	7/7	0.78	0.43	217,217,217,217	7
87	MG	A1	3965	1/1	0.78	0.48	80,80,80,80	0
87	MG	A5	4418	1/1	0.78	0.36	91,91,91,91	0
87	MG	A5	3887	1/1	0.78	0.36	84,84,84,84	0
87	MG	A5	4153	1/1	0.78	0.29	83,83,83,83	0
87	MG	A2	2140	1/1	0.78	0.26	69,69,69,69	0
87	MG	A5	4172	1/1	0.78	0.25	67,67,67,67	0
87	MG	A1	4223	1/1	0.78	0.30	79,79,79,79	0
87	MG	A6	2245	1/1	0.78	0.20	82,82,82,82	0
87	MG	A5	4455	1/1	0.78	0.23	60,60,60,60	0
87	MG	A2	2169	1/1	0.78	0.20	105,105,105,105	0
87	MG	A1	4110	1/1	0.78	0.12	71,71,71,71	0
87	MG	A1	4228	1/1	0.78	0.24	82,82,82,82	0
87	MG	A5	4491	1/1	0.78	0.23	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2259	1/1	0.78	0.17	63,63,63,63	0
87	MG	A5	4196	1/1	0.78	0.12	66,66,66,66	0
87	MG	A1	4115	1/1	0.78	0.21	62,62,62,62	0
87	MG	A1	3978	1/1	0.78	0.39	73,73,73,73	0
87	MG	A6	2273	1/1	0.78	0.42	90,90,90,90	0
87	MG	A5	4520	1/1	0.78	0.35	81,81,81,81	0
87	MG	A1	3879	1/1	0.78	0.46	89,89,89,89	0
87	MG	A5	4525	1/1	0.78	0.30	66,66,66,66	0
87	MG	A1	3993	1/1	0.78	0.30	52,52,52,52	0
87	MG	A2	2121	1/1	0.78	0.49	61,61,61,61	0
87	MG	A1	4387	1/1	0.78	0.36	89,89,89,89	0
87	MG	AB	302	1/1	0.78	0.07	63,63,63,63	0
87	MG	A5	4231	1/1	0.78	0.34	105,105,105,105	0
87	MG	A5	4249	1/1	0.78	0.41	40,40,40,40	0
87	MG	A1	4141	1/1	0.78	0.19	53,53,53,53	0
87	MG	A6	2299	1/1	0.78	0.24	84,84,84,84	0
87	MG	A2	2157	1/1	0.78	0.30	82,82,82,82	0
87	MG	A5	4265	1/1	0.78	0.36	80,80,80,80	0
87	MG	A1	3907	1/1	0.78	0.23	50,50,50,50	0
87	MG	A5	3989	1/1	0.78	0.48	76,76,76,76	0
86	OHX	A2	2037	7/7	0.78	0.24	197,197,197,197	7
87	MG	A5	4292	1/1	0.78	0.30	113,113,113,113	0
87	MG	A1	4046	1/1	0.78	0.20	50,50,50,50	0
87	MG	A2	2197	1/1	0.78	0.25	80,80,80,80	0
87	MG	A4	242	1/1	0.78	0.19	81,81,81,81	0
87	MG	A4	245	1/1	0.78	0.17	90,90,90,90	0
87	MG	A4	248	1/1	0.78	0.16	114,114,114,114	0
87	MG	A5	4042	1/1	0.78	0.41	75,75,75,75	0
87	MG	A1	4277	1/1	0.78	0.33	89,89,89,89	0
87	MG	DO	207	1/1	0.78	0.40	109,109,109,109	0
87	MG	A5	4054	1/1	0.78	0.45	71,71,71,71	0
87	MG	A1	4171	1/1	0.78	0.28	79,79,79,79	0
87	MG	A2	2176	1/1	0.78	0.35	64,64,64,64	0
87	MG	A1	4458	1/1	0.78	0.27	92,92,92,92	0
87	MG	A6	2163	1/1	0.79	0.36	58,58,58,58	0
87	MG	A1	4352	1/1	0.79	0.28	93,93,93,93	0
87	MG	A5	3923	1/1	0.79	0.18	68,68,68,68	0
87	MG	A3	221	1/1	0.79	0.15	69,69,69,69	0
87	MG	A6	2331	1/1	0.79	0.26	79,79,79,79	0
86	OHX	A2	2084	7/7	0.79	0.13	183,183,183,183	7
87	MG	A6	2335	1/1	0.79	0.22	84,84,84,84	0
87	MG	Bl	4500	1/1	0.79	0.23	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	4224	1/1	0.79	0.25	72,72,72,72	0
87	MG	A1	3845	1/1	0.79	0.35	70,70,70,70	0
86	OHX	A6	2031	6/7	0.79	0.14	195,195,195,195	6
87	MG	A5	3958	1/1	0.79	0.36	64,64,64,64	0
87	MG	A5	4165	1/1	0.79	0.15	73,73,73,73	0
87	MG	A5	4167	1/1	0.79	0.26	71,71,71,71	0
86	OHX	A5	3763	7/7	0.79	0.29	197,197,197,197	7
87	MG	A5	3979	1/1	0.79	0.41	61,61,61,61	0
87	MG	A1	4229	1/1	0.79	0.28	89,89,89,89	0
87	MG	A5	4530	1/1	0.79	0.46	113,113,113,113	0
87	MG	A5	4540	1/1	0.79	0.25	94,94,94,94	0
87	MG	A6	2277	1/1	0.79	0.22	79,79,79,79	0
87	MG	A1	4162	1/1	0.79	0.33	79,79,79,79	0
87	MG	A1	4011	1/1	0.79	0.22	50,50,50,50	0
87	MG	A6	2125	1/1	0.79	0.15	47,47,47,47	0
87	MG	A5	4194	1/1	0.79	0.42	88,88,88,88	0
87	MG	A5	3838	1/1	0.79	0.31	39,39,39,39	0
86	OHX	A6	2089	7/7	0.79	0.16	212,212,212,212	7
87	MG	A5	4375	1/1	0.79	0.25	65,65,65,65	0
87	MG	A5	4024	1/1	0.79	0.36	42,42,42,42	0
87	MG	A6	2129	1/1	0.79	0.35	66,66,66,66	0
87	MG	A2	2134	1/1	0.79	0.26	74,74,74,74	0
87	MG	A2	2215	1/1	0.79	0.30	86,86,86,86	0
87	MG	Aa	201	1/1	0.79	0.34	82,82,82,82	0
86	OHX	A1	3745	7/7	0.79	0.30	178,178,178,178	7
87	MG	A5	3893	1/1	0.79	0.25	73,73,73,73	0
87	MG	A5	4230	1/1	0.79	0.28	78,78,78,78	0
87	MG	A2	2122	1/1	0.79	0.23	74,74,74,74	0
87	MG	A1	3826	1/1	0.79	0.23	51,51,51,51	0
87	MG	A1	4449	1/1	0.79	0.15	98,98,98,98	0
87	MG	A5	4425	1/1	0.79	0.13	65,65,65,65	0
87	MG	DY	201	1/1	0.79	0.15	59,59,59,59	0
87	MG	A1	3976	1/1	0.79	0.38	66,66,66,66	0
87	MG	A2	2155	1/1	0.79	0.30	86,86,86,86	0
86	OHX	A1	3774	7/7	0.79	0.15	206,206,206,206	7
87	MG	A1	3918	1/1	0.80	0.27	83,83,83,83	0
87	MG	A5	4331	1/1	0.80	0.30	104,104,104,104	0
87	MG	A1	4249	1/1	0.80	0.21	73,73,73,73	0
87	MG	AS	201	1/1	0.80	0.14	105,105,105,105	0
87	MG	A6	2122	1/1	0.80	0.30	55,55,55,55	0
87	MG	A5	4021	1/1	0.80	0.23	35,35,35,35	0
87	MG	A1	4461	1/1	0.80	0.13	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2232	1/1	0.80	0.26	125,125,125,125	0
87	MG	A2	2206	1/1	0.80	0.20	78,78,78,78	0
87	MG	A5	4040	1/1	0.80	0.16	46,46,46,46	0
87	MG	A5	4348	1/1	0.80	0.16	58,58,58,58	0
87	MG	A1	4259	1/1	0.80	0.19	102,102,102,102	0
87	MG	A2	2207	1/1	0.80	0.19	76,76,76,76	0
87	MG	A1	4111	1/1	0.80	0.26	65,65,65,65	0
87	MG	A6	2136	1/1	0.80	0.27	48,48,48,48	0
87	MG	A2	2237	1/1	0.80	0.30	90,90,90,90	0
87	MG	A1	3932	1/1	0.80	0.26	30,30,30,30	0
86	OHX	A2	2080	7/7	0.80	0.13	191,191,191,191	7
87	MG	A1	3936	1/1	0.80	0.34	34,34,34,34	0
87	MG	A1	4483	1/1	0.80	0.12	72,72,72,72	0
87	MG	A5	4383	1/1	0.80	0.30	69,69,69,69	0
86	OHX	A1	3797	7/7	0.80	0.14	171,171,171,171	7
87	MG	A5	4392	1/1	0.80	0.20	64,64,64,64	0
87	MG	A2	2162	1/1	0.80	0.53	84,84,84,84	0
87	MG	A1	4136	1/1	0.80	0.25	53,53,53,53	0
87	MG	A6	2338	1/1	0.80	0.12	80,80,80,80	0
86	OHX	A1	3750	7/7	0.80	0.33	118,118,118,118	7
86	OHX	A2	2062	7/7	0.80	0.25	196,196,196,196	7
87	MG	A5	4126	1/1	0.80	0.17	100,100,100,100	0
86	OHX	A6	2068	7/7	0.80	0.29	217,217,217,217	7
87	MG	A1	3854	1/1	0.80	0.23	57,57,57,57	0
87	MG	A1	3857	1/1	0.80	0.24	53,53,53,53	0
87	MG	A1	4154	1/1	0.80	0.22	91,91,91,91	0
87	MG	A2	2254	1/1	0.80	0.17	61,61,61,61	0
87	MG	A1	3980	1/1	0.80	0.24	38,38,38,38	0
87	MG	A1	4317	1/1	0.80	0.22	92,92,92,92	0
87	MG	A1	4161	1/1	0.80	0.17	73,73,73,73	0
87	MG	A5	4478	1/1	0.80	0.28	81,81,81,81	0
87	MG	A1	4326	1/1	0.80	0.40	80,80,80,80	0
87	MG	A5	3852	1/1	0.80	0.22	49,49,49,49	0
87	MG	A1	3984	1/1	0.80	0.33	51,51,51,51	0
87	MG	A2	2189	1/1	0.80	0.26	55,55,55,55	0
87	MG	A1	3866	1/1	0.80	0.16	87,87,87,87	0
86	OHX	A6	2069	7/7	0.80	0.17	206,206,206,206	7
87	MG	A1	3995	1/1	0.80	0.28	63,63,63,63	0
87	MG	A5	4506	1/1	0.80	0.31	80,80,80,80	0
87	MG	A5	4510	1/1	0.80	0.32	86,86,86,86	0
87	MG	A5	4187	1/1	0.80	0.22	78,78,78,78	0
87	MG	A5	4517	1/1	0.80	0.33	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4188	1/1	0.80	0.29	78,78,78,78	0
87	MG	A5	3889	1/1	0.80	0.47	86,86,86,86	0
87	MG	A5	4522	1/1	0.80	0.19	73,73,73,73	0
87	MG	A6	2209	1/1	0.80	0.28	79,79,79,79	0
87	MG	A4	230	1/1	0.80	0.28	71,71,71,71	0
87	MG	A1	3875	1/1	0.80	0.26	60,60,60,60	0
87	MG	A4	234	1/1	0.80	0.25	74,74,74,74	0
87	MG	A1	3878	1/1	0.80	0.32	45,45,45,45	0
87	MG	A1	4019	1/1	0.80	0.38	42,42,42,42	0
87	MG	A5	4208	1/1	0.80	0.22	75,75,75,75	0
87	MG	A5	4561	1/1	0.80	0.25	111,111,111,111	0
86	OHX	A5	3753	7/7	0.80	0.13	207,207,207,207	7
86	OHX	A1	3792	7/7	0.80	0.32	213,213,213,213	7
86	OHX	A6	2080	7/7	0.80	0.22	167,167,167,167	7
87	MG	A5	4574	1/1	0.80	0.33	74,74,74,74	0
87	MG	A5	4575	1/1	0.80	0.16	68,68,68,68	0
87	MG	A1	4039	1/1	0.80	0.37	65,65,65,65	0
87	MG	A5	4227	1/1	0.80	0.24	46,46,46,46	0
87	MG	A1	4374	1/1	0.80	0.35	60,60,60,60	0
87	MG	A5	3926	1/1	0.80	0.32	53,53,53,53	0
87	MG	A1	4041	1/1	0.80	0.34	70,70,70,70	0
87	MG	A1	3889	1/1	0.80	0.31	74,74,74,74	0
87	MG	A1	3894	1/1	0.80	0.29	43,43,43,43	0
87	MG	A5	4253	1/1	0.80	0.19	75,75,75,75	0
87	MG	A8	235	1/1	0.80	0.23	79,79,79,79	0
87	MG	A1	3896	1/1	0.80	0.21	40,40,40,40	0
87	MG	A1	3898	1/1	0.80	0.20	64,64,64,64	0
87	MG	A1	4068	1/1	0.80	0.33	78,78,78,78	0
87	MG	AI	302	1/1	0.80	0.21	66,66,66,66	0
87	MG	A5	3951	1/1	0.80	0.28	40,40,40,40	0
87	MG	A5	3955	1/1	0.80	0.40	62,62,62,62	0
87	MG	A1	4437	1/1	0.80	0.20	60,60,60,60	0
87	MG	A1	4442	1/1	0.80	0.35	91,91,91,91	0
87	MG	DQ	202	1/1	0.80	0.23	88,88,88,88	0
87	MG	A5	3977	1/1	0.80	0.41	69,69,69,69	0
86	OHX	A2	2083	7/7	0.80	0.30	185,185,185,185	7
87	MG	De	202	1/1	0.80	0.28	52,52,52,52	0
86	OHX	A6	2082	7/7	0.80	0.38	180,180,180,180	7
87	MG	A5	4322	1/1	0.80	0.29	61,61,61,61	0
87	MG	A1	3914	1/1	0.80	0.30	73,73,73,73	0
87	MG	A1	4037	1/1	0.81	0.31	83,83,83,83	0
87	MG	A5	4109	1/1	0.81	0.35	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2188	1/1	0.81	0.27	82,82,82,82	0
87	MG	A1	3824	1/1	0.81	0.18	65,65,65,65	0
86	OHX	A6	2090	7/7	0.81	0.26	212,212,212,212	7
87	MG	A5	4135	1/1	0.81	0.18	73,73,73,73	0
86	OHX	A6	2058	7/7	0.81	0.14	196,196,196,196	7
87	MG	A6	2220	1/1	0.81	0.15	91,91,91,91	0
87	MG	BV	202	1/1	0.81	0.17	73,73,73,73	0
87	MG	A2	2160	1/1	0.81	0.12	66,66,66,66	0
87	MG	A1	4293	1/1	0.81	0.30	110,110,110,110	0
87	MG	A5	4151	1/1	0.81	0.14	64,64,64,64	0
87	MG	A2	2132	1/1	0.81	0.24	77,77,77,77	0
87	MG	A2	2133	1/1	0.81	0.23	72,72,72,72	0
87	MG	A1	3928	1/1	0.81	0.44	88,88,88,88	0
87	MG	A5	3902	1/1	0.81	0.18	31,31,31,31	0
87	MG	A5	4169	1/1	0.81	0.46	90,90,90,90	0
87	MG	A1	4196	1/1	0.81	0.23	71,71,71,71	0
87	MG	A1	4303	1/1	0.81	0.28	105,105,105,105	0
87	MG	A5	4427	1/1	0.81	0.30	102,102,102,102	0
86	OHX	A1	3809	7/7	0.81	0.14	192,192,192,192	7
87	MG	A5	4179	1/1	0.81	0.29	71,71,71,71	0
87	MG	A6	2105	1/1	0.81	0.20	78,78,78,78	0
87	MG	A2	2199	1/1	0.81	0.25	72,72,72,72	0
86	OHX	A5	3798	7/7	0.81	0.28	202,202,202,202	7
87	MG	A5	4476	1/1	0.81	0.19	86,86,86,86	0
87	MG	A1	4102	1/1	0.81	0.17	61,61,61,61	0
87	MG	A2	2205	1/1	0.81	0.28	83,83,83,83	0
87	MG	A6	2255	1/1	0.81	0.32	81,81,81,81	0
87	MG	A1	3952	1/1	0.81	0.41	89,89,89,89	0
87	MG	A6	2261	1/1	0.81	0.37	76,76,76,76	0
87	MG	A6	2127	1/1	0.81	0.32	41,41,41,41	0
87	MG	A1	4490	1/1	0.81	0.31	77,77,77,77	0
86	OHX	A5	3810	7/7	0.81	0.33	199,199,199,199	7
87	MG	A5	4503	1/1	0.81	0.20	72,72,72,72	0
87	MG	A6	2130	1/1	0.81	0.29	74,74,74,74	0
87	MG	A2	2105	1/1	0.81	0.32	55,55,55,55	0
87	MG	A5	4212	1/1	0.81	0.21	73,73,73,73	0
86	OHX	A2	2070	7/7	0.81	0.19	202,202,202,202	7
86	OHX	A5	3816	7/7	0.81	0.15	195,195,195,195	7
87	MG	A1	3873	1/1	0.81	0.34	62,62,62,62	0
87	MG	A6	2137	1/1	0.81	0.40	71,71,71,71	0
87	MG	A2	2256	1/1	0.81	0.24	80,80,80,80	0
87	MG	A5	3971	1/1	0.81	0.30	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3759	7/7	0.81	0.28	149,149,149,149	7
87	MG	A5	4235	1/1	0.81	0.34	75,75,75,75	0
87	MG	A5	4241	1/1	0.81	0.38	106,106,106,106	0
87	MG	A5	4243	1/1	0.81	0.24	45,45,45,45	0
87	MG	A5	4246	1/1	0.81	0.30	38,38,38,38	0
87	MG	A5	4543	1/1	0.81	0.14	78,78,78,78	0
86	OHX	A2	2076	7/7	0.81	0.17	185,185,185,185	7
87	MG	A5	3985	1/1	0.81	0.39	51,51,51,51	0
86	OHX	A1	3664	7/7	0.81	0.14	207,207,207,207	7
87	MG	A6	2309	1/1	0.81	0.36	105,105,105,105	0
87	MG	A1	4242	1/1	0.81	0.18	84,84,84,84	0
87	MG	A6	2155	1/1	0.81	0.28	41,41,41,41	0
87	MG	A1	4369	1/1	0.81	0.18	85,85,85,85	0
87	MG	A1	3987	1/1	0.81	0.10	57,57,57,57	0
87	MG	A1	4126	1/1	0.81	0.28	84,84,84,84	0
86	OHX	A1	3725	7/7	0.81	0.18	191,191,191,191	7
87	MG	A7	232	1/1	0.81	0.24	91,91,91,91	0
86	OHX	A1	3726	7/7	0.81	0.21	178,178,178,178	7
87	MG	A1	4395	1/1	0.81	0.26	97,97,97,97	0
87	MG	A5	4311	1/1	0.81	0.21	78,78,78,78	0
87	MG	A6	2172	1/1	0.81	0.33	66,66,66,66	0
87	MG	A8	231	1/1	0.81	0.15	71,71,71,71	0
87	MG	A8	234	1/1	0.81	0.14	64,64,64,64	0
87	MG	A2	2152	1/1	0.81	0.20	88,88,88,88	0
87	MG	A2	2217	1/1	0.81	0.24	117,117,117,117	0
87	MG	A5	4053	1/1	0.81	0.26	65,65,65,65	0
87	MG	A1	3897	1/1	0.81	0.23	75,75,75,75	0
87	MG	A6	2181	1/1	0.81	0.27	77,77,77,77	0
86	OHX	A6	2088	7/7	0.81	0.18	160,160,160,160	7
87	MG	A5	4062	1/1	0.81	0.20	37,37,37,37	0
87	MG	A5	4067	1/1	0.81	0.21	61,61,61,61	0
87	MG	CG	304	1/1	0.81	0.32	72,72,72,72	0
87	MG	DP	202	1/1	0.81	0.25	56,56,56,56	0
87	MG	A6	2187	1/1	0.81	0.25	64,64,64,64	0
87	MG	A1	4432	1/1	0.81	0.28	79,79,79,79	0
87	MG	AS	202	1/1	0.81	0.12	63,63,63,63	0
87	MG	A1	4268	1/1	0.81	0.27	65,65,65,65	0
87	MG	Do	202	1/1	0.81	0.18	50,50,50,50	0
86	OHX	A6	2056	7/7	0.81	0.14	178,178,178,178	7
87	MG	A2	2092	1/1	0.81	0.37	69,69,69,69	0
88	ZN	Ab	101	1/1	0.81	0.09	327,327,327,327	0
87	MG	A1	4447	1/1	0.81	0.30	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4164	1/1	0.82	0.07	87,87,87,87	0
86	OHX	A6	2075	7/7	0.82	0.16	194,194,194,194	7
86	OHX	A5	3733	7/7	0.82	0.24	162,162,162,162	7
87	MG	A1	4101	1/1	0.82	0.37	86,86,86,86	0
86	OHX	A5	3735	7/7	0.82	0.23	149,149,149,149	7
87	MG	A1	4383	1/1	0.82	0.11	62,62,62,62	0
86	OHX	A5	3748	7/7	0.82	0.29	183,183,183,183	7
87	MG	A1	4276	1/1	0.82	0.28	95,95,95,95	0
87	MG	A5	4181	1/1	0.82	0.35	80,80,80,80	0
87	MG	A1	3836	1/1	0.82	0.29	48,48,48,48	0
86	OHX	A2	2060	7/7	0.82	0.29	168,168,168,168	7
87	MG	A1	4401	1/1	0.82	0.33	69,69,69,69	0
86	OHX	AC	301	7/7	0.82	0.29	213,213,213,213	7
87	MG	A4	217	1/1	0.82	0.29	69,69,69,69	0
87	MG	A6	2144	1/1	0.82	0.29	51,51,51,51	0
87	MG	A5	4444	1/1	0.82	0.18	66,66,66,66	0
86	OHX	A1	3604	7/7	0.82	0.12	254,254,254,254	7
87	MG	A6	2147	1/1	0.82	0.26	44,44,44,44	0
87	MG	A5	4464	1/1	0.82	0.20	85,85,85,85	0
87	MG	A5	4473	1/1	0.82	0.38	94,94,94,94	0
87	MG	A5	4474	1/1	0.82	0.22	44,44,44,44	0
87	MG	A5	4198	1/1	0.82	0.23	58,58,58,58	0
86	OHX	DJ	201	7/7	0.82	0.13	185,185,185,185	7
86	OHX	A6	2044	7/7	0.82	0.17	178,178,178,178	7
86	OHX	DR	201	7/7	0.82	0.16	171,171,171,171	7
86	OHX	A1	3744	7/7	0.82	0.23	205,205,205,205	7
86	OHX	A2	2069	7/7	0.82	0.22	191,191,191,191	7
86	OHX	A2	2085	7/7	0.82	0.36	200,200,200,200	7
87	MG	A5	4497	1/1	0.82	0.19	76,76,76,76	0
87	MG	A6	2165	1/1	0.82	0.37	51,51,51,51	0
86	OHX	A2	2047	7/7	0.82	0.23	188,188,188,188	7
87	MG	AI	303	1/1	0.82	0.18	73,73,73,73	0
86	OHX	CB	301	7/7	0.82	0.20	162,162,162,162	7
87	MG	A5	3998	1/1	0.82	0.38	41,41,41,41	0
87	MG	A5	4229	1/1	0.82	0.25	81,81,81,81	0
87	MG	A1	3876	1/1	0.82	0.34	68,68,68,68	0
87	MG	A6	2327	1/1	0.82	0.39	108,108,108,108	0
87	MG	A5	4232	1/1	0.82	0.23	53,53,53,53	0
87	MG	A5	4014	1/1	0.82	0.29	54,54,54,54	0
87	MG	BB	403	1/1	0.82	0.17	53,53,53,53	0
87	MG	BC	406	1/1	0.82	0.16	61,61,61,61	0
87	MG	A6	2332	1/1	0.82	0.19	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	BD	302	1/1	0.82	0.28	79,79,79,79	0
87	MG	A5	4039	1/1	0.82	0.32	63,63,63,63	0
87	MG	A1	4043	1/1	0.82	0.29	62,62,62,62	0
87	MG	A1	4233	1/1	0.82	0.26	79,79,79,79	0
87	MG	A1	4324	1/1	0.82	0.28	79,79,79,79	0
87	MG	A5	4549	1/1	0.82	0.19	70,70,70,70	0
87	MG	A5	4556	1/1	0.82	0.22	73,73,73,73	0
87	MG	A5	4050	1/1	0.82	0.13	39,39,39,39	0
87	MG	CE	301	1/1	0.82	0.17	57,57,57,57	0
87	MG	BP	207	1/1	0.82	0.33	65,65,65,65	0
87	MG	A1	4463	1/1	0.82	0.24	76,76,76,76	0
86	OHX	A5	3796	7/7	0.82	0.21	176,176,176,176	7
87	MG	BQ	202	1/1	0.82	0.35	80,80,80,80	0
87	MG	A5	4577	1/1	0.82	0.12	76,76,76,76	0
86	OHX	BB	402	7/7	0.82	0.17	173,173,173,173	7
87	MG	A1	4329	1/1	0.82	0.33	85,85,85,85	0
87	MG	A5	4312	1/1	0.82	0.19	87,87,87,87	0
87	MG	BV	205	1/1	0.82	0.19	68,68,68,68	0
87	MG	Ba	207	1/1	0.82	0.28	89,89,89,89	0
87	MG	Bg	201	1/1	0.82	0.19	63,63,63,63	0
87	MG	A1	4334	1/1	0.82	0.22	104,104,104,104	0
87	MG	A5	4327	1/1	0.82	0.29	94,94,94,94	0
87	MG	A5	4090	1/1	0.82	0.28	45,45,45,45	0
87	MG	A1	4336	1/1	0.82	0.24	80,80,80,80	0
87	MG	A8	232	1/1	0.82	0.16	43,43,43,43	0
87	MG	A8	233	1/1	0.82	0.32	78,78,78,78	0
87	MG	A5	4332	1/1	0.82	0.13	73,73,73,73	0
87	MG	A5	4096	1/1	0.82	0.31	72,72,72,72	0
87	MG	A6	2218	1/1	0.82	0.12	53,53,53,53	0
87	MG	DB	411	1/1	0.82	0.42	61,61,61,61	0
86	OHX	BI	302	7/7	0.82	0.24	177,177,177,177	7
87	MG	A1	4052	1/1	0.82	0.26	71,71,71,71	0
87	MG	A5	3867	1/1	0.82	0.22	27,27,27,27	0
87	MG	A5	4115	1/1	0.82	0.27	69,69,69,69	0
87	MG	A1	4343	1/1	0.82	0.21	78,78,78,78	0
87	MG	Bo	204	1/1	0.82	0.10	76,76,76,76	0
87	MG	A2	2143	1/1	0.82	0.26	82,82,82,82	0
87	MG	A1	4347	1/1	0.82	0.44	86,86,86,86	0
87	MG	A1	4060	1/1	0.82	0.21	67,67,67,67	0
87	MG	DR	202	1/1	0.82	0.47	67,67,67,67	0
87	MG	A2	2106	1/1	0.82	0.33	57,57,57,57	0
87	MG	A6	2240	1/1	0.82	0.45	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2238	1/1	0.82	0.28	92,92,92,92	0
87	MG	A1	4257	1/1	0.82	0.20	88,88,88,88	0
87	MG	A5	4148	1/1	0.82	0.50	75,75,75,75	0
87	MG	A6	2120	1/1	0.82	0.37	51,51,51,51	0
87	MG	A1	4086	1/1	0.82	0.28	58,58,58,58	0
87	MG	A1	4168	1/1	0.82	0.14	44,44,44,44	0
87	MG	A1	4178	1/1	0.83	0.11	70,70,70,70	0
87	MG	A6	2216	1/1	0.83	0.10	64,64,64,64	0
87	MG	A5	3883	1/1	0.83	0.21	36,36,36,36	0
87	MG	A5	4386	1/1	0.83	0.20	65,65,65,65	0
87	MG	A5	4142	1/1	0.83	0.25	91,91,91,91	0
86	OHX	A6	2077	7/7	0.83	0.17	197,197,197,197	7
86	OHX	A6	2078	7/7	0.83	0.24	185,185,185,185	7
87	MG	Ba	208	1/1	0.83	0.24	68,68,68,68	0
87	MG	A5	3890	1/1	0.83	0.32	82,82,82,82	0
87	MG	A5	4406	1/1	0.83	0.30	75,75,75,75	0
87	MG	Be	201	1/1	0.83	0.21	88,88,88,88	0
87	MG	A1	4071	1/1	0.83	0.20	71,71,71,71	0
87	MG	A5	3898	1/1	0.83	0.16	44,44,44,44	0
87	MG	A1	4464	1/1	0.83	0.15	63,63,63,63	0
87	MG	A1	4192	1/1	0.83	0.46	86,86,86,86	0
87	MG	A1	4467	1/1	0.83	0.15	68,68,68,68	0
87	MG	A1	4075	1/1	0.83	0.17	62,62,62,62	0
86	OHX	A1	3702	7/7	0.83	0.14	141,141,141,141	7
87	MG	A1	4084	1/1	0.83	0.14	67,67,67,67	0
87	MG	A1	4198	1/1	0.83	0.12	79,79,79,79	0
87	MG	A5	4434	1/1	0.83	0.23	72,72,72,72	0
87	MG	A5	4440	1/1	0.83	0.38	76,76,76,76	0
87	MG	A1	4205	1/1	0.83	0.13	63,63,63,63	0
87	MG	A5	4450	1/1	0.83	0.38	73,73,73,73	0
87	MG	A1	4207	1/1	0.83	0.15	85,85,85,85	0
87	MG	A6	2247	1/1	0.83	0.23	88,88,88,88	0
87	MG	A1	4213	1/1	0.83	0.44	79,79,79,79	0
87	MG	A6	2110	1/1	0.83	0.32	65,65,65,65	0
87	MG	A1	4215	1/1	0.83	0.25	65,65,65,65	0
87	MG	A5	4191	1/1	0.83	0.29	99,99,99,99	0
86	OHX	A5	3698	7/7	0.83	0.23	173,173,173,173	7
87	MG	A6	2118	1/1	0.83	0.22	57,57,57,57	0
87	MG	A5	4480	1/1	0.83	0.23	76,76,76,76	0
87	MG	A5	4482	1/1	0.83	0.25	79,79,79,79	0
87	MG	A5	4485	1/1	0.83	0.24	77,77,77,77	0
87	MG	A1	4486	1/1	0.83	0.16	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3787	7/7	0.83	0.15	195,195,195,195	7
86	OHX	A5	3789	7/7	0.83	0.27	165,165,165,165	7
86	OHX	A1	3732	7/7	0.83	0.19	166,166,166,166	7
87	MG	A5	4495	1/1	0.83	0.31	88,88,88,88	0
87	MG	A5	3954	1/1	0.83	0.37	46,46,46,46	0
87	MG	A6	2282	1/1	0.83	0.13	83,83,83,83	0
86	OHX	A5	3794	7/7	0.83	0.16	179,179,179,179	7
87	MG	A5	3960	1/1	0.83	0.32	49,49,49,49	0
87	MG	A1	4339	1/1	0.83	0.31	97,97,97,97	0
87	MG	A2	2249	1/1	0.83	0.30	85,85,85,85	0
87	MG	A1	3901	1/1	0.83	0.39	74,74,74,74	0
87	MG	A5	4226	1/1	0.83	0.39	76,76,76,76	0
87	MG	A1	3989	1/1	0.83	0.27	42,42,42,42	0
87	MG	A5	3982	1/1	0.83	0.27	52,52,52,52	0
87	MG	A2	2184	1/1	0.83	0.24	109,109,109,109	0
86	OHX	A2	2081	7/7	0.83	0.14	199,199,199,199	7
87	MG	A1	3842	1/1	0.83	0.56	77,77,77,77	0
86	OHX	A2	2040	7/7	0.83	0.15	171,171,171,171	7
87	MG	A6	2138	1/1	0.83	0.26	94,94,94,94	0
86	OHX	A1	3799	7/7	0.83	0.18	165,165,165,165	7
86	OHX	A1	3784	7/7	0.83	0.22	169,169,169,169	7
87	MG	A5	4536	1/1	0.83	0.34	73,73,73,73	0
87	MG	A1	4014	1/1	0.83	0.36	56,56,56,56	0
87	MG	A5	4247	1/1	0.83	0.14	64,64,64,64	0
87	MG	A1	4015	1/1	0.83	0.40	63,63,63,63	0
87	MG	A5	4552	1/1	0.83	0.28	84,84,84,84	0
87	MG	A1	4016	1/1	0.83	0.30	40,40,40,40	0
87	MG	A6	2320	1/1	0.83	0.29	117,117,117,117	0
87	MG	A2	2257	1/1	0.83	0.21	75,75,75,75	0
87	MG	A1	4250	1/1	0.83	0.11	56,56,56,56	0
87	MG	A5	4263	1/1	0.83	0.16	72,72,72,72	0
87	MG	A1	4376	1/1	0.83	0.18	71,71,71,71	0
87	MG	A1	4133	1/1	0.83	0.28	91,91,91,91	0
87	MG	A2	2218	1/1	0.83	0.19	63,63,63,63	0
87	MG	A5	4289	1/1	0.83	0.35	112,112,112,112	0
87	MG	A6	2330	1/1	0.83	0.32	80,80,80,80	0
87	MG	A5	4048	1/1	0.83	0.12	34,34,34,34	0
87	MG	A1	4030	1/1	0.83	0.17	37,37,37,37	0
87	MG	A7	228	1/1	0.83	0.21	85,85,85,85	0
86	OHX	A5	3813	7/7	0.83	0.15	191,191,191,191	7
87	MG	A7	233	1/1	0.83	0.12	60,60,60,60	0
86	OHX	A5	3815	7/7	0.83	0.25	221,221,221,221	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3760	7/7	0.83	0.12	202,202,202,202	7
87	MG	A1	3930	1/1	0.83	0.26	38,38,38,38	0
86	OHX	A1	3806	7/7	0.83	0.18	198,198,198,198	7
86	OHX	A1	3754	7/7	0.83	0.23	159,159,159,159	7
86	OHX	A6	2097	7/7	0.83	0.23	181,181,181,181	7
87	MG	BB	404	1/1	0.83	0.21	57,57,57,57	0
87	MG	CL	203	1/1	0.83	0.21	61,61,61,61	0
87	MG	A5	4330	1/1	0.83	0.23	86,86,86,86	0
87	MG	DA	301	1/1	0.83	0.31	86,86,86,86	0
87	MG	A5	4084	1/1	0.83	0.37	112,112,112,112	0
87	MG	DB	407	1/1	0.83	0.28	72,72,72,72	0
87	MG	A1	4274	1/1	0.83	0.34	87,87,87,87	0
87	MG	A1	4156	1/1	0.83	0.31	75,75,75,75	0
87	MG	BF	4102	1/1	0.83	0.28	76,76,76,76	0
87	MG	A2	2233	1/1	0.83	0.18	80,80,80,80	0
87	MG	BI	305	1/1	0.83	0.29	84,84,84,84	0
87	MG	A1	3944	1/1	0.83	0.40	45,45,45,45	0
87	MG	A1	3877	1/1	0.83	0.31	34,34,34,34	0
87	MG	DM	203	1/1	0.83	0.21	94,94,94,94	0
87	MG	A1	4448	1/1	0.83	0.21	66,66,66,66	0
87	MG	A5	3835	1/1	0.83	0.31	49,49,49,49	0
87	MG	A5	4113	1/1	0.83	0.18	39,39,39,39	0
87	MG	A5	4114	1/1	0.83	0.15	38,38,38,38	0
87	MG	A5	4355	1/1	0.83	0.23	66,66,66,66	0
87	MG	A1	4057	1/1	0.83	0.27	63,63,63,63	0
87	MG	A1	4058	1/1	0.83	0.39	97,97,97,97	0
87	MG	De	203	1/1	0.83	0.31	109,109,109,109	0
87	MG	A1	3956	1/1	0.83	0.29	45,45,45,45	0
87	MG	A5	4370	1/1	0.83	0.37	59,59,59,59	0
87	MG	A5	4128	1/1	0.83	0.21	66,66,66,66	0
87	MG	BR	202	1/1	0.83	0.17	58,58,58,58	0
87	MG	A1	4455	1/1	0.83	0.14	79,79,79,79	0
87	MG	A3	222	1/1	0.84	0.12	66,66,66,66	0
87	MG	A6	2263	1/1	0.84	0.21	89,89,89,89	0
87	MG	A5	4178	1/1	0.84	0.19	83,83,83,83	0
87	MG	A5	4424	1/1	0.84	0.23	86,86,86,86	0
86	OHX	A5	3734	7/7	0.84	0.38	208,208,208,208	7
87	MG	A3	228	1/1	0.84	0.22	81,81,81,81	0
87	MG	A6	2132	1/1	0.84	0.29	81,81,81,81	0
87	MG	A6	2280	1/1	0.84	0.37	79,79,79,79	0
87	MG	A5	3936	1/1	0.84	0.56	62,62,62,62	0
87	MG	A1	4241	1/1	0.84	0.26	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3761	7/7	0.84	0.16	173,173,173,173	7
87	MG	A5	4441	1/1	0.84	0.10	61,61,61,61	0
86	OHX	A6	2091	7/7	0.84	0.26	165,165,165,165	7
86	OHX	A6	2094	7/7	0.84	0.21	180,180,180,180	7
87	MG	A5	4193	1/1	0.84	0.15	43,43,43,43	0
87	MG	A1	3921	1/1	0.84	0.36	87,87,87,87	0
87	MG	A2	2130	1/1	0.84	0.18	56,56,56,56	0
87	MG	A1	4253	1/1	0.84	0.27	110,110,110,110	0
87	MG	A1	4390	1/1	0.84	0.31	82,82,82,82	0
87	MG	A1	3923	1/1	0.84	0.21	44,44,44,44	0
87	MG	A1	4143	1/1	0.84	0.29	70,70,70,70	0
86	OHX	A5	3756	7/7	0.84	0.28	158,158,158,158	7
87	MG	A1	4149	1/1	0.84	0.14	74,74,74,74	0
87	MG	A2	2201	1/1	0.84	0.18	96,96,96,96	0
87	MG	A2	2246	1/1	0.84	0.24	100,100,100,100	0
87	MG	A4	249	1/1	0.84	0.26	75,75,75,75	0
87	MG	A5	4487	1/1	0.84	0.27	76,76,76,76	0
87	MG	A5	4488	1/1	0.84	0.28	81,81,81,81	0
87	MG	A5	4218	1/1	0.84	0.16	57,57,57,57	0
87	MG	A6	2158	1/1	0.84	0.40	66,66,66,66	0
87	MG	A5	3994	1/1	0.84	0.29	39,39,39,39	0
86	OHX	A5	3799	7/7	0.84	0.31	168,168,168,168	7
87	MG	A1	4264	1/1	0.84	0.16	65,65,65,65	0
87	MG	A6	2166	1/1	0.84	0.35	64,64,64,64	0
87	MG	A6	2325	1/1	0.84	0.25	106,106,106,106	0
86	OHX	A2	2027	7/7	0.84	0.23	166,166,166,166	7
87	MG	A2	2135	1/1	0.84	0.13	54,54,54,54	0
86	OHX	A1	3798	7/7	0.84	0.35	226,226,226,226	7
87	MG	A2	2102	1/1	0.84	0.38	60,60,60,60	0
86	OHX	A1	3813	7/7	0.84	0.14	201,201,201,201	7
87	MG	A1	4164	1/1	0.84	0.18	78,78,78,78	0
87	MG	A1	3945	1/1	0.84	0.33	50,50,50,50	0
87	MG	A1	3871	1/1	0.84	0.31	48,48,48,48	0
87	MG	A1	4285	1/1	0.84	0.20	64,64,64,64	0
87	MG	A5	4045	1/1	0.84	0.30	63,63,63,63	0
87	MG	A6	2183	1/1	0.84	0.35	64,64,64,64	0
87	MG	A5	4256	1/1	0.84	0.32	81,81,81,81	0
87	MG	A1	3953	1/1	0.84	0.30	43,43,43,43	0
87	MG	A2	2171	1/1	0.84	0.33	89,89,89,89	0
87	MG	A1	4063	1/1	0.84	0.28	73,73,73,73	0
86	OHX	A5	3768	7/7	0.84	0.28	198,198,198,198	7
87	MG	BS	202	1/1	0.84	0.27	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4058	1/1	0.84	0.18	59,59,59,59	0
87	MG	A5	4290	1/1	0.84	0.17	47,47,47,47	0
87	MG	A1	4188	1/1	0.84	0.20	82,82,82,82	0
87	MG	A1	4069	1/1	0.84	0.22	69,69,69,69	0
87	MG	BV	203	1/1	0.84	0.26	63,63,63,63	0
87	MG	A5	4073	1/1	0.84	0.26	66,66,66,66	0
86	OHX	CG	302	7/7	0.84	0.12	197,197,197,197	7
87	MG	A5	4572	1/1	0.84	0.37	77,77,77,77	0
87	MG	A6	2204	1/1	0.84	0.18	70,70,70,70	0
87	MG	A5	4315	1/1	0.84	0.27	106,106,106,106	0
87	MG	A5	4082	1/1	0.84	0.26	46,46,46,46	0
87	MG	A1	4072	1/1	0.84	0.23	73,73,73,73	0
86	OHX	A5	3772	7/7	0.84	0.27	137,137,137,137	7
87	MG	A1	4308	1/1	0.84	0.34	59,59,59,59	0
87	MG	A6	2213	1/1	0.84	0.16	65,65,65,65	0
87	MG	A5	3840	1/1	0.84	0.14	26,26,26,26	0
87	MG	A6	2214	1/1	0.84	0.24	53,53,53,53	0
87	MG	A2	2112	1/1	0.84	0.72	95,95,95,95	0
87	MG	A1	4079	1/1	0.84	0.36	75,75,75,75	0
87	MG	A7	236	1/1	0.84	0.20	102,102,102,102	0
86	OHX	AP	201	7/7	0.84	0.12	196,196,196,196	7
87	MG	A8	226	1/1	0.84	0.27	62,62,62,62	0
87	MG	A5	4103	1/1	0.84	0.29	74,74,74,74	0
87	MG	A1	3882	1/1	0.84	0.33	47,47,47,47	0
86	OHX	A6	2084	7/7	0.84	0.15	196,196,196,196	7
87	MG	A5	3882	1/1	0.84	0.12	74,74,74,74	0
87	MG	A1	4088	1/1	0.84	0.20	90,90,90,90	0
86	OHX	A7	213	7/7	0.84	0.18	181,181,181,181	7
87	MG	A6	2235	1/1	0.84	0.40	77,77,77,77	0
86	OHX	A8	217	7/7	0.84	0.22	169,169,169,169	7
87	MG	A2	2224	1/1	0.84	0.21	77,77,77,77	0
87	MG	A5	4132	1/1	0.84	0.36	66,66,66,66	0
87	MG	A5	4134	1/1	0.84	0.33	84,84,84,84	0
87	MG	A5	4360	1/1	0.84	0.32	85,85,85,85	0
87	MG	A2	2225	1/1	0.84	0.37	79,79,79,79	0
87	MG	A5	4365	1/1	0.84	0.28	80,80,80,80	0
87	MG	A1	3990	1/1	0.84	0.43	54,54,54,54	0
86	OHX	A6	2073	7/7	0.84	0.21	186,186,186,186	7
87	MG	A1	3992	1/1	0.84	0.30	41,41,41,41	0
87	MG	A2	2153	1/1	0.84	0.27	72,72,72,72	0
87	MG	A2	2228	1/1	0.84	0.12	85,85,85,85	0
87	MG	A5	3907	1/1	0.84	0.28	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	3909	1/1	0.84	0.23	70,70,70,70	0
87	MG	A2	2154	1/1	0.84	0.30	74,74,74,74	0
87	MG	DV	202	1/1	0.84	0.34	35,35,35,35	0
86	OHX	A1	3512	7/7	0.84	0.33	197,197,197,197	7
87	MG	A1	4004	1/1	0.84	0.53	57,57,57,57	0
87	MG	Da	201	1/1	0.84	0.24	54,54,54,54	0
87	MG	Da	203	1/1	0.84	0.21	54,54,54,54	0
87	MG	A5	4159	1/1	0.84	0.30	64,64,64,64	0
87	MG	A5	3918	1/1	0.84	0.33	79,79,79,79	0
87	MG	A6	2252	1/1	0.84	0.37	117,117,117,117	0
87	MG	A1	4008	1/1	0.84	0.32	36,36,36,36	0
86	OHX	A6	2046	7/7	0.84	0.18	204,204,204,204	7
87	MG	A1	4238	1/1	0.84	0.16	69,69,69,69	0
87	MG	A5	4174	1/1	0.84	0.25	75,75,75,75	0
87	MG	A1	4459	1/1	0.85	0.34	88,88,88,88	0
87	MG	A1	3934	1/1	0.85	0.29	46,46,46,46	0
87	MG	A5	3967	1/1	0.85	0.30	57,57,57,57	0
87	MG	A1	4319	1/1	0.85	0.23	76,76,76,76	0
87	MG	A5	3976	1/1	0.85	0.27	43,43,43,43	0
87	MG	A5	4432	1/1	0.85	0.36	95,95,95,95	0
86	OHX	A1	3722	7/7	0.85	0.21	150,150,150,150	7
87	MG	A5	3978	1/1	0.85	0.17	29,29,29,29	0
86	OHX	A6	2060	7/7	0.85	0.27	165,165,165,165	7
87	MG	A5	3981	1/1	0.85	0.59	79,79,79,79	0
87	MG	A6	2322	1/1	0.85	0.17	77,77,77,77	0
87	MG	A1	3941	1/1	0.85	0.42	52,52,52,52	0
87	MG	A6	2177	1/1	0.85	0.42	79,79,79,79	0
87	MG	A6	2179	1/1	0.85	0.16	47,47,47,47	0
86	OHX	A6	2066	7/7	0.85	0.16	119,119,119,119	7
86	OHX	A6	2067	7/7	0.85	0.30	136,136,136,136	7
87	MG	A1	3946	1/1	0.85	0.29	41,41,41,41	0
87	MG	A5	4477	1/1	0.85	0.12	66,66,66,66	0
87	MG	A6	2184	1/1	0.85	0.18	67,67,67,67	0
87	MG	A6	2186	1/1	0.85	0.26	104,104,104,104	0
87	MG	A2	2116	1/1	0.85	0.31	59,59,59,59	0
86	OHX	A2	2059	7/7	0.85	0.13	183,183,183,183	7
87	MG	Ba	203	1/1	0.85	0.25	70,70,70,70	0
87	MG	A5	4022	1/1	0.85	0.41	52,52,52,52	0
87	MG	A6	2336	1/1	0.85	0.34	93,93,93,93	0
86	OHX	A5	3767	7/7	0.85	0.21	185,185,185,185	7
87	MG	A5	4026	1/1	0.85	0.47	53,53,53,53	0
87	MG	A2	2230	1/1	0.85	0.18	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	Bd	201	1/1	0.85	0.31	106,106,106,106	0
87	MG	A1	4342	1/1	0.85	0.31	79,79,79,79	0
86	OHX	A5	3821	7/7	0.85	0.15	223,223,223,223	7
86	OHX	A1	3786	7/7	0.85	0.19	184,184,184,184	7
87	MG	A1	3969	1/1	0.85	0.35	49,49,49,49	0
87	MG	A1	4349	1/1	0.85	0.42	119,119,119,119	0
86	OHX	A1	3700	7/7	0.85	0.27	185,185,185,185	7
86	OHX	BR	201	7/7	0.85	0.11	181,181,181,181	7
86	OHX	A6	2003	7/7	0.85	0.23	177,177,177,177	7
87	MG	A6	2101	1/1	0.85	0.33	51,51,51,51	0
86	OHX	A6	2025	7/7	0.85	0.16	161,161,161,161	7
86	OHX	A1	3791	7/7	0.85	0.19	149,149,149,149	7
87	MG	A5	4061	1/1	0.85	0.39	83,83,83,83	0
87	MG	A5	3826	1/1	0.85	0.20	63,63,63,63	0
87	MG	A5	3827	1/1	0.85	0.27	67,67,67,67	0
87	MG	A5	4272	1/1	0.85	0.10	69,69,69,69	0
86	OHX	A5	3782	7/7	0.85	0.25	169,169,169,169	7
87	MG	A5	4069	1/1	0.85	0.36	88,88,88,88	0
86	OHX	A5	3591	7/7	0.85	0.15	209,209,209,209	7
87	MG	A5	4534	1/1	0.85	0.52	72,72,72,72	0
87	MG	A5	4535	1/1	0.85	0.28	68,68,68,68	0
87	MG	A5	4075	1/1	0.85	0.21	60,60,60,60	0
87	MG	A6	2106	1/1	0.85	0.31	64,64,64,64	0
87	MG	A1	4505	1/1	0.85	0.23	145,145,145,145	0
87	MG	A5	3851	1/1	0.85	0.27	45,45,45,45	0
87	MG	A6	2232	1/1	0.85	0.20	77,77,77,77	0
86	OHX	A5	3658	7/7	0.85	0.29	141,141,141,141	7
87	MG	A5	3862	1/1	0.85	0.40	82,82,82,82	0
87	MG	A5	4317	1/1	0.85	0.23	63,63,63,63	0
87	MG	A5	4089	1/1	0.85	0.30	81,81,81,81	0
87	MG	A5	3864	1/1	0.85	0.38	63,63,63,63	0
87	MG	A5	4321	1/1	0.85	0.24	77,77,77,77	0
87	MG	A5	4091	1/1	0.85	0.11	54,54,54,54	0
87	MG	A6	2234	1/1	0.85	0.20	92,92,92,92	0
87	MG	A1	4082	1/1	0.85	0.36	73,73,73,73	0
87	MG	A5	3872	1/1	0.85	0.33	81,81,81,81	0
87	MG	A1	4372	1/1	0.85	0.28	71,71,71,71	0
87	MG	A7	218	1/1	0.85	0.39	43,43,43,43	0
87	MG	A7	219	1/1	0.85	0.24	71,71,71,71	0
87	MG	A1	3910	1/1	0.85	0.41	58,58,58,58	0
87	MG	A2	2245	1/1	0.85	0.17	71,71,71,71	0
87	MG	A5	4106	1/1	0.85	0.26	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	3915	1/1	0.85	0.19	32,32,32,32	0
86	OHX	A5	3688	7/7	0.85	0.19	212,212,212,212	7
87	MG	A6	2126	1/1	0.85	0.32	78,78,78,78	0
86	OHX	A2	2029	7/7	0.85	0.26	150,150,150,150	7
86	OHX	A1	3768	7/7	0.85	0.29	137,137,137,137	7
87	MG	A5	3895	1/1	0.85	0.25	32,32,32,32	0
87	MG	A1	3853	1/1	0.85	0.08	43,43,43,43	0
86	OHX	A6	2050	7/7	0.85	0.12	206,206,206,206	7
87	MG	A4	220	1/1	0.85	0.39	70,70,70,70	0
87	MG	A1	4282	1/1	0.85	0.47	92,92,92,92	0
87	MG	A1	4199	1/1	0.85	0.26	74,74,74,74	0
87	MG	A6	2134	1/1	0.85	0.30	67,67,67,67	0
87	MG	A6	2256	1/1	0.85	0.33	73,73,73,73	0
87	MG	A8	237	1/1	0.85	0.13	85,85,85,85	0
87	MG	A1	4412	1/1	0.85	0.16	104,104,104,104	0
87	MG	DA	305	1/1	0.85	0.31	69,69,69,69	0
87	MG	A1	4200	1/1	0.85	0.28	71,71,71,71	0
87	MG	A1	4006	1/1	0.85	0.33	42,42,42,42	0
87	MG	A6	2270	1/1	0.85	0.23	90,90,90,90	0
87	MG	A2	2101	1/1	0.85	0.16	59,59,59,59	0
87	MG	A5	4374	1/1	0.85	0.34	95,95,95,95	0
86	OHX	A1	3708	7/7	0.85	0.18	158,158,158,158	7
87	MG	DD	302	1/1	0.85	0.11	66,66,66,66	0
87	MG	DD	304	1/1	0.85	0.21	71,71,71,71	0
87	MG	A1	3862	1/1	0.85	0.19	76,76,76,76	0
87	MG	DF	301	1/1	0.85	0.14	75,75,75,75	0
87	MG	A6	2278	1/1	0.85	0.12	64,64,64,64	0
87	MG	A1	4439	1/1	0.85	0.21	88,88,88,88	0
87	MG	A5	4163	1/1	0.85	0.17	58,58,58,58	0
87	MG	DO	205	1/1	0.85	0.18	52,52,52,52	0
87	MG	A1	3927	1/1	0.85	0.22	31,31,31,31	0
86	OHX	A6	2085	7/7	0.85	0.41	188,188,188,188	7
87	MG	DP	205	1/1	0.85	0.27	56,56,56,56	0
87	MG	A5	4393	1/1	0.85	0.28	97,97,97,97	0
86	OHX	A1	3752	7/7	0.85	0.10	207,207,207,207	7
87	MG	A5	4396	1/1	0.85	0.17	71,71,71,71	0
87	MG	A1	4300	1/1	0.85	0.36	76,76,76,76	0
86	OHX	A5	3752	7/7	0.85	0.28	127,127,127,127	7
87	MG	A1	4026	1/1	0.85	0.38	42,42,42,42	0
87	MG	A1	4452	1/1	0.85	0.33	112,112,112,112	0
87	MG	A1	4306	1/1	0.85	0.14	68,68,68,68	0
87	MG	A5	4416	1/1	0.85	0.32	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2109	1/1	0.85	0.42	56,56,56,56	0
87	MG	A5	4419	1/1	0.85	0.19	65,65,65,65	0
87	MG	A1	4225	1/1	0.85	0.22	67,67,67,67	0
87	MG	BJ	201	1/1	0.85	0.16	81,81,81,81	0
87	MG	A1	4033	1/1	0.85	0.27	48,48,48,48	0
87	MG	A5	4027	1/1	0.86	0.42	53,53,53,53	0
87	MG	A1	4384	1/1	0.86	0.21	61,61,61,61	0
86	OHX	A6	2030	7/7	0.86	0.20	170,170,170,170	7
87	MG	A5	4219	1/1	0.86	0.37	74,74,74,74	0
87	MG	A1	3986	1/1	0.86	0.32	41,41,41,41	0
87	MG	A5	4470	1/1	0.86	0.36	76,76,76,76	0
86	OHX	A1	3804	7/7	0.86	0.31	152,152,152,152	7
87	MG	A3	231	1/1	0.86	0.13	92,92,92,92	0
86	OHX	A6	2039	7/7	0.86	0.17	168,168,168,168	7
87	MG	A4	216	1/1	0.86	0.35	64,64,64,64	0
87	MG	A1	3832	1/1	0.86	0.31	65,65,65,65	0
87	MG	A1	3833	1/1	0.86	0.34	49,49,49,49	0
87	MG	A5	3857	1/1	0.86	0.23	53,53,53,53	0
86	OHX	A5	3808	7/7	0.86	0.27	182,182,182,182	7
87	MG	A5	4238	1/1	0.86	0.30	44,44,44,44	0
87	MG	A1	4407	1/1	0.86	0.32	113,113,113,113	0
86	OHX	A6	2043	7/7	0.86	0.21	156,156,156,156	7
87	MG	A1	4096	1/1	0.86	0.30	80,80,80,80	0
87	MG	A5	3869	1/1	0.86	0.36	58,58,58,58	0
87	MG	A5	4063	1/1	0.86	0.25	52,52,52,52	0
87	MG	A5	4064	1/1	0.86	0.12	30,30,30,30	0
87	MG	A2	2110	1/1	0.86	0.33	57,57,57,57	0
87	MG	A1	4431	1/1	0.86	0.20	59,59,59,59	0
87	MG	A5	3873	1/1	0.86	0.27	60,60,60,60	0
87	MG	A1	4204	1/1	0.86	0.10	59,59,59,59	0
87	MG	A1	4292	1/1	0.86	0.21	67,67,67,67	0
87	MG	A5	4076	1/1	0.86	0.21	64,64,64,64	0
87	MG	A5	4267	1/1	0.86	0.30	88,88,88,88	0
87	MG	A5	4511	1/1	0.86	0.22	68,68,68,68	0
87	MG	A5	4077	1/1	0.86	0.21	55,55,55,55	0
87	MG	A6	2258	1/1	0.86	0.18	71,71,71,71	0
87	MG	A6	2140	1/1	0.86	0.23	61,61,61,61	0
86	OHX	A1	3778	7/7	0.86	0.26	150,150,150,150	7
86	OHX	A1	3748	7/7	0.86	0.25	163,163,163,163	7
87	MG	A6	2269	1/1	0.86	0.21	60,60,60,60	0
86	OHX	A2	2043	7/7	0.86	0.15	192,192,192,192	7
87	MG	A5	4293	1/1	0.86	0.24	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	3894	1/1	0.86	0.38	67,67,67,67	0
87	MG	A6	2271	1/1	0.86	0.08	95,95,95,95	0
87	MG	A5	4302	1/1	0.86	0.30	72,72,72,72	0
87	MG	A5	4307	1/1	0.86	0.17	78,78,78,78	0
87	MG	A1	4443	1/1	0.86	0.26	65,65,65,65	0
87	MG	A1	3852	1/1	0.86	0.40	70,70,70,70	0
87	MG	A5	4537	1/1	0.86	0.36	83,83,83,83	0
86	OHX	A1	3811	7/7	0.86	0.21	183,183,183,183	7
87	MG	BB	405	1/1	0.86	0.29	51,51,51,51	0
87	MG	BC	403	1/1	0.86	0.18	72,72,72,72	0
87	MG	A1	4218	1/1	0.86	0.33	69,69,69,69	0
87	MG	A5	4101	1/1	0.86	0.18	64,64,64,64	0
86	OHX	A1	3812	7/7	0.86	0.33	187,187,187,187	7
87	MG	A1	4012	1/1	0.86	0.27	41,41,41,41	0
87	MG	A6	2289	1/1	0.86	0.18	96,96,96,96	0
87	MG	A5	3914	1/1	0.86	0.39	69,69,69,69	0
86	OHX	A1	3686	7/7	0.86	0.18	204,204,204,204	7
86	OHX	A2	2065	7/7	0.86	0.40	166,166,166,166	7
87	MG	A5	4121	1/1	0.86	0.13	55,55,55,55	0
87	MG	A5	4576	1/1	0.86	0.29	77,77,77,77	0
86	OHX	A5	3766	7/7	0.86	0.17	173,173,173,173	7
87	MG	BN	307	1/1	0.86	0.28	58,58,58,58	0
86	OHX	A5	3822	7/7	0.86	0.40	205,205,205,205	7
87	MG	A7	216	1/1	0.86	0.36	78,78,78,78	0
87	MG	A5	3924	1/1	0.86	0.27	39,39,39,39	0
87	MG	A6	2301	1/1	0.86	0.17	116,116,116,116	0
86	OHX	A5	3823	7/7	0.86	0.11	225,225,225,225	7
87	MG	A5	4343	1/1	0.86	0.23	56,56,56,56	0
87	MG	A1	3869	1/1	0.86	0.27	69,69,69,69	0
86	OHX	A7	210	7/7	0.86	0.32	114,114,114,114	7
86	OHX	A6	2061	7/7	0.86	0.22	172,172,172,172	7
87	MG	A1	3938	1/1	0.86	0.20	48,48,48,48	0
87	MG	A5	4353	1/1	0.86	0.20	71,71,71,71	0
86	OHX	A8	216	7/7	0.86	0.20	198,198,198,198	7
87	MG	A1	4331	1/1	0.86	0.17	62,62,62,62	0
86	OHX	A3	209	7/7	0.86	0.26	180,180,180,180	7
87	MG	A5	3940	1/1	0.86	0.35	39,39,39,39	0
87	MG	A8	230	1/1	0.86	0.14	68,68,68,68	0
87	MG	A6	2317	1/1	0.86	0.16	82,82,82,82	0
87	MG	A5	4152	1/1	0.86	0.28	79,79,79,79	0
87	MG	A6	2318	1/1	0.86	0.22	68,68,68,68	0
86	OHX	A6	2098	7/7	0.86	0.26	144,144,144,144	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3734	7/7	0.86	0.26	190,190,190,190	7
87	MG	A1	3951	1/1	0.86	0.34	46,46,46,46	0
86	OHX	A1	3758	7/7	0.86	0.32	139,139,139,139	7
87	MG	A5	4380	1/1	0.86	0.29	89,89,89,89	0
86	OHX	A5	3778	7/7	0.86	0.16	153,153,153,153	7
87	MG	A1	4244	1/1	0.86	0.13	52,52,52,52	0
87	MG	A1	3880	1/1	0.86	0.29	42,42,42,42	0
87	MG	A5	3973	1/1	0.86	0.28	38,38,38,38	0
87	MG	A2	2220	1/1	0.86	0.21	111,111,111,111	0
86	OHX	A2	2032	7/7	0.86	0.17	200,200,200,200	7
87	MG	A5	4176	1/1	0.86	0.17	89,89,89,89	0
86	OHX	A1	3737	7/7	0.86	0.12	183,183,183,183	7
87	MG	A1	4353	1/1	0.86	0.14	77,77,77,77	0
87	MG	A1	4355	1/1	0.86	0.29	53,53,53,53	0
86	OHX	A2	2025	7/7	0.86	0.19	219,219,219,219	7
87	MG	A5	4402	1/1	0.86	0.18	91,91,91,91	0
87	MG	A5	4182	1/1	0.86	0.29	66,66,66,66	0
86	OHX	A5	3647	7/7	0.86	0.15	204,204,204,204	7
87	MG	A1	4496	1/1	0.86	0.26	82,82,82,82	0
87	MG	DO	208	1/1	0.86	0.29	77,77,77,77	0
87	MG	A1	3974	1/1	0.86	0.15	35,35,35,35	0
87	MG	A6	2212	1/1	0.86	0.22	91,91,91,91	0
86	OHX	A1	3770	7/7	0.86	0.21	179,179,179,179	7
86	OHX	A1	3574	7/7	0.86	0.18	189,189,189,189	7
87	MG	CI	303	1/1	0.86	0.32	62,62,62,62	0
87	MG	A5	4000	1/1	0.86	0.39	53,53,53,53	0
86	OHX	A2	2018	7/7	0.86	0.16	176,176,176,176	7
87	MG	A5	4006	1/1	0.86	0.35	40,40,40,40	0
86	OHX	A5	3704	7/7	0.86	0.21	141,141,141,141	7
87	MG	A1	4176	1/1	0.86	0.09	84,84,84,84	0
87	MG	A1	4074	1/1	0.86	0.19	57,57,57,57	0
87	MG	Df	202	1/1	0.86	0.46	81,81,81,81	0
87	MG	Dj	101	1/1	0.86	0.23	38,38,38,38	0
87	MG	A3	214	1/1	0.86	0.27	70,70,70,70	0
87	MG	A1	4266	1/1	0.86	0.14	70,70,70,70	0
87	MG	A5	4435	1/1	0.86	0.15	87,87,87,87	0
87	MG	A1	4179	1/1	0.86	0.31	69,69,69,69	0
87	MG	A1	3981	1/1	0.86	0.38	41,41,41,41	0
87	MG	A2	2099	1/1	0.87	0.21	53,53,53,53	0
87	MG	A6	2264	1/1	0.87	0.15	62,62,62,62	0
87	MG	A5	4150	1/1	0.87	0.22	68,68,68,68	0
87	MG	A6	2265	1/1	0.87	0.23	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A6	2268	1/1	0.87	0.24	68,68,68,68	0
87	MG	A3	227	1/1	0.87	0.27	59,59,59,59	0
87	MG	A5	4417	1/1	0.87	0.29	50,50,50,50	0
87	MG	A1	4380	1/1	0.87	0.16	95,95,95,95	0
87	MG	A5	4156	1/1	0.87	0.22	65,65,65,65	0
86	OHX	A2	2057	7/7	0.87	0.18	173,173,173,173	7
87	MG	A1	4263	1/1	0.87	0.30	71,71,71,71	0
87	MG	A1	4386	1/1	0.87	0.19	78,78,78,78	0
87	MG	A1	4054	1/1	0.87	0.35	65,65,65,65	0
87	MG	A5	4166	1/1	0.87	0.19	57,57,57,57	0
87	MG	A1	4163	1/1	0.87	0.34	81,81,81,81	0
87	MG	A5	4168	1/1	0.87	0.46	74,74,74,74	0
87	MG	A2	2204	1/1	0.87	0.26	109,109,109,109	0
86	OHX	A1	3785	7/7	0.87	0.29	183,183,183,183	7
87	MG	A4	225	1/1	0.87	0.41	65,65,65,65	0
86	OHX	A2	2004	7/7	0.87	0.23	164,164,164,164	7
87	MG	A5	3931	1/1	0.87	0.23	35,35,35,35	0
87	MG	A2	2104	1/1	0.87	0.24	63,63,63,63	0
87	MG	A1	4402	1/1	0.87	0.16	65,65,65,65	0
87	MG	A6	2142	1/1	0.87	0.28	46,46,46,46	0
87	MG	A5	4180	1/1	0.87	0.34	81,81,81,81	0
87	MG	A6	2143	1/1	0.87	0.26	45,45,45,45	0
87	MG	A5	4457	1/1	0.87	0.25	78,78,78,78	0
87	MG	A6	2294	1/1	0.87	0.12	54,54,54,54	0
87	MG	A5	4469	1/1	0.87	0.12	70,70,70,70	0
86	OHX	A1	3739	7/7	0.87	0.15	185,185,185,185	7
86	OHX	A5	3741	7/7	0.87	0.16	185,185,185,185	7
87	MG	A2	2108	1/1	0.87	0.28	56,56,56,56	0
87	MG	A6	2148	1/1	0.87	0.27	39,39,39,39	0
87	MG	A4	237	1/1	0.87	0.18	94,94,94,94	0
87	MG	A1	3973	1/1	0.87	0.28	37,37,37,37	0
86	OHX	A5	3746	7/7	0.87	0.22	151,151,151,151	7
87	MG	A1	3975	1/1	0.87	0.29	67,67,67,67	0
86	OHX	A1	3709	7/7	0.87	0.18	176,176,176,176	7
86	OHX	A1	3765	7/7	0.87	0.29	173,173,173,173	7
87	MG	A1	3890	1/1	0.87	0.28	61,61,61,61	0
87	MG	BA	303	1/1	0.87	0.13	30,30,30,30	0
87	MG	BA	306	1/1	0.87	0.19	74,74,74,74	0
87	MG	A1	4195	1/1	0.87	0.57	83,83,83,83	0
87	MG	A6	2321	1/1	0.87	0.53	93,93,93,93	0
86	OHX	A6	2100	7/7	0.87	0.23	206,206,206,206	7
87	MG	A5	4493	1/1	0.87	0.11	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	3984	1/1	0.87	0.40	56,56,56,56	0
87	MG	A5	4496	1/1	0.87	0.21	77,77,77,77	0
87	MG	A1	3895	1/1	0.87	0.27	92,92,92,92	0
87	MG	A1	4297	1/1	0.87	0.25	94,94,94,94	0
87	MG	A1	4085	1/1	0.87	0.12	35,35,35,35	0
87	MG	A5	3990	1/1	0.87	0.47	68,68,68,68	0
87	MG	A5	4505	1/1	0.87	0.49	71,71,71,71	0
87	MG	A5	3991	1/1	0.87	0.39	46,46,46,46	0
87	MG	A5	4224	1/1	0.87	0.12	58,58,58,58	0
86	OHX	A5	3755	7/7	0.87	0.19	174,174,174,174	7
87	MG	A5	3993	1/1	0.87	0.18	25,25,25,25	0
87	MG	BE	201	1/1	0.87	0.10	55,55,55,55	0
87	MG	A1	3985	1/1	0.87	0.41	51,51,51,51	0
86	OHX	A2	2045	7/7	0.87	0.22	164,164,164,164	7
86	OHX	A1	3628	7/7	0.87	0.17	154,154,154,154	7
87	MG	A5	4002	1/1	0.87	0.27	40,40,40,40	0
87	MG	A5	4003	1/1	0.87	0.30	46,46,46,46	0
87	MG	A1	4206	1/1	0.87	0.10	55,55,55,55	0
87	MG	BL	201	1/1	0.87	0.12	51,51,51,51	0
87	MG	BN	304	1/1	0.87	0.40	80,80,80,80	0
87	MG	A5	4245	1/1	0.87	0.20	66,66,66,66	0
86	OHX	A5	3761	7/7	0.87	0.18	146,146,146,146	7
87	MG	A5	4015	1/1	0.87	0.38	45,45,45,45	0
87	MG	A1	4097	1/1	0.87	0.39	73,73,73,73	0
87	MG	A1	4100	1/1	0.87	0.12	34,34,34,34	0
87	MG	A6	2190	1/1	0.87	0.20	74,74,74,74	0
87	MG	Ad	103	1/1	0.87	0.22	67,67,67,67	0
87	MG	A1	4460	1/1	0.87	0.20	67,67,67,67	0
86	OHX	A2	2071	7/7	0.87	0.20	162,162,162,162	7
86	OHX	A2	2053	7/7	0.87	0.17	173,173,173,173	7
86	OHX	A5	3406	7/7	0.87	0.10	170,170,170,170	7
87	MG	A6	2197	1/1	0.87	0.17	74,74,74,74	0
87	MG	BR	204	1/1	0.87	0.20	67,67,67,67	0
87	MG	A5	4570	1/1	0.87	0.16	76,76,76,76	0
87	MG	A1	3912	1/1	0.87	0.14	84,84,84,84	0
87	MG	A5	4044	1/1	0.87	0.19	35,35,35,35	0
87	MG	A5	4286	1/1	0.87	0.22	58,58,58,58	0
87	MG	A1	4466	1/1	0.87	0.11	80,80,80,80	0
87	MG	CX	201	1/1	0.87	0.23	68,68,68,68	0
86	OHX	A6	2054	7/7	0.87	0.23	169,169,169,169	7
87	MG	CZ	201	1/1	0.87	0.23	74,74,74,74	0
86	OHX	A1	3687	7/7	0.87	0.18	182,182,182,182	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4294	1/1	0.87	0.19	62,62,62,62	0
86	OHX	A5	3769	7/7	0.87	0.23	169,169,169,169	7
87	MG	A5	3410	1/1	0.87	0.23	61,61,61,61	0
86	OHX	A8	213	7/7	0.87	0.20	146,146,146,146	7
86	OHX	A2	2041	7/7	0.87	0.14	184,184,184,184	7
86	OHX	A5	3671	7/7	0.87	0.21	171,171,171,171	7
86	OHX	A5	3680	7/7	0.87	0.27	134,134,134,134	7
86	OHX	DD	301	7/7	0.87	0.24	134,134,134,134	7
87	MG	A5	3841	1/1	0.87	0.35	44,44,44,44	0
87	MG	A5	3844	1/1	0.87	0.18	59,59,59,59	0
87	MG	A5	3845	1/1	0.87	0.31	51,51,51,51	0
87	MG	A8	223	1/1	0.87	0.29	50,50,50,50	0
86	OHX	A1	3783	7/7	0.87	0.16	152,152,152,152	7
87	MG	A5	3849	1/1	0.87	0.17	41,41,41,41	0
87	MG	A5	3850	1/1	0.87	0.31	55,55,55,55	0
87	MG	A6	2221	1/1	0.87	0.19	69,69,69,69	0
86	OHX	A5	3779	7/7	0.87	0.27	167,167,167,167	7
87	MG	A5	4079	1/1	0.87	0.25	67,67,67,67	0
87	MG	A5	3854	1/1	0.87	0.40	74,74,74,74	0
87	MG	A1	4484	1/1	0.87	0.35	106,106,106,106	0
86	OHX	A5	3689	7/7	0.87	0.28	134,134,134,134	7
87	MG	A1	4345	1/1	0.87	0.16	73,73,73,73	0
86	OHX	A5	3696	7/7	0.87	0.14	167,167,167,167	7
87	MG	A5	3865	1/1	0.87	0.26	37,37,37,37	0
87	MG	A5	4337	1/1	0.87	0.25	70,70,70,70	0
87	MG	Bo	202	1/1	0.87	0.30	82,82,82,82	0
87	MG	A2	2088	1/1	0.87	0.26	59,59,59,59	0
87	MG	A1	4491	1/1	0.87	0.30	80,80,80,80	0
87	MG	A5	4344	1/1	0.87	0.16	66,66,66,66	0
87	MG	A1	3856	1/1	0.87	0.27	38,38,38,38	0
87	MG	A1	4138	1/1	0.87	0.29	62,62,62,62	0
87	MG	A5	3874	1/1	0.87	0.21	32,32,32,32	0
87	MG	A5	4349	1/1	0.87	0.29	79,79,79,79	0
87	MG	A5	3876	1/1	0.87	0.28	66,66,66,66	0
87	MG	A5	3877	1/1	0.87	0.33	60,60,60,60	0
87	MG	A2	2190	1/1	0.87	0.23	82,82,82,82	0
87	MG	DL	201	1/1	0.87	0.23	94,94,94,94	0
87	MG	A5	4105	1/1	0.87	0.32	68,68,68,68	0
87	MG	A1	4142	1/1	0.87	0.14	68,68,68,68	0
86	OHX	A1	3805	7/7	0.87	0.30	209,209,209,209	7
87	MG	A5	4363	1/1	0.87	0.27	83,83,83,83	0
87	MG	A5	3885	1/1	0.87	0.29	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	3860	1/1	0.87	0.33	59,59,59,59	0
87	MG	A1	4503	1/1	0.87	0.24	77,77,77,77	0
87	MG	A6	2115	1/1	0.87	0.33	47,47,47,47	0
87	MG	DS	203	1/1	0.87	0.38	65,65,65,65	0
87	MG	A1	3861	1/1	0.87	0.23	34,34,34,34	0
86	OHX	A5	3785	7/7	0.87	0.34	126,126,126,126	7
87	MG	A6	2119	1/1	0.87	0.29	70,70,70,70	0
87	MG	A5	4130	1/1	0.87	0.19	49,49,49,49	0
87	MG	A1	4365	1/1	0.87	0.19	66,66,66,66	0
87	MG	Dd	201	1/1	0.87	0.33	77,77,77,77	0
86	OHX	A6	1991	7/7	0.87	0.27	149,149,149,149	7
86	OHX	A5	3711	7/7	0.87	0.17	164,164,164,164	7
87	MG	A5	3900	1/1	0.87	0.27	63,63,63,63	0
87	MG	Df	203	1/1	0.87	0.29	93,93,93,93	0
86	OHX	A5	3719	7/7	0.87	0.27	180,180,180,180	7
86	OHX	A5	3791	7/7	0.87	0.29	175,175,175,175	7
87	MG	A1	4158	1/1	0.87	0.38	87,87,87,87	0
87	MG	A6	2262	1/1	0.87	0.14	101,101,101,101	0
87	MG	A5	4143	1/1	0.87	0.33	70,70,70,70	0
87	MG	A5	3908	1/1	0.87	0.24	37,37,37,37	0
87	MG	A1	4216	1/1	0.88	0.30	93,93,93,93	0
86	OHX	A2	2064	7/7	0.88	0.25	169,169,169,169	7
86	OHX	A8	215	7/7	0.88	0.24	151,151,151,151	7
86	OHX	A1	3678	7/7	0.88	0.24	186,186,186,186	7
87	MG	A6	2292	1/1	0.88	0.11	75,75,75,75	0
87	MG	A3	216	1/1	0.88	0.17	67,67,67,67	0
87	MG	A5	4422	1/1	0.88	0.20	52,52,52,52	0
87	MG	A5	4171	1/1	0.88	0.22	108,108,108,108	0
87	MG	A3	219	1/1	0.88	0.28	40,40,40,40	0
86	OHX	A5	3665	7/7	0.88	0.22	184,184,184,184	7
87	MG	A1	4098	1/1	0.88	0.17	54,54,54,54	0
86	OHX	A2	2048	7/7	0.88	0.13	155,155,155,155	7
87	MG	A1	3982	1/1	0.88	0.36	43,43,43,43	0
87	MG	A5	3957	1/1	0.88	0.39	43,43,43,43	0
86	OHX	A3	212	7/7	0.88	0.21	159,159,159,159	7
87	MG	A5	4433	1/1	0.88	0.29	83,83,83,83	0
87	MG	A2	2198	1/1	0.88	0.20	80,80,80,80	0
87	MG	A2	2142	1/1	0.88	0.34	65,65,65,65	0
87	MG	A5	4438	1/1	0.88	0.10	58,58,58,58	0
87	MG	A1	3893	1/1	0.88	0.14	26,26,26,26	0
86	OHX	A5	3776	7/7	0.88	0.21	184,184,184,184	7
87	MG	A5	3972	1/1	0.88	0.35	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	AC	302	1/1	0.88	0.35	74,74,74,74	0
87	MG	A5	3975	1/1	0.88	0.31	41,41,41,41	0
86	OHX	A5	3685	7/7	0.88	0.22	141,141,141,141	7
87	MG	A2	2203	1/1	0.88	0.14	68,68,68,68	0
87	MG	A1	4112	1/1	0.88	0.16	58,58,58,58	0
87	MG	A6	2152	1/1	0.88	0.34	64,64,64,64	0
86	OHX	A6	2048	7/7	0.88	0.28	169,169,169,169	7
86	OHX	A6	2083	7/7	0.88	0.38	214,214,214,214	7
87	MG	A5	3983	1/1	0.88	0.34	47,47,47,47	0
87	MG	A1	4240	1/1	0.88	0.12	59,59,59,59	0
87	MG	A1	3903	1/1	0.88	0.36	85,85,85,85	0
86	OHX	A6	2049	7/7	0.88	0.20	175,175,175,175	7
86	OHX	A2	2058	7/7	0.88	0.26	201,201,201,201	7
87	MG	A5	4210	1/1	0.88	0.25	79,79,79,79	0
87	MG	A6	2164	1/1	0.88	0.35	57,57,57,57	0
87	MG	A5	4483	1/1	0.88	0.25	112,112,112,112	0
87	MG	A1	4125	1/1	0.88	0.14	56,56,56,56	0
86	OHX	A6	2086	7/7	0.88	0.32	215,215,215,215	7
87	MG	AX	201	1/1	0.88	0.20	70,70,70,70	0
87	MG	A1	4251	1/1	0.88	0.25	71,71,71,71	0
87	MG	A6	2170	1/1	0.88	0.20	49,49,49,49	0
87	MG	A4	243	1/1	0.88	0.20	48,48,48,48	0
87	MG	A5	4222	1/1	0.88	0.36	75,75,75,75	0
87	MG	A1	4010	1/1	0.88	0.39	61,61,61,61	0
86	OHX	A5	3784	7/7	0.88	0.19	173,173,173,173	7
86	OHX	A5	3706	7/7	0.88	0.21	139,139,139,139	7
86	OHX	A6	2051	7/7	0.88	0.17	167,167,167,167	7
87	MG	A1	3404	1/1	0.88	0.34	74,74,74,74	0
87	MG	A6	2178	1/1	0.88	0.21	71,71,71,71	0
87	MG	CI	302	1/1	0.88	0.20	63,63,63,63	0
87	MG	A1	4258	1/1	0.88	0.14	67,67,67,67	0
86	OHX	A1	3800	7/7	0.88	0.30	188,188,188,188	7
87	MG	A1	4018	1/1	0.88	0.30	38,38,38,38	0
87	MG	A1	4410	1/1	0.88	0.20	69,69,69,69	0
87	MG	A1	4411	1/1	0.88	0.35	94,94,94,94	0
87	MG	A1	3818	1/1	0.88	0.10	63,63,63,63	0
87	MG	A1	4148	1/1	0.88	0.34	94,94,94,94	0
87	MG	A5	4519	1/1	0.88	0.12	63,63,63,63	0
86	OHX	A5	3788	7/7	0.88	0.24	141,141,141,141	7
87	MG	A5	4248	1/1	0.88	0.35	99,99,99,99	0
87	MG	A5	4034	1/1	0.88	0.11	46,46,46,46	0
87	MG	A5	4038	1/1	0.88	0.13	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4252	1/1	0.88	0.22	68,68,68,68	0
87	MG	CX	202	1/1	0.88	0.21	81,81,81,81	0
86	OHX	A5	3722	7/7	0.88	0.18	164,164,164,164	7
87	MG	A1	4265	1/1	0.88	0.29	74,74,74,74	0
87	MG	A1	4029	1/1	0.88	0.12	29,29,29,29	0
87	MG	A5	4261	1/1	0.88	0.17	71,71,71,71	0
87	MG	A1	4436	1/1	0.88	0.13	115,115,115,115	0
86	OHX	A5	3790	7/7	0.88	0.17	157,157,157,157	7
87	MG	BL	202	1/1	0.88	0.26	78,78,78,78	0
87	MG	A1	4269	1/1	0.88	0.18	87,87,87,87	0
87	MG	A5	4546	1/1	0.88	0.11	66,66,66,66	0
87	MG	A5	4051	1/1	0.88	0.35	77,77,77,77	0
87	MG	A5	4276	1/1	0.88	0.21	60,60,60,60	0
87	MG	A5	4555	1/1	0.88	0.19	63,63,63,63	0
87	MG	A5	3831	1/1	0.88	0.13	37,37,37,37	0
87	MG	A5	4284	1/1	0.88	0.16	69,69,69,69	0
87	MG	A5	4285	1/1	0.88	0.16	68,68,68,68	0
87	MG	A1	4271	1/1	0.88	0.20	58,58,58,58	0
87	MG	A5	4567	1/1	0.88	0.16	59,59,59,59	0
87	MG	A6	2201	1/1	0.88	0.23	72,72,72,72	0
86	OHX	A5	3725	7/7	0.88	0.17	171,171,171,171	7
87	MG	BO	205	1/1	0.88	0.24	58,58,58,58	0
87	MG	A6	2205	1/1	0.88	0.28	72,72,72,72	0
86	OHX	A2	2034	7/7	0.88	0.14	173,173,173,173	7
86	OHX	A5	3732	7/7	0.88	0.19	209,209,209,209	7
86	OHX	A6	2055	7/7	0.88	0.27	131,131,131,131	7
87	MG	A6	2211	1/1	0.88	0.13	86,86,86,86	0
86	OHX	A2	2019	7/7	0.88	0.19	174,174,174,174	7
87	MG	A5	4304	1/1	0.88	0.14	66,66,66,66	0
87	MG	A1	4450	1/1	0.88	0.22	68,68,68,68	0
87	MG	A5	4309	1/1	0.88	0.29	64,64,64,64	0
87	MG	A5	4071	1/1	0.88	0.32	79,79,79,79	0
87	MG	A1	4278	1/1	0.88	0.11	67,67,67,67	0
87	MG	A7	225	1/1	0.88	0.28	45,45,45,45	0
87	MG	A7	226	1/1	0.88	0.26	74,74,74,74	0
86	OHX	A6	2093	7/7	0.88	0.15	149,149,149,149	7
87	MG	A7	230	1/1	0.88	0.15	61,61,61,61	0
86	OHX	A5	3800	7/7	0.88	0.20	203,203,203,203	7
87	MG	A1	4454	1/1	0.88	0.28	81,81,81,81	0
86	OHX	A5	3802	7/7	0.88	0.32	151,151,151,151	7
87	MG	A7	235	1/1	0.88	0.24	74,74,74,74	0
86	OHX	A5	3806	7/7	0.88	0.20	120,120,120,120	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	BV	204	1/1	0.88	0.30	40,40,40,40	0
87	MG	A6	2226	1/1	0.88	0.11	68,68,68,68	0
87	MG	A8	224	1/1	0.88	0.26	67,67,67,67	0
87	MG	A5	4083	1/1	0.88	0.23	70,70,70,70	0
86	OHX	A2	2073	7/7	0.88	0.23	147,147,147,147	7
87	MG	A1	4173	1/1	0.88	0.12	45,45,45,45	0
87	MG	Ba	205	1/1	0.88	0.19	69,69,69,69	0
87	MG	A1	4289	1/1	0.88	0.22	74,74,74,74	0
87	MG	A5	3875	1/1	0.88	0.56	78,78,78,78	0
87	MG	A1	4290	1/1	0.88	0.18	69,69,69,69	0
86	OHX	A5	3744	7/7	0.88	0.23	140,140,140,140	7
87	MG	A5	3879	1/1	0.88	0.17	61,61,61,61	0
87	MG	A1	4053	1/1	0.88	0.21	76,76,76,76	0
87	MG	A1	3940	1/1	0.88	0.30	51,51,51,51	0
87	MG	DA	303	1/1	0.88	0.20	53,53,53,53	0
87	MG	A1	4294	1/1	0.88	0.39	78,78,78,78	0
86	OHX	A1	3599	7/7	0.88	0.25	196,196,196,196	7
86	OHX	A1	3807	7/7	0.88	0.21	167,167,167,167	7
87	MG	Bj	110	1/1	0.88	0.21	94,94,94,94	0
87	MG	DB	412	1/1	0.88	0.16	70,70,70,70	0
87	MG	A1	4472	1/1	0.88	0.17	86,86,86,86	0
87	MG	A2	2118	1/1	0.88	0.28	47,47,47,47	0
86	OHX	A1	3789	7/7	0.88	0.18	189,189,189,189	7
87	MG	A1	4189	1/1	0.88	0.20	59,59,59,59	0
87	MG	DD	303	1/1	0.88	0.19	67,67,67,67	0
87	MG	A5	4352	1/1	0.88	0.27	67,67,67,67	0
87	MG	A2	2178	1/1	0.88	0.17	73,73,73,73	0
87	MG	A5	3896	1/1	0.88	0.32	67,67,67,67	0
87	MG	DH	202	1/1	0.88	0.16	73,73,73,73	0
87	MG	DH	203	1/1	0.88	0.16	72,72,72,72	0
86	OHX	A6	2023	7/7	0.88	0.17	177,177,177,177	7
87	MG	A6	2254	1/1	0.88	0.12	69,69,69,69	0
87	MG	A5	4127	1/1	0.88	0.26	68,68,68,68	0
87	MG	DM	202	1/1	0.88	0.16	70,70,70,70	0
87	MG	A5	3899	1/1	0.88	0.29	73,73,73,73	0
86	OHX	A1	3712	7/7	0.88	0.26	180,180,180,180	7
87	MG	A1	4307	1/1	0.88	0.16	71,71,71,71	0
87	MG	A1	3954	1/1	0.88	0.25	45,45,45,45	0
86	OHX	A6	2026	7/7	0.88	0.19	176,176,176,176	7
87	MG	A6	2107	1/1	0.88	0.31	52,52,52,52	0
87	MG	A1	4485	1/1	0.88	0.26	93,93,93,93	0
86	OHX	A5	3758	7/7	0.88	0.33	167,167,167,167	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A6	2113	1/1	0.88	0.20	48,48,48,48	0
87	MG	A1	3961	1/1	0.88	0.24	33,33,33,33	0
87	MG	A5	3913	1/1	0.88	0.11	68,68,68,68	0
87	MG	A2	2241	1/1	0.88	0.20	108,108,108,108	0
86	OHX	A6	2071	7/7	0.88	0.22	160,160,160,160	7
87	MG	Da	202	1/1	0.88	0.16	84,84,84,84	0
87	MG	A1	4201	1/1	0.88	0.20	65,65,65,65	0
87	MG	A5	4149	1/1	0.88	0.15	63,63,63,63	0
87	MG	A1	4080	1/1	0.88	0.14	60,60,60,60	0
87	MG	A2	2243	1/1	0.88	0.17	86,86,86,86	0
86	OHX	A2	2038	7/7	0.88	0.19	195,195,195,195	7
86	OHX	A2	2001	7/7	0.88	0.23	140,140,140,140	7
87	MG	Df	205	1/1	0.88	0.18	76,76,76,76	0
87	MG	A5	4398	1/1	0.88	0.12	54,54,54,54	0
87	MG	A1	4211	1/1	0.88	0.28	102,102,102,102	0
86	OHX	A5	3407	7/7	0.88	0.21	196,196,196,196	7
87	MG	A1	4214	1/1	0.88	0.26	55,55,55,55	0
87	MG	A5	4409	1/1	0.88	0.14	59,59,59,59	0
86	OHX	A6	2032	7/7	0.88	0.16	143,143,143,143	7
86	OHX	A5	3751	7/7	0.89	0.25	148,148,148,148	7
87	MG	Ad	104	1/1	0.89	0.11	65,65,65,65	0
87	MG	CQ	201	1/1	0.89	0.28	75,75,75,75	0
87	MG	A5	4005	1/1	0.89	0.31	31,31,31,31	0
87	MG	BN	302	1/1	0.89	0.21	44,44,44,44	0
87	MG	A5	4463	1/1	0.89	0.11	89,89,89,89	0
87	MG	A5	4215	1/1	0.89	0.18	52,52,52,52	0
86	OHX	A1	3667	7/7	0.89	0.29	92,92,92,92	7
87	MG	A5	4011	1/1	0.89	0.28	54,54,54,54	0
87	MG	A1	3406	1/1	0.89	0.29	67,67,67,67	0
87	MG	A1	4042	1/1	0.89	0.21	68,68,68,68	0
86	OHX	A2	2012	7/7	0.89	0.15	180,180,180,180	7
87	MG	A1	3925	1/1	0.89	0.21	40,40,40,40	0
87	MG	A6	2198	1/1	0.89	0.13	49,49,49,49	0
86	OHX	A5	3754	7/7	0.89	0.18	147,147,147,147	7
87	MG	BP	208	1/1	0.89	0.10	52,52,52,52	0
87	MG	A1	4184	1/1	0.89	0.20	81,81,81,81	0
86	OHX	A1	3762	7/7	0.89	0.14	144,144,144,144	7
87	MG	A5	4029	1/1	0.89	0.38	44,44,44,44	0
86	OHX	A1	3727	7/7	0.89	0.26	146,146,146,146	7
86	OHX	A1	3681	7/7	0.89	0.21	146,146,146,146	7
87	MG	A1	3931	1/1	0.89	0.27	40,40,40,40	0
87	MG	A5	4489	1/1	0.89	0.31	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	BR	205	1/1	0.89	0.22	99,99,99,99	0
86	OHX	A6	2047	7/7	0.89	0.27	156,156,156,156	7
87	MG	A5	4244	1/1	0.89	0.26	82,82,82,82	0
86	OHX	A1	3729	7/7	0.89	0.35	167,167,167,167	7
86	OHX	A1	3771	7/7	0.89	0.19	174,174,174,174	7
86	OHX	A1	3682	7/7	0.89	0.18	145,145,145,145	7
87	MG	A1	4302	1/1	0.89	0.24	114,114,114,114	0
87	MG	A5	4498	1/1	0.89	0.42	90,90,90,90	0
87	MG	A5	4049	1/1	0.89	0.34	70,70,70,70	0
87	MG	A5	4250	1/1	0.89	0.26	110,110,110,110	0
87	MG	A1	3838	1/1	0.89	0.22	67,67,67,67	0
87	MG	A1	3839	1/1	0.89	0.28	64,64,64,64	0
87	MG	A5	4052	1/1	0.89	0.16	46,46,46,46	0
87	MG	A5	4508	1/1	0.89	0.26	67,67,67,67	0
87	MG	A5	4509	1/1	0.89	0.30	134,134,134,134	0
87	MG	A1	3939	1/1	0.89	0.25	32,32,32,32	0
86	OHX	A1	3810	7/7	0.89	0.34	199,199,199,199	7
86	OHX	CI	301	7/7	0.89	0.12	172,172,172,172	7
87	MG	A1	3943	1/1	0.89	0.36	59,59,59,59	0
87	MG	A5	3858	1/1	0.89	0.26	43,43,43,43	0
87	MG	A5	4264	1/1	0.89	0.67	103,103,103,103	0
87	MG	A5	4060	1/1	0.89	0.33	57,57,57,57	0
87	MG	A1	4316	1/1	0.89	0.17	65,65,65,65	0
87	MG	A1	3844	1/1	0.89	0.20	48,48,48,48	0
86	OHX	A1	3683	7/7	0.89	0.14	159,159,159,159	7
86	OHX	A1	3685	7/7	0.89	0.22	150,150,150,150	7
87	MG	A5	4277	1/1	0.89	0.20	85,85,85,85	0
87	MG	A5	3866	1/1	0.89	0.20	51,51,51,51	0
87	MG	A1	3949	1/1	0.89	0.33	43,43,43,43	0
87	MG	A5	4531	1/1	0.89	0.18	65,65,65,65	0
87	MG	A6	2236	1/1	0.89	0.27	76,76,76,76	0
87	MG	A1	4325	1/1	0.89	0.13	67,67,67,67	0
87	MG	A1	3850	1/1	0.89	0.41	64,64,64,64	0
87	MG	A5	4074	1/1	0.89	0.14	51,51,51,51	0
87	MG	A2	2222	1/1	0.89	0.21	103,103,103,103	0
87	MG	A5	4542	1/1	0.89	0.48	59,59,59,59	0
86	OHX	A1	3564	7/7	0.89	0.23	136,136,136,136	7
86	OHX	A5	3771	7/7	0.89	0.22	176,176,176,176	7
87	MG	A6	2243	1/1	0.89	0.12	74,74,74,74	0
86	OHX	A1	3782	7/7	0.89	0.24	186,186,186,186	7
86	OHX	A5	3775	7/7	0.89	0.17	152,152,152,152	7
87	MG	A1	4488	1/1	0.89	0.31	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4303	1/1	0.89	0.18	57,57,57,57	0
86	OHX	A1	3815	7/7	0.89	0.38	183,183,183,183	7
87	MG	A6	2248	1/1	0.89	0.16	75,75,75,75	0
87	MG	A5	4085	1/1	0.89	0.35	79,79,79,79	0
87	MG	A2	2229	1/1	0.89	0.10	60,60,60,60	0
87	MG	A1	4340	1/1	0.89	0.35	96,96,96,96	0
86	OHX	A5	3615	7/7	0.89	0.20	147,147,147,147	7
87	MG	A6	2108	1/1	0.89	0.28	52,52,52,52	0
86	OHX	A2	2061	7/7	0.89	0.30	142,142,142,142	7
87	MG	A5	4319	1/1	0.89	0.15	86,86,86,86	0
87	MG	A1	4099	1/1	0.89	0.28	71,71,71,71	0
86	OHX	A3	210	7/7	0.89	0.20	175,175,175,175	7
87	MG	A6	2114	1/1	0.89	0.35	61,61,61,61	0
87	MG	A7	214	1/1	0.89	0.40	55,55,55,55	0
87	MG	A1	4499	1/1	0.89	0.13	65,65,65,65	0
86	OHX	A6	2062	7/7	0.89	0.20	163,163,163,163	7
86	OHX	A6	2063	7/7	0.89	0.21	176,176,176,176	7
87	MG	A1	4348	1/1	0.89	0.23	73,73,73,73	0
87	MG	A1	3868	1/1	0.89	0.22	55,55,55,55	0
86	OHX	A1	3697	7/7	0.89	0.23	182,182,182,182	7
87	MG	A5	3903	1/1	0.89	0.23	34,34,34,34	0
87	MG	A5	4112	1/1	0.89	0.40	65,65,65,65	0
86	OHX	A2	2049	7/7	0.89	0.18	140,140,140,140	7
87	MG	A1	4354	1/1	0.89	0.12	61,61,61,61	0
86	OHX	A4	214	7/7	0.89	0.21	167,167,167,167	7
87	MG	A5	4118	1/1	0.89	0.30	57,57,57,57	0
87	MG	A5	4340	1/1	0.89	0.17	61,61,61,61	0
87	MG	A3	215	1/1	0.89	0.35	77,77,77,77	0
87	MG	A1	4356	1/1	0.89	0.33	65,65,65,65	0
87	MG	A3	217	1/1	0.89	0.30	56,56,56,56	0
87	MG	A6	2276	1/1	0.89	0.15	105,105,105,105	0
87	MG	A1	3872	1/1	0.89	0.21	37,37,37,37	0
86	OHX	AI	301	7/7	0.89	0.10	156,156,156,156	7
87	MG	A1	4360	1/1	0.89	0.21	88,88,88,88	0
87	MG	A6	2281	1/1	0.89	0.12	75,75,75,75	0
86	OHX	A5	3693	7/7	0.89	0.22	181,181,181,181	7
87	MG	A3	223	1/1	0.89	0.21	75,75,75,75	0
87	MG	A2	2173	1/1	0.89	0.09	82,82,82,82	0
86	OHX	A6	2070	7/7	0.89	0.17	139,139,139,139	7
86	OHX	BC	401	7/7	0.89	0.14	130,130,130,130	7
86	OHX	A1	3746	7/7	0.89	0.18	142,142,142,142	7
87	MG	A2	2113	1/1	0.89	0.47	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4364	1/1	0.89	0.20	76,76,76,76	0
86	OHX	A2	1960	7/7	0.89	0.17	173,173,173,173	7
87	MG	DB	403	1/1	0.89	0.35	36,36,36,36	0
87	MG	A1	4371	1/1	0.89	0.17	63,63,63,63	0
87	MG	DB	406	1/1	0.89	0.23	47,47,47,47	0
86	OHX	A5	3708	7/7	0.89	0.13	141,141,141,141	7
87	MG	A5	3932	1/1	0.89	0.24	34,34,34,34	0
87	MG	A1	3887	1/1	0.89	0.14	54,54,54,54	0
87	MG	A4	219	1/1	0.89	0.23	59,59,59,59	0
87	MG	A1	4129	1/1	0.89	0.15	75,75,75,75	0
87	MG	A5	4377	1/1	0.89	0.29	85,85,85,85	0
87	MG	A4	223	1/1	0.89	0.35	44,44,44,44	0
87	MG	A5	4154	1/1	0.89	0.11	54,54,54,54	0
86	OHX	A1	3790	7/7	0.89	0.19	164,164,164,164	7
87	MG	A1	4134	1/1	0.89	0.42	69,69,69,69	0
87	MG	DD	307	1/1	0.89	0.16	77,77,77,77	0
87	MG	A5	3948	1/1	0.89	0.21	28,28,28,28	0
86	OHX	A5	3712	7/7	0.89	0.20	149,149,149,149	7
86	OHX	A5	3718	7/7	0.89	0.14	157,157,157,157	7
87	MG	A1	3891	1/1	0.89	0.23	58,58,58,58	0
86	OHX	A1	3749	7/7	0.89	0.21	177,177,177,177	7
86	OHX	A6	1988	7/7	0.89	0.25	138,138,138,138	7
86	OHX	A1	3655	7/7	0.89	0.24	150,150,150,150	7
87	MG	A5	3965	1/1	0.89	0.36	64,64,64,64	0
87	MG	DN	301	1/1	0.89	0.18	77,77,77,77	0
86	OHX	A6	1999	7/7	0.89	0.20	140,140,140,140	7
87	MG	A1	4398	1/1	0.89	0.17	49,49,49,49	0
87	MG	A5	4173	1/1	0.89	0.20	67,67,67,67	0
86	OHX	A5	3728	7/7	0.89	0.33	131,131,131,131	7
86	OHX	A1	3657	7/7	0.89	0.18	166,166,166,166	7
86	OHX	A6	2008	7/7	0.89	0.20	176,176,176,176	7
86	OHX	A6	2014	7/7	0.89	0.17	144,144,144,144	7
87	MG	DS	202	1/1	0.89	0.32	75,75,75,75	0
86	OHX	A1	3795	7/7	0.89	0.27	195,195,195,195	7
87	MG	DT	203	1/1	0.89	0.34	80,80,80,80	0
86	OHX	A5	3736	7/7	0.89	0.28	143,143,143,143	7
87	MG	BA	304	1/1	0.89	0.19	62,62,62,62	0
86	OHX	A1	3720	7/7	0.89	0.21	139,139,139,139	7
87	MG	DY	202	1/1	0.89	0.21	55,55,55,55	0
86	OHX	A1	3721	7/7	0.89	0.15	153,153,153,153	7
87	MG	A1	4422	1/1	0.89	0.22	68,68,68,68	0
87	MG	A6	2333	1/1	0.89	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
86	OHX	A1	3756	7/7	0.89	0.28	158,158,158,158	7
87	MG	A1	4426	1/1	0.89	0.22	82,82,82,82	0
87	MG	A1	4027	1/1	0.89	0.44	65,65,65,65	0
87	MG	A6	2180	1/1	0.89	0.21	87,87,87,87	0
87	MG	A2	2202	1/1	0.89	0.16	66,66,66,66	0
87	MG	A1	4434	1/1	0.89	0.42	55,55,55,55	0
87	MG	A2	2136	1/1	0.89	0.35	70,70,70,70	0
86	OHX	A1	3407	7/7	0.89	0.21	138,138,138,138	7
87	MG	A6	2185	1/1	0.89	0.29	71,71,71,71	0
87	MG	A2	2138	1/1	0.89	0.14	56,56,56,56	0
87	MG	CL	202	1/1	0.89	0.28	82,82,82,82	0
88	ZN	Bo	205	1/1	0.89	0.13	209,209,209,209	0
87	MG	A1	4165	1/1	0.89	0.16	57,57,57,57	0
87	MG	A5	3953	1/1	0.90	0.46	69,69,69,69	0
86	OHX	A1	3666	7/7	0.90	0.19	142,142,142,142	7
87	MG	A1	3955	1/1	0.90	0.33	42,42,42,42	0
87	MG	A2	2107	1/1	0.90	0.40	66,66,66,66	0
87	MG	A1	3957	1/1	0.90	0.39	50,50,50,50	0
87	MG	A6	2304	1/1	0.90	0.17	81,81,81,81	0
86	OHX	A1	3755	7/7	0.90	0.27	135,135,135,135	7
86	OHX	A5	3730	7/7	0.90	0.25	97,97,97,97	7
87	MG	A1	3962	1/1	0.90	0.41	61,61,61,61	0
87	MG	A5	3970	1/1	0.90	0.44	60,60,60,60	0
87	MG	A1	4094	1/1	0.90	0.15	34,34,34,34	0
87	MG	A5	4184	1/1	0.90	0.20	55,55,55,55	0
87	MG	A6	2311	1/1	0.90	0.19	76,76,76,76	0
87	MG	A5	4439	1/1	0.90	0.12	56,56,56,56	0
86	OHX	A5	3731	7/7	0.90	0.17	138,138,138,138	7
87	MG	A1	3967	1/1	0.90	0.33	40,40,40,40	0
86	OHX	A5	3793	7/7	0.90	0.28	158,158,158,158	7
87	MG	A5	4449	1/1	0.90	0.35	122,122,122,122	0
86	OHX	A1	3403	7/7	0.90	0.19	169,169,169,169	7
87	MG	A1	3971	1/1	0.90	0.28	35,35,35,35	0
87	MG	A5	4453	1/1	0.90	0.16	66,66,66,66	0
87	MG	A6	2319	1/1	0.90	0.12	64,64,64,64	0
86	OHX	A1	3723	7/7	0.90	0.26	161,161,161,161	7
87	MG	A5	4462	1/1	0.90	0.23	83,83,83,83	0
86	OHX	A6	2099	7/7	0.90	0.36	184,184,184,184	7
86	OHX	A6	2059	7/7	0.90	0.20	153,153,153,153	7
87	MG	A5	4466	1/1	0.90	0.13	79,79,79,79	0
87	MG	A5	4199	1/1	0.90	0.28	70,70,70,70	0
86	OHX	A1	3724	7/7	0.90	0.17	144,144,144,144	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2252	1/1	0.90	0.08	89,89,89,89	0
87	MG	A6	2160	1/1	0.90	0.37	45,45,45,45	0
87	MG	A1	4385	1/1	0.90	0.22	65,65,65,65	0
87	MG	A4	232	1/1	0.90	0.23	74,74,74,74	0
87	MG	A4	233	1/1	0.90	0.10	57,57,57,57	0
87	MG	A6	2329	1/1	0.90	0.34	138,138,138,138	0
87	MG	A1	4243	1/1	0.90	0.19	61,61,61,61	0
87	MG	A4	236	1/1	0.90	0.13	100,100,100,100	0
87	MG	A5	4216	1/1	0.90	0.21	80,80,80,80	0
87	MG	A1	4107	1/1	0.90	0.41	74,74,74,74	0
86	OHX	A5	3801	7/7	0.90	0.16	156,156,156,156	7
87	MG	A4	241	1/1	0.90	0.24	60,60,60,60	0
87	MG	A1	4248	1/1	0.90	0.19	78,78,78,78	0
86	OHX	BP	201	7/7	0.90	0.33	115,115,115,115	7
87	MG	A5	4223	1/1	0.90	0.29	78,78,78,78	0
87	MG	A6	2174	1/1	0.90	0.14	50,50,50,50	0
87	MG	A5	4225	1/1	0.90	0.28	66,66,66,66	0
87	MG	A1	3881	1/1	0.90	0.24	39,39,39,39	0
87	MG	CB	302	1/1	0.90	0.18	93,93,93,93	0
86	OHX	A5	3805	7/7	0.90	0.16	172,172,172,172	7
87	MG	A2	2186	1/1	0.90	0.26	76,76,76,76	0
87	MG	CG	303	1/1	0.90	0.29	54,54,54,54	0
87	MG	A1	4113	1/1	0.90	0.33	70,70,70,70	0
87	MG	A5	4016	1/1	0.90	0.21	42,42,42,42	0
87	MG	A5	4233	1/1	0.90	0.24	91,91,91,91	0
87	MG	A1	3983	1/1	0.90	0.17	65,65,65,65	0
87	MG	A1	4406	1/1	0.90	0.22	69,69,69,69	0
87	MG	A5	4507	1/1	0.90	0.24	92,92,92,92	0
87	MG	A2	2120	1/1	0.90	0.38	73,73,73,73	0
86	OHX	A5	3743	7/7	0.90	0.20	167,167,167,167	7
86	OHX	A2	2023	7/7	0.90	0.19	136,136,136,136	7
86	OHX	A5	3745	7/7	0.90	0.20	131,131,131,131	7
87	MG	A5	4513	1/1	0.90	0.20	53,53,53,53	0
87	MG	A1	4414	1/1	0.90	0.24	90,90,90,90	0
87	MG	BC	405	1/1	0.90	0.27	49,49,49,49	0
87	MG	A5	4030	1/1	0.90	0.30	39,39,39,39	0
87	MG	A1	4123	1/1	0.90	0.43	77,77,77,77	0
87	MG	A5	4037	1/1	0.90	0.34	67,67,67,67	0
87	MG	A1	3988	1/1	0.90	0.35	67,67,67,67	0
87	MG	A1	4424	1/1	0.90	0.10	50,50,50,50	0
86	OHX	A2	2056	7/7	0.90	0.15	130,130,130,130	7
87	MG	A2	2125	1/1	0.90	0.37	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4255	1/1	0.90	0.14	72,72,72,72	0
86	OHX	A5	3747	7/7	0.90	0.24	160,160,160,160	7
87	MG	A2	2127	1/1	0.90	0.31	49,49,49,49	0
87	MG	A1	4433	1/1	0.90	0.21	67,67,67,67	0
86	OHX	A6	2064	7/7	0.90	0.13	164,164,164,164	7
87	MG	BL	203	1/1	0.90	0.23	61,61,61,61	0
86	OHX	Cg	401	7/7	0.90	0.14	182,182,182,182	7
87	MG	A5	4266	1/1	0.90	0.26	72,72,72,72	0
87	MG	A5	3829	1/1	0.90	0.20	35,35,35,35	0
87	MG	AP	202	1/1	0.90	0.22	88,88,88,88	0
87	MG	A1	3999	1/1	0.90	0.31	37,37,37,37	0
87	MG	A5	4545	1/1	0.90	0.47	94,94,94,94	0
87	MG	A1	4140	1/1	0.90	0.32	56,56,56,56	0
87	MG	A5	4547	1/1	0.90	0.26	88,88,88,88	0
87	MG	A1	3900	1/1	0.90	0.21	78,78,78,78	0
87	MG	A5	4551	1/1	0.90	0.19	62,62,62,62	0
87	MG	BO	208	1/1	0.90	0.24	75,75,75,75	0
87	MG	A6	2208	1/1	0.90	0.18	56,56,56,56	0
86	OHX	A6	1990	7/7	0.90	0.20	177,177,177,177	7
87	MG	BP	205	1/1	0.90	0.19	53,53,53,53	0
87	MG	A5	4287	1/1	0.90	0.22	101,101,101,101	0
87	MG	A2	2131	1/1	0.90	0.19	65,65,65,65	0
87	MG	A1	4144	1/1	0.90	0.17	82,82,82,82	0
87	MG	A5	4569	1/1	0.90	0.21	103,103,103,103	0
87	MG	A1	4146	1/1	0.90	0.58	91,91,91,91	0
87	MG	A5	4066	1/1	0.90	0.28	73,73,73,73	0
86	OHX	A2	2002	7/7	0.90	0.15	169,169,169,169	7
87	MG	A6	2215	1/1	0.90	0.10	56,56,56,56	0
87	MG	A5	3855	1/1	0.90	0.29	55,55,55,55	0
86	OHX	A2	2086	7/7	0.90	0.22	156,156,156,156	7
87	MG	A1	3908	1/1	0.90	0.23	64,64,64,64	0
87	MG	BR	203	1/1	0.90	0.11	65,65,65,65	0
86	OHX	A2	2015	7/7	0.90	0.15	138,138,138,138	7
87	MG	A1	4151	1/1	0.90	0.27	71,71,71,71	0
86	OHX	A5	3638	7/7	0.90	0.20	135,135,135,135	7
87	MG	A7	217	1/1	0.90	0.30	55,55,55,55	0
86	OHX	A2	2036	7/7	0.90	0.23	162,162,162,162	7
87	MG	A1	3913	1/1	0.90	0.29	86,86,86,86	0
87	MG	A5	4314	1/1	0.90	0.15	56,56,56,56	0
87	MG	A5	4080	1/1	0.90	0.33	71,71,71,71	0
87	MG	A7	224	1/1	0.90	0.09	69,69,69,69	0
87	MG	A6	2231	1/1	0.90	0.19	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3607	7/7	0.90	0.12	204,204,204,204	7
87	MG	A7	227	1/1	0.90	0.22	100,100,100,100	0
86	OHX	A1	3773	7/7	0.90	0.24	159,159,159,159	7
87	MG	A1	3917	1/1	0.90	0.18	31,31,31,31	0
87	MG	Ba	201	1/1	0.90	0.09	66,66,66,66	0
87	MG	A1	4024	1/1	0.90	0.32	40,40,40,40	0
87	MG	A2	2139	1/1	0.90	0.38	81,81,81,81	0
87	MG	A5	4324	1/1	0.90	0.21	80,80,80,80	0
86	OHX	A5	3669	7/7	0.90	0.28	109,109,109,109	7
87	MG	A5	4328	1/1	0.90	0.15	72,72,72,72	0
87	MG	A8	221	1/1	0.90	0.14	33,33,33,33	0
87	MG	A5	3878	1/1	0.90	0.22	56,56,56,56	0
87	MG	A1	3819	1/1	0.90	0.09	63,63,63,63	0
86	OHX	A6	2024	7/7	0.90	0.17	156,156,156,156	7
86	OHX	A1	3688	7/7	0.90	0.16	181,181,181,181	7
87	MG	A1	4468	1/1	0.90	0.24	79,79,79,79	0
87	MG	A1	3827	1/1	0.90	0.28	47,47,47,47	0
86	OHX	A1	3696	7/7	0.90	0.18	143,143,143,143	7
86	OHX	A1	3619	7/7	0.90	0.24	128,128,128,128	7
86	OHX	DC	402	7/7	0.90	0.18	145,145,145,145	7
87	MG	A1	4177	1/1	0.90	0.18	76,76,76,76	0
87	MG	A5	4339	1/1	0.90	0.15	66,66,66,66	0
86	OHX	A2	2021	7/7	0.90	0.28	158,158,158,158	7
87	MG	A8	239	1/1	0.90	0.21	93,93,93,93	0
87	MG	A5	4107	1/1	0.90	0.27	66,66,66,66	0
87	MG	A5	4108	1/1	0.90	0.43	74,74,74,74	0
86	OHX	A5	3690	7/7	0.90	0.29	130,130,130,130	7
87	MG	A5	4111	1/1	0.90	0.28	65,65,65,65	0
87	MG	A1	4312	1/1	0.90	0.23	60,60,60,60	0
87	MG	A1	3929	1/1	0.90	0.28	75,75,75,75	0
87	MG	A1	4183	1/1	0.90	0.15	51,51,51,51	0
87	MG	A5	4350	1/1	0.90	0.34	58,58,58,58	0
87	MG	A1	4045	1/1	0.90	0.18	55,55,55,55	0
86	OHX	A1	3636	7/7	0.90	0.17	148,148,148,148	7
87	MG	A1	4321	1/1	0.90	0.24	88,88,88,88	0
87	MG	A1	4322	1/1	0.90	0.27	74,74,74,74	0
87	MG	A5	4357	1/1	0.90	0.31	75,75,75,75	0
86	OHX	A6	2034	7/7	0.90	0.19	137,137,137,137	7
86	OHX	DP	201	7/7	0.90	0.17	155,155,155,155	7
87	MG	A1	4049	1/1	0.90	0.21	59,59,59,59	0
86	OHX	A5	3773	7/7	0.90	0.14	141,141,141,141	7
86	OHX	A5	3697	7/7	0.90	0.15	167,167,167,167	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	DF	302	1/1	0.90	0.25	48,48,48,48	0
87	MG	A6	2267	1/1	0.90	0.15	72,72,72,72	0
87	MG	A5	4366	1/1	0.90	0.15	65,65,65,65	0
87	MG	A1	4493	1/1	0.90	0.19	66,66,66,66	0
87	MG	A5	4369	1/1	0.90	0.22	69,69,69,69	0
86	OHX	A1	3707	7/7	0.90	0.17	135,135,135,135	7
87	MG	A1	4056	1/1	0.90	0.22	61,61,61,61	0
87	MG	A1	3847	1/1	0.90	0.19	74,74,74,74	0
86	OHX	A1	3639	7/7	0.90	0.19	145,145,145,145	7
87	MG	DO	203	1/1	0.90	0.25	58,58,58,58	0
86	OHX	A2	2046	7/7	0.90	0.37	139,139,139,139	7
87	MG	DO	206	1/1	0.90	0.20	55,55,55,55	0
87	MG	A6	2274	1/1	0.90	0.20	95,95,95,95	0
87	MG	A6	2275	1/1	0.90	0.10	63,63,63,63	0
86	OHX	A1	3787	7/7	0.90	0.20	173,173,173,173	7
87	MG	A1	4062	1/1	0.90	0.31	72,72,72,72	0
87	MG	A2	2096	1/1	0.90	0.45	76,76,76,76	0
87	MG	A5	4385	1/1	0.90	0.23	74,74,74,74	0
87	MG	A1	4066	1/1	0.90	0.17	53,53,53,53	0
87	MG	A5	4389	1/1	0.90	0.21	66,66,66,66	0
87	MG	DS	204	1/1	0.90	0.15	63,63,63,63	0
87	MG	A1	4067	1/1	0.90	0.29	66,66,66,66	0
86	OHX	A1	3710	7/7	0.90	0.26	122,122,122,122	7
87	MG	A6	2285	1/1	0.90	0.30	74,74,74,74	0
87	MG	DW	201	1/1	0.90	0.35	85,85,85,85	0
87	MG	A6	2286	1/1	0.90	0.24	75,75,75,75	0
86	OHX	AN	201	7/7	0.90	0.11	192,192,192,192	7
86	OHX	A1	3719	7/7	0.90	0.18	154,154,154,154	7
87	MG	A5	4157	1/1	0.90	0.15	56,56,56,56	0
86	OHX	A4	213	7/7	0.90	0.18	164,164,164,164	7
87	MG	A5	4401	1/1	0.90	0.20	64,64,64,64	0
87	MG	A5	4162	1/1	0.90	0.24	70,70,70,70	0
87	MG	A5	4405	1/1	0.90	0.23	69,69,69,69	0
87	MG	A1	3947	1/1	0.90	0.39	42,42,42,42	0
86	OHX	A5	3721	7/7	0.90	0.22	167,167,167,167	7
86	OHX	A2	2072	7/7	0.90	0.30	207,207,207,207	7
86	OHX	A5	3724	7/7	0.90	0.30	124,124,124,124	7
87	MG	Dj	103	1/1	0.90	0.34	65,65,65,65	0
87	MG	Dl	101	1/1	0.90	0.31	112,112,112,112	0
87	MG	A5	4415	1/1	0.90	0.18	75,75,75,75	0
87	MG	A5	3943	1/1	0.90	0.37	38,38,38,38	0
87	MG	A5	3947	1/1	0.90	0.19	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A4	215	7/7	0.90	0.23	175,175,175,175	7
87	MG	A5	3950	1/1	0.90	0.38	38,38,38,38	0
87	MG	A6	2295	1/1	0.90	0.14	79,79,79,79	0
87	MG	A5	3870	1/1	0.91	0.29	56,56,56,56	0
87	MG	A1	4358	1/1	0.91	0.17	86,86,86,86	0
86	OHX	A2	2066	7/7	0.91	0.27	164,164,164,164	7
86	OHX	BA	301	7/7	0.91	0.29	217,217,217,217	7
87	MG	A1	4361	1/1	0.91	0.22	126,126,126,126	0
86	OHX	A2	2039	7/7	0.91	0.26	157,157,157,157	7
86	OHX	A1	3674	7/7	0.91	0.20	159,159,159,159	7
87	MG	A1	4508	1/1	0.91	0.12	58,58,58,58	0
87	MG	A1	4124	1/1	0.91	0.21	53,53,53,53	0
87	MG	A6	2257	1/1	0.91	0.34	65,65,65,65	0
86	OHX	A1	3704	7/7	0.91	0.14	176,176,176,176	7
87	MG	A1	4366	1/1	0.91	0.42	86,86,86,86	0
87	MG	A1	3911	1/1	0.91	0.08	58,58,58,58	0
86	OHX	A1	3730	7/7	0.91	0.21	135,135,135,135	7
87	MG	A5	3886	1/1	0.91	0.26	43,43,43,43	0
87	MG	A6	2117	1/1	0.91	0.34	64,64,64,64	0
87	MG	A1	4132	1/1	0.91	0.13	64,64,64,64	0
87	MG	A5	4278	1/1	0.91	0.20	82,82,82,82	0
87	MG	A1	4013	1/1	0.91	0.28	47,47,47,47	0
86	OHX	A1	3731	7/7	0.91	0.21	119,119,119,119	7
87	MG	Af	201	1/1	0.91	0.24	88,88,88,88	0
86	OHX	A1	3705	7/7	0.91	0.16	164,164,164,164	7
87	MG	A6	2123	1/1	0.91	0.25	51,51,51,51	0
87	MG	A3	226	1/1	0.91	0.26	69,69,69,69	0
87	MG	A1	4379	1/1	0.91	0.13	70,70,70,70	0
86	OHX	A1	3763	7/7	0.91	0.27	157,157,157,157	7
87	MG	A1	4382	1/1	0.91	0.15	81,81,81,81	0
86	OHX	A6	1977	7/7	0.91	0.16	128,128,128,128	7
87	MG	A1	4020	1/1	0.91	0.30	52,52,52,52	0
87	MG	A5	4092	1/1	0.91	0.41	82,82,82,82	0
86	OHX	A1	3733	7/7	0.91	0.25	125,125,125,125	7
86	OHX	A1	3767	7/7	0.91	0.24	158,158,158,158	7
87	MG	A5	4097	1/1	0.91	0.20	37,37,37,37	0
87	MG	A1	3820	1/1	0.91	0.31	47,47,47,47	0
87	MG	A5	4305	1/1	0.91	0.15	88,88,88,88	0
86	OHX	A1	3675	7/7	0.91	0.16	169,169,169,169	7
87	MG	A1	3825	1/1	0.91	0.21	47,47,47,47	0
87	MG	A5	4528	1/1	0.91	0.22	97,97,97,97	0
87	MG	A1	4392	1/1	0.91	0.25	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A6	1998	7/7	0.91	0.17	147,147,147,147	7
87	MG	A5	4104	1/1	0.91	0.29	52,52,52,52	0
86	OHX	A5	3624	7/7	0.91	0.25	82,82,82,82	7
87	MG	A5	4316	1/1	0.91	0.19	57,57,57,57	0
87	MG	A4	227	1/1	0.91	0.11	53,53,53,53	0
86	OHX	A5	3750	7/7	0.91	0.25	199,199,199,199	7
86	OHX	A5	3637	7/7	0.91	0.15	178,178,178,178	7
87	MG	A5	3916	1/1	0.91	0.28	49,49,49,49	0
86	OHX	A1	3623	7/7	0.91	0.16	147,147,147,147	7
87	MG	A1	4403	1/1	0.91	0.15	71,71,71,71	0
86	OHX	A7	212	7/7	0.91	0.44	165,165,165,165	7
86	OHX	A5	3639	7/7	0.91	0.14	157,157,157,157	7
87	MG	A1	3837	1/1	0.91	0.34	68,68,68,68	0
87	MG	A5	4116	1/1	0.91	0.17	56,56,56,56	0
86	OHX	A8	212	7/7	0.91	0.18	172,172,172,172	7
87	MG	A5	4554	1/1	0.91	0.21	86,86,86,86	0
87	MG	A1	4157	1/1	0.91	0.24	87,87,87,87	0
87	MG	A6	2300	1/1	0.91	0.27	56,56,56,56	0
87	MG	A5	4557	1/1	0.91	0.11	69,69,69,69	0
87	MG	A5	4125	1/1	0.91	0.29	67,67,67,67	0
86	OHX	A1	3679	7/7	0.91	0.26	114,114,114,114	7
87	MG	A4	240	1/1	0.91	0.25	72,72,72,72	0
87	MG	A5	3930	1/1	0.91	0.15	29,29,29,29	0
87	MG	A5	4129	1/1	0.91	0.20	94,94,94,94	0
87	MG	A6	2303	1/1	0.91	0.22	60,60,60,60	0
86	OHX	A5	3654	7/7	0.91	0.15	116,116,116,116	7
87	MG	A1	4415	1/1	0.91	0.20	85,85,85,85	0
87	MG	A1	4419	1/1	0.91	0.14	79,79,79,79	0
86	OHX	A5	3656	7/7	0.91	0.13	169,169,169,169	7
87	MG	A1	3843	1/1	0.91	0.21	46,46,46,46	0
87	MG	A5	3938	1/1	0.91	0.29	45,45,45,45	0
87	MG	A5	4345	1/1	0.91	0.18	77,77,77,77	0
86	OHX	A5	3757	7/7	0.91	0.09	192,192,192,192	7
87	MG	A1	4050	1/1	0.91	0.23	63,63,63,63	0
87	MG	A6	2313	1/1	0.91	0.30	78,78,78,78	0
87	MG	A5	3944	1/1	0.91	0.18	36,36,36,36	0
87	MG	A5	3946	1/1	0.91	0.39	41,41,41,41	0
86	OHX	A6	2005	7/7	0.91	0.23	145,145,145,145	7
87	MG	A1	4427	1/1	0.91	0.18	77,77,77,77	0
86	OHX	A8	219	7/7	0.91	0.26	166,166,166,166	7
86	OHX	DB	402	7/7	0.91	0.12	145,145,145,145	7
87	MG	A1	4055	1/1	0.91	0.22	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A2	2223	1/1	0.91	0.31	156,156,156,156	0
87	MG	BC	402	1/1	0.91	0.14	54,54,54,54	0
86	OHX	A6	2007	7/7	0.91	0.18	164,164,164,164	7
86	OHX	A1	3738	7/7	0.91	0.23	138,138,138,138	7
86	OHX	A2	2078	7/7	0.91	0.33	169,169,169,169	7
87	MG	BC	407	1/1	0.91	0.20	58,58,58,58	0
87	MG	A5	4160	1/1	0.91	0.14	53,53,53,53	0
87	MG	A5	4367	1/1	0.91	0.26	74,74,74,74	0
86	OHX	DI	302	7/7	0.91	0.22	160,160,160,160	7
87	MG	A7	238	1/1	0.91	0.21	95,95,95,95	0
87	MG	A1	4180	1/1	0.91	0.19	79,79,79,79	0
87	MG	BF	4101	1/1	0.91	0.16	64,64,64,64	0
86	OHX	A5	3673	7/7	0.91	0.22	144,144,144,144	7
86	OHX	A5	3679	7/7	0.91	0.17	174,174,174,174	7
87	MG	A1	3858	1/1	0.91	0.39	64,64,64,64	0
87	MG	A5	3974	1/1	0.91	0.32	40,40,40,40	0
87	MG	BI	307	1/1	0.91	0.19	81,81,81,81	0
86	OHX	A6	2017	7/7	0.91	0.18	132,132,132,132	7
87	MG	A1	4187	1/1	0.91	0.22	90,90,90,90	0
86	OHX	A6	2019	7/7	0.91	0.20	127,127,127,127	7
86	OHX	Dg	201	7/7	0.91	0.28	153,153,153,153	7
87	MG	A5	3980	1/1	0.91	0.33	58,58,58,58	0
86	OHX	A2	2003	7/7	0.91	0.14	147,147,147,147	7
87	MG	A5	4387	1/1	0.91	0.15	93,93,93,93	0
86	OHX	A1	3776	7/7	0.91	0.26	123,123,123,123	7
87	MG	A1	3864	1/1	0.91	0.17	46,46,46,46	0
87	MG	A1	4310	1/1	0.91	0.36	67,67,67,67	0
87	MG	BO	203	1/1	0.91	0.22	74,74,74,74	0
87	MG	A2	2235	1/1	0.91	0.17	80,80,80,80	0
87	MG	A1	3867	1/1	0.91	0.27	61,61,61,61	0
86	OHX	A1	3777	7/7	0.91	0.22	137,137,137,137	7
87	MG	BP	203	1/1	0.91	0.32	71,71,71,71	0
86	OHX	A5	3692	7/7	0.91	0.12	170,170,170,170	7
86	OHX	A6	2079	7/7	0.91	0.16	161,161,161,161	7
87	MG	A1	4083	1/1	0.91	0.21	44,44,44,44	0
87	MG	DB	415	1/1	0.91	0.37	91,91,91,91	0
87	MG	A5	4403	1/1	0.91	0.13	81,81,81,81	0
86	OHX	A1	3714	7/7	0.91	0.31	118,118,118,118	7
87	MG	A5	3996	1/1	0.91	0.38	46,46,46,46	0
87	MG	A5	4407	1/1	0.91	0.39	95,95,95,95	0
87	MG	A5	3997	1/1	0.91	0.37	43,43,43,43	0
87	MG	A5	4410	1/1	0.91	0.25	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	4203	1/1	0.91	0.10	69,69,69,69	0
87	MG	A5	3999	1/1	0.91	0.23	32,32,32,32	0
87	MG	A5	4195	1/1	0.91	0.16	72,72,72,72	0
87	MG	DG	302	1/1	0.91	0.28	65,65,65,65	0
87	MG	BQ	201	1/1	0.91	0.16	65,65,65,65	0
86	OHX	A2	2014	7/7	0.91	0.20	166,166,166,166	7
86	OHX	A1	3780	7/7	0.91	0.18	136,136,136,136	7
86	OHX	A5	3700	7/7	0.91	0.32	146,146,146,146	7
87	MG	A2	2100	1/1	0.91	0.25	67,67,67,67	0
87	MG	A5	4421	1/1	0.91	0.22	55,55,55,55	0
86	OHX	A1	3641	7/7	0.91	0.21	137,137,137,137	7
87	MG	A1	4328	1/1	0.91	0.37	76,76,76,76	0
87	MG	A1	4474	1/1	0.91	0.30	72,72,72,72	0
87	MG	A5	4012	1/1	0.91	0.33	43,43,43,43	0
86	OHX	A5	3705	7/7	0.91	0.22	152,152,152,152	7
86	OHX	A1	3747	7/7	0.91	0.21	118,118,118,118	7
87	MG	A5	4429	1/1	0.91	0.13	58,58,58,58	0
87	MG	A5	3411	1/1	0.91	0.21	82,82,82,82	0
87	MG	DP	203	1/1	0.91	0.32	37,37,37,37	0
86	OHX	A5	3707	7/7	0.91	0.34	135,135,135,135	7
87	MG	DP	207	1/1	0.91	0.24	64,64,64,64	0
86	OHX	A6	2037	7/7	0.91	0.22	138,138,138,138	7
87	MG	BY	201	1/1	0.91	0.13	56,56,56,56	0
86	OHX	A5	3710	7/7	0.91	0.15	132,132,132,132	7
87	MG	A5	3834	1/1	0.91	0.26	59,59,59,59	0
87	MG	A2	2177	1/1	0.91	0.25	83,83,83,83	0
87	MG	A6	2225	1/1	0.91	0.17	59,59,59,59	0
87	MG	A5	3839	1/1	0.91	0.15	48,48,48,48	0
86	OHX	A1	3643	7/7	0.91	0.15	153,153,153,153	7
87	MG	A6	2227	1/1	0.91	0.12	67,67,67,67	0
87	MG	A5	4447	1/1	0.91	0.18	61,61,61,61	0
86	OHX	A6	2041	7/7	0.91	0.24	145,145,145,145	7
87	MG	A6	2229	1/1	0.91	0.27	65,65,65,65	0
87	MG	A2	2180	1/1	0.91	0.29	101,101,101,101	0
86	OHX	A5	3713	7/7	0.91	0.25	122,122,122,122	7
87	MG	Da	204	1/1	0.91	0.21	52,52,52,52	0
86	OHX	A5	3715	7/7	0.91	0.25	100,100,100,100	7
87	MG	Be	202	1/1	0.91	0.15	67,67,67,67	0
87	MG	A5	4458	1/1	0.91	0.22	76,76,76,76	0
86	OHX	A6	2042	7/7	0.91	0.19	169,169,169,169	7
86	OHX	A2	2042	7/7	0.91	0.15	155,155,155,155	7
86	OHX	A2	1988	7/7	0.91	0.21	189,189,189,189	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	Bj	108	1/1	0.91	0.28	66,66,66,66	0
86	OHX	A6	2045	7/7	0.91	0.24	124,124,124,124	7
87	MG	A1	4351	1/1	0.91	0.11	97,97,97,97	0
86	OHX	A5	3723	7/7	0.91	0.17	180,180,180,180	7
86	OHX	A1	3751	7/7	0.91	0.13	189,189,189,189	7
86	OHX	A5	3797	7/7	0.91	0.30	130,130,130,130	7
86	OHX	A1	3691	7/7	0.91	0.25	175,175,175,175	7
86	OHX	A2	2008	7/7	0.91	0.20	135,135,135,135	7
87	MG	A1	4116	1/1	0.91	0.09	65,65,65,65	0
87	MG	A5	4242	1/1	0.92	0.22	65,65,65,65	0
87	MG	A5	4047	1/1	0.92	0.28	57,57,57,57	0
86	OHX	A1	3690	7/7	0.92	0.25	178,178,178,178	7
86	OHX	A2	1999	7/7	0.92	0.16	168,168,168,168	7
87	MG	A1	4332	1/1	0.92	0.25	74,74,74,74	0
87	MG	A5	3859	1/1	0.92	0.17	50,50,50,50	0
87	MG	A5	4481	1/1	0.92	0.20	60,60,60,60	0
86	OHX	A1	3694	7/7	0.92	0.26	131,131,131,131	7
86	OHX	A1	3695	7/7	0.92	0.13	163,163,163,163	7
87	MG	A5	4484	1/1	0.92	0.21	89,89,89,89	0
86	OHX	A1	3573	7/7	0.92	0.24	120,120,120,120	7
87	MG	A1	4338	1/1	0.92	0.18	84,84,84,84	0
86	OHX	A1	3644	7/7	0.92	0.20	139,139,139,139	7
87	MG	A5	4057	1/1	0.92	0.26	82,82,82,82	0
86	OHX	A1	3647	7/7	0.92	0.17	129,129,129,129	7
87	MG	A5	4059	1/1	0.92	0.43	71,71,71,71	0
87	MG	A1	3979	1/1	0.92	0.31	52,52,52,52	0
87	MG	A1	4091	1/1	0.92	0.33	65,65,65,65	0
87	MG	A1	4093	1/1	0.92	0.25	55,55,55,55	0
87	MG	A5	4494	1/1	0.92	0.21	111,111,111,111	0
86	OHX	A6	2038	7/7	0.92	0.21	169,169,169,169	7
86	OHX	A2	2016	7/7	0.92	0.15	156,156,156,156	7
87	MG	A5	4065	1/1	0.92	0.22	68,68,68,68	0
86	OHX	A3	211	7/7	0.92	0.21	137,137,137,137	7
87	MG	A1	4494	1/1	0.92	0.10	87,87,87,87	0
87	MG	A5	4500	1/1	0.92	0.15	82,82,82,82	0
86	OHX	A5	3709	7/7	0.92	0.11	171,171,171,171	7
86	OHX	A1	3740	7/7	0.92	0.27	107,107,107,107	7
86	OHX	A1	3703	7/7	0.92	0.25	93,93,93,93	7
86	OHX	A4	211	7/7	0.92	0.22	108,108,108,108	7
87	MG	A1	4500	1/1	0.92	0.14	106,106,106,106	0
86	OHX	A1	3743	7/7	0.92	0.33	148,148,148,148	7
87	MG	A5	4280	1/1	0.92	0.20	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4283	1/1	0.92	0.17	79,79,79,79	0
86	OHX	A2	2068	7/7	0.92	0.28	177,177,177,177	7
86	OHX	A1	3660	7/7	0.92	0.24	137,137,137,137	7
86	OHX	A2	2017	7/7	0.92	0.14	186,186,186,186	7
87	MG	A6	2109	1/1	0.92	0.32	54,54,54,54	0
86	OHX	A1	3606	7/7	0.92	0.19	132,132,132,132	7
86	OHX	A2	1947	7/7	0.92	0.15	157,157,157,157	7
86	OHX	A1	3670	7/7	0.92	0.18	152,152,152,152	7
87	MG	A2	2195	1/1	0.92	0.20	90,90,90,90	0
86	OHX	A1	3711	7/7	0.92	0.26	155,155,155,155	7
86	OHX	CP	201	7/7	0.92	0.10	177,177,177,177	7
86	OHX	A1	3673	7/7	0.92	0.21	154,154,154,154	7
87	MG	A5	4296	1/1	0.92	0.15	54,54,54,54	0
87	MG	A1	4234	1/1	0.92	0.42	82,82,82,82	0
87	MG	A5	4298	1/1	0.92	0.18	106,106,106,106	0
87	MG	A3	218	1/1	0.92	0.20	46,46,46,46	0
87	MG	A1	4235	1/1	0.92	0.20	62,62,62,62	0
87	MG	A5	4532	1/1	0.92	0.22	95,95,95,95	0
87	MG	A5	4533	1/1	0.92	0.20	83,83,83,83	0
86	OHX	CY	202	7/7	0.92	0.13	130,130,130,130	7
86	OHX	A5	3729	7/7	0.92	0.16	165,165,165,165	7
87	MG	A5	4094	1/1	0.92	0.23	69,69,69,69	0
86	OHX	A1	3608	7/7	0.92	0.13	160,160,160,160	7
87	MG	A5	4538	1/1	0.92	0.17	67,67,67,67	0
87	MG	A6	2124	1/1	0.92	0.10	55,55,55,55	0
87	MG	A5	4541	1/1	0.92	0.26	107,107,107,107	0
86	OHX	A5	3403	7/7	0.92	0.20	171,171,171,171	7
87	MG	A6	2279	1/1	0.92	0.15	81,81,81,81	0
87	MG	A5	4544	1/1	0.92	0.27	79,79,79,79	0
86	OHX	A5	3405	7/7	0.92	0.31	118,118,118,118	7
86	OHX	BP	202	7/7	0.92	0.15	139,139,139,139	7
87	MG	A5	3910	1/1	0.92	0.37	57,57,57,57	0
87	MG	A1	4120	1/1	0.92	0.13	26,26,26,26	0
87	MG	A6	2283	1/1	0.92	0.12	75,75,75,75	0
87	MG	A6	2284	1/1	0.92	0.25	107,107,107,107	0
87	MG	A1	4122	1/1	0.92	0.25	57,57,57,57	0
87	MG	A1	4377	1/1	0.92	0.30	54,54,54,54	0
87	MG	A1	3823	1/1	0.92	0.24	60,60,60,60	0
86	OHX	A1	3609	7/7	0.92	0.20	122,122,122,122	7
87	MG	A5	4110	1/1	0.92	0.28	63,63,63,63	0
87	MG	A1	4381	1/1	0.92	0.18	65,65,65,65	0
87	MG	A1	3916	1/1	0.92	0.42	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3518	7/7	0.92	0.18	159,159,159,159	7
87	MG	A1	4128	1/1	0.92	0.18	63,63,63,63	0
87	MG	A1	4017	1/1	0.92	0.34	48,48,48,48	0
87	MG	A1	4130	1/1	0.92	0.26	69,69,69,69	0
87	MG	A5	4117	1/1	0.92	0.20	49,49,49,49	0
87	MG	A5	4573	1/1	0.92	0.27	56,56,56,56	0
87	MG	A4	224	1/1	0.92	0.17	30,30,30,30	0
87	MG	A5	4120	1/1	0.92	0.10	49,49,49,49	0
87	MG	A1	4254	1/1	0.92	0.28	72,72,72,72	0
87	MG	A1	4389	1/1	0.92	0.19	46,46,46,46	0
87	MG	A5	4579	1/1	0.92	0.19	57,57,57,57	0
86	OHX	A5	3551	7/7	0.92	0.16	142,142,142,142	7
86	OHX	A5	3584	7/7	0.92	0.21	119,119,119,119	7
87	MG	A1	3828	1/1	0.92	0.21	43,43,43,43	0
87	MG	A7	215	1/1	0.92	0.20	46,46,46,46	0
86	OHX	A5	3742	7/7	0.92	0.27	143,143,143,143	7
87	MG	A5	3934	1/1	0.92	0.17	61,61,61,61	0
87	MG	A1	4022	1/1	0.92	0.18	40,40,40,40	0
87	MG	A1	3830	1/1	0.92	0.30	60,60,60,60	0
87	MG	A1	4399	1/1	0.92	0.14	85,85,85,85	0
86	OHX	A5	3585	7/7	0.92	0.20	163,163,163,163	7
87	MG	A7	222	1/1	0.92	0.24	94,94,94,94	0
86	OHX	A1	3677	7/7	0.92	0.26	115,115,115,115	7
87	MG	A5	4136	1/1	0.92	0.08	46,46,46,46	0
87	MG	A1	4028	1/1	0.92	0.29	28,28,28,28	0
86	OHX	A5	3604	7/7	0.92	0.23	113,113,113,113	7
87	MG	A1	4405	1/1	0.92	0.12	61,61,61,61	0
87	MG	A1	3834	1/1	0.92	0.07	44,44,44,44	0
86	OHX	A5	3612	7/7	0.92	0.23	147,147,147,147	7
87	MG	A1	4408	1/1	0.92	0.21	81,81,81,81	0
87	MG	A5	4145	1/1	0.92	0.22	57,57,57,57	0
87	MG	A4	244	1/1	0.92	0.27	61,61,61,61	0
87	MG	A5	4147	1/1	0.92	0.18	63,63,63,63	0
87	MG	A1	4267	1/1	0.92	0.14	82,82,82,82	0
87	MG	A1	4145	1/1	0.92	0.14	54,54,54,54	0
87	MG	A1	4034	1/1	0.92	0.16	46,46,46,46	0
86	OHX	A6	1986	7/7	0.92	0.18	165,165,165,165	7
87	MG	A5	3956	1/1	0.92	0.23	39,39,39,39	0
87	MG	A1	4036	1/1	0.92	0.42	71,71,71,71	0
87	MG	A1	4416	1/1	0.92	0.25	57,57,57,57	0
86	OHX	A5	3622	7/7	0.92	0.13	136,136,136,136	7
87	MG	A5	3963	1/1	0.92	0.35	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3794	7/7	0.92	0.28	150,150,150,150	7
87	MG	A1	3840	1/1	0.92	0.31	59,59,59,59	0
87	MG	A5	4376	1/1	0.92	0.13	67,67,67,67	0
87	MG	A1	4423	1/1	0.92	0.15	85,85,85,85	0
87	MG	BB	406	1/1	0.92	0.19	59,59,59,59	0
86	OHX	A5	3630	7/7	0.92	0.17	128,128,128,128	7
86	OHX	A1	3615	7/7	0.92	0.26	139,139,139,139	7
86	OHX	A1	3616	7/7	0.92	0.29	117,117,117,117	7
87	MG	A1	4044	1/1	0.92	0.24	44,44,44,44	0
87	MG	DA	304	1/1	0.92	0.21	69,69,69,69	0
87	MG	A1	4430	1/1	0.92	0.15	67,67,67,67	0
86	OHX	A1	3618	7/7	0.92	0.23	158,158,158,158	7
86	OHX	A6	2065	7/7	0.92	0.22	156,156,156,156	7
86	OHX	A5	3648	7/7	0.92	0.19	111,111,111,111	7
87	MG	A1	4160	1/1	0.92	0.24	70,70,70,70	0
87	MG	DB	409	1/1	0.92	0.14	56,56,56,56	0
86	OHX	A8	220	7/7	0.92	0.27	111,111,111,111	7
86	OHX	A2	2011	7/7	0.92	0.20	154,154,154,154	7
86	OHX	A6	2001	7/7	0.92	0.16	149,149,149,149	7
87	MG	A1	4438	1/1	0.92	0.13	82,82,82,82	0
87	MG	DC	403	1/1	0.92	0.13	65,65,65,65	0
87	MG	A2	2151	1/1	0.92	0.08	49,49,49,49	0
86	OHX	A2	1995	7/7	0.92	0.15	171,171,171,171	7
87	MG	A1	4167	1/1	0.92	0.25	66,66,66,66	0
86	OHX	A1	3627	7/7	0.92	0.21	130,130,130,130	7
87	MG	A1	3855	1/1	0.92	0.20	40,40,40,40	0
87	MG	BN	305	1/1	0.92	0.32	56,56,56,56	0
86	OHX	DH	201	7/7	0.92	0.13	142,142,142,142	7
87	MG	A1	4174	1/1	0.92	0.22	57,57,57,57	0
86	OHX	DI	301	7/7	0.92	0.20	118,118,118,118	7
86	OHX	A5	3762	7/7	0.92	0.21	153,153,153,153	7
87	MG	BO	206	1/1	0.92	0.14	69,69,69,69	0
87	MG	BO	207	1/1	0.92	0.23	56,56,56,56	0
86	OHX	A5	3666	7/7	0.92	0.19	127,127,127,127	7
87	MG	A6	2207	1/1	0.92	0.11	57,57,57,57	0
86	OHX	A5	3764	7/7	0.92	0.30	120,120,120,120	7
87	MG	A5	4001	1/1	0.92	0.42	48,48,48,48	0
87	MG	Ca	201	1/1	0.92	0.15	67,67,67,67	0
86	OHX	A2	2022	7/7	0.92	0.20	138,138,138,138	7
87	MG	A5	4197	1/1	0.92	0.21	84,84,84,84	0
87	MG	Ch	301	1/1	0.92	0.12	44,44,44,44	0
87	MG	BP	204	1/1	0.92	0.38	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4200	1/1	0.92	0.16	70,70,70,70	0
87	MG	A5	3409	1/1	0.92	0.23	45,45,45,45	0
87	MG	A5	4205	1/1	0.92	0.35	79,79,79,79	0
86	OHX	A1	3764	7/7	0.92	0.17	159,159,159,159	7
87	MG	A5	4008	1/1	0.92	0.37	42,42,42,42	0
87	MG	A1	4456	1/1	0.92	0.12	76,76,76,76	0
86	OHX	A6	2009	7/7	0.92	0.20	136,136,136,136	7
87	MG	A1	4309	1/1	0.92	0.23	99,99,99,99	0
86	OHX	A2	2074	7/7	0.92	0.12	191,191,191,191	7
86	OHX	A6	2015	7/7	0.92	0.15	159,159,159,159	7
87	MG	A5	4017	1/1	0.92	0.50	62,62,62,62	0
87	MG	A5	4436	1/1	0.92	0.33	90,90,90,90	0
87	MG	A5	4020	1/1	0.92	0.35	33,33,33,33	0
87	MG	A1	4185	1/1	0.92	0.22	65,65,65,65	0
87	MG	A1	3960	1/1	0.92	0.25	54,54,54,54	0
87	MG	A5	3837	1/1	0.92	0.32	58,58,58,58	0
87	MG	A1	4070	1/1	0.92	0.32	76,76,76,76	0
87	MG	A5	4446	1/1	0.92	0.18	64,64,64,64	0
86	OHX	A5	3681	7/7	0.92	0.27	112,112,112,112	7
86	OHX	A1	3766	7/7	0.92	0.26	135,135,135,135	7
87	MG	A1	4073	1/1	0.92	0.13	57,57,57,57	0
87	MG	A1	4191	1/1	0.92	0.13	58,58,58,58	0
86	OHX	A2	1997	7/7	0.92	0.20	121,121,121,121	7
87	MG	A5	3846	1/1	0.92	0.16	37,37,37,37	0
86	OHX	A6	2021	7/7	0.92	0.18	131,131,131,131	7
87	MG	A5	3848	1/1	0.92	0.35	77,77,77,77	0
87	MG	A5	4461	1/1	0.92	0.23	62,62,62,62	0
87	MG	Dg	202	1/1	0.92	0.12	50,50,50,50	0
87	MG	A1	4077	1/1	0.92	0.33	77,77,77,77	0
87	MG	A6	2230	1/1	0.92	0.14	86,86,86,86	0
86	OHX	A5	3774	7/7	0.92	0.24	148,148,148,148	7
87	MG	A5	4465	1/1	0.92	0.16	62,62,62,62	0
86	OHX	A1	3689	7/7	0.92	0.21	99,99,99,99	7
87	MG	A5	3853	1/1	0.92	0.22	67,67,67,67	0
86	OHX	A1	3769	7/7	0.92	0.24	142,142,142,142	7
87	MG	A5	4472	1/1	0.92	0.24	75,75,75,75	0
87	MG	A5	4046	1/1	0.92	0.13	39,39,39,39	0
86	OHX	A2	1946	7/7	0.93	0.12	156,156,156,156	7
87	MG	A5	3949	1/1	0.93	0.23	37,37,37,37	0
87	MG	BP	206	1/1	0.93	0.31	86,86,86,86	0
86	OHX	A5	3687	7/7	0.93	0.23	109,109,109,109	7
86	OHX	A2	2030	7/7	0.93	0.27	155,155,155,155	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4119	1/1	0.93	0.26	65,65,65,65	0
87	MG	AL	202	1/1	0.93	0.17	78,78,78,78	0
87	MG	A5	4308	1/1	0.93	0.26	52,52,52,52	0
87	MG	A1	4346	1/1	0.93	0.08	53,53,53,53	0
87	MG	A1	4002	1/1	0.93	0.25	37,37,37,37	0
87	MG	A6	2202	1/1	0.93	0.41	71,71,71,71	0
86	OHX	Bj	103	7/7	0.93	0.24	138,138,138,138	7
87	MG	A5	3959	1/1	0.93	0.42	61,61,61,61	0
87	MG	A5	4514	1/1	0.93	0.37	98,98,98,98	0
86	OHX	A6	2096	7/7	0.93	0.17	156,156,156,156	7
86	OHX	A1	3601	7/7	0.93	0.13	184,184,184,184	7
87	MG	A1	3902	1/1	0.93	0.19	47,47,47,47	0
86	OHX	A1	3651	7/7	0.93	0.16	131,131,131,131	7
87	MG	A1	3905	1/1	0.93	0.10	19,19,19,19	0
87	MG	A5	4133	1/1	0.93	0.08	54,54,54,54	0
87	MG	A5	4523	1/1	0.93	0.18	65,65,65,65	0
87	MG	A5	3968	1/1	0.93	0.22	50,50,50,50	0
86	OHX	A1	3692	7/7	0.93	0.23	124,124,124,124	7
86	OHX	A2	2055	7/7	0.93	0.20	116,116,116,116	7
86	OHX	A1	3605	7/7	0.93	0.12	166,166,166,166	7
86	OHX	A5	3783	7/7	0.93	0.19	154,154,154,154	7
86	OHX	A6	2053	7/7	0.93	0.25	123,123,123,123	7
86	OHX	A6	1993	7/7	0.93	0.16	129,129,129,129	7
86	OHX	CJ	201	7/7	0.93	0.27	105,105,105,105	7
87	MG	A1	4127	1/1	0.93	0.15	65,65,65,65	0
87	MG	A6	2217	1/1	0.93	0.20	87,87,87,87	0
87	MG	A1	3405	1/1	0.93	0.11	71,71,71,71	0
86	OHX	A6	1996	7/7	0.93	0.18	148,148,148,148	7
86	OHX	A2	2031	7/7	0.93	0.12	140,140,140,140	7
86	OHX	A1	3661	7/7	0.93	0.19	118,118,118,118	7
87	MG	A2	2196	1/1	0.93	0.32	131,131,131,131	0
87	MG	A1	4245	1/1	0.93	0.23	73,73,73,73	0
86	OHX	CY	201	7/7	0.93	0.17	121,121,121,121	7
87	MG	A5	3986	1/1	0.93	0.17	53,53,53,53	0
87	MG	A5	4342	1/1	0.93	0.10	50,50,50,50	0
87	MG	Bj	105	1/1	0.93	0.23	64,64,64,64	0
87	MG	A1	3821	1/1	0.93	0.40	71,71,71,71	0
87	MG	A1	3822	1/1	0.93	0.28	50,50,50,50	0
86	OHX	A1	3662	7/7	0.93	0.25	119,119,119,119	7
87	MG	A5	4158	1/1	0.93	0.24	62,62,62,62	0
87	MG	A1	4375	1/1	0.93	0.15	51,51,51,51	0
86	OHX	A2	1982	7/7	0.93	0.17	125,125,125,125	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A2	1983	7/7	0.93	0.13	166,166,166,166	7
87	MG	A5	3836	1/1	0.93	0.44	66,66,66,66	0
87	MG	A1	4378	1/1	0.93	0.25	51,51,51,51	0
86	OHX	Ag	401	7/7	0.93	0.10	167,167,167,167	7
87	MG	A5	4559	1/1	0.93	0.18	74,74,74,74	0
87	MG	A5	4560	1/1	0.93	0.26	108,108,108,108	0
87	MG	A5	4354	1/1	0.93	0.15	60,60,60,60	0
87	MG	Bo	203	1/1	0.93	0.23	79,79,79,79	0
87	MG	A5	4563	1/1	0.93	0.31	89,89,89,89	0
87	MG	A5	4564	1/1	0.93	0.12	79,79,79,79	0
86	OHX	A1	3668	7/7	0.93	0.17	151,151,151,151	7
86	OHX	A1	3669	7/7	0.93	0.21	130,130,130,130	7
87	MG	A5	4568	1/1	0.93	0.27	64,64,64,64	0
87	MG	A5	3843	1/1	0.93	0.21	50,50,50,50	0
86	OHX	A6	2010	7/7	0.93	0.11	181,181,181,181	7
86	OHX	A5	3541	7/7	0.93	0.25	113,113,113,113	7
86	OHX	A6	2013	7/7	0.93	0.25	180,180,180,180	7
86	OHX	A5	3557	7/7	0.93	0.17	154,154,154,154	7
86	OHX	A1	3610	7/7	0.93	0.20	121,121,121,121	7
87	MG	A3	225	1/1	0.93	0.12	61,61,61,61	0
86	OHX	A5	3804	7/7	0.93	0.23	162,162,162,162	7
87	MG	A1	4388	1/1	0.93	0.18	78,78,78,78	0
86	OHX	A2	1987	7/7	0.93	0.22	147,147,147,147	7
87	MG	A5	4013	1/1	0.93	0.30	44,44,44,44	0
86	OHX	A5	3726	7/7	0.93	0.10	135,135,135,135	7
87	MG	A5	4373	1/1	0.93	0.20	74,74,74,74	0
87	MG	A6	2112	1/1	0.93	0.38	64,64,64,64	0
87	MG	A1	4152	1/1	0.93	0.19	34,34,34,34	0
86	OHX	A1	3781	7/7	0.93	0.23	122,122,122,122	7
87	MG	A5	4185	1/1	0.93	0.16	49,49,49,49	0
87	MG	A5	4378	1/1	0.93	0.32	75,75,75,75	0
87	MG	A5	4018	1/1	0.93	0.32	40,40,40,40	0
86	OHX	A5	3603	7/7	0.93	0.25	107,107,107,107	7
86	OHX	A2	2024	7/7	0.93	0.21	174,174,174,174	7
86	OHX	A5	3609	7/7	0.93	0.11	153,153,153,153	7
87	MG	A5	4384	1/1	0.93	0.27	77,77,77,77	0
87	MG	A5	3861	1/1	0.93	0.23	65,65,65,65	0
86	OHX	A1	3617	7/7	0.93	0.16	144,144,144,144	7
87	MG	A5	3863	1/1	0.93	0.43	51,51,51,51	0
86	OHX	A5	3613	7/7	0.93	0.20	137,137,137,137	7
87	MG	A4	221	1/1	0.93	0.20	43,43,43,43	0
87	MG	A1	3942	1/1	0.93	0.31	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A6	2072	7/7	0.93	0.32	133,133,133,133	7
87	MG	A5	4394	1/1	0.93	0.26	73,73,73,73	0
87	MG	A5	4031	1/1	0.93	0.37	39,39,39,39	0
87	MG	A5	4032	1/1	0.93	0.43	41,41,41,41	0
86	OHX	A5	3620	7/7	0.93	0.23	113,113,113,113	7
87	MG	A5	4201	1/1	0.93	0.10	49,49,49,49	0
87	MG	A5	4202	1/1	0.93	0.15	45,45,45,45	0
86	OHX	A1	3453	7/7	0.93	0.33	134,134,134,134	0
87	MG	A8	225	1/1	0.93	0.29	58,58,58,58	0
86	OHX	A5	3820	7/7	0.93	0.23	80,80,80,80	7
87	MG	A1	3849	1/1	0.93	0.35	56,56,56,56	0
86	OHX	A2	2006	7/7	0.93	0.18	162,162,162,162	7
87	MG	A1	4166	1/1	0.93	0.13	74,74,74,74	0
87	MG	A1	4061	1/1	0.93	0.23	35,35,35,35	0
86	OHX	A5	3626	7/7	0.93	0.24	147,147,147,147	7
87	MG	A1	4413	1/1	0.93	0.19	106,106,106,106	0
87	MG	A5	4411	1/1	0.93	0.27	94,94,94,94	0
87	MG	A1	4169	1/1	0.93	0.17	80,80,80,80	0
87	MG	A1	4170	1/1	0.93	0.13	50,50,50,50	0
86	OHX	A5	3629	7/7	0.93	0.26	100,100,100,100	7
86	OHX	A7	207	7/7	0.93	0.19	145,145,145,145	7
87	MG	A4	239	1/1	0.93	0.20	70,70,70,70	0
87	MG	A5	3884	1/1	0.93	0.24	54,54,54,54	0
86	OHX	A1	3715	7/7	0.93	0.22	120,120,120,120	7
87	MG	A5	4221	1/1	0.93	0.24	88,88,88,88	0
86	OHX	A5	3634	7/7	0.93	0.16	130,130,130,130	7
86	OHX	A4	212	7/7	0.93	0.27	118,118,118,118	7
86	OHX	A6	2029	7/7	0.93	0.23	141,141,141,141	7
86	OHX	A1	3542	7/7	0.93	0.15	159,159,159,159	7
86	OHX	A5	3645	7/7	0.93	0.16	141,141,141,141	7
87	MG	A5	3891	1/1	0.93	0.17	50,50,50,50	0
87	MG	A4	247	1/1	0.93	0.39	56,56,56,56	0
86	OHX	A5	3749	7/7	0.93	0.11	178,178,178,178	7
86	OHX	A1	3680	7/7	0.93	0.20	127,127,127,127	7
86	OHX	A1	3626	7/7	0.93	0.15	162,162,162,162	7
86	OHX	A5	3650	7/7	0.93	0.22	133,133,133,133	7
87	MG	DC	407	1/1	0.93	0.15	75,75,75,75	0
86	OHX	A5	3653	7/7	0.93	0.24	130,130,130,130	7
86	OHX	DA	302	7/7	0.93	0.21	157,157,157,157	7
87	MG	A6	2153	1/1	0.93	0.37	54,54,54,54	0
87	MG	A5	4239	1/1	0.93	0.10	44,44,44,44	0
87	MG	DD	306	1/1	0.93	0.13	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3548	7/7	0.93	0.18	136,136,136,136	7
86	OHX	DC	401	7/7	0.93	0.09	148,148,148,148	7
86	OHX	A6	2036	7/7	0.93	0.25	122,122,122,122	7
87	MG	DF	303	1/1	0.93	0.29	73,73,73,73	0
86	OHX	A1	3557	7/7	0.93	0.19	121,121,121,121	7
87	MG	A5	4443	1/1	0.93	0.25	64,64,64,64	0
86	OHX	A5	3661	7/7	0.93	0.14	134,134,134,134	7
87	MG	A5	4445	1/1	0.93	0.26	65,65,65,65	0
86	OHX	A5	3662	7/7	0.93	0.19	148,148,148,148	7
87	MG	A6	2161	1/1	0.93	0.46	55,55,55,55	0
87	MG	A5	4448	1/1	0.93	0.14	64,64,64,64	0
87	MG	A6	2162	1/1	0.93	0.48	63,63,63,63	0
86	OHX	A5	3663	7/7	0.93	0.25	136,136,136,136	7
86	OHX	A1	3684	7/7	0.93	0.12	143,143,143,143	7
87	MG	A1	4315	1/1	0.93	0.22	62,62,62,62	0
87	MG	A6	2305	1/1	0.93	0.12	76,76,76,76	0
87	MG	A5	4456	1/1	0.93	0.43	79,79,79,79	0
86	OHX	BD	301	7/7	0.93	0.18	138,138,138,138	7
87	MG	A6	2307	1/1	0.93	0.19	94,94,94,94	0
87	MG	A2	2250	1/1	0.93	0.04	97,97,97,97	0
86	OHX	A5	3668	7/7	0.93	0.24	163,163,163,163	7
87	MG	A5	4259	1/1	0.93	0.10	56,56,56,56	0
87	MG	DP	208	1/1	0.93	0.17	42,42,42,42	0
87	MG	A1	4320	1/1	0.93	0.28	59,59,59,59	0
87	MG	A5	3922	1/1	0.93	0.16	54,54,54,54	0
87	MG	DS	201	1/1	0.93	0.19	61,61,61,61	0
86	OHX	A6	2040	7/7	0.93	0.24	87,87,87,87	7
87	MG	A5	4468	1/1	0.93	0.15	73,73,73,73	0
87	MG	A5	4088	1/1	0.93	0.09	41,41,41,41	0
87	MG	A1	4095	1/1	0.93	0.24	56,56,56,56	0
87	MG	BI	306	1/1	0.93	0.12	32,32,32,32	0
87	MG	DV	203	1/1	0.93	0.18	65,65,65,65	0
86	OHX	DQ	201	7/7	0.93	0.23	147,147,147,147	7
87	MG	A5	4268	1/1	0.93	0.17	96,96,96,96	0
87	MG	A1	4202	1/1	0.93	0.18	67,67,67,67	0
86	OHX	A2	2000	7/7	0.93	0.18	140,140,140,140	7
86	OHX	A1	3760	7/7	0.93	0.20	136,136,136,136	7
86	OHX	A5	3674	7/7	0.93	0.29	100,100,100,100	7
87	MG	A1	3884	1/1	0.93	0.24	64,64,64,64	0
87	MG	A2	2089	1/1	0.93	0.26	49,49,49,49	0
87	MG	Db	102	1/1	0.93	0.24	70,70,70,70	0
87	MG	A1	4208	1/1	0.93	0.21	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4282	1/1	0.93	0.15	52,52,52,52	0
87	MG	A1	4209	1/1	0.93	0.29	76,76,76,76	0
87	MG	A1	4333	1/1	0.93	0.23	68,68,68,68	0
86	OHX	A5	3678	7/7	0.93	0.23	111,111,111,111	7
87	MG	A1	4335	1/1	0.93	0.15	86,86,86,86	0
87	MG	A1	4212	1/1	0.93	0.18	67,67,67,67	0
87	MG	A5	4288	1/1	0.93	0.23	49,49,49,49	0
86	OHX	A1	3566	7/7	0.93	0.20	122,122,122,122	7
86	OHX	A2	2009	7/7	0.93	0.12	144,144,144,144	7
87	MG	A5	3942	1/1	0.93	0.33	38,38,38,38	0
87	MG	Dp	101	1/1	0.93	0.11	54,54,54,54	0
86	OHX	A6	2092	7/7	0.93	0.23	182,182,182,182	7
87	MG	Dp	103	1/1	0.93	0.15	72,72,72,72	0
87	MG	A1	4106	1/1	0.93	0.33	69,69,69,69	0
87	MG	A5	3945	1/1	0.93	0.17	56,56,56,56	0
86	OHX	A5	3683	7/7	0.93	0.17	119,119,119,119	7
87	MG	A6	2193	1/1	0.93	0.14	75,75,75,75	0
87	MG	A5	4516	1/1	0.94	0.29	74,74,74,74	0
87	MG	A1	3886	1/1	0.94	0.35	72,72,72,72	0
87	MG	BQ	204	1/1	0.94	0.23	99,99,99,99	0
87	MG	A1	4222	1/1	0.94	0.16	73,73,73,73	0
87	MG	A5	4325	1/1	0.94	0.44	57,57,57,57	0
86	OHX	A5	3642	7/7	0.94	0.16	118,118,118,118	7
86	OHX	A5	3643	7/7	0.94	0.12	150,150,150,150	7
87	MG	A5	4141	1/1	0.94	0.21	66,66,66,66	0
86	OHX	A5	3644	7/7	0.94	0.20	135,135,135,135	7
87	MG	A1	3996	1/1	0.94	0.44	48,48,48,48	0
87	MG	A1	3997	1/1	0.94	0.29	40,40,40,40	0
87	MG	A1	4350	1/1	0.94	0.21	76,76,76,76	0
86	OHX	A2	2010	7/7	0.94	0.20	119,119,119,119	7
87	MG	A1	4000	1/1	0.94	0.12	18,18,18,18	0
86	OHX	A5	3646	7/7	0.94	0.14	135,135,135,135	7
87	MG	Ch	302	1/1	0.94	0.11	53,53,53,53	0
86	OHX	A1	3569	7/7	0.94	0.12	144,144,144,144	7
86	OHX	A1	3629	7/7	0.94	0.18	128,128,128,128	7
86	OHX	A1	3630	7/7	0.94	0.17	119,119,119,119	7
87	MG	Ba	204	1/1	0.94	0.17	74,74,74,74	0
87	MG	A5	3987	1/1	0.94	0.41	59,59,59,59	0
86	OHX	A1	3631	7/7	0.94	0.14	141,141,141,141	7
87	MG	A5	4539	1/1	0.94	0.21	77,77,77,77	0
86	OHX	A1	3633	7/7	0.94	0.24	101,101,101,101	7
87	MG	A6	2224	1/1	0.94	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	4237	1/1	0.94	0.11	46,46,46,46	0
87	MG	A5	3832	1/1	0.94	0.13	35,35,35,35	0
87	MG	A5	3833	1/1	0.94	0.36	54,54,54,54	0
86	OHX	A1	3635	7/7	0.94	0.21	84,84,84,84	7
86	OHX	A5	3657	7/7	0.94	0.23	83,83,83,83	7
86	OHX	A2	1986	7/7	0.94	0.17	124,124,124,124	7
87	MG	AL	203	1/1	0.94	0.16	80,80,80,80	0
87	MG	Bj	104	1/1	0.94	0.25	86,86,86,86	0
86	OHX	A5	3660	7/7	0.94	0.19	108,108,108,108	7
86	OHX	Dh	201	7/7	0.94	0.16	129,129,129,129	7
86	OHX	A6	2035	7/7	0.94	0.12	129,129,129,129	7
87	MG	A1	4367	1/1	0.94	0.12	69,69,69,69	0
86	OHX	A2	2020	7/7	0.94	0.19	118,118,118,118	7
87	MG	A5	4558	1/1	0.94	0.14	63,63,63,63	0
86	OHX	A1	3580	7/7	0.94	0.14	149,149,149,149	7
86	OHX	A1	3582	7/7	0.94	0.22	92,92,92,92	7
87	MG	A2	2093	1/1	0.94	0.18	47,47,47,47	0
86	OHX	A1	3583	7/7	0.94	0.19	147,147,147,147	7
87	MG	A1	4373	1/1	0.94	0.29	56,56,56,56	0
87	MG	A5	4010	1/1	0.94	0.32	50,50,50,50	0
87	MG	A6	2241	1/1	0.94	0.19	112,112,112,112	0
87	MG	A1	4023	1/1	0.94	0.31	42,42,42,42	0
86	OHX	A1	3742	7/7	0.94	0.23	140,140,140,140	7
86	OHX	A1	3646	7/7	0.94	0.17	110,110,110,110	7
86	OHX	A1	3587	7/7	0.94	0.13	147,147,147,147	7
86	OHX	A5	3672	7/7	0.94	0.18	142,142,142,142	7
87	MG	A5	3856	1/1	0.94	0.24	54,54,54,54	0
86	OHX	A1	3648	7/7	0.94	0.17	102,102,102,102	7
86	OHX	A1	3649	7/7	0.94	0.19	167,167,167,167	7
87	MG	A1	4031	1/1	0.94	0.20	32,32,32,32	0
86	OHX	A5	3676	7/7	0.94	0.21	155,155,155,155	7
87	MG	A5	4379	1/1	0.94	0.19	45,45,45,45	0
86	OHX	A2	1965	7/7	0.94	0.18	138,138,138,138	7
86	OHX	A2	1980	7/7	0.94	0.17	152,152,152,152	7
86	OHX	A2	2007	7/7	0.94	0.25	146,146,146,146	7
86	OHX	A1	3659	7/7	0.94	0.13	156,156,156,156	7
86	OHX	A6	1947	7/7	0.94	0.17	134,134,134,134	7
86	OHX	A6	1963	7/7	0.94	0.20	103,103,103,103	7
87	MG	A1	4040	1/1	0.94	0.06	40,40,40,40	0
86	OHX	A1	3506	7/7	0.94	0.17	103,103,103,103	7
86	OHX	A6	1978	7/7	0.94	0.17	146,146,146,146	7
86	OHX	A6	1982	7/7	0.94	0.17	123,123,123,123	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4035	1/1	0.94	0.07	39,39,39,39	0
87	MG	A5	4036	1/1	0.94	0.12	60,60,60,60	0
87	MG	A7	223	1/1	0.94	0.30	69,69,69,69	0
86	OHX	A2	1993	7/7	0.94	0.10	159,159,159,159	7
87	MG	A1	4272	1/1	0.94	0.11	53,53,53,53	0
86	OHX	A5	3691	7/7	0.94	0.21	155,155,155,155	7
86	OHX	A1	3524	7/7	0.94	0.19	139,139,139,139	7
87	MG	A5	4041	1/1	0.94	0.20	47,47,47,47	0
87	MG	A5	4399	1/1	0.94	0.14	64,64,64,64	0
87	MG	A1	4400	1/1	0.94	0.12	70,70,70,70	0
86	OHX	A5	3404	7/7	0.94	0.19	111,111,111,111	7
86	OHX	A5	3694	7/7	0.94	0.17	127,127,127,127	7
86	OHX	A5	3695	7/7	0.94	0.18	158,158,158,158	7
86	OHX	A1	3663	7/7	0.94	0.22	126,126,126,126	7
87	MG	A7	237	1/1	0.94	0.12	69,69,69,69	0
87	MG	A1	4280	1/1	0.94	0.07	51,51,51,51	0
87	MG	A1	3835	1/1	0.94	0.19	41,41,41,41	0
86	OHX	A6	2057	7/7	0.94	0.27	134,134,134,134	7
87	MG	A8	222	1/1	0.94	0.30	47,47,47,47	0
87	MG	A1	4283	1/1	0.94	0.33	91,91,91,91	0
86	OHX	A1	3539	7/7	0.94	0.20	103,103,103,103	7
87	MG	A4	235	1/1	0.94	0.09	119,119,119,119	0
86	OHX	A1	3665	7/7	0.94	0.26	104,104,104,104	7
86	OHX	A5	3703	7/7	0.94	0.27	123,123,123,123	7
87	MG	A1	4287	1/1	0.94	0.13	61,61,61,61	0
86	OHX	A5	3532	7/7	0.94	0.14	164,164,164,164	7
87	MG	A5	3892	1/1	0.94	0.15	45,45,45,45	0
86	OHX	A6	1994	7/7	0.94	0.15	133,133,133,133	7
86	OHX	A6	1995	7/7	0.94	0.12	143,143,143,143	7
86	OHX	A5	3556	7/7	0.94	0.20	111,111,111,111	7
87	MG	A2	2216	1/1	0.94	0.08	63,63,63,63	0
86	OHX	A2	2044	7/7	0.94	0.16	162,162,162,162	7
87	MG	A1	3846	1/1	0.94	0.17	37,37,37,37	0
87	MG	A1	4295	1/1	0.94	0.18	62,62,62,62	0
86	OHX	A6	1997	7/7	0.94	0.17	125,125,125,125	7
87	MG	A5	4237	1/1	0.94	0.09	51,51,51,51	0
87	MG	A5	3901	1/1	0.94	0.22	85,85,85,85	0
87	MG	A1	3950	1/1	0.94	0.16	48,48,48,48	0
86	OHX	A1	3801	7/7	0.94	0.23	125,125,125,125	7
87	MG	A6	2150	1/1	0.94	0.30	48,48,48,48	0
87	MG	A5	4070	1/1	0.94	0.33	56,56,56,56	0
87	MG	DB	408	1/1	0.94	0.15	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3802	7/7	0.94	0.20	146,146,146,146	7
87	MG	DB	410	1/1	0.94	0.17	54,54,54,54	0
87	MG	A5	4072	1/1	0.94	0.20	56,56,56,56	0
87	MG	A1	4181	1/1	0.94	0.22	61,61,61,61	0
87	MG	A6	2297	1/1	0.94	0.22	68,68,68,68	0
87	MG	BA	305	1/1	0.94	0.17	61,61,61,61	0
86	OHX	A5	3593	7/7	0.94	0.13	134,134,134,134	7
86	OHX	A5	3595	7/7	0.94	0.22	125,125,125,125	7
87	MG	A5	4442	1/1	0.94	0.25	76,76,76,76	0
86	OHX	A5	3600	7/7	0.94	0.16	133,133,133,133	7
87	MG	A1	4305	1/1	0.94	0.16	65,65,65,65	0
86	OHX	A5	3717	7/7	0.94	0.18	108,108,108,108	7
86	OHX	A6	2000	7/7	0.94	0.21	128,128,128,128	7
86	OHX	A1	3713	7/7	0.94	0.27	101,101,101,101	7
87	MG	A5	3917	1/1	0.94	0.14	44,44,44,44	0
87	MG	A5	4258	1/1	0.94	0.26	70,70,70,70	0
86	OHX	A1	3544	7/7	0.94	0.22	96,96,96,96	7
87	MG	A1	4441	1/1	0.94	0.23	61,61,61,61	0
86	OHX	A5	3814	7/7	0.94	0.18	114,114,114,114	7
87	MG	A5	4454	1/1	0.94	0.13	68,68,68,68	0
87	MG	A5	4262	1/1	0.94	0.19	60,60,60,60	0
86	OHX	A5	3611	7/7	0.94	0.18	115,115,115,115	7
86	OHX	A1	3546	7/7	0.94	0.16	106,106,106,106	7
87	MG	A6	2167	1/1	0.94	0.20	46,46,46,46	0
87	MG	A1	4445	1/1	0.94	0.12	69,69,69,69	0
87	MG	A1	4081	1/1	0.94	0.12	56,56,56,56	0
87	MG	A6	2314	1/1	0.94	0.17	112,112,112,112	0
87	MG	A5	4093	1/1	0.94	0.15	64,64,64,64	0
87	MG	A5	4271	1/1	0.94	0.15	68,68,68,68	0
87	MG	A1	3966	1/1	0.94	0.41	60,60,60,60	0
87	MG	A5	4467	1/1	0.94	0.23	70,70,70,70	0
86	OHX	A2	2035	7/7	0.94	0.18	120,120,120,120	7
86	OHX	A5	3614	7/7	0.94	0.21	120,120,120,120	7
87	MG	DO	209	1/1	0.94	0.29	62,62,62,62	0
86	OHX	A1	3549	7/7	0.94	0.19	139,139,139,139	7
86	OHX	A5	3616	7/7	0.94	0.23	102,102,102,102	7
86	OHX	A5	3619	7/7	0.94	0.18	119,119,119,119	7
86	OHX	A1	3554	7/7	0.94	0.18	159,159,159,159	7
86	OHX	A2	2067	7/7	0.94	0.20	108,108,108,108	7
87	MG	A5	4102	1/1	0.94	0.35	71,71,71,71	0
87	MG	BL	204	1/1	0.94	0.17	72,72,72,72	0
87	MG	BL	205	1/1	0.94	0.13	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A1	4090	1/1	0.94	0.36	78,78,78,78	0
87	MG	BN	303	1/1	0.94	0.21	72,72,72,72	0
86	OHX	A5	3623	7/7	0.94	0.22	156,156,156,156	7
87	MG	DT	201	1/1	0.94	0.17	63,63,63,63	0
87	MG	DT	202	1/1	0.94	0.20	89,89,89,89	0
86	OHX	A1	3620	7/7	0.94	0.12	139,139,139,139	7
86	OHX	A7	211	7/7	0.94	0.19	117,117,117,117	7
86	OHX	A1	3676	7/7	0.94	0.23	148,148,148,148	7
86	OHX	A1	3621	7/7	0.94	0.19	119,119,119,119	7
87	MG	BO	204	1/1	0.94	0.12	53,53,53,53	0
87	MG	A6	2188	1/1	0.94	0.17	38,38,38,38	0
87	MG	A1	4462	1/1	0.94	0.09	71,71,71,71	0
87	MG	A1	4330	1/1	0.94	0.21	82,82,82,82	0
86	OHX	A1	3562	7/7	0.94	0.15	143,143,143,143	7
87	MG	A5	4299	1/1	0.94	0.15	80,80,80,80	0
87	MG	A5	4300	1/1	0.94	0.18	51,51,51,51	0
87	MG	A5	4301	1/1	0.94	0.08	71,71,71,71	0
87	MG	A1	3874	1/1	0.94	0.33	60,60,60,60	0
87	MG	A2	2244	1/1	0.94	0.18	99,99,99,99	0
87	MG	A6	2339	1/1	0.94	0.25	64,64,64,64	0
86	OHX	A5	3633	7/7	0.94	0.22	126,126,126,126	7
87	MG	A5	4306	1/1	0.94	0.17	72,72,72,72	0
86	OHX	A5	3740	7/7	0.94	0.17	155,155,155,155	7
87	MG	A5	4122	1/1	0.94	0.26	52,52,52,52	0
87	MG	CF	301	1/1	0.94	0.19	87,87,87,87	0
86	OHX	A6	2018	7/7	0.94	0.18	153,153,153,153	7
87	MG	A2	2248	1/1	0.94	0.12	69,69,69,69	0
87	MG	Dn	101	1/1	0.94	0.15	84,84,84,84	0
86	OHX	A5	3635	7/7	0.94	0.14	147,147,147,147	7
87	MG	A5	3961	1/1	0.94	0.35	55,55,55,55	0
86	OHX	A1	3624	7/7	0.94	0.22	137,137,137,137	7
87	MG	A5	3964	1/1	0.94	0.26	57,57,57,57	0
87	MG	BP	210	1/1	0.94	0.17	46,46,46,46	0
86	OHX	A2	1984	7/7	0.94	0.18	108,108,108,108	7
86	OHX	A3	207	7/7	0.94	0.14	167,167,167,167	7
86	OHX	A5	3640	7/7	0.94	0.14	147,147,147,147	7
88	ZN	Do	203	1/1	0.94	0.10	181,181,181,181	0
86	OHX	A6	1967	7/7	0.95	0.21	112,112,112,112	7
87	MG	A2	2163	1/1	0.95	0.12	80,80,80,80	0
87	MG	A2	2164	1/1	0.95	0.17	74,74,74,74	0
87	MG	A5	4204	1/1	0.95	0.15	56,56,56,56	0
87	MG	A6	2296	1/1	0.95	0.21	119,119,119,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3590	7/7	0.95	0.20	114,114,114,114	7
86	OHX	A5	3714	7/7	0.95	0.16	126,126,126,126	7
86	OHX	A6	1970	7/7	0.95	0.15	160,160,160,160	7
87	MG	A5	4209	1/1	0.95	0.15	53,53,53,53	0
86	OHX	A6	1972	7/7	0.95	0.19	109,109,109,109	7
87	MG	A5	3904	1/1	0.95	0.19	60,60,60,60	0
86	OHX	A8	206	7/7	0.95	0.13	136,136,136,136	7
87	MG	A5	4213	1/1	0.95	0.17	52,52,52,52	0
86	OHX	A8	207	7/7	0.95	0.14	126,126,126,126	7
86	OHX	A8	211	7/7	0.95	0.12	135,135,135,135	7
86	OHX	A5	3594	7/7	0.95	0.15	131,131,131,131	7
86	OHX	A1	3638	7/7	0.95	0.15	141,141,141,141	7
87	MG	A2	2174	1/1	0.95	0.14	53,53,53,53	0
86	OHX	A1	3575	7/7	0.95	0.15	120,120,120,120	7
86	OHX	A5	3602	7/7	0.95	0.23	109,109,109,109	7
86	OHX	A6	1980	7/7	0.95	0.20	133,133,133,133	7
86	OHX	A6	1981	7/7	0.95	0.17	110,110,110,110	7
86	OHX	A5	3607	7/7	0.95	0.16	142,142,142,142	7
86	OHX	A5	3608	7/7	0.95	0.13	125,125,125,125	7
87	MG	A1	4446	1/1	0.95	0.07	62,62,62,62	0
86	OHX	A2	2026	7/7	0.95	0.12	140,140,140,140	7
87	MG	A5	3919	1/1	0.95	0.36	66,66,66,66	0
87	MG	A1	4065	1/1	0.95	0.12	47,47,47,47	0
86	OHX	A6	1984	7/7	0.95	0.13	174,174,174,174	7
86	OHX	A1	3642	7/7	0.95	0.14	139,139,139,139	7
86	OHX	A2	2005	7/7	0.95	0.16	134,134,134,134	7
86	OHX	A6	1989	7/7	0.95	0.18	122,122,122,122	7
87	MG	A5	4578	1/1	0.95	0.16	74,74,74,74	0
86	OHX	A2	1981	7/7	0.95	0.17	132,132,132,132	7
87	MG	A5	4234	1/1	0.95	0.16	67,67,67,67	0
87	MG	A1	4193	1/1	0.95	0.36	72,72,72,72	0
86	OHX	A1	3645	7/7	0.95	0.18	102,102,102,102	7
86	OHX	A5	3617	7/7	0.95	0.11	154,154,154,154	7
86	OHX	A5	3618	7/7	0.95	0.19	101,101,101,101	7
87	MG	A5	4240	1/1	0.95	0.14	77,77,77,77	0
87	MG	A1	3948	1/1	0.95	0.36	55,55,55,55	0
86	OHX	A1	3585	7/7	0.95	0.15	122,122,122,122	7
87	MG	A5	4413	1/1	0.95	0.23	80,80,80,80	0
87	MG	A1	4076	1/1	0.95	0.35	64,64,64,64	0
86	OHX	A1	3698	7/7	0.95	0.16	105,105,105,105	7
86	OHX	A5	3621	7/7	0.95	0.20	123,123,123,123	7
86	OHX	A2	1931	7/7	0.95	0.14	143,143,143,143	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3589	7/7	0.95	0.17	97,97,97,97	7
86	OHX	A1	3595	7/7	0.95	0.20	120,120,120,120	7
86	OHX	A1	3597	7/7	0.95	0.15	123,123,123,123	7
86	OHX	A5	3628	7/7	0.95	0.19	129,129,129,129	7
86	OHX	A1	3652	7/7	0.95	0.23	115,115,115,115	7
87	MG	A7	231	1/1	0.95	0.30	87,87,87,87	0
86	OHX	A1	3757	7/7	0.95	0.16	73,73,73,73	7
87	MG	A1	4471	1/1	0.95	0.22	88,88,88,88	0
86	OHX	A5	3632	7/7	0.95	0.25	106,106,106,106	7
87	MG	A1	4210	1/1	0.95	0.27	44,44,44,44	0
86	OHX	A2	2052	7/7	0.95	0.19	117,117,117,117	7
87	MG	A6	2199	1/1	0.95	0.12	62,62,62,62	0
86	OHX	A2	1940	7/7	0.95	0.18	100,100,100,100	7
87	MG	A7	239	1/1	0.95	0.10	71,71,71,71	0
87	MG	A1	3963	1/1	0.95	0.23	56,56,56,56	0
86	OHX	A1	3658	7/7	0.95	0.16	118,118,118,118	7
86	OHX	A1	3511	7/7	0.95	0.13	154,154,154,154	0
86	OHX	A2	1954	7/7	0.95	0.16	162,162,162,162	7
86	OHX	A1	3518	7/7	0.95	0.15	140,140,140,140	7
86	OHX	A2	1956	7/7	0.95	0.14	128,128,128,128	7
87	MG	A5	4437	1/1	0.95	0.12	86,86,86,86	0
87	MG	A8	227	1/1	0.95	0.11	65,65,65,65	0
87	MG	A1	3970	1/1	0.95	0.29	69,69,69,69	0
86	OHX	A5	3641	7/7	0.95	0.18	127,127,127,127	7
86	OHX	A6	2011	7/7	0.95	0.20	120,120,120,120	7
87	MG	BT	202	1/1	0.95	0.23	89,89,89,89	0
86	OHX	A6	2012	7/7	0.95	0.14	149,149,149,149	7
86	OHX	A1	3531	7/7	0.95	0.16	140,140,140,140	7
87	MG	A5	4274	1/1	0.95	0.08	51,51,51,51	0
86	OHX	A1	3532	7/7	0.95	0.17	87,87,87,87	7
86	OHX	A1	3816	7/7	0.95	0.12	150,150,150,150	7
87	MG	A8	238	1/1	0.95	0.20	93,93,93,93	0
86	OHX	A1	3716	7/7	0.95	0.18	113,113,113,113	7
86	OHX	A3	208	7/7	0.95	0.18	126,126,126,126	7
86	OHX	A2	1959	7/7	0.95	0.13	147,147,147,147	7
87	MG	Ba	202	1/1	0.95	0.14	63,63,63,63	0
87	MG	A5	3969	1/1	0.95	0.30	37,37,37,37	0
86	OHX	A6	2020	7/7	0.95	0.22	88,88,88,88	7
86	OHX	A2	1941	7/7	0.95	0.17	117,117,117,117	7
87	MG	DB	405	1/1	0.95	0.13	62,62,62,62	0
87	MG	A1	4231	1/1	0.95	0.12	82,82,82,82	0
87	MG	A5	4123	1/1	0.95	0.07	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	Ba	206	1/1	0.95	0.13	61,61,61,61	0
86	OHX	A5	3655	7/7	0.95	0.20	124,124,124,124	7
87	MG	A5	4460	1/1	0.95	0.15	74,74,74,74	0
87	MG	A1	4498	1/1	0.95	0.08	60,60,60,60	0
86	OHX	A2	1991	7/7	0.95	0.17	113,113,113,113	7
86	OHX	A2	1961	7/7	0.95	0.12	150,150,150,150	7
87	MG	DB	414	1/1	0.95	0.19	76,76,76,76	0
86	OHX	A1	3547	7/7	0.95	0.20	99,99,99,99	7
87	MG	A5	3828	1/1	0.95	0.07	34,34,34,34	0
86	OHX	A5	3659	7/7	0.95	0.17	106,106,106,106	7
87	MG	A5	3830	1/1	0.95	0.16	39,39,39,39	0
86	OHX	A4	209	7/7	0.95	0.10	153,153,153,153	7
86	OHX	A6	2028	7/7	0.95	0.30	136,136,136,136	7
86	OHX	A4	210	7/7	0.95	0.11	131,131,131,131	7
87	MG	A5	4471	1/1	0.95	0.14	61,61,61,61	0
86	OHX	A2	1994	7/7	0.95	0.16	118,118,118,118	7
86	OHX	A1	3672	7/7	0.95	0.20	99,99,99,99	7
86	OHX	CG	301	7/7	0.95	0.10	147,147,147,147	7
87	MG	DD	308	1/1	0.95	0.17	70,70,70,70	0
86	OHX	A2	1962	7/7	0.95	0.18	136,136,136,136	7
86	OHX	A1	3550	7/7	0.95	0.18	130,130,130,130	7
86	OHX	A1	3552	7/7	0.95	0.20	115,115,115,115	7
87	MG	A1	4246	1/1	0.95	0.16	80,80,80,80	0
86	OHX	CL	201	7/7	0.95	0.19	134,134,134,134	7
86	OHX	A2	1943	7/7	0.95	0.15	123,123,123,123	7
86	OHX	A2	1998	7/7	0.95	0.20	135,135,135,135	7
87	MG	A5	4310	1/1	0.95	0.13	69,69,69,69	0
86	OHX	A5	3675	7/7	0.95	0.22	132,132,132,132	7
86	OHX	A1	3558	7/7	0.95	0.15	139,139,139,139	7
87	MG	A5	4313	1/1	0.95	0.14	66,66,66,66	0
86	OHX	CS	201	7/7	0.95	0.13	129,129,129,129	7
87	MG	DO	202	1/1	0.95	0.12	61,61,61,61	0
86	OHX	A2	1966	7/7	0.95	0.18	101,101,101,101	7
86	OHX	A2	1967	7/7	0.95	0.19	120,120,120,120	7
86	OHX	A1	3565	7/7	0.95	0.15	127,127,127,127	7
86	OHX	A5	3682	7/7	0.95	0.22	110,110,110,110	7
86	OHX	A2	1969	7/7	0.95	0.15	144,144,144,144	7
87	MG	A6	2251	1/1	0.95	0.11	73,73,73,73	0
86	OHX	A5	3684	7/7	0.95	0.21	122,122,122,122	7
86	OHX	BN	301	7/7	0.95	0.17	116,116,116,116	7
87	MG	DP	204	1/1	0.95	0.29	78,78,78,78	0
87	MG	A1	3892	1/1	0.95	0.47	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	DP	206	1/1	0.95	0.25	55,55,55,55	0
86	OHX	A1	3632	7/7	0.95	0.09	170,170,170,170	7
87	MG	A1	4139	1/1	0.95	0.17	56,56,56,56	0
87	MG	A5	4326	1/1	0.95	0.22	75,75,75,75	0
87	MG	A5	4161	1/1	0.95	0.15	51,51,51,51	0
86	OHX	A2	1977	7/7	0.95	0.09	174,174,174,174	7
87	MG	A4	218	1/1	0.95	0.28	59,59,59,59	0
86	OHX	A1	3634	7/7	0.95	0.14	133,133,133,133	7
86	OHX	A2	1979	7/7	0.95	0.17	121,121,121,121	7
87	MG	A1	4393	1/1	0.95	0.20	78,78,78,78	0
87	MG	A4	222	1/1	0.95	0.27	43,43,43,43	0
86	OHX	A5	3521	7/7	0.95	0.18	150,150,150,150	7
86	OHX	A5	3528	7/7	0.95	0.12	163,163,163,163	0
87	MG	A6	2266	1/1	0.95	0.14	106,106,106,106	0
87	MG	A5	3868	1/1	0.95	0.17	44,44,44,44	0
87	MG	A1	3899	1/1	0.95	0.24	57,57,57,57	0
86	OHX	A6	1942	7/7	0.95	0.18	114,114,114,114	7
87	MG	A1	4270	1/1	0.95	0.08	57,57,57,57	0
86	OHX	A5	3540	7/7	0.95	0.15	119,119,119,119	7
87	MG	A5	4025	1/1	0.95	0.26	38,38,38,38	0
86	OHX	A2	1945	7/7	0.95	0.15	140,140,140,140	7
86	OHX	A5	3807	7/7	0.95	0.20	107,107,107,107	7
87	MG	A5	4521	1/1	0.95	0.16	68,68,68,68	0
87	MG	A1	3904	1/1	0.95	0.26	43,43,43,43	0
86	OHX	A5	3547	7/7	0.95	0.21	104,104,104,104	7
86	OHX	A6	1955	7/7	0.95	0.12	153,153,153,153	7
86	OHX	A6	1961	7/7	0.95	0.20	132,132,132,132	7
86	OHX	A6	1962	7/7	0.95	0.16	126,126,126,126	7
87	MG	A1	4409	1/1	0.95	0.42	58,58,58,58	0
87	MG	A1	4032	1/1	0.95	0.06	46,46,46,46	0
86	OHX	A5	3702	7/7	0.95	0.27	121,121,121,121	7
86	OHX	A5	3562	7/7	0.95	0.19	104,104,104,104	7
86	OHX	A5	3564	7/7	0.95	0.12	143,143,143,143	7
87	MG	Dm	201	1/1	0.95	0.16	75,75,75,75	0
86	OHX	A5	3567	7/7	0.95	0.20	106,106,106,106	7
86	OHX	A5	3571	7/7	0.95	0.14	143,143,143,143	7
86	OHX	A5	3572	7/7	0.95	0.16	145,145,145,145	7
87	MG	A1	4417	1/1	0.95	0.17	94,94,94,94	0
87	MG	A1	4418	1/1	0.95	0.12	48,48,48,48	0
87	MG	A4	246	1/1	0.95	0.19	91,91,91,91	0
86	OHX	A5	3574	7/7	0.95	0.12	154,154,154,154	7
86	OHX	A5	3581	7/7	0.95	0.15	148,148,148,148	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3583	7/7	0.95	0.14	137,137,137,137	7
88	ZN	Cf	501	1/1	0.95	0.09	152,152,152,152	0
86	OHX	A1	3637	7/7	0.95	0.10	146,146,146,146	7
87	MG	BQ	203	1/1	0.96	0.12	63,63,63,63	0
87	MG	A5	4356	1/1	0.96	0.12	74,74,74,74	0
86	OHX	A8	210	7/7	0.96	0.11	133,133,133,133	7
86	OHX	A1	3520	7/7	0.96	0.17	129,129,129,129	7
86	OHX	A5	3544	7/7	0.96	0.17	97,97,97,97	7
86	OHX	A5	3545	7/7	0.96	0.16	133,133,133,133	7
86	OHX	A1	3523	7/7	0.96	0.16	111,111,111,111	7
87	MG	BS	201	1/1	0.96	0.10	64,64,64,64	0
86	OHX	A1	3706	7/7	0.96	0.13	135,135,135,135	7
87	MG	A5	4550	1/1	0.96	0.27	83,83,83,83	0
86	OHX	A5	3552	7/7	0.96	0.10	138,138,138,138	7
87	MG	A5	4019	1/1	0.96	0.43	48,48,48,48	0
87	MG	A5	4553	1/1	0.96	0.25	73,73,73,73	0
86	OHX	A5	3554	7/7	0.96	0.16	130,130,130,130	7
87	MG	A1	4469	1/1	0.96	0.16	66,66,66,66	0
86	OHX	A5	3555	7/7	0.96	0.10	152,152,152,152	0
86	OHX	A1	3584	7/7	0.96	0.18	88,88,88,88	7
86	OHX	A2	1934	7/7	0.96	0.14	123,123,123,123	7
86	OHX	A5	3560	7/7	0.96	0.19	106,106,106,106	7
87	MG	BY	202	1/1	0.96	0.18	85,85,85,85	0
86	OHX	A5	3561	7/7	0.96	0.18	121,121,121,121	7
86	OHX	A1	3526	7/7	0.96	0.14	126,126,126,126	7
86	OHX	A1	3588	7/7	0.96	0.18	104,104,104,104	7
86	OHX	A5	3565	7/7	0.96	0.15	105,105,105,105	7
87	MG	A1	3885	1/1	0.96	0.26	61,61,61,61	0
87	MG	A5	4566	1/1	0.96	0.10	74,74,74,74	0
86	OHX	A2	1952	7/7	0.96	0.13	127,127,127,127	7
86	OHX	A5	3568	7/7	0.96	0.19	103,103,103,103	7
86	OHX	A1	3590	7/7	0.96	0.12	135,135,135,135	7
86	OHX	A1	3650	7/7	0.96	0.15	120,120,120,120	7
86	OHX	Bf	201	7/7	0.96	0.20	85,85,85,85	7
86	OHX	A5	3575	7/7	0.96	0.21	81,81,81,81	7
86	OHX	A5	3577	7/7	0.96	0.14	128,128,128,128	7
86	OHX	A5	3716	7/7	0.96	0.24	115,115,115,115	7
86	OHX	A5	3578	7/7	0.96	0.09	159,159,159,159	7
86	OHX	A5	3580	7/7	0.96	0.14	121,121,121,121	7
86	OHX	A1	3592	7/7	0.96	0.15	108,108,108,108	7
86	OHX	A5	3720	7/7	0.96	0.13	101,101,101,101	7
87	MG	A2	2090	1/1	0.96	0.20	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3594	7/7	0.96	0.11	144,144,144,144	7
86	OHX	A1	3653	7/7	0.96	0.13	153,153,153,153	7
86	OHX	A6	1951	7/7	0.96	0.15	115,115,115,115	7
86	OHX	A5	3587	7/7	0.96	0.18	96,96,96,96	7
86	OHX	A5	3588	7/7	0.96	0.23	106,106,106,106	7
87	MG	A6	2260	1/1	0.96	0.21	62,62,62,62	0
87	MG	A5	3881	1/1	0.96	0.31	60,60,60,60	0
86	OHX	A5	3589	7/7	0.96	0.21	93,93,93,93	7
86	OHX	A1	3717	7/7	0.96	0.15	141,141,141,141	7
87	MG	A5	4404	1/1	0.96	0.29	54,54,54,54	0
87	MG	A1	4051	1/1	0.96	0.13	71,71,71,71	0
86	OHX	A6	1956	7/7	0.96	0.13	130,130,130,130	7
86	OHX	A1	3718	7/7	0.96	0.14	94,94,94,94	7
87	MG	A5	4408	1/1	0.96	0.08	65,65,65,65	0
86	OHX	A2	1953	7/7	0.96	0.16	120,120,120,120	7
86	OHX	A1	3656	7/7	0.96	0.17	114,114,114,114	7
86	OHX	A5	3598	7/7	0.96	0.11	143,143,143,143	7
87	MG	A7	229	1/1	0.96	0.16	98,98,98,98	0
86	OHX	A5	3599	7/7	0.96	0.12	120,120,120,120	7
86	OHX	A6	1964	7/7	0.96	0.17	132,132,132,132	7
86	OHX	A5	3601	7/7	0.96	0.17	96,96,96,96	7
86	OHX	A6	1965	7/7	0.96	0.12	123,123,123,123	7
86	OHX	A1	3596	7/7	0.96	0.15	120,120,120,120	7
87	MG	A5	4236	1/1	0.96	0.09	19,19,19,19	0
86	OHX	A6	1968	7/7	0.96	0.18	101,101,101,101	7
86	OHX	A5	3605	7/7	0.96	0.20	112,112,112,112	7
86	OHX	A5	3606	7/7	0.96	0.15	130,130,130,130	7
86	OHX	A1	3534	7/7	0.96	0.16	106,106,106,106	7
86	OHX	A1	3598	7/7	0.96	0.15	139,139,139,139	7
86	OHX	A6	1973	7/7	0.96	0.19	87,87,87,87	7
86	OHX	A6	1974	7/7	0.96	0.16	116,116,116,116	7
86	OHX	A1	3536	7/7	0.96	0.12	136,136,136,136	7
87	MG	A5	4426	1/1	0.96	0.11	70,70,70,70	0
86	OHX	A2	1964	7/7	0.96	0.14	135,135,135,135	7
86	OHX	A6	1979	7/7	0.96	0.17	116,116,116,116	7
86	OHX	A1	3602	7/7	0.96	0.20	99,99,99,99	7
86	OHX	A1	3603	7/7	0.96	0.15	136,136,136,136	7
86	OHX	A1	3540	7/7	0.96	0.10	141,141,141,141	7
86	OHX	A6	1983	7/7	0.96	0.18	133,133,133,133	7
86	OHX	A1	3541	7/7	0.96	0.16	109,109,109,109	7
86	OHX	A2	1935	7/7	0.96	0.17	120,120,120,120	7
86	OHX	A6	1987	7/7	0.96	0.18	113,113,113,113	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A6	2076	7/7	0.96	0.15	90,90,90,90	7
86	OHX	A2	1937	7/7	0.96	0.14	122,122,122,122	7
87	MG	A8	236	1/1	0.96	0.28	75,75,75,75	0
86	OHX	A2	1985	7/7	0.96	0.16	144,144,144,144	7
86	OHX	A2	1957	7/7	0.96	0.20	101,101,101,101	7
86	OHX	A2	1968	7/7	0.96	0.18	134,134,134,134	7
86	OHX	A6	1992	7/7	0.96	0.13	125,125,125,125	7
86	OHX	A1	3671	7/7	0.96	0.18	96,96,96,96	7
86	OHX	A5	3631	7/7	0.96	0.17	89,89,89,89	7
86	OHX	A1	3612	7/7	0.96	0.09	146,146,146,146	7
86	OHX	A1	3613	7/7	0.96	0.18	98,98,98,98	7
86	OHX	A1	3614	7/7	0.96	0.21	112,112,112,112	7
86	OHX	A2	1958	7/7	0.96	0.15	139,139,139,139	7
87	MG	A1	4092	1/1	0.96	0.25	66,66,66,66	0
86	OHX	A5	3636	7/7	0.96	0.15	111,111,111,111	7
86	OHX	A1	3402	7/7	0.96	0.21	130,130,130,130	7
87	MG	A6	2145	1/1	0.96	0.23	46,46,46,46	0
87	MG	A5	4452	1/1	0.96	0.20	57,57,57,57	0
86	OHX	A2	1989	7/7	0.96	0.11	131,131,131,131	7
87	MG	A5	4273	1/1	0.96	0.18	75,75,75,75	0
86	OHX	A2	1971	7/7	0.96	0.15	110,110,110,110	7
87	MG	A5	4275	1/1	0.96	0.21	63,63,63,63	0
86	OHX	A1	3555	7/7	0.96	0.17	125,125,125,125	7
87	MG	A6	2149	1/1	0.96	0.30	49,49,49,49	0
86	OHX	A1	3556	7/7	0.96	0.18	128,128,128,128	7
86	OHX	A6	2004	7/7	0.96	0.17	105,105,105,105	7
87	MG	A1	4394	1/1	0.96	0.13	58,58,58,58	0
86	OHX	A2	1973	7/7	0.96	0.16	136,136,136,136	7
86	OHX	A1	3454	7/7	0.96	0.15	106,106,106,106	7
87	MG	A1	4397	1/1	0.96	0.16	80,80,80,80	0
86	OHX	A1	3560	7/7	0.96	0.14	116,116,116,116	7
86	OHX	A1	3625	7/7	0.96	0.21	92,92,92,92	7
86	OHX	A1	3561	7/7	0.96	0.18	110,110,110,110	7
87	MG	A6	2159	1/1	0.96	0.20	33,33,33,33	0
86	OHX	A1	3490	7/7	0.96	0.16	126,126,126,126	0
86	OHX	A5	3649	7/7	0.96	0.19	129,129,129,129	7
86	OHX	A1	3563	7/7	0.96	0.16	131,131,131,131	7
86	OHX	A5	3651	7/7	0.96	0.20	137,137,137,137	7
86	OHX	A5	3652	7/7	0.96	0.18	150,150,150,150	7
87	MG	A1	3964	1/1	0.96	0.33	50,50,50,50	0
86	OHX	A3	202	7/7	0.96	0.15	103,103,103,103	7
86	OHX	A3	205	7/7	0.96	0.14	113,113,113,113	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A3	206	7/7	0.96	0.13	140,140,140,140	7
86	OHX	A1	3493	7/7	0.96	0.12	148,148,148,148	0
86	OHX	A1	3494	7/7	0.96	0.12	133,133,133,133	0
86	OHX	A1	3504	7/7	0.96	0.16	105,105,105,105	7
86	OHX	A1	3568	7/7	0.96	0.11	133,133,133,133	7
86	OHX	A5	3795	7/7	0.96	0.17	117,117,117,117	7
87	MG	DO	204	1/1	0.96	0.09	57,57,57,57	0
86	OHX	A2	1975	7/7	0.96	0.12	141,141,141,141	7
86	OHX	A6	2022	7/7	0.96	0.10	145,145,145,145	7
86	OHX	A1	3572	7/7	0.96	0.17	114,114,114,114	7
87	MG	BC	404	1/1	0.96	0.21	67,67,67,67	0
87	MG	A5	3962	1/1	0.96	0.32	41,41,41,41	0
86	OHX	A1	3508	7/7	0.96	0.16	93,93,93,93	7
86	OHX	A5	3664	7/7	0.96	0.20	106,106,106,106	7
86	OHX	A4	205	7/7	0.96	0.14	122,122,122,122	7
87	MG	A1	4421	1/1	0.96	0.13	63,63,63,63	0
86	OHX	A4	207	7/7	0.96	0.13	129,129,129,129	7
86	OHX	A5	3803	7/7	0.96	0.19	107,107,107,107	7
86	OHX	A5	3667	7/7	0.96	0.16	100,100,100,100	7
86	OHX	A6	2027	7/7	0.96	0.09	189,189,189,189	7
87	MG	A5	4140	1/1	0.96	0.06	56,56,56,56	0
86	OHX	A5	3402	7/7	0.96	0.14	116,116,116,116	7
87	MG	A1	4131	1/1	0.96	0.22	75,75,75,75	0
87	MG	A5	4501	1/1	0.96	0.21	56,56,56,56	0
87	MG	A1	4429	1/1	0.96	0.13	54,54,54,54	0
87	MG	BI	308	1/1	0.96	0.08	57,57,57,57	0
87	MG	A5	4504	1/1	0.96	0.12	84,84,84,84	0
86	OHX	A5	3670	7/7	0.96	0.20	109,109,109,109	7
86	OHX	A2	1976	7/7	0.96	0.11	139,139,139,139	7
87	MG	A1	4279	1/1	0.96	0.26	54,54,54,54	0
86	OHX	A2	2013	7/7	0.96	0.20	116,116,116,116	7
86	OHX	A1	3577	7/7	0.96	0.20	122,122,122,122	7
86	OHX	A1	3699	7/7	0.96	0.21	107,107,107,107	7
86	OHX	A1	3578	7/7	0.96	0.17	112,112,112,112	7
86	OHX	A5	3472	7/7	0.96	0.19	105,105,105,105	0
87	MG	CY	204	1/1	0.96	0.11	56,56,56,56	0
86	OHX	A5	3677	7/7	0.96	0.19	113,113,113,113	7
86	OHX	A5	3488	7/7	0.96	0.14	125,125,125,125	0
86	OHX	A5	3493	7/7	0.96	0.17	102,102,102,102	7
86	OHX	A5	3502	7/7	0.96	0.13	141,141,141,141	0
86	OHX	A5	3513	7/7	0.96	0.14	115,115,115,115	7
86	OHX	A6	2033	7/7	0.96	0.20	133,133,133,133	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3701	7/7	0.96	0.17	112,112,112,112	7
86	OHX	A5	3522	7/7	0.96	0.11	123,123,123,123	7
87	MG	Df	204	1/1	0.96	0.12	61,61,61,61	0
86	OHX	A5	3524	7/7	0.96	0.17	92,92,92,92	7
87	MG	A5	3412	1/1	0.96	0.18	68,68,68,68	0
87	MG	Dg	203	1/1	0.96	0.18	88,88,88,88	0
87	MG	A5	3824	1/1	0.96	0.22	37,37,37,37	0
87	MG	Dj	102	1/1	0.96	0.15	74,74,74,74	0
86	OHX	A7	209	7/7	0.96	0.19	115,115,115,115	7
86	OHX	A5	3686	7/7	0.96	0.17	121,121,121,121	7
87	MG	A1	4003	1/1	0.96	0.33	48,48,48,48	0
86	OHX	A1	3640	7/7	0.96	0.10	153,153,153,153	7
87	MG	A1	4005	1/1	0.96	0.27	42,42,42,42	0
86	OHX	A5	3529	7/7	0.96	0.15	93,93,93,93	7
87	MG	A1	4007	1/1	0.96	0.21	29,29,29,29	0
86	OHX	A5	3530	7/7	0.96	0.17	105,105,105,105	7
87	MG	A1	4009	1/1	0.96	0.38	51,51,51,51	0
86	OHX	A8	204	7/7	0.96	0.17	101,101,101,101	7
87	MG	A1	4304	1/1	0.96	0.13	102,102,102,102	0
86	OHX	A2	1932	7/7	0.96	0.12	117,117,117,117	7
87	MG	A6	2219	1/1	0.96	0.07	50,50,50,50	0
86	OHX	BB	401	7/7	0.96	0.13	111,111,111,111	7
86	OHX	A6	1945	7/7	0.97	0.12	148,148,148,148	0
86	OHX	A6	1946	7/7	0.97	0.13	105,105,105,105	7
86	OHX	A5	3441	7/7	0.97	0.20	96,96,96,96	0
87	MG	A5	3952	1/1	0.97	0.38	43,43,43,43	0
86	OHX	A5	3447	7/7	0.97	0.19	107,107,107,107	0
87	MG	A1	4475	1/1	0.97	0.15	64,64,64,64	0
87	MG	A1	4476	1/1	0.97	0.08	68,68,68,68	0
86	OHX	A5	3463	7/7	0.97	0.15	130,130,130,130	0
87	MG	A5	4257	1/1	0.97	0.20	70,70,70,70	0
86	OHX	A5	3466	7/7	0.97	0.15	120,120,120,120	0
86	OHX	A5	3467	7/7	0.97	0.13	104,104,104,104	7
86	OHX	A1	3476	7/7	0.97	0.13	129,129,129,129	0
86	OHX	A6	1950	7/7	0.97	0.09	140,140,140,140	0
87	MG	A1	4064	1/1	0.97	0.17	69,69,69,69	0
86	OHX	A5	3491	7/7	0.97	0.16	106,106,106,106	7
86	OHX	A1	3479	7/7	0.97	0.13	117,117,117,117	7
86	OHX	A5	3495	7/7	0.97	0.15	92,92,92,92	7
86	OHX	A5	3501	7/7	0.97	0.12	106,106,106,106	7
86	OHX	A6	1952	7/7	0.97	0.12	123,123,123,123	7
86	OHX	A5	3508	7/7	0.97	0.14	119,119,119,119	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
87	MG	A5	4269	1/1	0.97	0.21	66,66,66,66	0
86	OHX	A5	3509	7/7	0.97	0.17	97,97,97,97	7
86	OHX	A5	3511	7/7	0.97	0.10	142,142,142,142	0
87	MG	A1	3935	1/1	0.97	0.41	59,59,59,59	0
86	OHX	A6	1954	7/7	0.97	0.13	141,141,141,141	7
86	OHX	A1	3482	7/7	0.97	0.14	106,106,106,106	7
86	OHX	A1	3559	7/7	0.97	0.20	116,116,116,116	7
86	OHX	A6	1957	7/7	0.97	0.11	144,144,144,144	7
86	OHX	A6	1959	7/7	0.97	0.16	107,107,107,107	7
86	OHX	A5	3527	7/7	0.97	0.18	105,105,105,105	7
86	OHX	A6	1960	7/7	0.97	0.12	120,120,120,120	7
86	OHX	A1	3484	7/7	0.97	0.12	126,126,126,126	0
87	MG	A5	4281	1/1	0.97	0.19	56,56,56,56	0
86	OHX	A1	3488	7/7	0.97	0.15	109,109,109,109	7
87	MG	Bf	202	1/1	0.97	0.15	69,69,69,69	0
86	OHX	A5	3531	7/7	0.97	0.14	106,106,106,106	7
86	OHX	A1	3622	7/7	0.97	0.16	112,112,112,112	7
86	OHX	A5	3533	7/7	0.97	0.13	118,118,118,118	7
86	OHX	A5	3534	7/7	0.97	0.13	92,92,92,92	7
86	OHX	A5	3536	7/7	0.97	0.15	97,97,97,97	7
86	OHX	A5	3537	7/7	0.97	0.13	115,115,115,115	7
86	OHX	A5	3539	7/7	0.97	0.14	125,125,125,125	7
86	OHX	A2	1949	7/7	0.97	0.10	135,135,135,135	7
86	OHX	A2	1950	7/7	0.97	0.12	122,122,122,122	7
87	MG	A5	3842	1/1	0.97	0.04	34,34,34,34	0
86	OHX	A5	3542	7/7	0.97	0.13	103,103,103,103	7
86	OHX	A5	3543	7/7	0.97	0.15	109,109,109,109	7
86	OHX	A2	1951	7/7	0.97	0.14	126,126,126,126	7
86	OHX	A1	3503	7/7	0.97	0.11	111,111,111,111	7
86	OHX	A5	3546	7/7	0.97	0.13	132,132,132,132	7
86	OHX	A6	1969	7/7	0.97	0.17	90,90,90,90	7
86	OHX	A5	3548	7/7	0.97	0.14	134,134,134,134	7
87	MG	A5	4459	1/1	0.97	0.14	84,84,84,84	0
86	OHX	A5	3549	7/7	0.97	0.17	107,107,107,107	7
86	OHX	A5	3550	7/7	0.97	0.17	119,119,119,119	7
86	OHX	A2	1921	7/7	0.97	0.13	113,113,113,113	7
86	OHX	A6	1971	7/7	0.97	0.12	108,108,108,108	7
86	OHX	A1	3505	7/7	0.97	0.11	124,124,124,124	7
86	OHX	A2	1992	7/7	0.97	0.16	123,123,123,123	7
86	OHX	A1	3570	7/7	0.97	0.17	100,100,100,100	7
86	OHX	A5	3809	7/7	0.97	0.14	91,91,91,91	7
86	OHX	A6	1975	7/7	0.97	0.15	106,106,106,106	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A6	1976	7/7	0.97	0.18	105,105,105,105	7
86	OHX	A5	3812	7/7	0.97	0.12	135,135,135,135	7
87	MG	A5	4009	1/1	0.97	0.32	45,45,45,45	0
86	OHX	A1	3571	7/7	0.97	0.10	119,119,119,119	7
86	OHX	A2	1970	7/7	0.97	0.12	138,138,138,138	7
86	OHX	A5	3563	7/7	0.97	0.15	98,98,98,98	7
86	OHX	A1	3510	7/7	0.97	0.15	92,92,92,92	7
86	OHX	A2	1936	7/7	0.97	0.18	112,112,112,112	7
86	OHX	A5	3566	7/7	0.97	0.18	99,99,99,99	7
86	OHX	A2	1924	7/7	0.97	0.14	111,111,111,111	7
86	OHX	A2	1996	7/7	0.97	0.16	113,113,113,113	7
86	OHX	A5	3570	7/7	0.97	0.19	97,97,97,97	7
86	OHX	A1	3519	7/7	0.97	0.15	137,137,137,137	7
86	OHX	A1	3579	7/7	0.97	0.18	97,97,97,97	7
87	MG	A5	4170	1/1	0.97	0.14	69,69,69,69	0
86	OHX	A7	206	7/7	0.97	0.13	115,115,115,115	7
86	OHX	A5	3573	7/7	0.97	0.18	107,107,107,107	7
87	MG	DC	405	1/1	0.97	0.09	72,72,72,72	0
86	OHX	A6	1985	7/7	0.97	0.18	114,114,114,114	7
86	OHX	A2	1974	7/7	0.97	0.08	170,170,170,170	7
86	OHX	A5	3699	7/7	0.97	0.18	107,107,107,107	7
86	OHX	A5	3576	7/7	0.97	0.21	124,124,124,124	7
86	OHX	A5	3701	7/7	0.97	0.25	57,57,57,57	7
86	OHX	A3	201	7/7	0.97	0.12	109,109,109,109	0
86	OHX	A8	205	7/7	0.97	0.13	107,107,107,107	7
86	OHX	A2	1955	7/7	0.97	0.16	123,123,123,123	7
86	OHX	A3	204	7/7	0.97	0.12	125,125,125,125	7
86	OHX	A8	208	7/7	0.97	0.14	115,115,115,115	7
87	MG	A5	4033	1/1	0.97	0.05	31,31,31,31	0
86	OHX	A8	209	7/7	0.97	0.15	130,130,130,130	7
86	OHX	A2	1939	7/7	0.97	0.13	144,144,144,144	7
87	MG	A1	3998	1/1	0.97	0.16	28,28,28,28	0
86	OHX	A5	3582	7/7	0.97	0.18	95,95,95,95	7
86	OHX	A1	3525	7/7	0.97	0.17	101,101,101,101	7
86	OHX	A2	1927	7/7	0.97	0.14	115,115,115,115	7
87	MG	A5	4190	1/1	0.97	0.16	58,58,58,58	0
86	OHX	A8	214	7/7	0.97	0.10	125,125,125,125	7
86	OHX	A1	3586	7/7	0.97	0.17	117,117,117,117	7
86	OHX	A5	3586	7/7	0.97	0.14	112,112,112,112	7
86	OHX	A1	3527	7/7	0.97	0.15	94,94,94,94	7
86	OHX	A1	3529	7/7	0.97	0.18	77,77,77,77	7
86	OHX	A1	3530	7/7	0.97	0.14	125,125,125,125	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A2	1978	7/7	0.97	0.14	108,108,108,108	7
87	MG	A5	4512	1/1	0.97	0.10	56,56,56,56	0
86	OHX	AL	201	7/7	0.97	0.15	119,119,119,119	7
86	OHX	A4	204	7/7	0.97	0.12	122,122,122,122	7
86	OHX	A1	3593	7/7	0.97	0.14	113,113,113,113	7
86	OHX	A1	3533	7/7	0.97	0.20	104,104,104,104	7
86	OHX	A5	3596	7/7	0.97	0.17	84,84,84,84	7
86	OHX	A6	2002	7/7	0.97	0.15	96,96,96,96	7
87	MG	A1	4428	1/1	0.97	0.34	58,58,58,58	0
86	OHX	A4	208	7/7	0.97	0.17	90,90,90,90	7
86	OHX	A2	1928	7/7	0.97	0.12	126,126,126,126	7
87	MG	A5	4362	1/1	0.97	0.11	60,60,60,60	0
86	OHX	A1	3535	7/7	0.97	0.17	102,102,102,102	7
86	OHX	A6	2006	7/7	0.97	0.18	87,87,87,87	7
86	OHX	A1	3654	7/7	0.97	0.09	149,149,149,149	7
86	OHX	A2	1942	7/7	0.97	0.17	113,113,113,113	7
86	OHX	A1	3538	7/7	0.97	0.14	105,105,105,105	7
86	OHX	Ad	101	7/7	0.97	0.14	130,130,130,130	7
86	OHX	DV	201	7/7	0.97	0.11	126,126,126,126	7
86	OHX	Df	201	7/7	0.97	0.17	99,99,99,99	7
86	OHX	A1	3600	7/7	0.97	0.15	100,100,100,100	7
87	MG	A1	4440	1/1	0.97	0.19	55,55,55,55	0
86	OHX	A2	1930	7/7	0.97	0.14	120,120,120,120	7
86	OHX	A2	1908	7/7	0.97	0.16	115,115,115,115	0
86	OHX	A5	3610	7/7	0.97	0.12	161,161,161,161	7
86	OHX	A2	1911	7/7	0.97	0.15	124,124,124,124	0
86	OHX	A1	3543	7/7	0.97	0.11	137,137,137,137	7
86	OHX	A6	2016	7/7	0.97	0.10	124,124,124,124	7
86	OHX	A2	1963	7/7	0.97	0.21	129,129,129,129	7
86	OHX	A5	3738	7/7	0.97	0.17	101,101,101,101	7
86	OHX	A5	3739	7/7	0.97	0.16	105,105,105,105	7
86	OHX	BI	301	7/7	0.97	0.14	94,94,94,94	7
86	OHX	A1	3447	7/7	0.97	0.14	98,98,98,98	0
86	OHX	A2	1913	7/7	0.97	0.15	129,129,129,129	0
86	OHX	A2	1948	7/7	0.97	0.15	108,108,108,108	7
87	MG	BN	306	1/1	0.97	0.09	55,55,55,55	0
87	MG	A1	4314	1/1	0.97	0.12	78,78,78,78	0
87	MG	A5	4548	1/1	0.97	0.11	74,74,74,74	0
87	MG	A5	4388	1/1	0.97	0.15	47,47,47,47	0
86	OHX	A1	3458	7/7	0.97	0.13	111,111,111,111	7
86	OHX	A1	3460	7/7	0.97	0.12	111,111,111,111	0
87	MG	A5	4391	1/1	0.97	0.16	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3611	7/7	0.97	0.16	96,96,96,96	7
87	MG	A1	4318	1/1	0.97	0.12	66,66,66,66	0
86	OHX	A1	3469	7/7	0.97	0.15	122,122,122,122	0
86	OHX	A1	3553	7/7	0.97	0.12	110,110,110,110	7
86	OHX	Bj	101	7/7	0.97	0.13	100,100,100,100	7
86	OHX	A5	3625	7/7	0.97	0.15	117,117,117,117	7
86	OHX	A1	3472	7/7	0.97	0.14	109,109,109,109	7
86	OHX	A5	3627	7/7	0.97	0.18	80,80,80,80	7
86	OHX	Cd	101	7/7	0.97	0.14	135,135,135,135	7
86	OHX	A6	1927	7/7	0.97	0.14	129,129,129,129	0
86	OHX	A6	1933	7/7	0.97	0.15	104,104,104,104	7
86	OHX	A6	1934	7/7	0.97	0.16	105,105,105,105	7
87	MG	BP	209	1/1	0.97	0.10	59,59,59,59	0
86	OHX	A6	1940	7/7	0.97	0.12	129,129,129,129	7
86	OHX	A1	3475	7/7	0.97	0.19	98,98,98,98	7
86	OHX	A5	3481	7/7	0.98	0.12	92,92,92,92	7
86	OHX	A5	3483	7/7	0.98	0.11	103,103,103,103	7
86	OHX	A5	3486	7/7	0.98	0.14	75,75,75,75	7
86	OHX	A5	3487	7/7	0.98	0.14	94,94,94,94	7
86	OHX	A6	1937	7/7	0.98	0.13	96,96,96,96	7
86	OHX	A5	3490	7/7	0.98	0.11	113,113,113,113	7
86	OHX	A6	1938	7/7	0.98	0.12	96,96,96,96	7
86	OHX	A6	1939	7/7	0.98	0.08	134,134,134,134	0
86	OHX	A5	3494	7/7	0.98	0.15	97,97,97,97	7
86	OHX	A2	1915	7/7	0.98	0.10	109,109,109,109	7
86	OHX	A5	3497	7/7	0.98	0.13	81,81,81,81	7
86	OHX	A5	3498	7/7	0.98	0.11	89,89,89,89	7
86	OHX	A5	3499	7/7	0.98	0.14	84,84,84,84	7
86	OHX	A5	3500	7/7	0.98	0.12	88,88,88,88	7
86	OHX	A6	1941	7/7	0.98	0.13	112,112,112,112	7
86	OHX	A1	3489	7/7	0.98	0.10	90,90,90,90	7
86	OHX	A5	3504	7/7	0.98	0.12	101,101,101,101	7
86	OHX	A5	3505	7/7	0.98	0.12	94,94,94,94	7
86	OHX	A5	3506	7/7	0.98	0.12	102,102,102,102	7
86	OHX	A6	1943	7/7	0.98	0.11	106,106,106,106	7
86	OHX	A6	1944	7/7	0.98	0.11	115,115,115,115	7
86	OHX	A5	3510	7/7	0.98	0.14	90,90,90,90	7
86	OHX	A2	1916	7/7	0.98	0.12	110,110,110,110	7
86	OHX	A5	3512	7/7	0.98	0.11	111,111,111,111	7
86	OHX	A1	3735	7/7	0.98	0.12	83,83,83,83	7
86	OHX	A5	3515	7/7	0.98	0.12	121,121,121,121	7
86	OHX	A5	3516	7/7	0.98	0.13	89,89,89,89	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3517	7/7	0.98	0.13	80,80,80,80	7
86	OHX	A1	3551	7/7	0.98	0.16	100,100,100,100	7
86	OHX	A5	3519	7/7	0.98	0.14	78,78,78,78	7
86	OHX	A5	3520	7/7	0.98	0.14	113,113,113,113	7
86	OHX	A6	1948	7/7	0.98	0.11	114,114,114,114	7
86	OHX	A6	1949	7/7	0.98	0.12	102,102,102,102	7
86	OHX	A1	3401	7/7	0.98	0.11	121,121,121,121	7
86	OHX	A5	3525	7/7	0.98	0.09	112,112,112,112	7
86	OHX	A2	1933	7/7	0.98	0.12	109,109,109,109	7
86	OHX	A1	3495	7/7	0.98	0.13	101,101,101,101	7
87	MG	A5	3825	1/1	0.98	0.10	29,29,29,29	0
86	OHX	A6	1953	7/7	0.98	0.08	136,136,136,136	7
86	OHX	A1	3496	7/7	0.98	0.14	97,97,97,97	7
86	OHX	A1	3497	7/7	0.98	0.16	100,100,100,100	7
86	OHX	A1	3498	7/7	0.98	0.15	89,89,89,89	7
86	OHX	A1	3500	7/7	0.98	0.14	87,87,87,87	7
86	OHX	A6	1958	7/7	0.98	0.11	133,133,133,133	7
86	OHX	A5	3535	7/7	0.98	0.14	77,77,77,77	7
86	OHX	A1	3501	7/7	0.98	0.14	94,94,94,94	7
86	OHX	A1	3502	7/7	0.98	0.12	78,78,78,78	7
86	OHX	A5	3538	7/7	0.98	0.12	104,104,104,104	7
86	OHX	A2	1917	7/7	0.98	0.11	111,111,111,111	7
87	MG	A1	3865	1/1	0.98	0.03	31,31,31,31	0
86	OHX	A2	1918	7/7	0.98	0.13	99,99,99,99	7
87	MG	A1	4172	1/1	0.98	0.36	54,54,54,54	0
86	OHX	A1	3432	7/7	0.98	0.12	90,90,90,90	0
86	OHX	A1	3441	7/7	0.98	0.10	93,93,93,93	0
86	OHX	A1	3507	7/7	0.98	0.14	75,75,75,75	7
86	OHX	A6	1966	7/7	0.98	0.12	92,92,92,92	7
86	OHX	A1	3442	7/7	0.98	0.12	95,95,95,95	0
86	OHX	A7	201	7/7	0.98	0.13	107,107,107,107	0
87	MG	A1	4025	1/1	0.98	0.42	39,39,39,39	0
86	OHX	A7	202	7/7	0.98	0.13	81,81,81,81	7
86	OHX	A7	203	7/7	0.98	0.13	105,105,105,105	7
86	OHX	A7	205	7/7	0.98	0.12	106,106,106,106	7
87	MG	A5	4475	1/1	0.98	0.17	127,127,127,127	0
86	OHX	A1	3567	7/7	0.98	0.14	88,88,88,88	7
86	OHX	A1	3509	7/7	0.98	0.13	98,98,98,98	7
86	OHX	A7	208	7/7	0.98	0.18	105,105,105,105	7
86	OHX	A2	1919	7/7	0.98	0.10	106,106,106,106	7
86	OHX	A3	203	7/7	0.98	0.12	118,118,118,118	7
86	OHX	A1	3450	7/7	0.98	0.12	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3693	7/7	0.98	0.14	100,100,100,100	7
86	OHX	A1	3451	7/7	0.98	0.12	105,105,105,105	0
86	OHX	A8	203	7/7	0.98	0.10	111,111,111,111	7
86	OHX	A5	3553	7/7	0.98	0.14	75,75,75,75	7
86	OHX	A1	3513	7/7	0.98	0.13	101,101,101,101	7
86	OHX	A1	3514	7/7	0.98	0.13	99,99,99,99	7
86	OHX	A1	3515	7/7	0.98	0.13	115,115,115,115	7
86	OHX	A1	3516	7/7	0.98	0.12	86,86,86,86	7
86	OHX	A5	3558	7/7	0.98	0.14	85,85,85,85	7
86	OHX	A5	3559	7/7	0.98	0.14	109,109,109,109	7
86	OHX	A1	3576	7/7	0.98	0.16	83,83,83,83	7
86	OHX	A1	3517	7/7	0.98	0.12	99,99,99,99	7
86	OHX	A2	1907	7/7	0.98	0.13	104,104,104,104	7
86	OHX	A4	203	7/7	0.98	0.13	93,93,93,93	7
86	OHX	A2	2033	7/7	0.98	0.13	97,97,97,97	7
86	OHX	A2	1922	7/7	0.98	0.10	99,99,99,99	7
86	OHX	A4	206	7/7	0.98	0.13	104,104,104,104	7
86	OHX	A1	3581	7/7	0.98	0.14	73,73,73,73	7
86	OHX	A1	3521	7/7	0.98	0.15	84,84,84,84	7
86	OHX	A5	3569	7/7	0.98	0.12	110,110,110,110	7
87	MG	DF	304	1/1	0.98	0.12	57,57,57,57	0
86	OHX	A1	3522	7/7	0.98	0.14	79,79,79,79	7
86	OHX	DB	401	7/7	0.98	0.11	98,98,98,98	7
86	OHX	A1	3459	7/7	0.98	0.12	86,86,86,86	7
86	OHX	A2	1923	7/7	0.98	0.12	110,110,110,110	7
86	OHX	A1	3461	7/7	0.98	0.12	104,104,104,104	0
86	OHX	A1	3462	7/7	0.98	0.11	91,91,91,91	7
86	OHX	A1	3463	7/7	0.98	0.09	110,110,110,110	7
86	OHX	A1	3528	7/7	0.98	0.15	81,81,81,81	7
86	OHX	A1	3464	7/7	0.98	0.13	88,88,88,88	7
86	OHX	A1	3591	7/7	0.98	0.14	95,95,95,95	7
86	OHX	A5	3579	7/7	0.98	0.14	105,105,105,105	7
86	OHX	A1	3465	7/7	0.98	0.12	94,94,94,94	7
86	OHX	DO	201	7/7	0.98	0.13	93,93,93,93	7
86	OHX	A2	1902	7/7	0.98	0.16	102,102,102,102	0
87	MG	A5	4358	1/1	0.98	0.12	54,54,54,54	0
86	OHX	A1	3471	7/7	0.98	0.13	107,107,107,107	7
86	OHX	A2	1926	7/7	0.98	0.11	112,112,112,112	7
86	OHX	A1	3473	7/7	0.98	0.14	85,85,85,85	7
86	OHX	De	201	7/7	0.98	0.13	91,91,91,91	7
86	OHX	A2	1903	7/7	0.98	0.13	94,94,94,94	0
86	OHX	A2	1990	7/7	0.98	0.12	105,105,105,105	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3537	7/7	0.98	0.15	119,119,119,119	7
86	OHX	Dj	104	7/7	0.98	0.13	105,105,105,105	7
86	OHX	Do	201	7/7	0.98	0.12	89,89,89,89	7
86	OHX	BO	201	7/7	0.98	0.11	97,97,97,97	7
86	OHX	A1	3477	7/7	0.98	0.12	83,83,83,83	7
86	OHX	A1	3478	7/7	0.98	0.11	112,112,112,112	7
86	OHX	A2	1944	7/7	0.98	0.13	109,109,109,109	7
86	OHX	A5	3592	7/7	0.98	0.15	102,102,102,102	7
86	OHX	A1	3480	7/7	0.98	0.15	96,96,96,96	7
86	OHX	A1	3481	7/7	0.98	0.12	97,97,97,97	7
86	OHX	Bj	102	7/7	0.98	0.15	102,102,102,102	7
86	OHX	A2	1912	7/7	0.98	0.13	115,115,115,115	0
86	OHX	A5	3597	7/7	0.98	0.14	95,95,95,95	7
86	OHX	Bo	201	7/7	0.98	0.11	97,97,97,97	7
86	OHX	A6	1908	7/7	0.98	0.16	101,101,101,101	0
86	OHX	A6	1911	7/7	0.98	0.17	100,100,100,100	0
86	OHX	A6	1914	7/7	0.98	0.12	111,111,111,111	0
86	OHX	A6	1917	7/7	0.98	0.12	100,100,100,100	7
86	OHX	A6	1919	7/7	0.98	0.11	104,104,104,104	7
86	OHX	A6	1921	7/7	0.98	0.12	92,92,92,92	7
86	OHX	A5	3401	7/7	0.98	0.13	102,102,102,102	0
86	OHX	A6	1922	7/7	0.98	0.11	108,108,108,108	0
86	OHX	A6	1925	7/7	0.98	0.10	112,112,112,112	7
86	OHX	A1	3483	7/7	0.98	0.12	103,103,103,103	7
86	OHX	A6	1928	7/7	0.98	0.12	73,73,73,73	7
86	OHX	A6	1929	7/7	0.98	0.12	128,128,128,128	0
86	OHX	A6	1930	7/7	0.98	0.11	120,120,120,120	7
86	OHX	A6	1931	7/7	0.98	0.12	84,84,84,84	7
86	OHX	A5	3446	7/7	0.98	0.11	82,82,82,82	0
86	OHX	A6	1932	7/7	0.98	0.12	109,109,109,109	7
86	OHX	A5	3454	7/7	0.98	0.10	103,103,103,103	0
86	OHX	A5	3455	7/7	0.98	0.12	100,100,100,100	0
86	OHX	A5	3459	7/7	0.98	0.12	100,100,100,100	0
86	OHX	A5	3462	7/7	0.98	0.12	102,102,102,102	0
86	OHX	A2	1906	7/7	0.98	0.12	98,98,98,98	0
86	OHX	A5	3759	7/7	0.98	0.13	80,80,80,80	7
86	OHX	A5	3464	7/7	0.98	0.12	98,98,98,98	7
86	OHX	A5	3465	7/7	0.98	0.12	91,91,91,91	7
86	OHX	A1	3485	7/7	0.98	0.12	113,113,113,113	7
86	OHX	A6	1935	7/7	0.98	0.13	102,102,102,102	7
86	OHX	A5	3470	7/7	0.98	0.12	118,118,118,118	0
86	OHX	A6	1936	7/7	0.98	0.13	100,100,100,100	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3475	7/7	0.98	0.12	95,95,95,95	7
87	MG	A5	3939	1/1	0.98	0.35	42,42,42,42	0
88	ZN	Ad	105	1/1	0.98	0.04	83,83,83,83	0
86	OHX	A5	3477	7/7	0.98	0.11	108,108,108,108	7
86	OHX	A5	3479	7/7	0.98	0.10	110,110,110,110	0
86	OHX	A5	3480	7/7	0.98	0.11	101,101,101,101	7
87	MG	A1	4121	1/1	0.98	0.08	74,74,74,74	0
86	OHX	A1	3455	7/7	0.99	0.10	100,100,100,100	0
86	OHX	A1	3456	7/7	0.99	0.11	100,100,100,100	7
86	OHX	Bb	101	7/7	0.99	0.10	77,77,77,77	0
86	OHX	A1	3457	7/7	0.99	0.13	97,97,97,97	7
86	OHX	A2	1904	7/7	0.99	0.11	99,99,99,99	0
86	OHX	A2	1905	7/7	0.99	0.09	88,88,88,88	0
86	OHX	A5	3468	7/7	0.99	0.10	75,75,75,75	7
86	OHX	A5	3469	7/7	0.99	0.09	107,107,107,107	7
86	OHX	A2	1920	7/7	0.99	0.12	115,115,115,115	7
86	OHX	A5	3471	7/7	0.99	0.10	90,90,90,90	7
86	OHX	A1	3408	7/7	0.99	0.15	66,66,66,66	0
86	OHX	A5	3473	7/7	0.99	0.09	82,82,82,82	7
86	OHX	A5	3474	7/7	0.99	0.09	81,81,81,81	7
86	OHX	A6	1901	7/7	0.99	0.14	78,78,78,78	0
86	OHX	A5	3476	7/7	0.99	0.10	103,103,103,103	7
86	OHX	A6	1902	7/7	0.99	0.15	90,90,90,90	0
86	OHX	A5	3478	7/7	0.99	0.12	76,76,76,76	7
86	OHX	A6	1903	7/7	0.99	0.12	84,84,84,84	0
86	OHX	A6	1904	7/7	0.99	0.11	88,88,88,88	0
86	OHX	A5	3737	7/7	0.99	0.10	75,75,75,75	7
86	OHX	A6	1905	7/7	0.99	0.12	88,88,88,88	0
86	OHX	A5	3482	7/7	0.99	0.11	85,85,85,85	7
86	OHX	A6	1906	7/7	0.99	0.09	85,85,85,85	0
86	OHX	A5	3484	7/7	0.99	0.09	99,99,99,99	7
86	OHX	Db	101	7/7	0.99	0.11	86,86,86,86	0
86	OHX	A5	3485	7/7	0.99	0.09	85,85,85,85	7
86	OHX	A6	1907	7/7	0.99	0.12	91,91,91,91	0
86	OHX	A1	3412	7/7	0.99	0.14	76,76,76,76	0
86	OHX	A6	1909	7/7	0.99	0.10	84,84,84,84	0
86	OHX	A5	3489	7/7	0.99	0.11	88,88,88,88	7
86	OHX	A1	3414	7/7	0.99	0.12	77,77,77,77	0
86	OHX	A6	1912	7/7	0.99	0.10	96,96,96,96	0
86	OHX	A5	3492	7/7	0.99	0.11	89,89,89,89	7
86	OHX	A6	1913	7/7	0.99	0.08	91,91,91,91	0
86	OHX	A1	3416	7/7	0.99	0.09	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A6	1915	7/7	0.99	0.08	87,87,87,87	7
86	OHX	A5	3496	7/7	0.99	0.10	73,73,73,73	7
86	OHX	A6	1916	7/7	0.99	0.11	87,87,87,87	7
86	OHX	A1	3417	7/7	0.99	0.13	82,82,82,82	0
86	OHX	A6	1918	7/7	0.99	0.09	100,100,100,100	0
86	OHX	A1	3466	7/7	0.99	0.12	90,90,90,90	7
86	OHX	A6	1920	7/7	0.99	0.08	87,87,87,87	7
86	OHX	A1	3467	7/7	0.99	0.11	91,91,91,91	7
86	OHX	A5	3503	7/7	0.99	0.12	97,97,97,97	7
86	OHX	A1	3468	7/7	0.99	0.10	74,74,74,74	7
86	OHX	A6	1923	7/7	0.99	0.11	76,76,76,76	7
86	OHX	A6	1924	7/7	0.99	0.10	83,83,83,83	7
86	OHX	A5	3507	7/7	0.99	0.12	75,75,75,75	7
86	OHX	A1	3418	7/7	0.99	0.10	81,81,81,81	0
86	OHX	A6	1926	7/7	0.99	0.11	82,82,82,82	7
86	OHX	A1	3470	7/7	0.99	0.12	96,96,96,96	7
86	OHX	A1	3419	7/7	0.99	0.09	76,76,76,76	0
86	OHX	A1	3421	7/7	0.99	0.09	80,80,80,80	0
86	OHX	A1	3422	7/7	0.99	0.10	78,78,78,78	0
86	OHX	A5	3514	7/7	0.99	0.13	90,90,90,90	7
86	OHX	A1	3474	7/7	0.99	0.10	92,92,92,92	7
86	OHX	A1	3423	7/7	0.99	0.07	75,75,75,75	0
86	OHX	A1	3424	7/7	0.99	0.10	81,81,81,81	0
86	OHX	A1	3425	7/7	0.99	0.11	85,85,85,85	0
86	OHX	A1	3426	7/7	0.99	0.09	73,73,73,73	0
86	OHX	A1	3427	7/7	0.99	0.10	86,86,86,86	0
86	OHX	A1	3428	7/7	0.99	0.10	87,87,87,87	0
86	OHX	A1	3429	7/7	0.99	0.10	87,87,87,87	0
86	OHX	A5	3523	7/7	0.99	0.12	79,79,79,79	7
86	OHX	A1	3430	7/7	0.99	0.13	93,93,93,93	0
86	OHX	A1	3431	7/7	0.99	0.10	89,89,89,89	0
86	OHX	A5	3526	7/7	0.99	0.10	85,85,85,85	7
86	OHX	A2	1938	7/7	0.99	0.09	111,111,111,111	7
86	OHX	A1	3433	7/7	0.99	0.09	85,85,85,85	0
86	OHX	A1	3486	7/7	0.99	0.10	92,92,92,92	7
86	OHX	A1	3487	7/7	0.99	0.12	94,94,94,94	7
86	OHX	A4	201	7/7	0.99	0.13	77,77,77,77	0
86	OHX	A4	202	7/7	0.99	0.10	80,80,80,80	0
86	OHX	A1	3435	7/7	0.99	0.08	85,85,85,85	0
86	OHX	A1	3545	7/7	0.99	0.14	78,78,78,78	7
86	OHX	A1	3436	7/7	0.99	0.07	69,69,69,69	7
86	OHX	A1	3775	7/7	0.99	0.12	69,69,69,69	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3437	7/7	0.99	0.10	74,74,74,74	7
86	OHX	A1	3491	7/7	0.99	0.11	90,90,90,90	7
86	OHX	A1	3492	7/7	0.99	0.12	98,98,98,98	7
86	OHX	A1	3438	7/7	0.99	0.09	91,91,91,91	7
86	OHX	A1	3439	7/7	0.99	0.10	81,81,81,81	7
86	OHX	A1	3440	7/7	0.99	0.11	86,86,86,86	0
86	OHX	A2	1929	7/7	0.99	0.10	90,90,90,90	7
86	OHX	A2	1914	7/7	0.99	0.08	92,92,92,92	7
86	OHX	A1	3443	7/7	0.99	0.09	76,76,76,76	0
86	OHX	A1	3499	7/7	0.99	0.11	83,83,83,83	7
86	OHX	A1	3444	7/7	0.99	0.10	84,84,84,84	0
86	OHX	A1	3445	7/7	0.99	0.09	81,81,81,81	0
86	OHX	A1	3446	7/7	0.99	0.11	79,79,79,79	7
86	OHX	A2	1909	7/7	0.99	0.10	93,93,93,93	7
86	OHX	A1	3448	7/7	0.99	0.10	85,85,85,85	7
86	OHX	A5	3418	7/7	0.99	0.14	77,77,77,77	0
86	OHX	A5	3419	7/7	0.99	0.13	79,79,79,79	0
86	OHX	A5	3420	7/7	0.99	0.10	74,74,74,74	0
86	OHX	A5	3421	7/7	0.99	0.13	81,81,81,81	0
86	OHX	A5	3422	7/7	0.99	0.11	75,75,75,75	0
86	OHX	A5	3424	7/7	0.99	0.15	86,86,86,86	0
86	OHX	A5	3426	7/7	0.99	0.08	67,67,67,67	0
86	OHX	A5	3427	7/7	0.99	0.11	79,79,79,79	0
86	OHX	A5	3428	7/7	0.99	0.11	88,88,88,88	0
86	OHX	A5	3429	7/7	0.99	0.13	84,84,84,84	0
86	OHX	A5	3431	7/7	0.99	0.11	83,83,83,83	0
86	OHX	A5	3433	7/7	0.99	0.09	81,81,81,81	0
87	MG	A1	3959	1/1	0.99	0.33	43,43,43,43	0
86	OHX	A5	3434	7/7	0.99	0.10	85,85,85,85	0
86	OHX	A5	3435	7/7	0.99	0.07	70,70,70,70	0
86	OHX	A5	3436	7/7	0.99	0.09	82,82,82,82	0
86	OHX	A5	3437	7/7	0.99	0.12	83,83,83,83	0
86	OHX	A5	3438	7/7	0.99	0.13	91,91,91,91	0
86	OHX	A5	3439	7/7	0.99	0.09	81,81,81,81	0
86	OHX	A7	204	7/7	0.99	0.10	75,75,75,75	7
86	OHX	A1	3449	7/7	0.99	0.10	99,99,99,99	0
86	OHX	A5	3442	7/7	0.99	0.08	85,85,85,85	0
86	OHX	A5	3443	7/7	0.99	0.08	75,75,75,75	7
86	OHX	A5	3444	7/7	0.99	0.10	74,74,74,74	7
86	OHX	A2	1972	7/7	0.99	0.10	138,138,138,138	7
86	OHX	A2	1910	7/7	0.99	0.11	104,104,104,104	0
86	OHX	A5	3448	7/7	0.99	0.09	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A5	3449	7/7	0.99	0.09	85,85,85,85	7
86	OHX	A5	3450	7/7	0.99	0.07	76,76,76,76	7
86	OHX	A5	3451	7/7	0.99	0.08	81,81,81,81	7
86	OHX	A5	3452	7/7	0.99	0.10	86,86,86,86	7
86	OHX	A5	3453	7/7	0.99	0.12	102,102,102,102	0
86	OHX	A1	3452	7/7	0.99	0.07	81,81,81,81	7
86	OHX	A2	1901	7/7	0.99	0.14	95,95,95,95	0
88	ZN	Aa	202	1/1	0.99	0.04	92,92,92,92	0
86	OHX	A5	3456	7/7	0.99	0.11	85,85,85,85	7
86	OHX	A5	3457	7/7	0.99	0.09	86,86,86,86	7
88	ZN	Af	202	1/1	0.99	0.03	113,113,113,113	0
88	ZN	Bm	202	1/1	0.99	0.03	56,56,56,56	0
86	OHX	A5	3458	7/7	0.99	0.11	91,91,91,91	0
88	ZN	Bp	501	1/1	0.99	0.03	68,68,68,68	0
86	OHX	A2	1925	7/7	0.99	0.07	138,138,138,138	0
88	ZN	Cd	103	1/1	0.99	0.02	71,71,71,71	0
86	OHX	A5	3460	7/7	0.99	0.09	80,80,80,80	7
86	OHX	A5	3461	7/7	0.99	0.09	82,82,82,82	7
88	ZN	Dp	104	1/1	0.99	0.03	79,79,79,79	0
86	OHX	A5	3413	7/7	1.00	0.16	71,71,71,71	0
86	OHX	A5	3430	7/7	1.00	0.08	80,80,80,80	0
86	OHX	A5	3414	7/7	1.00	0.15	69,69,69,69	0
86	OHX	A5	3432	7/7	1.00	0.07	73,73,73,73	0
86	OHX	A5	3415	7/7	1.00	0.13	67,67,67,67	0
86	OHX	A5	3416	7/7	1.00	0.11	68,68,68,68	0
86	OHX	A5	3417	7/7	1.00	0.13	72,72,72,72	0
86	OHX	A1	3411	7/7	1.00	0.11	71,71,71,71	0
86	OHX	A8	202	7/7	1.00	0.12	77,77,77,77	0
86	OHX	A1	3409	7/7	1.00	0.13	70,70,70,70	0
86	OHX	A1	3413	7/7	1.00	0.13	75,75,75,75	0
86	OHX	A1	3410	7/7	1.00	0.11	68,68,68,68	0
86	OHX	A5	3440	7/7	1.00	0.07	63,63,63,63	7
88	ZN	Bj	111	1/1	1.00	0.02	44,44,44,44	0
86	OHX	A6	1910	7/7	1.00	0.07	84,84,84,84	0
86	OHX	A5	3423	7/7	1.00	0.07	68,68,68,68	0
86	OHX	BT	201	7/7	1.00	0.08	78,78,78,78	0
88	ZN	Ca	202	1/1	1.00	0.03	73,73,73,73	0
86	OHX	A5	3425	7/7	1.00	0.08	72,72,72,72	0
86	OHX	A5	3445	7/7	1.00	0.07	73,73,73,73	0
86	OHX	A1	3420	7/7	1.00	0.07	69,69,69,69	0
88	ZN	Dj	105	1/1	1.00	0.02	48,48,48,48	0
88	ZN	Dm	202	1/1	1.00	0.01	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	A1	3415	7/7	1.00	0.07	68,68,68,68	0
86	OHX	A1	3434	7/7	1.00	0.07	72,72,72,72	7

6.5 Other polymers (i)

There are no such residues in this entry.