



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 08:35 AM EDT

PDB ID : 4V8E  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-tyr complex).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-07  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

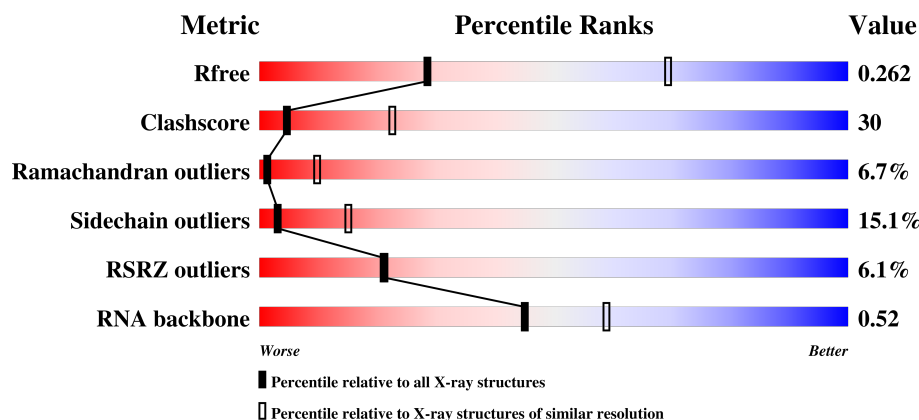
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)
RNA backbone	2636	1009 (3.74-2.86)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	<div> <div>2%</div> <div>36% 47% 17%</div> </div>
1	CA	2912	<div> <div>%</div> <div>33% 49% 17%</div> </div>
2	AB	122	<div> <div>2%</div> <div>43% 45% 11%</div> </div>
2	CB	122	<div> <div>%</div> <div>30% 49% 20%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AD	276	
3	CD	276	
4	AE	206	
4	CE	206	
5	AF	210	
5	CF	210	
6	AG	182	
6	CG	182	
7	AH	180	
7	CH	180	
8	AK	148	
8	CK	148	
9	AM	140	
9	CM	140	
10	AN	122	
10	CN	122	
11	AO	150	
11	CO	150	
12	AP	141	
12	CP	141	
13	A0	118	
13	C0	118	
14	AQ	112	
14	CQ	112	
15	AR	146	



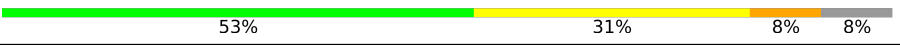
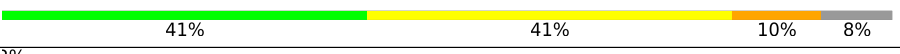
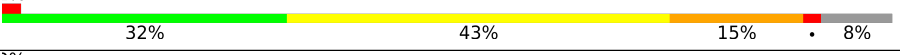
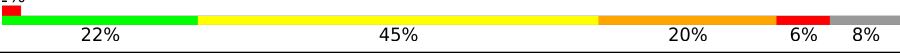
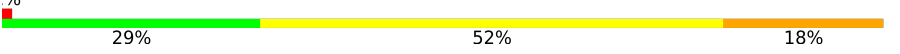
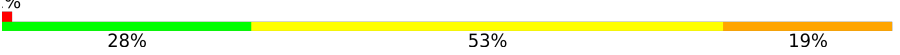

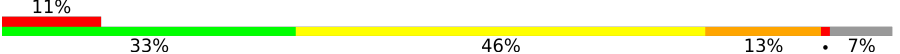
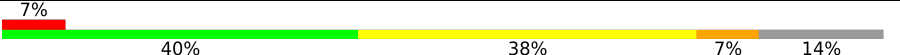
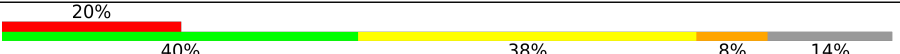

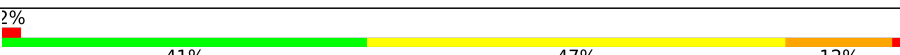
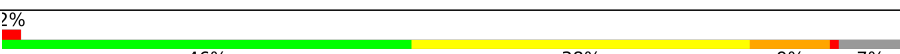
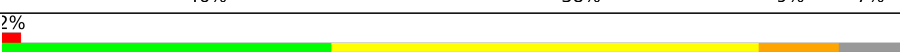


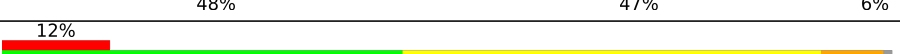

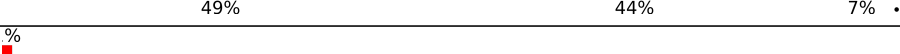




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CR	146	
16	A1	118	
16	C1	118	
17	A2	101	
17	C2	101	
18	AS	113	
18	CS	113	
19	AT	96	
19	CT	96	
20	AU	110	
20	CU	110	
21	AV	206	
21	CV	206	
22	A3	85	
22	C3	85	
23	AZ	98	
23	CZ	98	
24	AW	72	
24	CW	72	
25	AX	60	
25	CX	60	
26	A4	71	
26	C4	71	
27	A5	60	
27	C5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A6	54	
28	C6	54	
29	A7	49	
29	C7	49	
30	A8	65	
30	C8	65	
31	BA	1506	
31	DA	1506	
32	BE	256	
32	DE	256	
33	BF	239	
33	DF	239	
34	BG	208	
34	DG	208	
35	BH	162	
35	DH	162	
36	BI	101	
36	DI	101	
37	BJ	156	
37	DJ	156	
38	BK	138	
38	DK	138	
39	BL	128	
39	DL	128	
40	BM	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DM	105	
41	BN	129	
41	DN	129	
42	BO	132	
42	DO	132	
43	BP	126	
43	DP	126	
44	BQ	61	
44	DQ	61	
45	BR	89	
45	DR	89	
46	BS	88	
46	DS	88	
47	BT	105	
47	DT	105	
48	BU	88	
48	DU	88	
49	BV	93	
49	DV	93	
50	BW	106	
50	DW	106	
51	BX	27	
51	DX	27	
52	BB	85	
52	BD	85	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	DB	85	
52	DD	85	
53	BC	77	
53	DC	77	
54	B1	16	
54	D1	16	

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
55	MG	AA	3009	-	-	-	X
55	MG	AA	3015	-	-	-	X
55	MG	AA	3035	-	-	-	X
55	MG	AA	3044	-	-	-	X
55	MG	AA	3048	-	-	-	X
55	MG	AA	3052	-	-	-	X
55	MG	AA	3059	-	-	-	X
55	MG	AA	3079	-	-	-	X
55	MG	AA	3087	-	-	-	X
55	MG	AA	3105	-	-	-	X
55	MG	AA	3107	-	-	-	X
55	MG	AA	3132	-	-	-	X
55	MG	AA	3137	-	-	-	X
55	MG	AA	3165	-	-	-	X
55	MG	AA	3174	-	-	-	X
55	MG	AA	3199	-	-	-	X
55	MG	AA	3220	-	-	-	X
55	MG	AA	3224	-	-	-	X
55	MG	AA	3264	-	-	-	X
55	MG	AA	3347	-	-	-	X
55	MG	BA	1627	-	-	-	X
55	MG	BA	1646	-	-	-	X
55	MG	BA	1648	-	-	-	X
55	MG	BA	1699	-	-	-	X
55	MG	BA	1703	-	-	-	X
55	MG	BA	1710	-	-	-	X
55	MG	BA	1711	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	1720	-	-	-	X
55	MG	BA	1727	-	-	-	X
55	MG	BA	1730	-	-	-	X
55	MG	BA	1751	-	-	-	X
55	MG	BB	104	-	-	-	X
55	MG	CA	3136	-	-	-	X
55	MG	CA	3164	-	-	-	X
55	MG	CA	3187	-	-	-	X
55	MG	CA	3202	-	-	-	X
55	MG	CA	3206	-	-	-	X
55	MG	CA	3455	-	-	-	X
55	MG	CA	3477	-	-	-	X
55	MG	DA	1628	-	-	-	X
55	MG	DA	1631	-	-	-	X
55	MG	DA	1641	-	-	-	X
55	MG	DA	1642	-	-	-	X
55	MG	DA	1660	-	-	-	X
55	MG	DA	1661	-	-	-	X
55	MG	DA	1695	-	-	-	X
55	MG	DA	1698	-	-	-	X
55	MG	DA	1701	-	-	-	X
55	MG	DA	1708	-	-	-	X
55	MG	DA	1720	-	-	-	X
55	MG	DA	1725	-	-	-	X
55	MG	DB	101	-	-	-	X
56	OHX	AA	3568	-	-	X	-
56	OHX	BA	1673	-	-	X	-
56	OHX	BA	1684	-	-	X	-
56	OHX	C6	101	-	-	X	-
56	OHX	DA	1731	-	-	X	-
56	OHX	DA	1760	-	-	X	-
56	OHX	DA	1767	-	-	X	-
56	OHX	DC	107	-	-	X	-



## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 303952 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 RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	CA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	INSERTION	GB AP008226.1
AA	654A	A	G	CONFLICT	GB AP008226.1
AA	654E	C	G	CONFLICT	GB AP008226.1
AA	654P	G	C	CONFLICT	GB AP008226.1
AA	654T	A	C	CONFLICT	GB AP008226.1
AA	1058	U	G	CONFLICT	GB AP008226.1
AA	1080	A	C	CONFLICT	GB AP008226.1
CA	156	U	-	INSERTION	GB AP008226.1
CA	681	A	G	CONFLICT	GB AP008226.1
CA	685	C	G	CONFLICT	GB AP008226.1
CA	696	G	C	CONFLICT	GB AP008226.1
CA	700	A	C	CONFLICT	GB AP008226.1
CA	1105	U	G	CONFLICT	GB AP008226.1
CA	1127	A	C	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	CB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
3	CD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
4	CE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
5	CF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
7	CH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	CK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
9	CM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	CN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	CO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	CP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	C0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	CQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
15	CR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	C1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	C2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	CS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			725	471	131	123			
19	CT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
20	CU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	CV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	C3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	CZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	CX	59	Total	C	N	O		0	0	0
			469	298	90	81				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	C4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	C5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	C6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
29	C7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
30	C8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
31	DA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	DE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	DF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	DG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	DH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	DI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	DJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	DK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	DL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	DN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	DO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	DP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
44	DQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	DR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	DS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	DT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	DU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
49	DV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	DW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	DX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
52	BB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	BD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	DB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	DD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	CONFLICT	GB AP012306.1
DC	18	C	U	CONFLICT	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			
54	D1	16	Total	C	N	O	P	0	0	0
			347	156	69	106	16			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

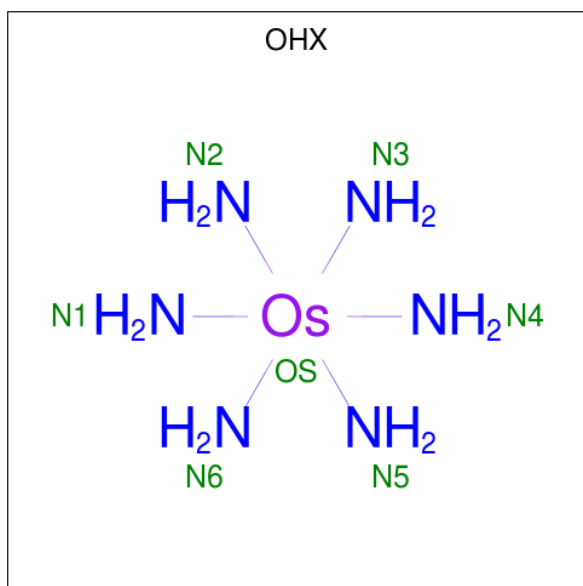
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	115	Total Mg 115 115	0	0
55	CA	274	Total Mg 274 274	0	0
55	C5	1	Total Mg 1 1	0	0
55	AB	6	Total Mg 6 6	0	0
55	B1	1	Total Mg 1 1	0	0
55	DN	1	Total Mg 1 1	0	0
55	DC	6	Total Mg 6 6	0	0
55	BB	5	Total Mg 5 5	0	0
55	AE	3	Total Mg 3 3	0	0
55	DL	1	Total Mg 1 1	0	0
55	C0	1	Total Mg 1 1	0	0
55	AA	331	Total Mg 331 331	0	0
55	BQ	1	Total Mg 1 1	0	0
55	A5	1	Total Mg 1 1	0	0
55	BC	5	Total Mg 5 5	0	0
55	A1	1	Total Mg 1 1	0	0
55	BN	1	Total Mg 1 1	0	0
55	C7	1	Total Mg 1 1	0	0
55	DA	119	Total Mg 119 119	0	0
55	AO	3	Total Mg 3 3	0	0
55	A0	1	Total Mg 1 1	0	0
55	D1	1	Total Mg 1 1	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CB	7	Total 7	Mg 7	0	0
55	BS	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	CE	1	Total 1	Mg 1	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	2	Total 2	Mg 2	0	0
55	DB	2	Total 2	Mg 2	0	0

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0
56	AA	1	Total 7	N 6	Os 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AA	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AB	1	Total	N	Os	0	0
			7	6	1		
56	AE	1	Total	N	Os	0	0
			7	6	1		
56	AF	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	AO	1	Total	N	Os	0	0
			7	6	1		
56	A1	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	A1	1	Total	N	Os	0	0
			7	6	1		
56	A3	1	Total	N	Os	0	0
			7	6	1		
56	AW	1	Total	N	Os	0	0
			7	6	1		
56	A6	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		
56	BA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BG	1	Total	N	Os	0	0
			7	6	1		
56	BR	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
			7	6	1		
56	BB	1	Total	N	Os	0	0
			7	6	1		
56	BC	1	Total	N	Os	0	0
			7	6	1		
56	BC	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	BD	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CA	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CB	1	Total	N	Os	0	0
			7	6	1		
56	CF	1	Total	N	Os	0	0
			7	6	1		
56	CO	1	Total	N	Os	0	0
			7	6	1		
56	C1	1	Total	N	Os	0	0
			7	6	1		
56	C3	1	Total	N	Os	0	0
			7	6	1		
56	C5	1	Total	N	Os	0	0
			7	6	1		
56	C6	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DG	1	Total	N	Os	0	0
			7	6	1		
56	DK	1	Total	N	Os	0	0
			7	6	1		
56	DR	1	Total	N	Os	0	0
			7	6	1		
56	DV	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DC	1	Total	N	Os	0	0
			7	6	1		
56	DD	1	Total	N	Os	0	0
			7	6	1		

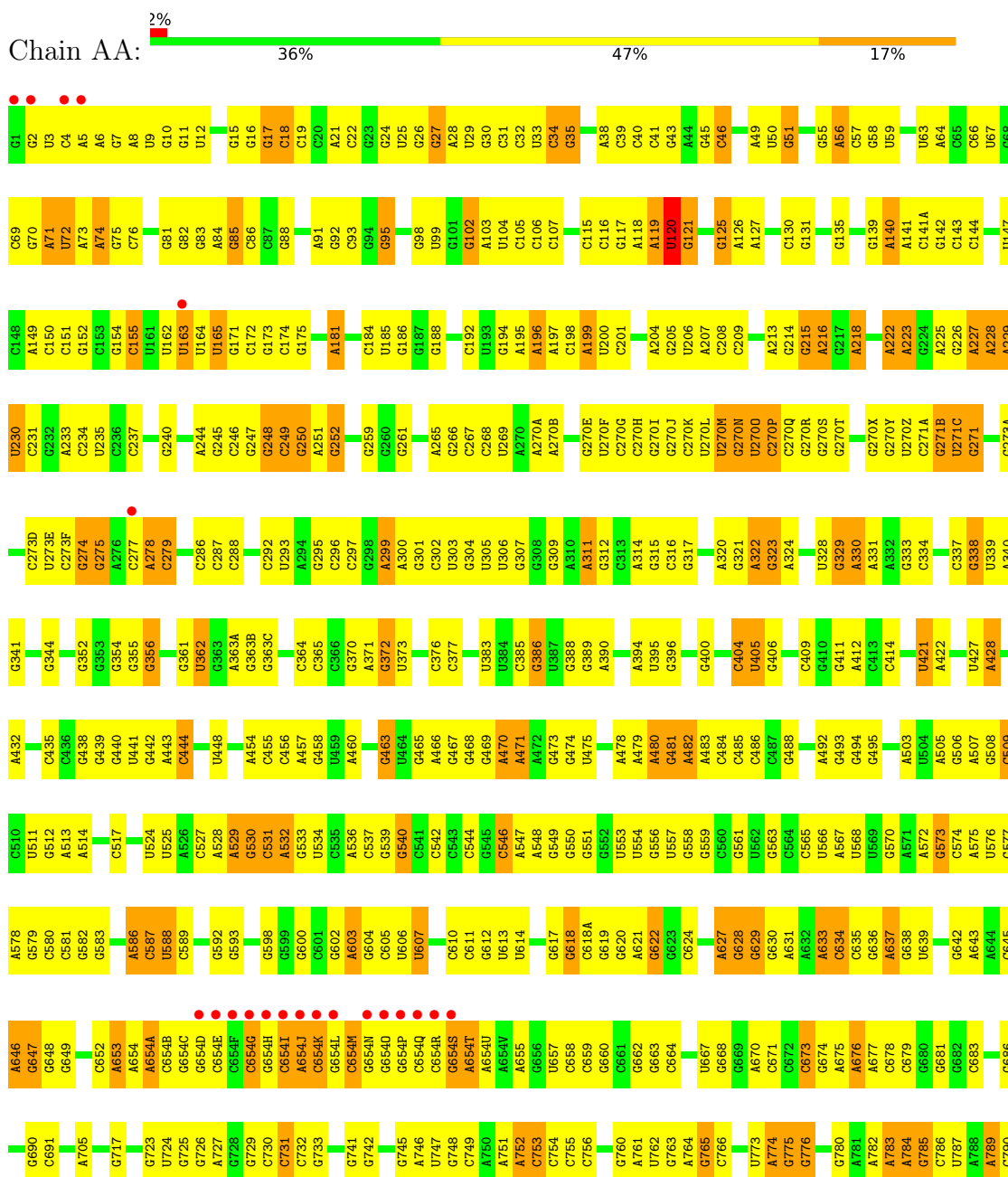
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DG	1	Total	Zn	0	0
			1	1		
57	BG	1	Total	Zn	0	0
			1	1		
57	BQ	1	Total	Zn	0	0
			1	1		
57	DQ	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

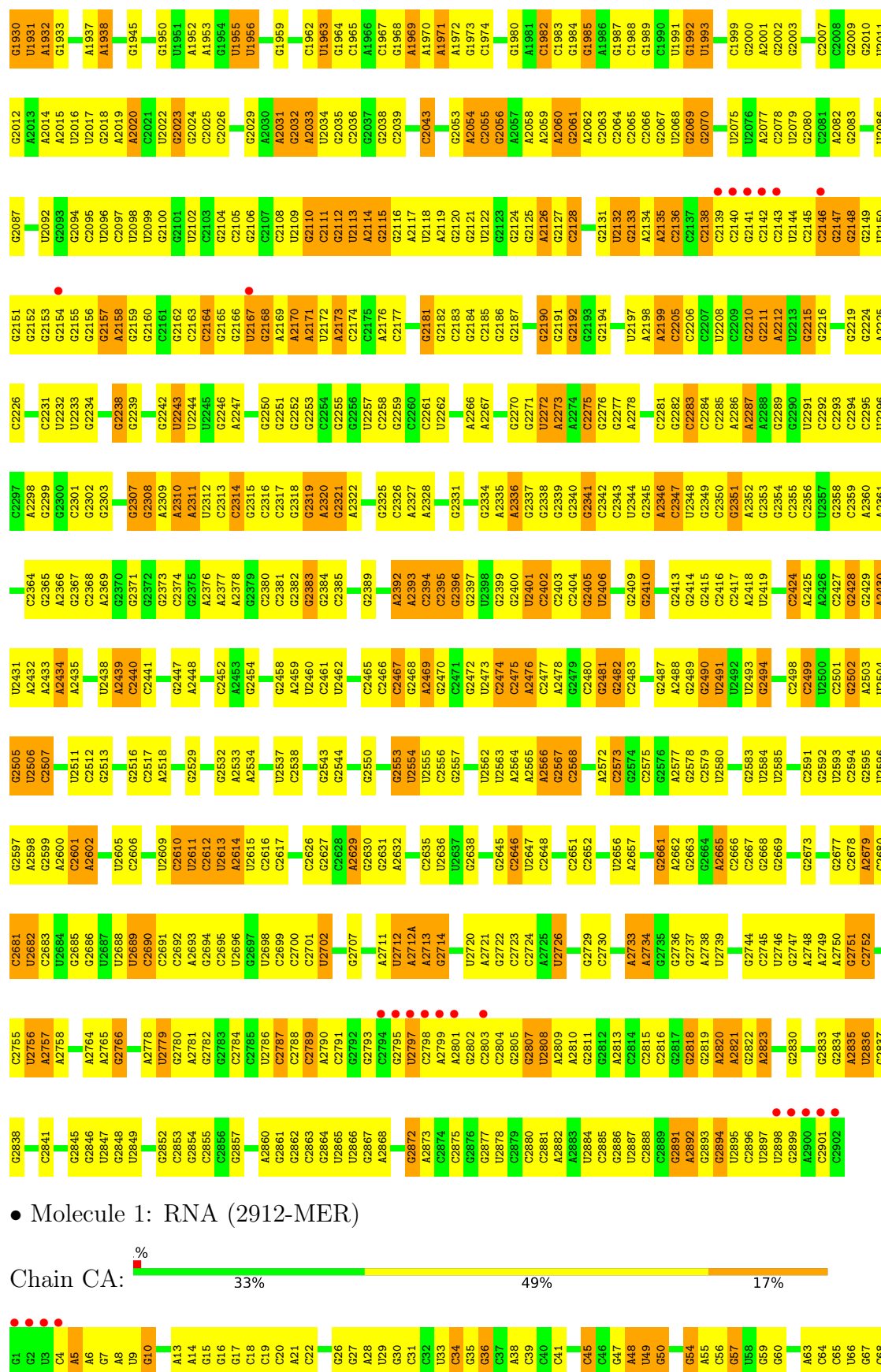
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: RNA (2912-MER)



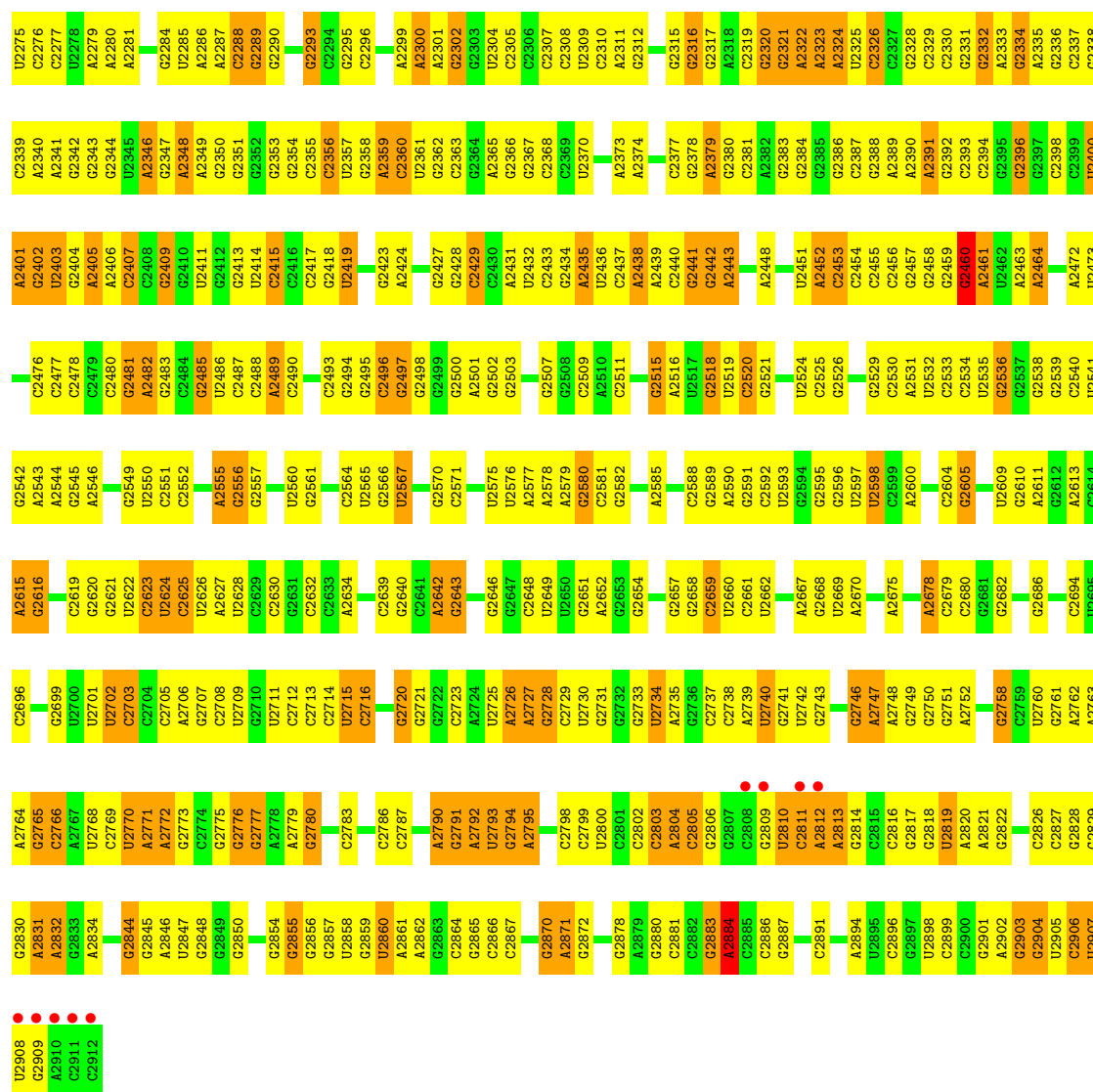




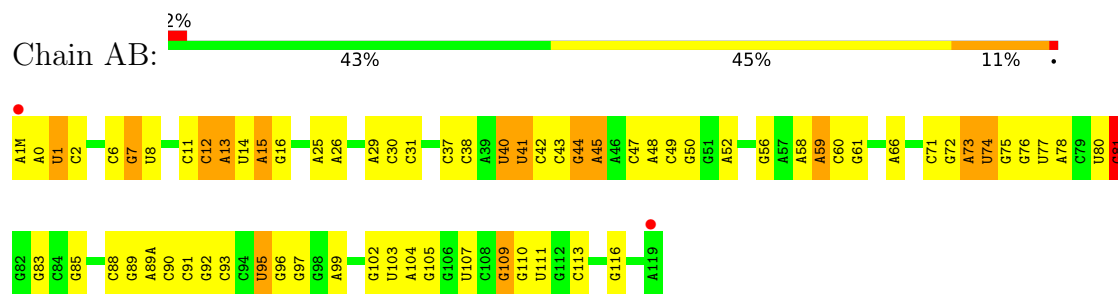


G1062	G1063	A1127	G1435	G216	G358	U493	A507	U579	G651	C721	C801	A877	G939	G1000	G1062
G1083	G1084	U1128	G1436	A217	C359	G424	G508	G580	U652	G722	C802	G878	C940	C1001	G1083
G1085	G1086		U147	A218	C360	A429	G509	U581	A653	A723	U810	G879	C941	G1002	G1084
A1131	A1132	A1131	G151	U220	C362	U433	C512	C584	G655	G728	A812	U881	C942	A1003	G1085
A1133	A1134	A1132	G152	A223	C365	U434	C513	C587	G656	G729	A813	C882	C943	U1004	A1066
A1133	A1133	A1133	G153	C224	C366	G435	C514	C588	G657	C730	C814	C884	C944	A1005	A1068
G1134	G1135	G1134	G154	U225	C367	G436	G515	C589	A658	G731		C885	A946	A1006	G1069
A1136	A1136	A1136	U	C226	C368	G437	G516	C590	A659	G732	U821	C886	A947	G1007	U1070
G1137	G1137	G1137	U	C227	C369	G439	G517	U590	C661	A733	A822	U887	C948	U1009	G1072
G1138	G1138	G1138	U	C228	C370	A440	A518		G662	G734	G823	C888	C950		U1073
A1139	A1139	A1139	U		C302	C441	A519	A595	A663		G824		C951	G1012	A1074
A1075	A1075	A1075	U		A303	C442	G520	A596	G664	C739	A825	C892	U952	G1013	A1075
A1076	A1076	A1076	U		A304		G521	A597			A826	G893	G953	G1014	A1076
A1079	A1079	A1079	G161	A231	C305	U455		C598	C671	G744	U827	G894	U954	U1015	
U1141	U1141	U1141	G162	U233	C306	A456	A527	C599	A672	C745	A827	G895	U955	C1016	
U1143	U1143	U1143	G163	A234	G306			A599	A673	C746	U830	U896	C956	C1017	
U1144	U1144	U1144	G164	G235	A307			A599	G673	A747	A831	G897	A956	G1018	
A1145	A1145	A1145	U89	C236	A308	C463	A531	U600	G674	G748	A832	C898	A957	A1019	
U1082	U1082	U1082	G165	G237	A309	C464	G532		G675	G749	A833	C899	A958	G1020	
C1147	C1147	C1147	G166	U238	U309	C465	G533	G603	G676	G750	A834	U899	A959	C1021	
U1148	U1148	U1148	G167	C239	C310	U465	G534	G604	G677	G751	A835	G900	U960	G1022	
C1149	C1149	C1149	G170	G240	C311	G466	G535	C605	G678	G752	U836	G901	C961	G1023	
A1150	A1150	A1150	U89	A241	C312	U467	C536	G606	C679	G755	A837	G902	C962	G1024	
U1151	U1151	U1151	A171	G242	C313	U468	C537	G607	G680	G756	A838	G903	G963	G1025	
U1152	U1152	U1152	A172		C314	C469	U537		A681	U757	C838	C904	A964	G1026	
G1153	G1153	G1153	U175	A245	C321	A470	G538	A610	G682	G758	C839	C905	A965	A1027	
G1154	G1154	G1154	G176	G248	G388	C471	A539	C611	G683	G759	U840	U906	U966	A1028	
U1155	U1155	U1155	G177	C249	A389	C472	A540	U612	G684	G763	A841	G907	C967	C1029	
C1156	C1156	C1156	G178	G249	G390	C473	A541	C613	G685	G764	A842	U908	G968	G1030	
U1157	U1157	U1157	U179		G391	U474	C543	G616	C686	C767	C844	A909	U969	A1031	
A1095	A1095	A1095	A180	C254	C392	U475	U544	G617	C687	C768	C845	G910	C970		
C1096	C1096	C1096	G188	C255	U393	A476	U545		G688	C769	C846	A911	C971		
A1097	A1097	A1097	A189	A256	G394	C477	G546		G689	A770	A847	G912	C972		
U1098	U1098	U1098	G184	G256	G395	C478	C549	U620	C690	A771	A848	G913	C973		
A1104	A1104	A1104	A185		C396	C479	U550	U621	A690	G772	A849	G914	C974		
U1105	U1105	U1105	A186	U259	U331	C480	U551	G622	C691	U773	A850	C915	G975		
G1106	G1106	G1106	A187	A260	G397	C481	A552	G623	C692	G774	A851	U916	U976		
U1107	U1107	U1107	C188		C398	C482	C553	G626	G694	A775	A852	G917	C977		
U1108	U1108	U1108	A190	G265	G399	C483	C554	A627	G695	G776	A853	A918	C978		
G1109	G1109	G1109	U190	U266	A400	A484	A554	G628	G696	G777	C854	U919	C979		
C1111	C1111	C1111	C191	C267	U401	U485	A555		G697	G778	C855	A920	C980		
U1112	U1112	U1112	U192	C268	U402	U486	G556	U631	C698	C779	U855	G921	C981		
U1113	U1113	U1113	C193	G269	C403	C487	C557		C698		C856	G922			
A1114	A1114	A1114	A194	G270	C404	C488	A558	G634	G699	A782		G923	G984		
G1115	G1115	G1115	G195	C271	C405	C489	G559		A700		U859	G924	G985		
A1116	A1116	A1116	U196	C272	C406	G490	U560	G637	A701		C860	U925	G986		
U1117	U1117	U1117	U197	U273	G407	U491	C561	U638	C706	G787		C926	A987		
G1118	G1118	G1118	C198	G274	U408	C492	A562	U639	C707	U788		A927	G988		
C1119	C1119	C1119	C199	U275	G409	A493	C563	G640	C708	G790	C863	G928	U989		
A1120	A1120	A1120	G204	C276	C410	G494	G564	A641	G709	G791	C864	G929	G990		
U1121	U1121	U1121	G205	C277	U411	G495	G565	G642	G710	G792	C865	G930	A991		
G1122	G1122	G1122	G206	G278	U412	G496	C566	G643	G711	G793	C866	G931	C992		
U1187	U1187	U1187	A206	C279	C413	A497	C567	G644	G714	A794	A867	G932	G993		
A1189	A1189	A1189	G207	G280	G351	U498	C568	C644	G715	G795	C868	C932	C994		
			A208	C281	U415	A499	G569	G645	U716	G796	A869	C933	G994		
			G209	G282	U416	G500	A572	G646	G717	C797	C873	C934	C995		
			G210	G283	U417	G501	A573	G647	G718	A798	U874	A935	G996		
			A211		C354	U502	A577	G648	G719	A799	U875	C937	G997		
			A212		A356		G577	G649	C720	A800	U876	A938	C998		
			C143		A357		U578	C650					A999		
			C144												

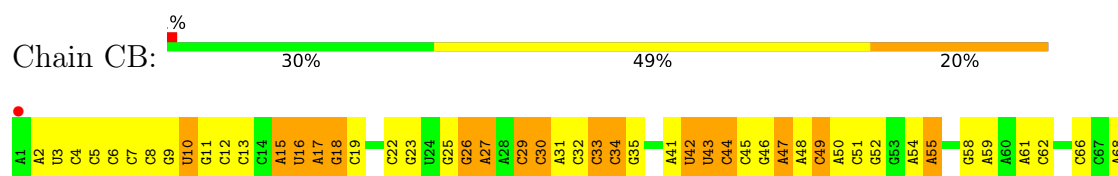




### ● Molecule 2: 5S RIBOSOMAL RNA

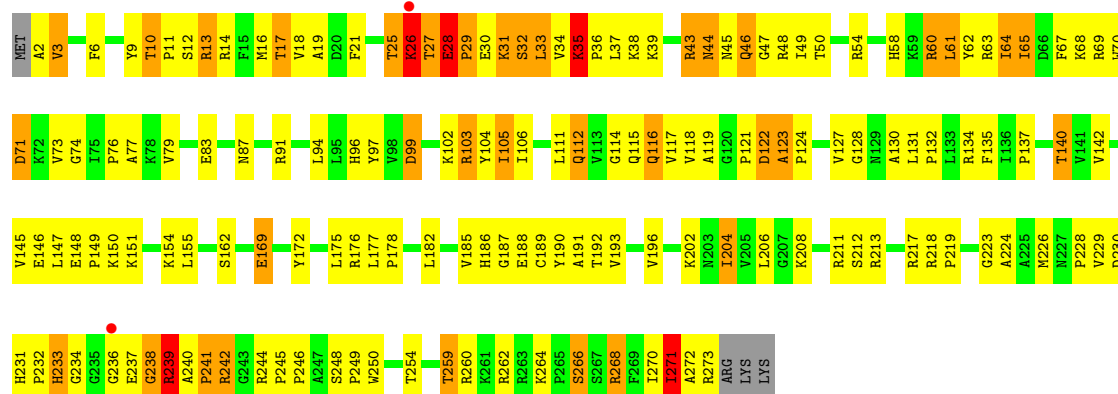
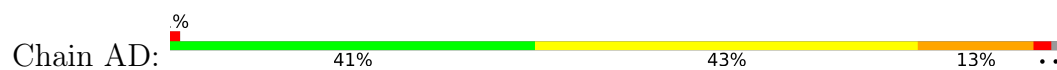


### ● Molecule 2: 5S RIBOSOMAL RNA

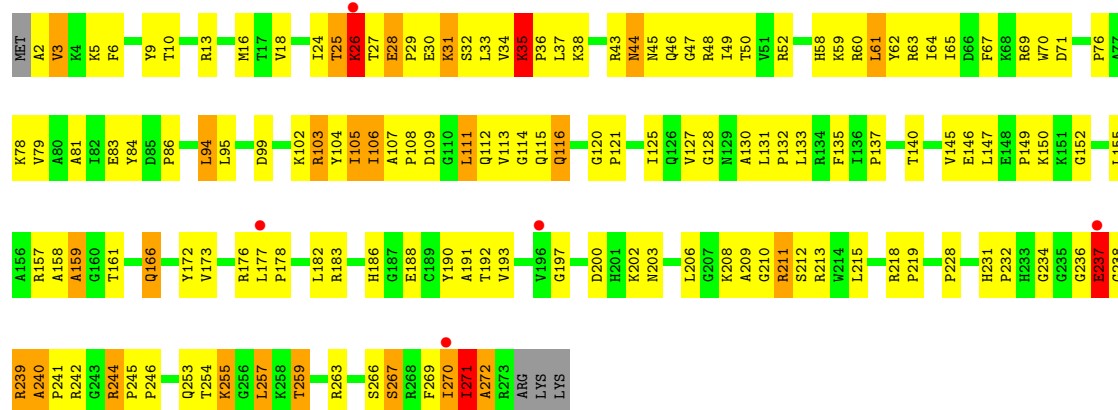




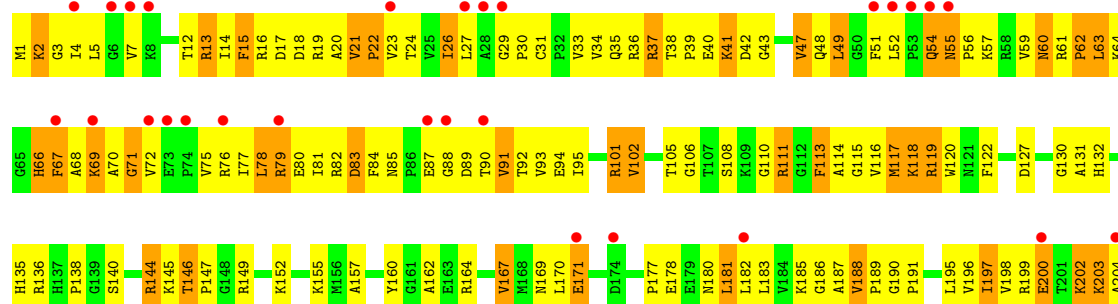
### • Molecule 3: 50S ribosomal protein L2



### • Molecule 3: 50S ribosomal protein L2

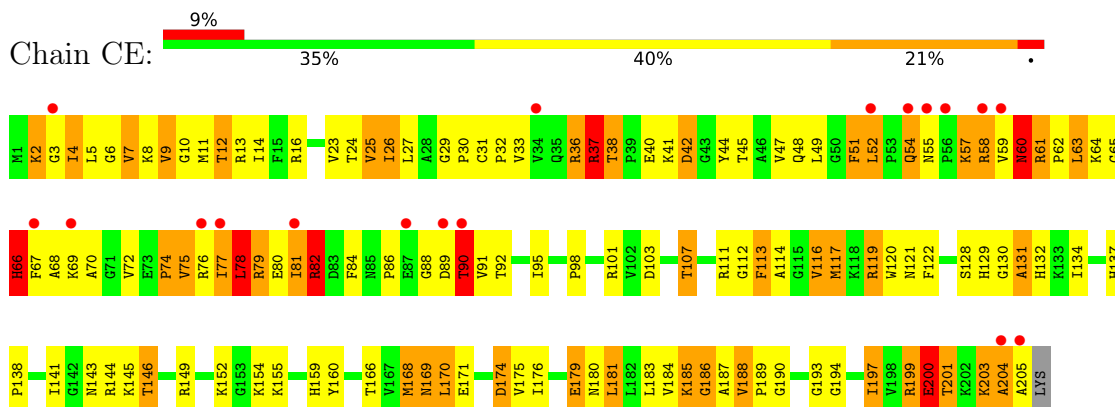


### • Molecule 4: 50S ribosomal protein L3

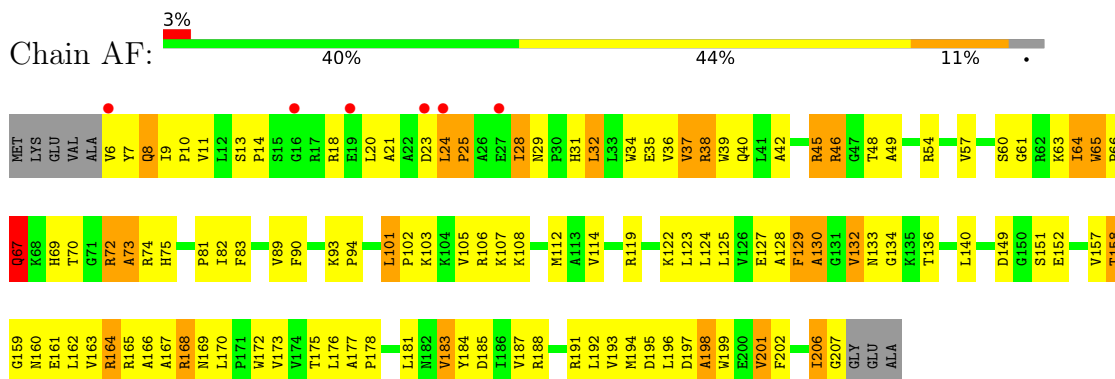




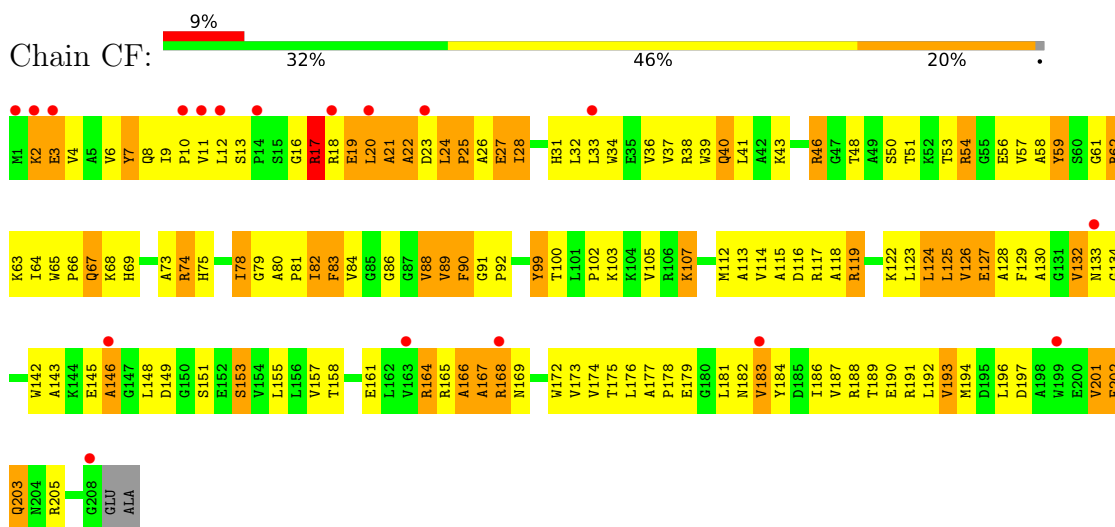
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

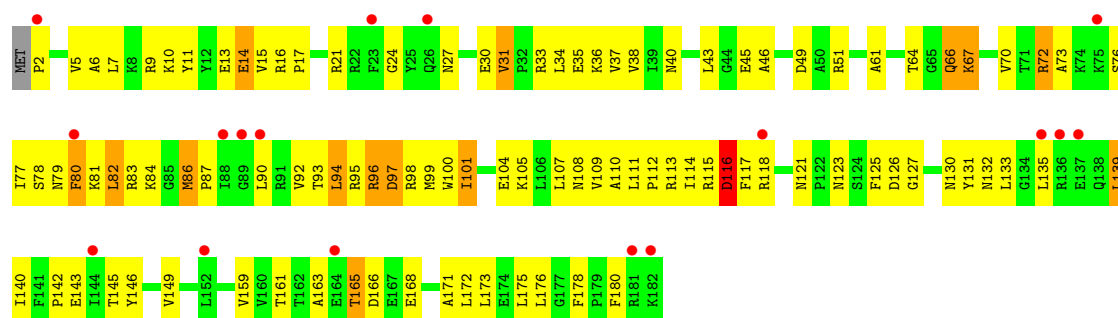


• Molecule 5: 50S ribosomal protein L4

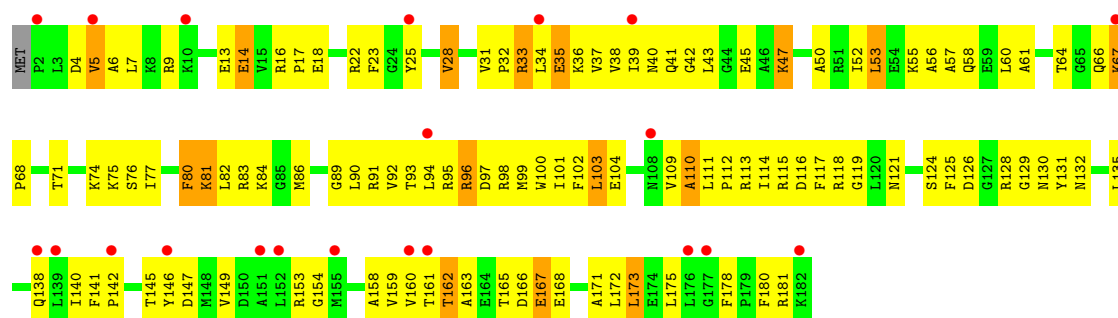


• Molecule 6: 50S ribosomal protein L5

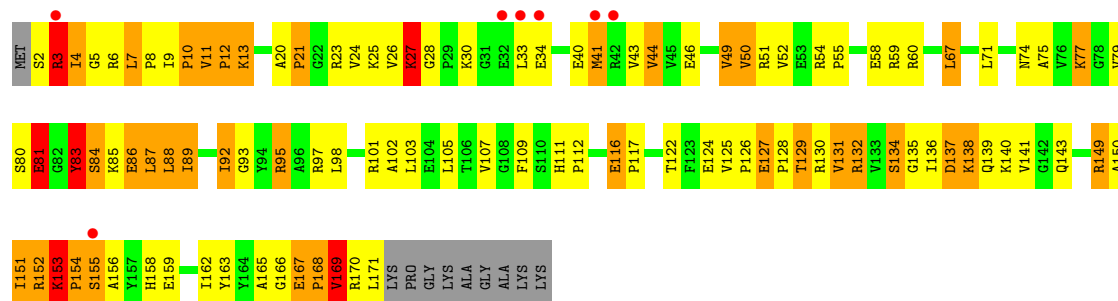




• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

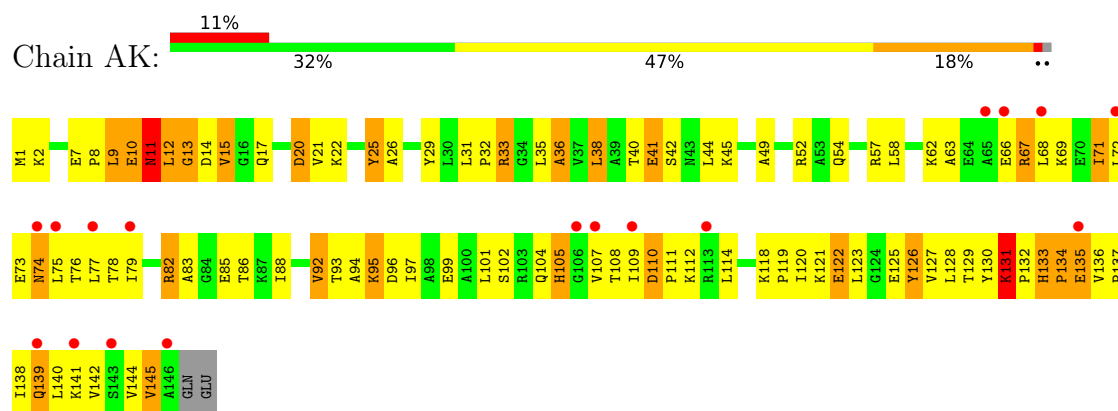


• Molecule 7: 50S ribosomal protein L6

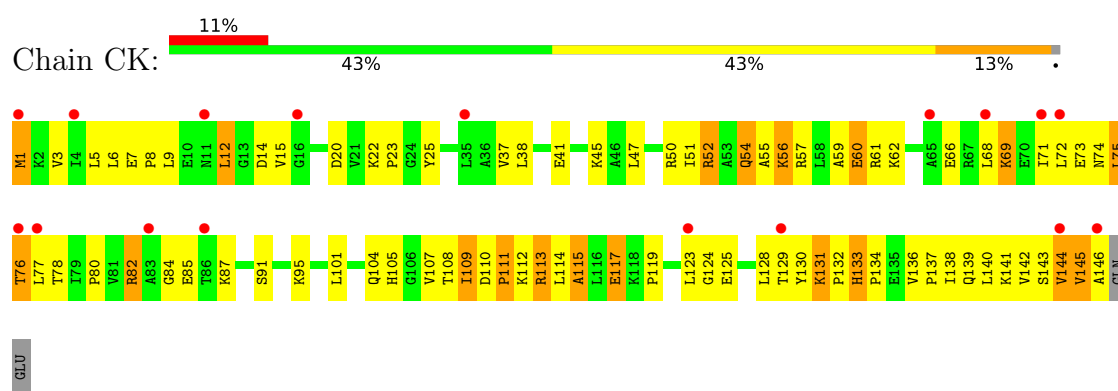




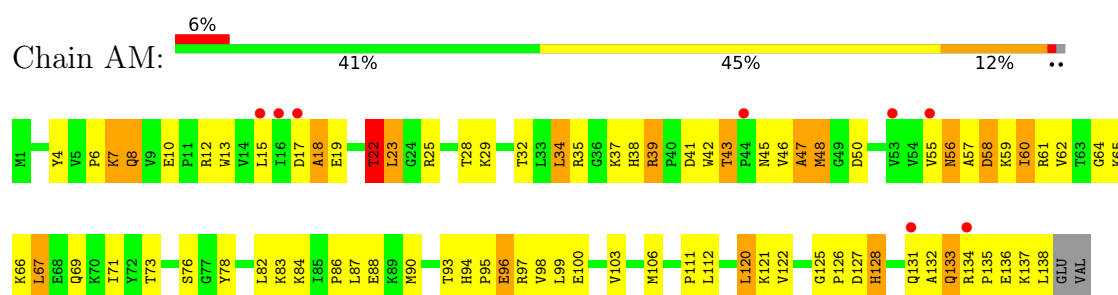
- Molecule 8: 50S ribosomal protein L9



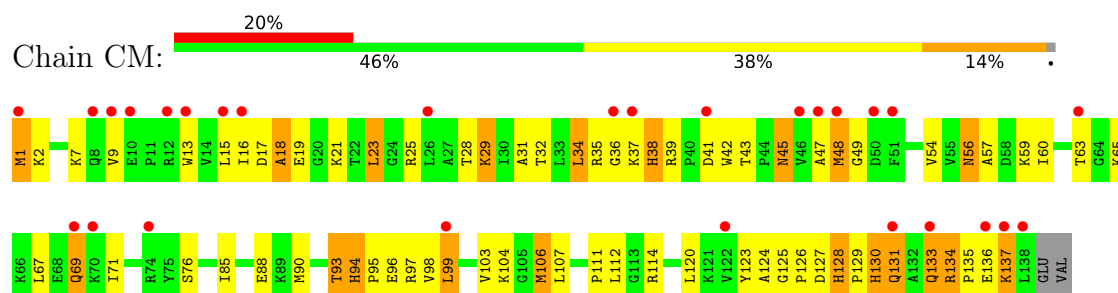
- Molecule 8: 50S ribosomal protein L9



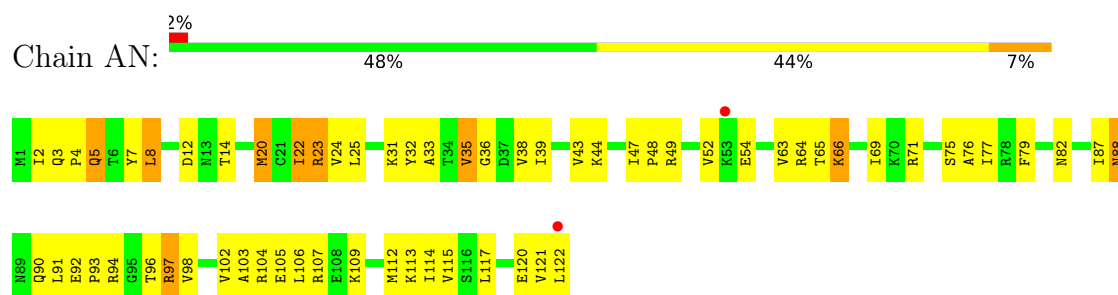
- Molecule 9: 50S ribosomal protein L13



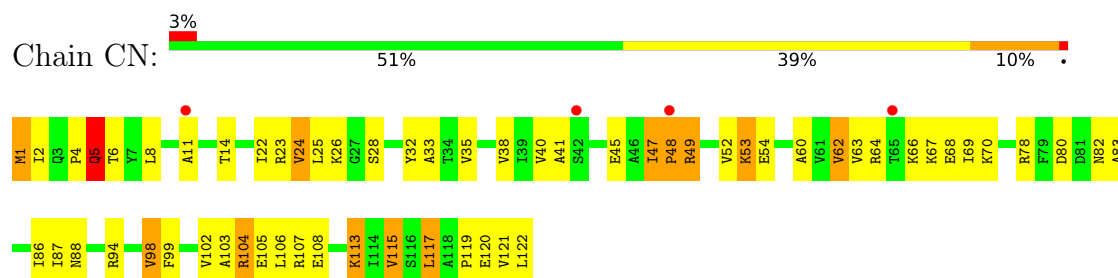
- Molecule 9: 50S ribosomal protein L13



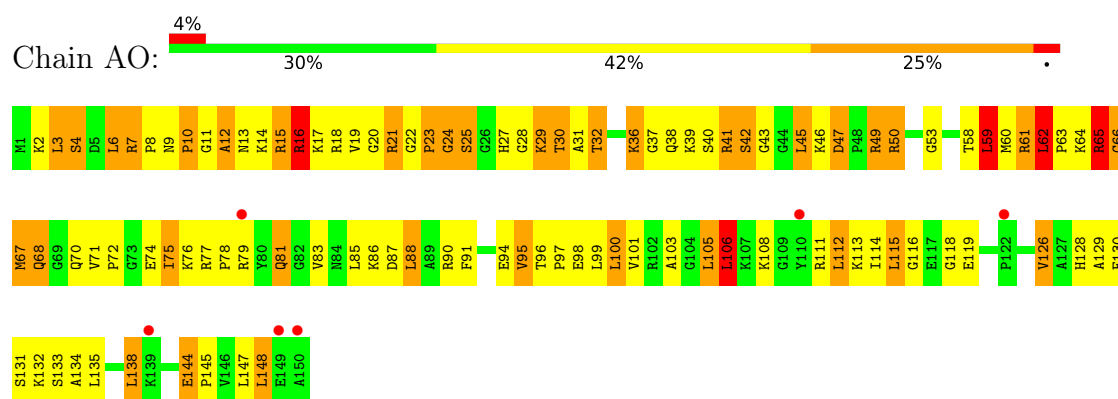
- Molecule 10: 50S ribosomal protein L14



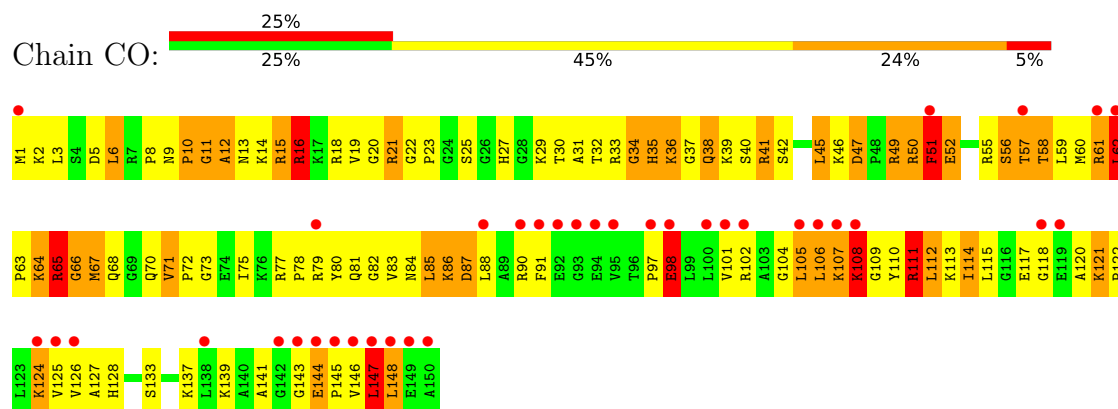
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15

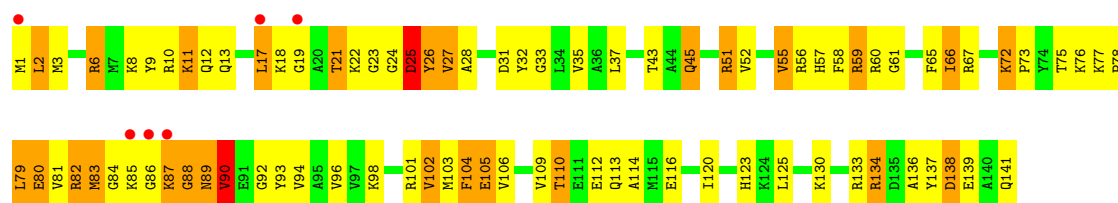


• Molecule 11: 50S ribosomal protein L15

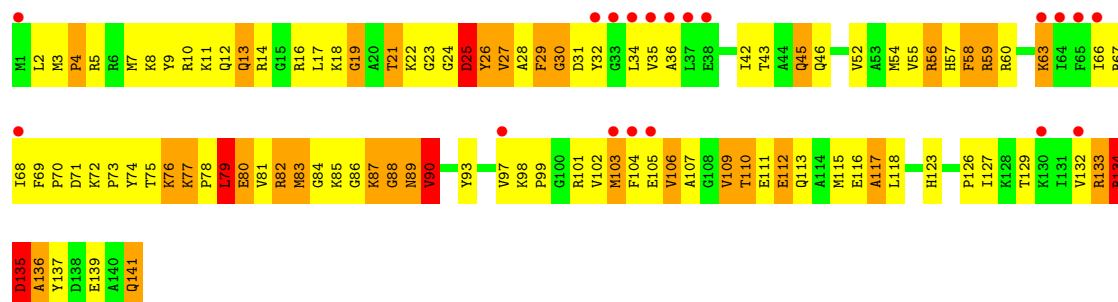


• Molecule 12: 50S ribosomal protein L16

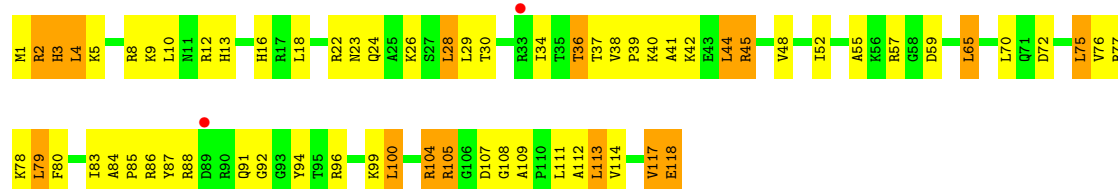




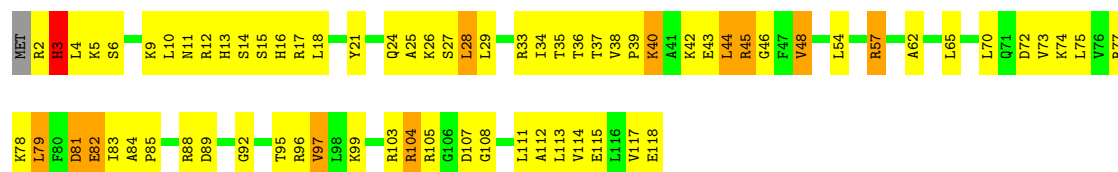
• Molecule 12: 50S ribosomal protein L16



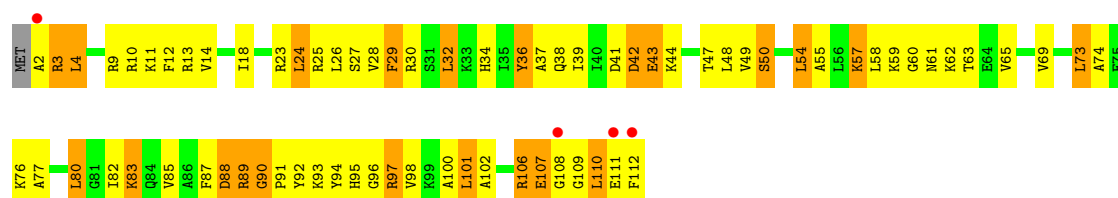
• Molecule 13: 50S ribosomal protein L17



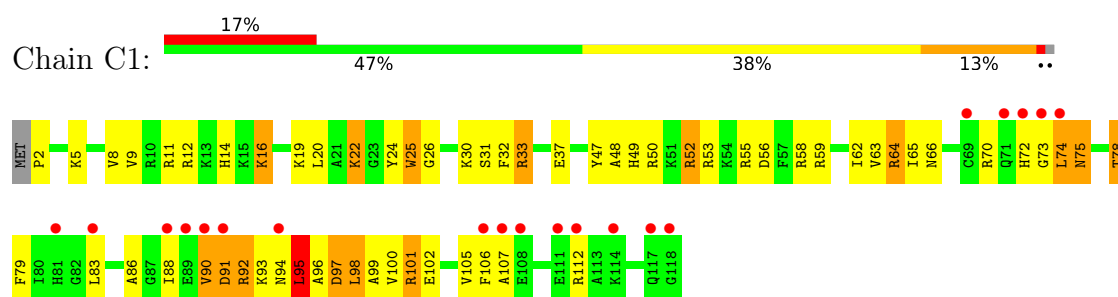
• Molecule 13: 50S ribosomal protein L17



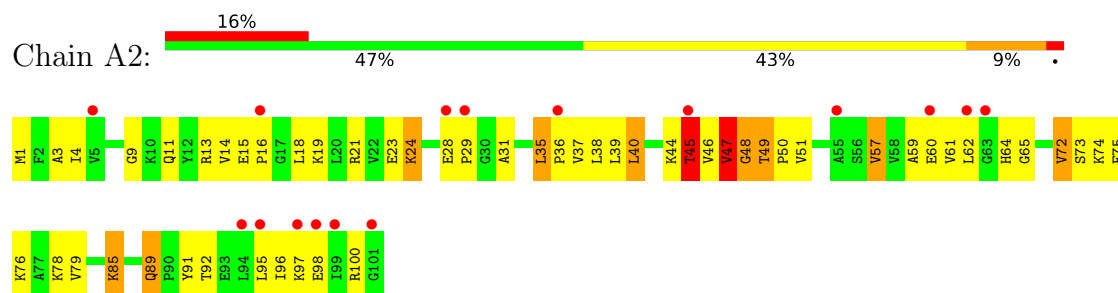
• Molecule 14: 50S ribosomal protein L18



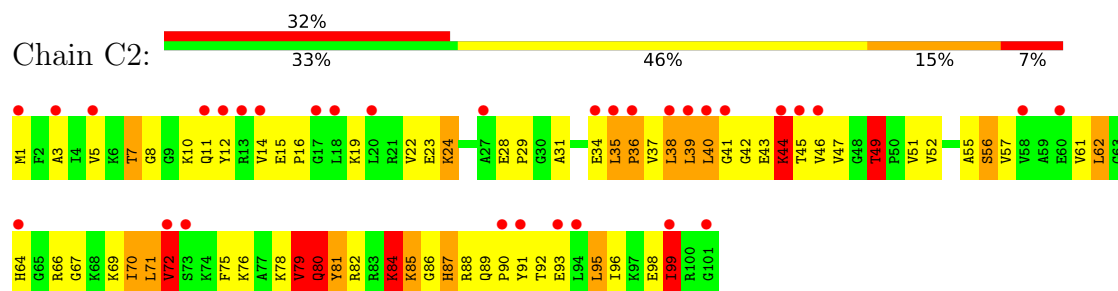




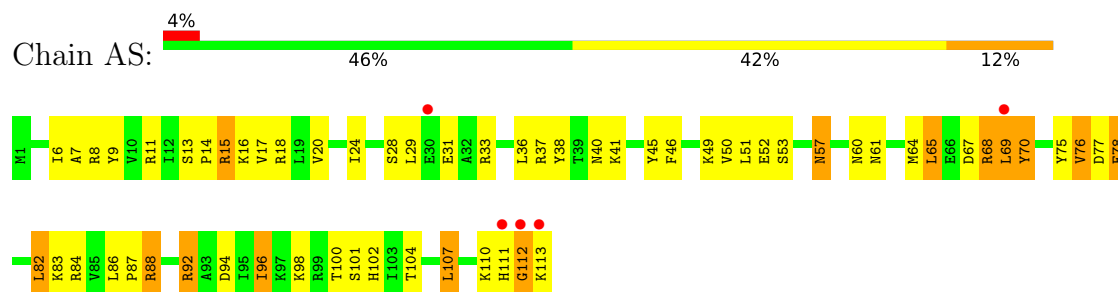
- Molecule 17: 50S ribosomal protein L21



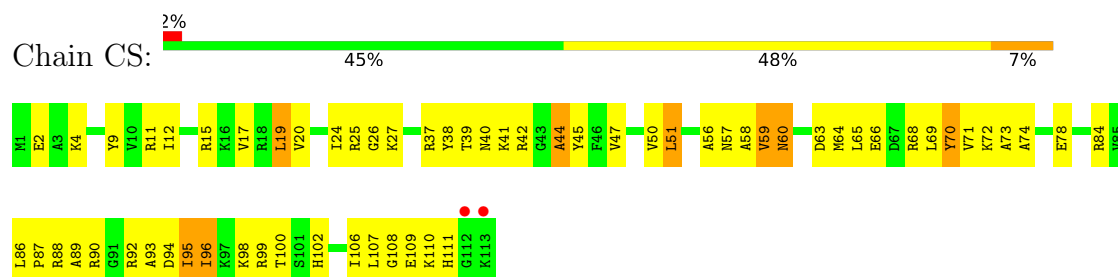
- Molecule 17: 50S ribosomal protein L21



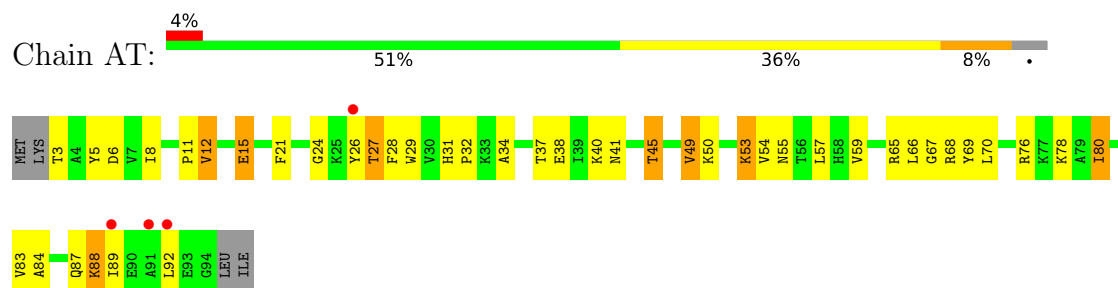
- Molecule 18: 50S ribosomal protein L22



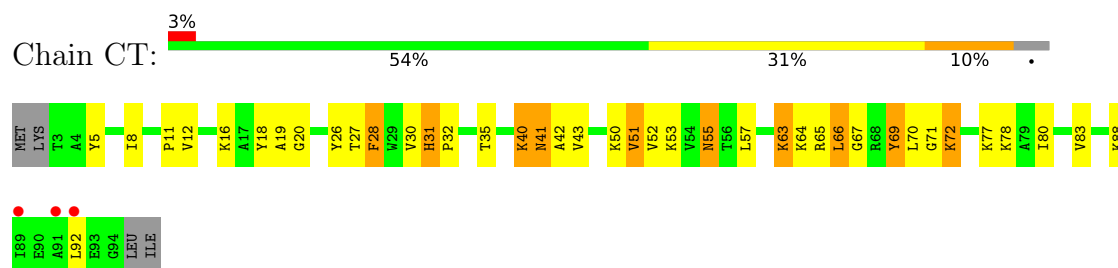
- Molecule 18: 50S ribosomal protein L22



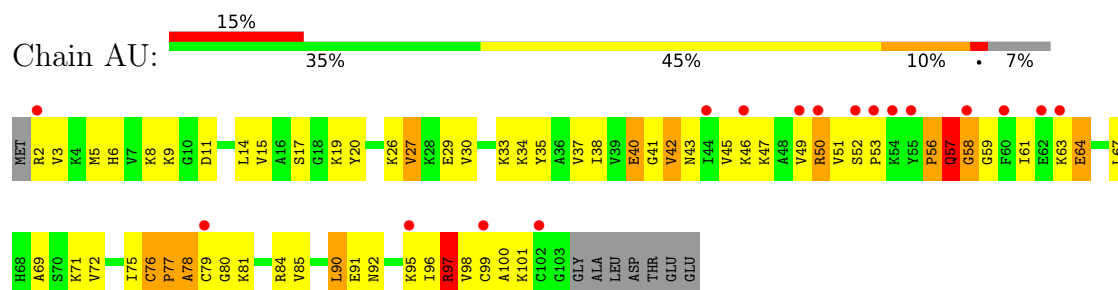
- Molecule 19: 50S ribosomal protein L23



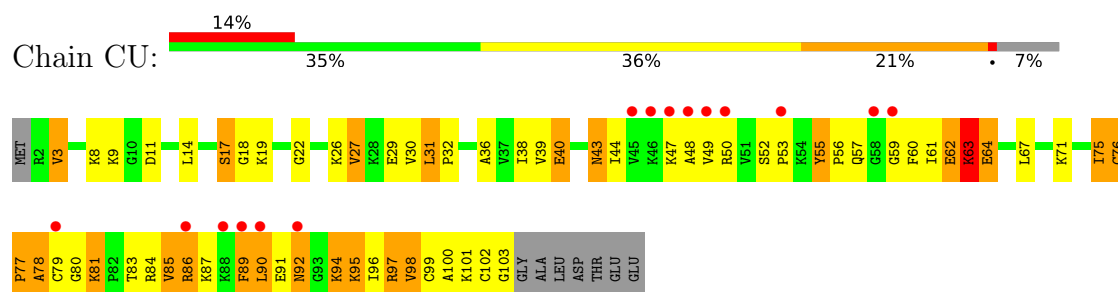
- Molecule 19: 50S ribosomal protein L23



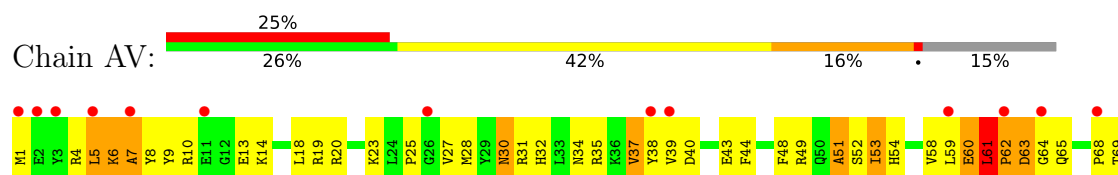
- Molecule 20: 50S ribosomal protein L24

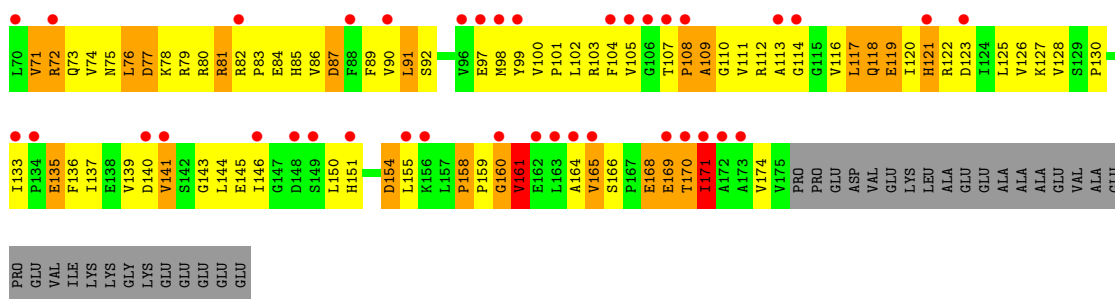


- Molecule 20: 50S ribosomal protein L24

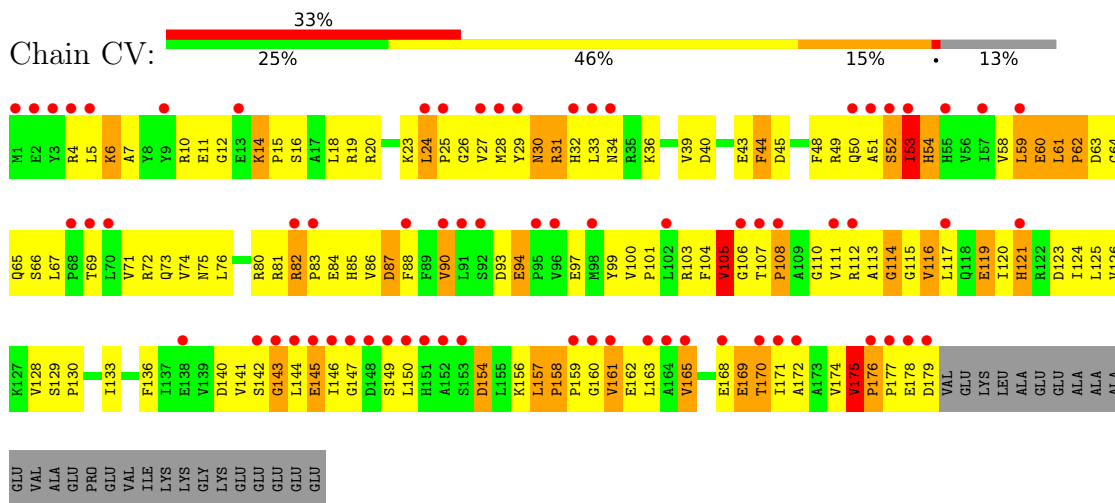


- Molecule 21: 50S ribosomal protein L25

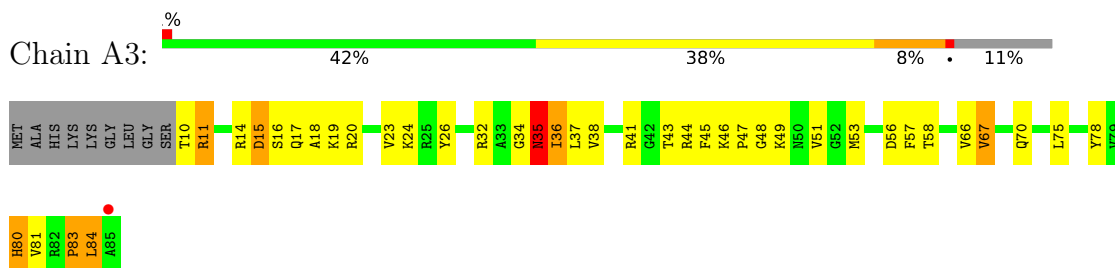




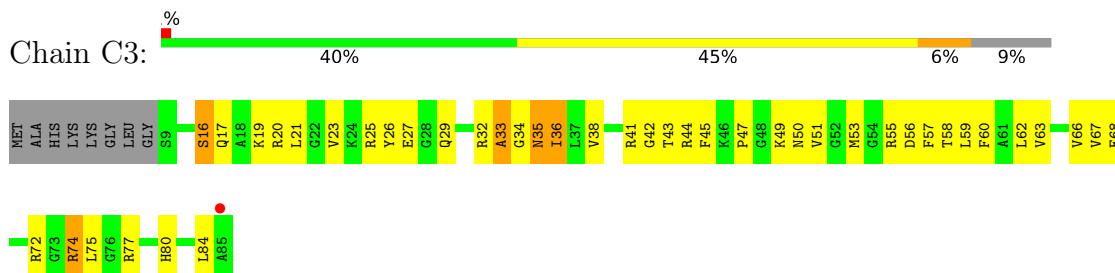
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

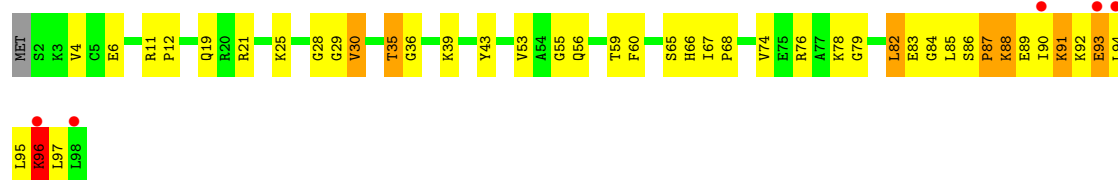


- Molecule 23: 50S ribosomal protein L28

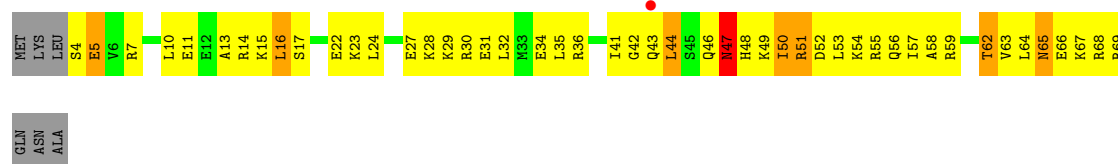




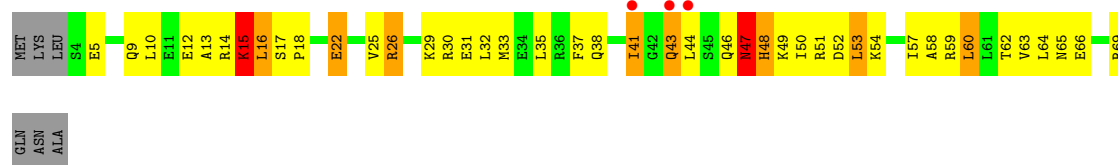
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



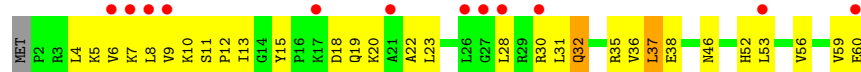
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

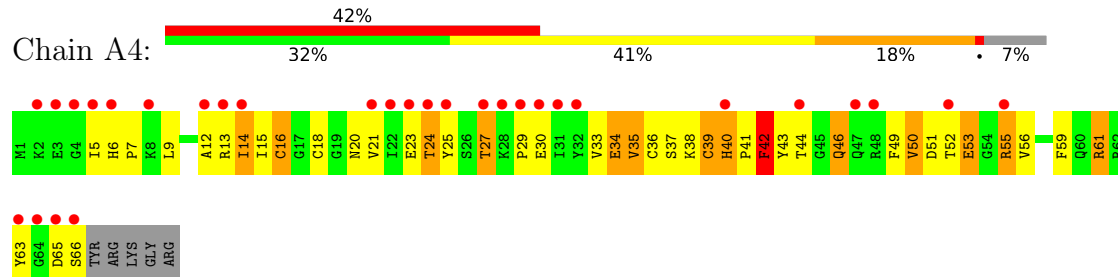


- Molecule 25: 50S ribosomal protein L30

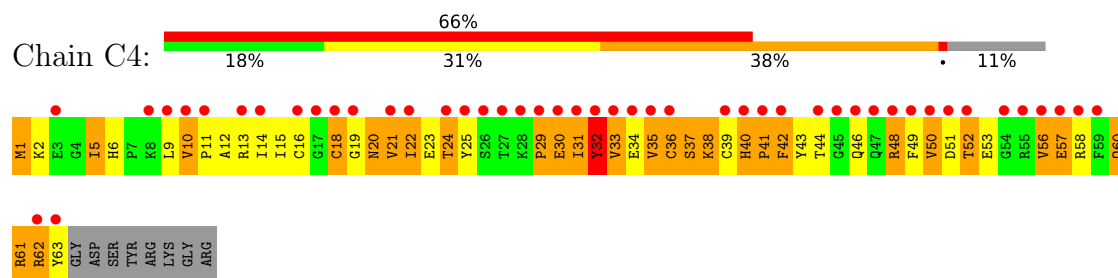




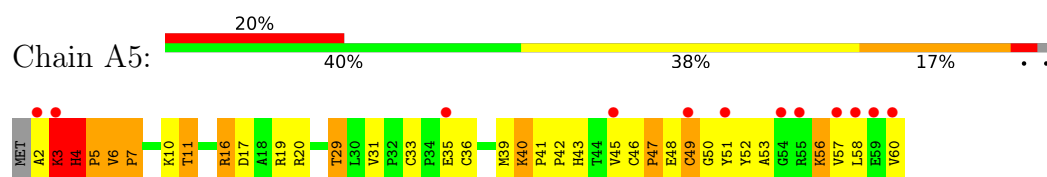
- Molecule 26: 50S ribosomal protein L31



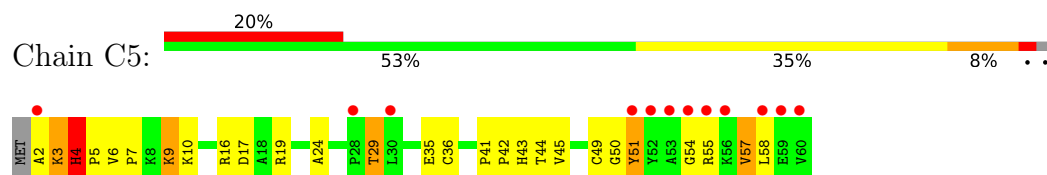
- Molecule 26: 50S ribosomal protein L31



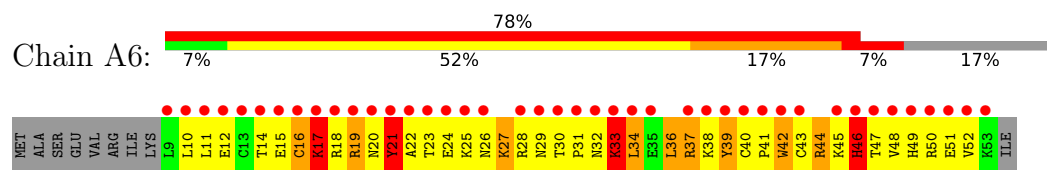
- Molecule 27: 50S ribosomal protein L32



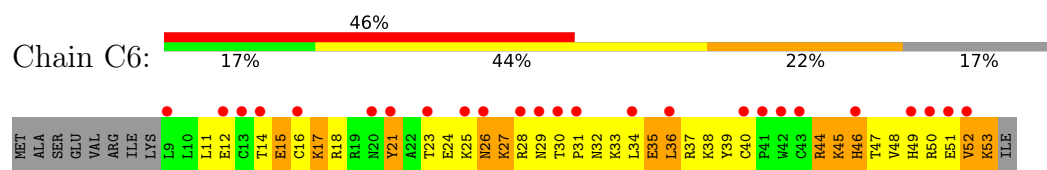
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

Chain A7:  53% 31% 8% 8%



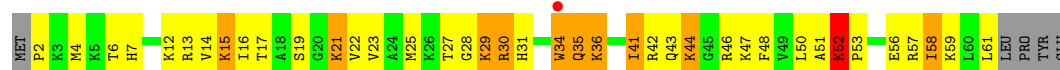
- Molecule 29: 50S ribosomal protein L34

Chain C7:  41% 41% 10% 8%

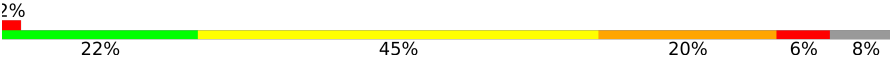


- Molecule 30: 50S ribosomal protein L35

Chain A8:  2% 32% 43% 15% 8%



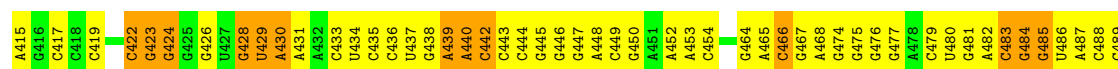
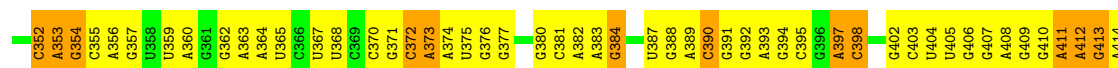
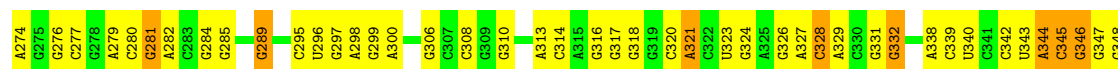
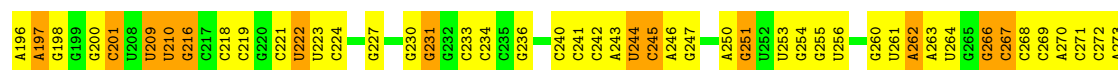
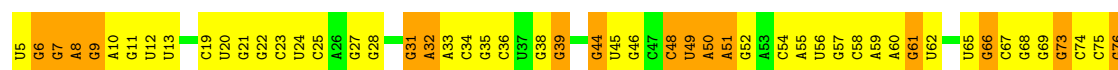
- Molecule 30: 50S ribosomal protein L35

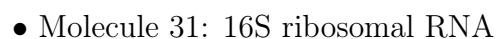
Chain C8:  2% 22% 45% 20% 6% 8%



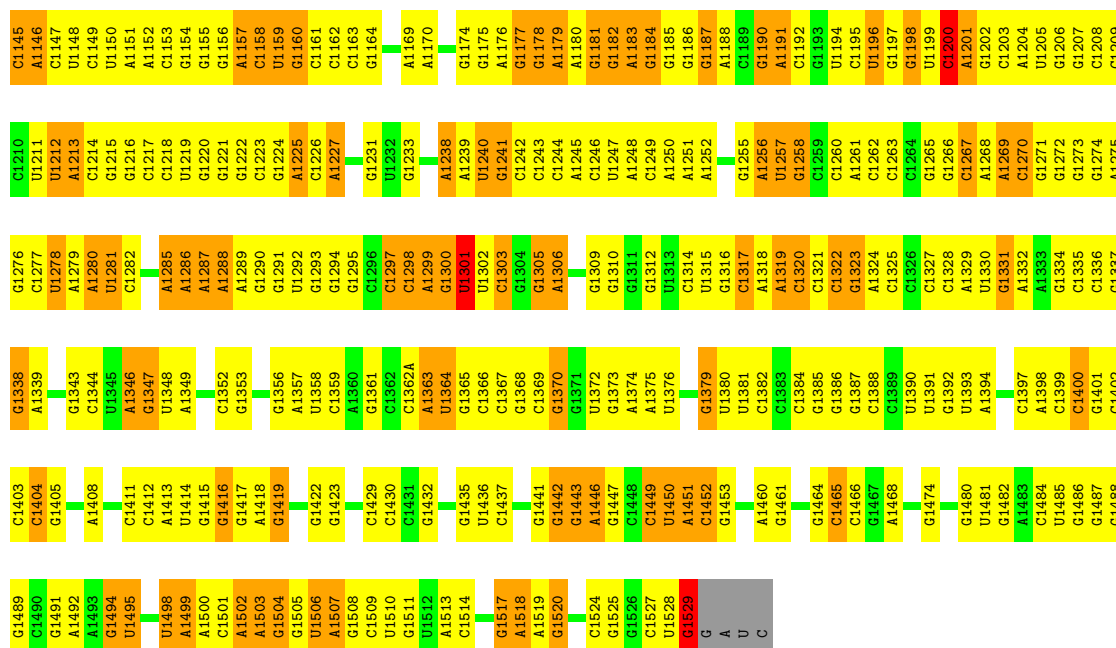
- Molecule 31: 16S ribosomal RNA

Chain BA:  29% 52% 18%

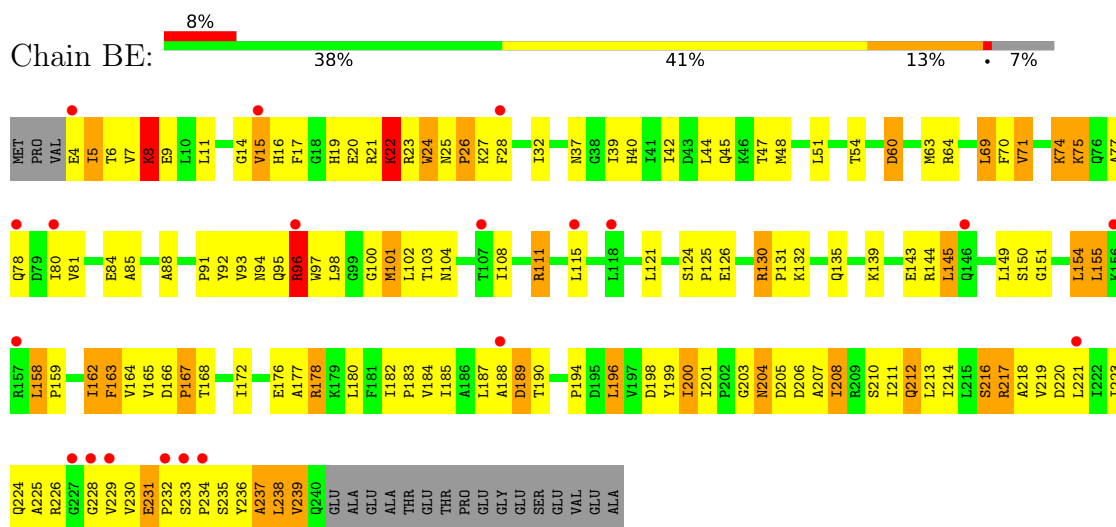




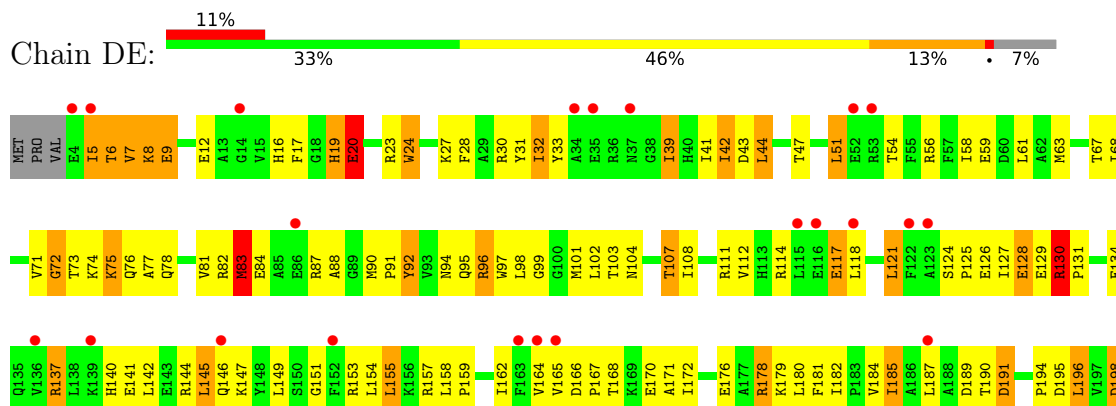
A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	G1022	G1023	G1024	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	A1101	A1102	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1123	U1124	U1125	U1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	U1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144																																																																																
G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960																																																																										
U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021																																																																																								
G1022	G1023	G1024	U1083	U1084	U1085	U1086	U1087	G1028A	G1028B	G1029	G1030	G1031	G1032	G1032A	G1032B	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	U1086	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	U1070	G1071	G1072	U1073	G1074	G1075	U1076	G1077	U1078	U1079																																																																																						
U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	U20	U21	U22	U23	U24	U25	U26	U27	U28	U29	U30	U31	U32	U33	U34	U35	U36	U37	U38	U39	U40	U41	U42	U43	U44	U45	U46	U47	U48	U49	U50	U51	U52	U53	U54	U55	U56	U57	U58	U59	U60	U61	U62	U63	U64	U65	U66	U67	U68	U69	U70	U71	U72	U73	U74	U75	U76	U77	U78	U79	U80																																																																									
G81	U82	U84	U85	U86	U87	C88	C89	C90	C91	C92	C93	C94	C95	C96	C97	C98	C99	C100	C101	C102	C103	C104	C105	C106	C107	C108	C109	C110	C111	C112	C113	C114	C115	C116	C117	C118	C119	C120	C121	C122	C123	C124	C125	C126	C127	C128	C129	C130	C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150																																																																																
C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180	C181	C182	C183	C184	C185	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217																																																																																				
C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301																																																																				
G302	A303	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451																																																																												
A452	A453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600
C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739										
U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807																																																																																	
C808	C809	C812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890																																																																				
G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960																																																																										
U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021																																																																																								
G1022	G1023	G1024	U1083	U1084	U1085	U1086	U1087	G1028A	G1028B	G1029	G1030	G1031	G1032	G1032A	G1032B	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	U1086	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	U1070	G1071	G1072	U1073	G1074	G1075	U1076	G1077	U1078	U1079																																																																																						

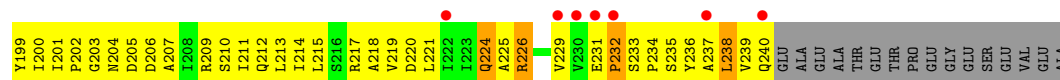


### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

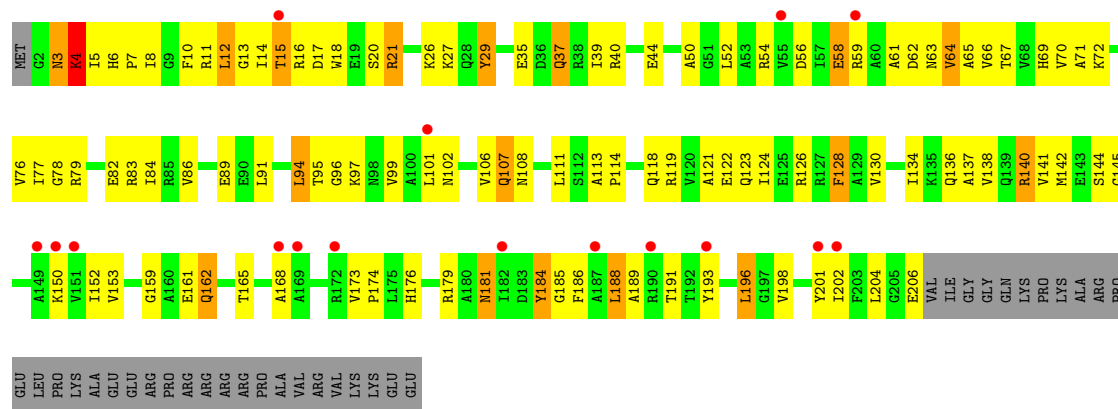


### • Molecule 32: 30S RIBOSOMAL PROTEIN S2

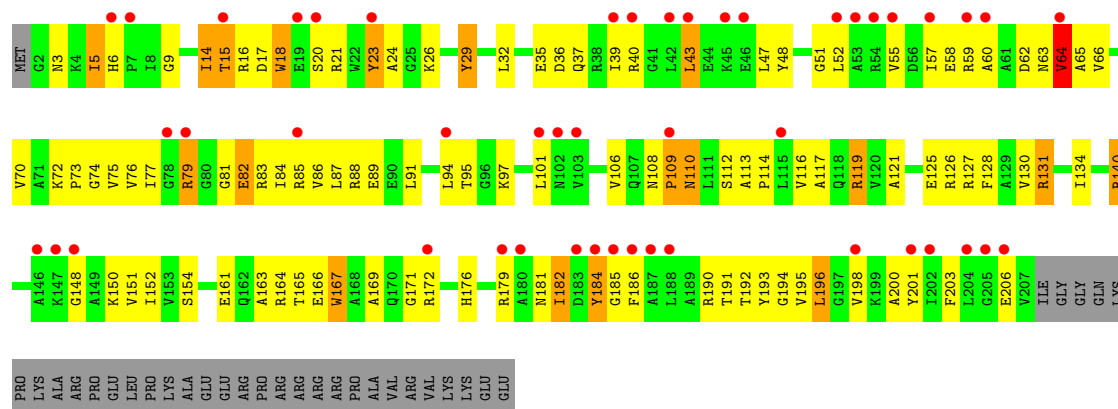
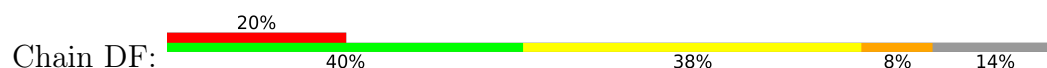




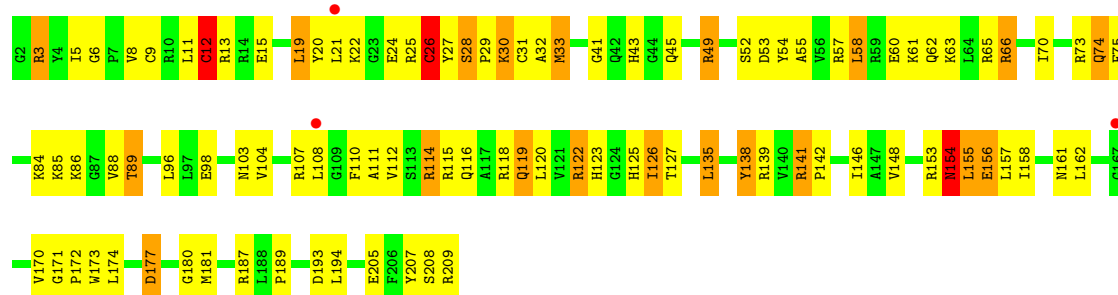
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



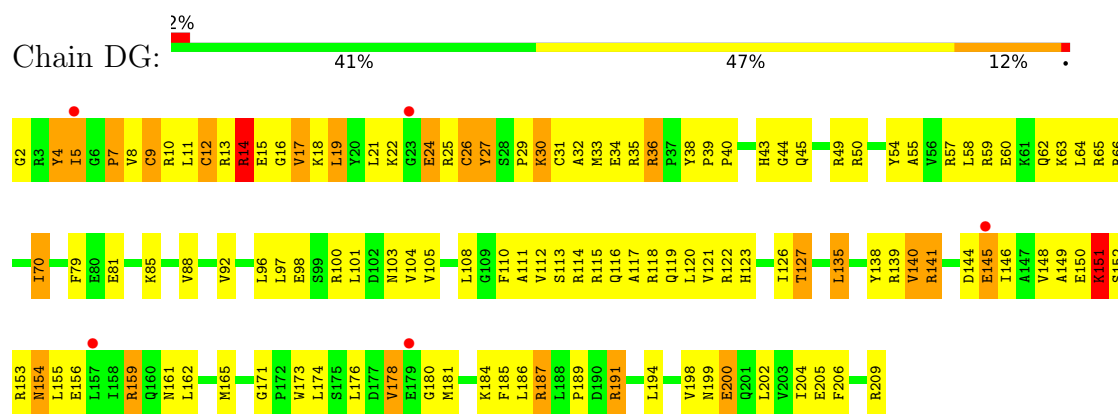
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



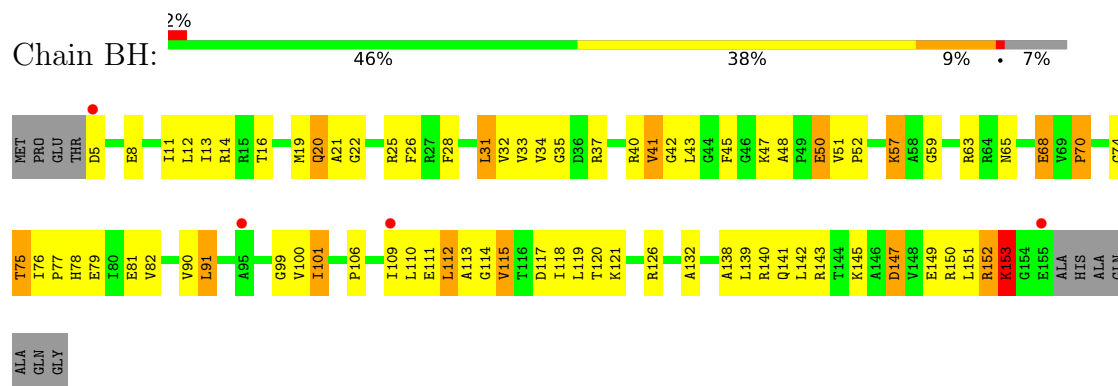
• Molecule 34: 30S RIBOSOMAL PROTEIN S4

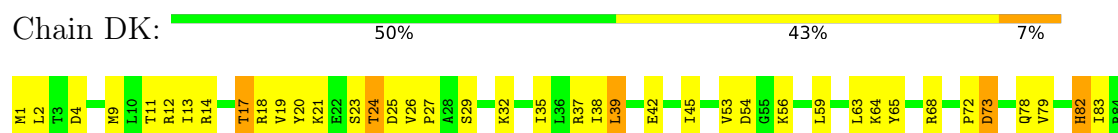


• Molecule 34: 30S RIBOSOMAL PROTEIN S4



• Molecule 35: 30S RIBOSOMAL PROTEIN S5



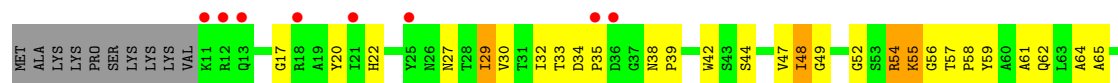








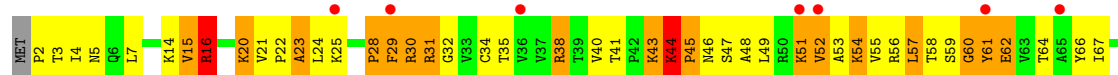
• Molecule 41: 30S RIBOSOMAL PROTEIN S11



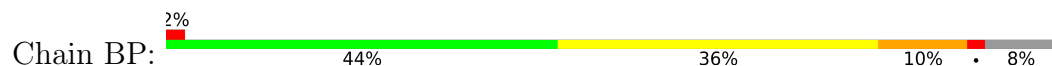
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



• Molecule 43: 30S RIBOSOMAL PROTEIN S13

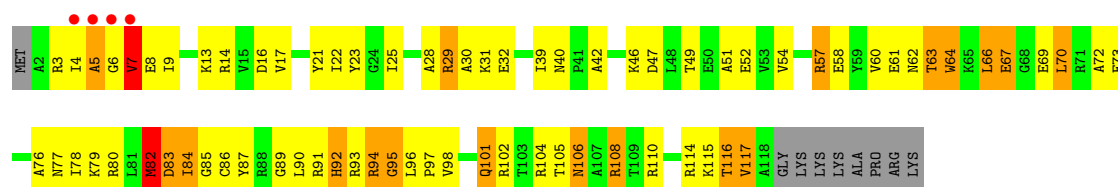


• Molecule 44: 30S RIBOSOMAL PROTEIN S14



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

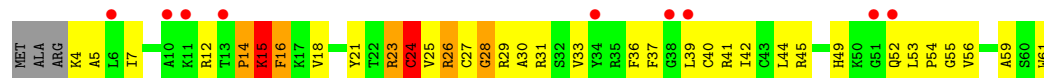




• Molecule 44: 30S RIBOSOMAL PROTEIN S14



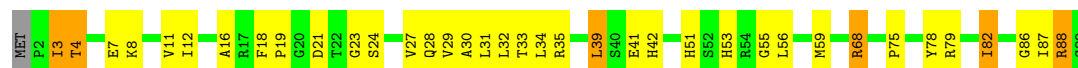
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



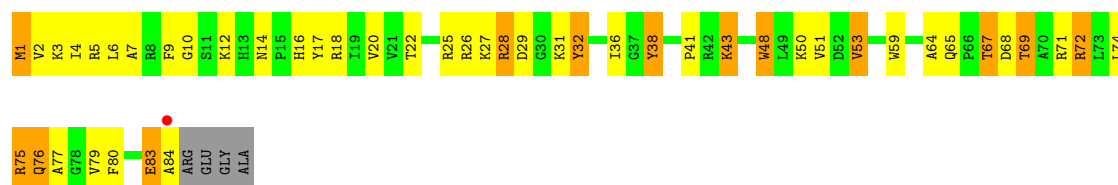
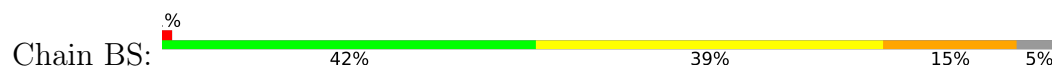
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

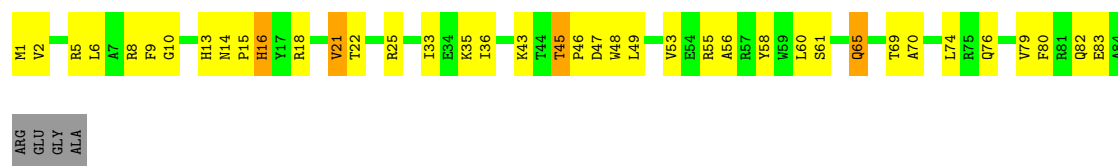


• Molecule 46: 30S RIBOSOMAL PROTEIN S16

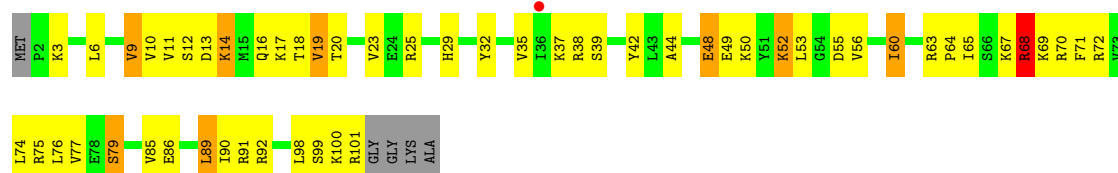
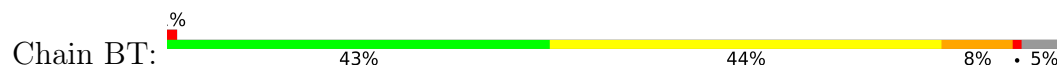


• Molecule 46: 30S RIBOSOMAL PROTEIN S16

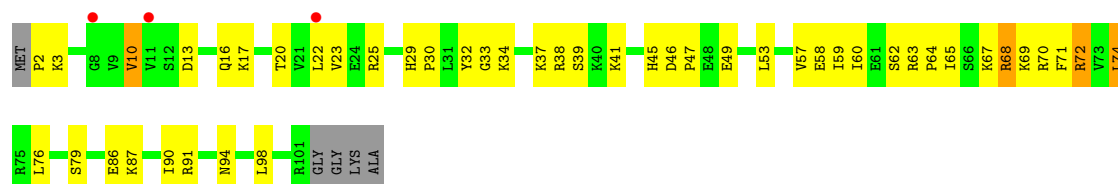




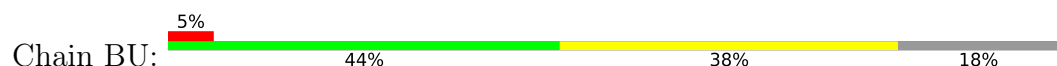
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



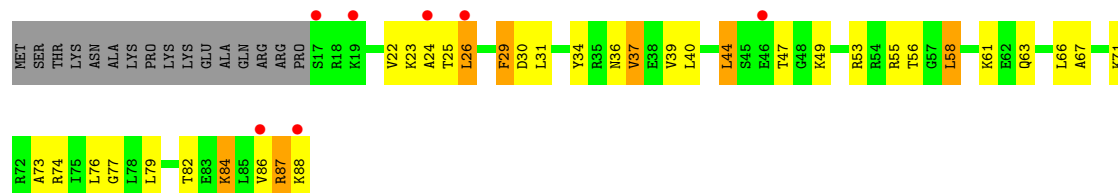
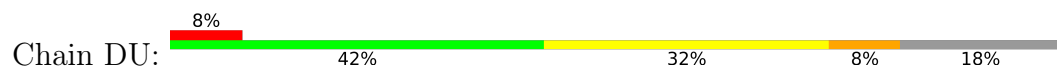
- Molecule 47: 30S RIBOSOMAL PROTEIN S17



- Molecule 48: 30S RIBOSOMAL PROTEIN S18

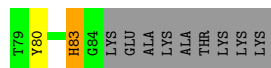


- Molecule 48: 30S RIBOSOMAL PROTEIN S18



- Molecule 49: 30S RIBOSOMAL PROTEIN S19

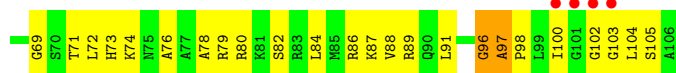




● Molecule 49: 30S RIBOSOMAL PROTEIN S19



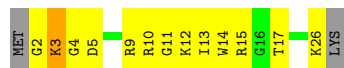
● Molecule 50: 30S RIBOSOMAL PROTEIN S20



• Molecule 50: 30S RIBOSOMAL PROTEIN S20



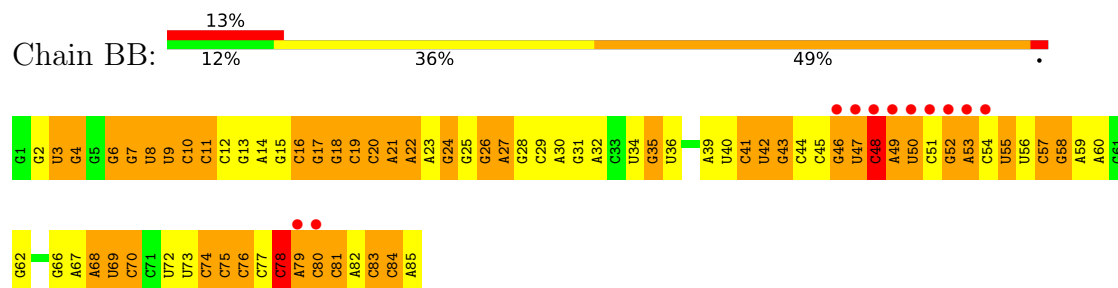
● Molecule 51: 30S RIBOSOMAL PROTEIN THX



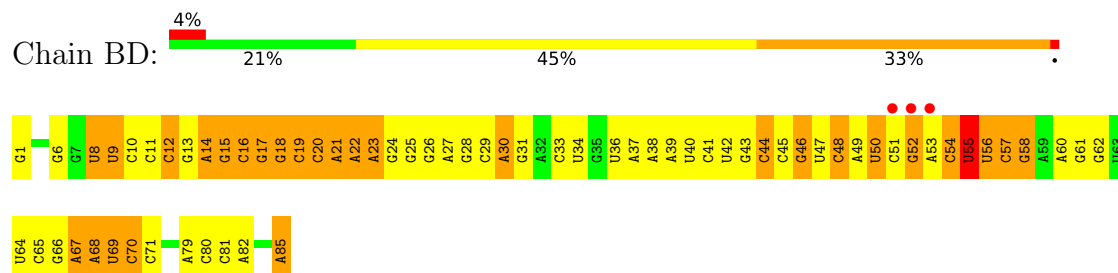
● Molecule 51: 30S RIBOSOMAL PROTEIN THX



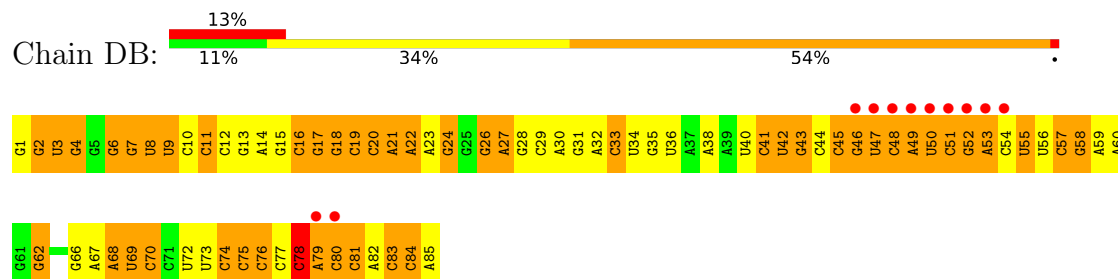
## • Molecule 52: TRNA-TYR



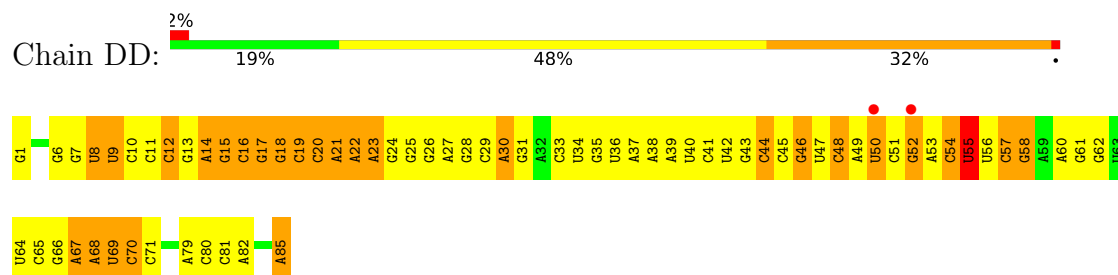
## • Molecule 52: TRNA-TYR



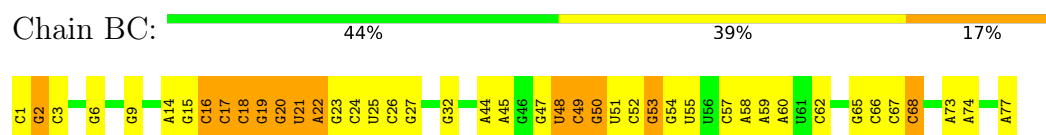
## • Molecule 52: TRNA-TYR



## • Molecule 52: TRNA-TYR



## • Molecule 53: TRNA-FMET

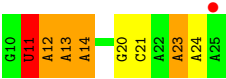


## • Molecule 53: TRNA-FMET

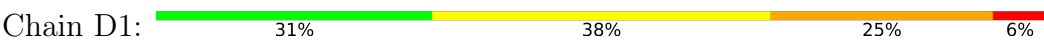




● Molecule 54: MRNA



● Molecule 54: MRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.25Å 450.87Å 622.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.19 – 3.30 256.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (256.19-3.30) 92.8 (256.19-3.20)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, $R_{free}$	0.206 , 0.259 0.206 , 0.262	Depositor DCC
$R_{free}$ test set	2000 reflections (0.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 91.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	303952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	AA	0.34	0/70233	0.73	38/109643 (0.0%)
1	CA	0.30	1/70122 (0.0%)	0.70	35/109469 (0.0%)
2	AB	0.32	0/2928	0.79	11/4568 (0.2%)
2	CB	0.27	0/2928	0.70	1/4568 (0.0%)
3	AD	0.30	0/2165	0.56	0/2919
3	CD	0.28	0/2165	0.50	0/2919
4	AE	0.27	0/1601	0.53	0/2160
4	CE	0.26	0/1601	0.51	0/2160
5	AF	0.27	0/1620	0.49	0/2194
5	CF	0.25	0/1662	0.54	0/2249
6	AG	0.23	0/1499	0.45	0/2016
6	CG	0.21	0/1499	0.42	0/2016
7	AH	0.27	0/1332	0.51	0/1802
7	CH	0.23	0/1332	0.47	0/1802
8	AK	0.24	0/1151	0.50	0/1558
8	CK	0.22	0/1151	0.50	0/1558
9	AM	0.26	0/1131	0.48	0/1525
9	CM	0.23	0/1131	0.45	0/1525
10	AN	0.26	0/943	0.47	0/1269
10	CN	0.25	0/943	0.45	0/1269
11	AO	0.27	0/1162	0.60	1/1544 (0.1%)
11	CO	0.24	0/1162	0.47	0/1544
12	AP	0.27	0/1143	0.45	0/1527
12	CP	0.23	0/1143	0.43	0/1527
13	A0	0.25	0/982	0.48	0/1312
13	C0	0.24	0/974	0.44	0/1302
14	AQ	0.25	0/892	0.47	0/1187
14	CQ	0.24	0/892	0.47	0/1187
15	AR	0.27	0/1155	0.50	0/1542
15	CR	0.24	0/1155	0.44	0/1542
16	A1	0.27	0/982	0.50	0/1306
16	C1	0.24	0/982	0.41	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	A2	0.26	0/790	0.50	0/1057
17	C2	0.26	0/790	0.53	0/1057
18	AS	0.26	0/911	0.46	0/1220
18	CS	0.25	0/911	0.46	0/1220
19	AT	0.31	0/739	0.49	0/993
19	CT	0.28	0/739	0.47	0/993
20	AU	0.27	0/798	0.49	0/1064
20	CU	0.25	0/798	0.48	0/1064
21	AV	0.25	0/1427	0.50	1/1935 (0.1%)
21	CV	0.22	0/1460	0.45	0/1982
22	A3	0.27	0/615	0.50	0/819
22	C3	0.25	0/621	0.48	0/827
23	AZ	0.26	0/770	0.50	0/1022
23	CZ	0.26	0/770	0.51	0/1022
24	AW	0.29	0/560	0.54	0/741
24	CW	0.24	0/560	0.45	0/741
25	AX	0.24	0/474	0.40	0/635
25	CX	0.21	0/474	0.40	0/635
26	A4	0.25	0/545	0.58	0/733
26	C4	0.26	0/527	0.55	0/709
27	A5	0.24	0/473	0.49	0/639
27	C5	0.25	0/473	0.51	0/639
28	A6	0.28	0/396	0.54	0/529
28	C6	0.25	0/396	0.58	0/529
29	A7	0.31	0/399	0.48	0/526
29	C7	0.25	0/399	0.45	0/526
30	A8	0.34	0/486	0.61	0/638
30	C8	0.27	0/486	0.51	0/638
31	BA	0.28	0/36139	0.68	22/56406 (0.0%)
31	DA	0.26	0/36142	0.65	20/56410 (0.0%)
32	BE	0.22	0/1959	0.43	0/2642
32	DE	0.22	0/1959	0.43	0/2642
33	BF	0.23	0/1629	0.41	0/2195
33	DF	0.21	0/1636	0.40	0/2205
34	BG	0.26	0/1733	0.45	0/2318
34	DG	0.24	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	DH	0.22	0/1171	0.43	0/1576
36	BI	0.24	0/856	0.43	0/1154
36	DI	0.23	0/856	0.44	0/1154
37	BJ	0.23	0/1276	0.38	0/1709
37	DJ	0.21	0/1276	0.37	0/1709
38	BK	0.23	0/1136	0.47	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.21	0/1136	0.42	0/1527
39	BL	0.22	0/1029	0.41	0/1379
39	DL	0.23	0/1029	0.44	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	DM	0.21	0/814	0.44	0/1095
41	BN	0.24	0/900	0.47	0/1213
41	DN	0.23	0/900	0.45	0/1213
42	BO	0.26	0/991	0.47	0/1327
42	DO	0.24	0/991	0.47	0/1327
43	BP	0.22	0/938	0.47	0/1258
43	DP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/485	0.45	0/643
44	DQ	0.23	0/485	0.46	0/643
45	BR	0.24	0/745	0.41	0/992
45	DR	0.22	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	DS	0.22	0/721	0.43	0/970
47	BT	0.24	0/847	0.41	0/1131
47	DT	0.23	0/847	0.40	0/1131
48	BU	0.24	0/596	0.45	0/790
48	DU	0.24	0/596	0.43	0/790
49	BV	0.22	0/638	0.44	0/860
49	DV	0.23	0/638	0.46	0/860
50	BW	0.22	0/765	0.42	0/1007
50	DW	0.23	0/765	0.47	0/1007
51	BX	0.22	0/221	0.39	0/288
51	DX	0.21	0/221	0.41	0/288
52	BB	0.35	0/1992	0.71	2/3099 (0.1%)
52	BD	0.32	0/1992	0.66	2/3099 (0.1%)
52	DB	0.35	0/1992	0.68	1/3099 (0.0%)
52	DD	0.32	0/1992	0.64	2/3099 (0.1%)
53	BC	0.26	0/1835	0.61	0/2859
53	DC	0.24	0/1835	0.56	0/2859
54	B1	0.33	0/390	0.59	1/606 (0.2%)
54	D1	0.34	0/390	0.63	1/606 (0.2%)
All	All	0.29	1/324159 (0.0%)	0.65	138/485455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	2884	A	N7-C5	-5.57	1.35	1.39

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1495	U	N1-C2-O2	9.65	129.55	122.80
1	AA	673	C	C2-N3-C4	-8.89	115.45	119.90
2	AB	81	G	C5-C6-O6	-8.73	123.36	128.60
1	CA	979	A	C4-N9-C1'	8.38	141.38	126.30
1	CA	1922	G	N3-C4-N9	-8.15	121.11	126.00

There are no chirality outliers.

There are no planarity outliers.

## 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	AA	62707	0	31613	2349	0
1	CA	62607	0	31564	2395	0
2	AB	2617	0	1328	88	0
2	CB	2617	0	1328	126	0
3	AD	2115	0	2195	232	0
3	CD	2115	0	2195	198	0
4	AE	1568	0	1634	155	0
4	CE	1568	0	1634	162	0
5	AF	1585	0	1632	122	0
5	CF	1627	0	1680	182	0
6	AG	1474	0	1535	112	0
6	CG	1474	0	1535	112	0
7	AH	1307	0	1382	129	0
7	CH	1307	0	1382	110	1
8	AK	1136	0	1223	92	0
8	CK	1136	0	1223	77	0
9	AM	1104	0	1180	81	0
9	CM	1104	0	1180	64	0
10	AN	933	0	996	64	0
10	CN	933	0	996	53	0
11	AO	1145	0	1228	178	0
11	CO	1145	0	1228	265	0
12	AP	1122	0	1179	168	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CP	1122	0	1179	189	0
13	A0	968	0	1033	74	0
13	C0	960	0	1021	70	0
14	AQ	882	0	943	83	0
14	CQ	882	0	943	89	0
15	AR	1141	0	1202	107	0
15	CR	1141	0	1202	94	0
16	A1	964	0	1022	87	0
16	C1	964	0	1022	83	0
17	A2	779	0	852	63	0
17	C2	779	0	852	99	0
18	AS	900	0	964	55	0
18	CS	900	0	964	54	0
19	AT	725	0	778	43	0
19	CT	725	0	778	39	0
20	AU	785	0	878	75	0
20	CU	785	0	878	80	0
21	AV	1397	0	1430	140	0
21	CV	1428	0	1454	149	0
22	A3	607	0	628	42	0
22	C3	613	0	633	47	0
23	AZ	763	0	848	49	0
23	CZ	763	0	848	44	0
24	AW	558	0	610	45	0
24	CW	558	0	610	51	0
25	AX	469	0	518	28	0
25	CX	469	0	518	27	0
26	A4	533	0	522	72	0
26	C4	515	0	510	96	0
27	A5	459	0	480	88	0
27	C5	459	0	478	33	0
28	A6	389	0	404	59	0
28	C6	389	0	404	51	0
29	A7	391	0	432	21	0
29	C7	391	0	432	33	0
30	A8	480	0	549	67	0
30	C8	480	0	549	114	0
31	BA	32284	0	16296	1465	1
31	DA	32287	0	16295	1435	0
32	BE	1924	0	1975	137	0
32	DE	1924	0	1975	162	0
33	BF	1605	0	1668	95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DF	1612	0	1677	110	0
34	BG	1703	0	1763	120	0
34	DG	1703	0	1763	129	0
35	BH	1155	0	1213	71	0
35	DH	1155	0	1213	79	0
36	BI	843	0	857	36	0
36	DI	843	0	857	46	0
37	BJ	1257	0	1296	70	0
37	DJ	1257	0	1296	91	0
38	BK	1116	0	1177	83	0
38	DK	1116	0	1177	56	0
39	BL	1010	0	1037	72	0
39	DL	1010	0	1037	112	0
40	BM	801	0	849	79	0
40	DM	801	0	849	87	0
41	BN	885	0	904	54	0
41	DN	885	0	904	58	0
42	BO	975	0	1062	53	0
42	DO	975	0	1062	89	0
43	BP	928	0	987	74	0
43	DP	933	0	992	81	0
44	BQ	476	0	511	43	0
44	DQ	476	0	511	53	0
45	BR	734	0	771	34	0
45	DR	734	0	771	38	0
46	BS	705	0	725	54	0
46	DS	705	0	725	35	0
47	BT	834	0	904	53	0
47	DT	834	0	904	41	0
48	BU	591	0	662	38	0
48	DU	591	0	662	40	0
49	BV	624	0	636	50	0
49	DV	624	0	636	77	0
50	BW	763	0	861	59	0
50	DW	763	0	861	48	0
51	BX	217	0	234	12	0
51	DX	217	0	234	21	0
52	BB	1814	0	932	159	0
52	BD	1814	0	932	154	0
52	DB	1814	0	932	174	0
52	DD	1814	0	932	173	0
53	BC	1643	0	837	47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DC	1643	0	837	51	0
54	B1	347	0	174	24	0
54	D1	347	0	174	25	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0
55	AA	331	0	0	0	0
55	AB	6	0	0	0	0
55	AE	3	0	0	0	0
55	AF	2	0	0	0	0
55	AO	3	0	0	0	0
55	B1	1	0	0	0	0
55	BA	115	0	0	0	0
55	BB	5	0	0	0	0
55	BC	5	0	0	0	0
55	BD	1	0	0	0	0
55	BN	1	0	0	0	0
55	BQ	1	0	0	0	0
55	BS	1	0	0	0	0
55	C0	1	0	0	0	0
55	C5	1	0	0	0	0
55	C7	1	0	0	0	0
55	CA	274	0	0	0	0
55	CB	7	0	0	0	0
55	CE	1	0	0	0	0
55	D1	1	0	0	0	0
55	DA	119	0	0	0	0
55	DB	2	0	0	0	0
55	DC	6	0	0	0	0
55	DL	1	0	0	0	0
55	DN	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	0	0
56	A6	7	0	0	3	0
56	AA	1666	0	0	98	0
56	AB	91	0	0	4	0
56	AE	7	0	0	0	0
56	AF	7	0	0	1	0
56	AO	14	0	0	1	0
56	AW	7	0	0	0	0
56	BA	707	0	0	51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BB	14	0	0	1	0
56	BC	14	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BR	7	0	0	0	0
56	C1	7	0	0	0	0
56	C3	7	0	0	0	0
56	C5	7	0	0	1	0
56	C6	7	0	0	4	0
56	CA	1526	0	0	72	0
56	CB	91	0	0	4	0
56	CF	7	0	0	0	0
56	CO	7	0	0	0	0
56	DA	651	0	0	55	0
56	DB	21	0	0	1	0
56	DC	28	0	0	10	0
56	DD	7	0	0	1	0
56	DG	7	0	0	2	0
56	DK	7	0	0	1	0
56	DR	7	0	0	0	0
56	DV	7	0	0	1	0
57	BG	1	0	0	0	0
57	BQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	303952	0	200977	14995	1

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 30.

The worst 5 of 14995 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)
1:CA:2320:G:C8	1:CA:2324:A:C2	1.85	1.64
1:CA:216:G:N2	1:CA:218:A:H61	1.09	1.47
1:AA:2308:G:N1	1:AA:2311:A:N1	1.63	1.43
1:CA:216:G:H21	1:CA:218:A:N6	0.92	1.42
1:AA:2308:G:N2	1:AA:2311:A:H2	1.02	1.42

All (1) 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)
31:BA:85:U:O2'	7:CH:100:GLY:O[3_555]	1.93	0.27

## 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	
3	AD	270/276 (98%)	218 (81%)	35 (13%)	17 (6%)	1	11
3	CD	270/276 (98%)	218 (81%)	40 (15%)	12 (4%)	3	18
4	AE	203/206 (98%)	141 (70%)	39 (19%)	23 (11%)	0	3
4	CE	203/206 (98%)	131 (64%)	46 (23%)	26 (13%)	0	2
5	AF	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	3	18
5	CF	206/210 (98%)	144 (70%)	35 (17%)	27 (13%)	0	2
6	AG	179/182 (98%)	147 (82%)	25 (14%)	7 (4%)	3	21
6	CG	179/182 (98%)	144 (80%)	27 (15%)	8 (4%)	3	18
7	AH	168/180 (93%)	123 (73%)	20 (12%)	25 (15%)	0	1
7	CH	168/180 (93%)	111 (66%)	41 (24%)	16 (10%)	1	4
8	AK	144/148 (97%)	99 (69%)	31 (22%)	14 (10%)	1	4
8	CK	144/148 (97%)	104 (72%)	32 (22%)	8 (6%)	2	13
9	AM	136/140 (97%)	108 (79%)	17 (12%)	11 (8%)	1	7
9	CM	136/140 (97%)	106 (78%)	23 (17%)	7 (5%)	2	16
10	AN	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	10	40
10	CN	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	4	25
11	AO	148/150 (99%)	93 (63%)	35 (24%)	20 (14%)	0	2
11	CO	148/150 (99%)	91 (62%)	32 (22%)	25 (17%)	0	1
12	AP	139/141 (99%)	101 (73%)	21 (15%)	17 (12%)	0	2
12	CP	139/141 (99%)	95 (68%)	24 (17%)	20 (14%)	0	1
13	A0	116/118 (98%)	96 (83%)	15 (13%)	5 (4%)	3	19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C0	115/118 (98%)	97 (84%)	12 (10%)	6 (5%)	2	15
14	AQ	109/112 (97%)	86 (79%)	14 (13%)	9 (8%)	1	6
14	CQ	109/112 (97%)	72 (66%)	24 (22%)	13 (12%)	0	2
15	AR	135/146 (92%)	107 (79%)	22 (16%)	6 (4%)	3	18
15	CR	135/146 (92%)	112 (83%)	15 (11%)	8 (6%)	2	12
16	A1	115/118 (98%)	96 (84%)	13 (11%)	6 (5%)	2	15
16	C1	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1	6
17	A2	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	2	16
17	C2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0	2
18	AS	111/113 (98%)	97 (87%)	13 (12%)	1 (1%)	19	53
18	CS	111/113 (98%)	99 (89%)	9 (8%)	3 (3%)	5	29
19	AT	90/96 (94%)	84 (93%)	5 (6%)	1 (1%)	16	50
19	CT	90/96 (94%)	73 (81%)	14 (16%)	3 (3%)	4	25
20	AU	100/110 (91%)	76 (76%)	13 (13%)	11 (11%)	0	3
20	CU	100/110 (91%)	62 (62%)	27 (27%)	11 (11%)	0	3
21	AV	173/206 (84%)	113 (65%)	40 (23%)	20 (12%)	0	2
21	CV	177/206 (86%)	112 (63%)	40 (23%)	25 (14%)	0	1
22	A3	74/85 (87%)	62 (84%)	7 (10%)	5 (7%)	1	9
22	C3	75/85 (88%)	59 (79%)	13 (17%)	3 (4%)	3	21
23	AZ	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	1	11
23	CZ	95/98 (97%)	76 (80%)	9 (10%)	10 (10%)	0	3
24	AW	64/72 (89%)	57 (89%)	4 (6%)	3 (5%)	2	17
24	CW	64/72 (89%)	52 (81%)	7 (11%)	5 (8%)	1	7
25	AX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
25	CX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	A4	64/71 (90%)	39 (61%)	13 (20%)	12 (19%)	0	1
26	C4	61/71 (86%)	23 (38%)	20 (33%)	18 (30%)	0	0
27	A5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	0	3
27	C5	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	4	24
28	A6	43/54 (80%)	23 (54%)	13 (30%)	7 (16%)	0	1
28	C6	43/54 (80%)	23 (54%)	11 (26%)	9 (21%)	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	A7	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
29	C7	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
30	A8	58/65 (89%)	47 (81%)	8 (14%)	3 (5%)	2	15
30	C8	58/65 (89%)	41 (71%)	6 (10%)	11 (19%)	0	1
32	BE	235/256 (92%)	181 (77%)	38 (16%)	16 (7%)	1	9
32	DE	235/256 (92%)	177 (75%)	40 (17%)	18 (8%)	1	7
33	BF	203/239 (85%)	161 (79%)	36 (18%)	6 (3%)	5	27
33	DF	204/239 (85%)	163 (80%)	35 (17%)	6 (3%)	5	28
34	BG	206/208 (99%)	179 (87%)	19 (9%)	8 (4%)	3	21
34	DG	206/208 (99%)	159 (77%)	35 (17%)	12 (6%)	2	12
35	BH	149/162 (92%)	127 (85%)	16 (11%)	6 (4%)	3	21
35	DH	149/162 (92%)	132 (89%)	15 (10%)	2 (1%)	13	45
36	BI	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	5	27
36	DI	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	8	37
37	BJ	153/156 (98%)	128 (84%)	21 (14%)	4 (3%)	6	30
37	DJ	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	13	45
38	BK	136/138 (99%)	116 (85%)	16 (12%)	4 (3%)	5	28
38	DK	136/138 (99%)	116 (85%)	15 (11%)	5 (4%)	4	23
39	BL	125/128 (98%)	95 (76%)	25 (20%)	5 (4%)	3	21
39	DL	125/128 (98%)	97 (78%)	21 (17%)	7 (6%)	2	13
40	BM	97/105 (92%)	83 (86%)	13 (13%)	1 (1%)	17	51
40	DM	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	17	51
41	BN	117/129 (91%)	99 (85%)	12 (10%)	6 (5%)	2	16
41	DN	117/129 (91%)	103 (88%)	8 (7%)	6 (5%)	2	16
42	BO	123/132 (93%)	100 (81%)	17 (14%)	6 (5%)	2	16
42	DO	123/132 (93%)	94 (76%)	17 (14%)	12 (10%)	1	4
43	BP	114/126 (90%)	82 (72%)	22 (19%)	10 (9%)	1	5
43	DP	115/126 (91%)	85 (74%)	18 (16%)	12 (10%)	0	3
44	BQ	56/61 (92%)	40 (71%)	10 (18%)	6 (11%)	0	3
44	DQ	56/61 (92%)	41 (73%)	8 (14%)	7 (12%)	0	2
45	BR	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	7	33

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DR	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	14	47
46	BS	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	6	32
46	DS	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	14	47
47	BT	98/105 (93%)	82 (84%)	13 (13%)	3 (3%)	4	27
47	DT	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	8	37
48	BU	70/88 (80%)	59 (84%)	10 (14%)	1 (1%)	12	43
48	DU	70/88 (80%)	57 (81%)	12 (17%)	1 (1%)	12	43
49	BV	76/93 (82%)	59 (78%)	14 (18%)	3 (4%)	3	21
49	DV	76/93 (82%)	55 (72%)	17 (22%)	4 (5%)	2	14
50	BW	97/106 (92%)	78 (80%)	16 (16%)	3 (3%)	4	27
50	DW	97/106 (92%)	82 (84%)	9 (9%)	6 (6%)	1	12
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	19
51	DX	23/27 (85%)	21 (91%)	0	2 (9%)	1	6
All	All	11319/12052 (94%)	8877 (78%)	1684 (15%)	758 (7%)	1	10

5 of 758 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	28	GLU
3	AD	32	SER
3	AD	122	ASP
3	AD	123	ALA
3	AD	238	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/218 (98%)	172 (80%)	42 (20%)	1	6
3	CD	214/218 (98%)	187 (87%)	27 (13%)	5	21
4	AE	165/166 (99%)	137 (83%)	28 (17%)	2	11

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	165/166 (99%)	125 (76%)	40 (24%)	1	3
5	AF	161/166 (97%)	137 (85%)	24 (15%)	3	15
5	CF	165/166 (99%)	137 (83%)	28 (17%)	2	11
6	AG	155/156 (99%)	136 (88%)	19 (12%)	5	22
6	CG	155/156 (99%)	139 (90%)	16 (10%)	8	29
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1	5
7	CH	142/148 (96%)	123 (87%)	19 (13%)	4	19
8	AK	122/124 (98%)	98 (80%)	24 (20%)	1	6
8	CK	122/124 (98%)	104 (85%)	18 (15%)	3	16
9	AM	117/119 (98%)	98 (84%)	19 (16%)	2	12
9	CM	117/119 (98%)	95 (81%)	22 (19%)	1	8
10	AN	100/100 (100%)	92 (92%)	8 (8%)	13	41
10	CN	100/100 (100%)	88 (88%)	12 (12%)	5	23
11	AO	116/116 (100%)	84 (72%)	32 (28%)	0	1
11	CO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	91 (82%)	20 (18%)	2	9
12	CP	111/111 (100%)	88 (79%)	23 (21%)	1	5
13	A0	101/101 (100%)	83 (82%)	18 (18%)	2	9
13	C0	100/101 (99%)	84 (84%)	16 (16%)	2	13
14	AQ	87/88 (99%)	70 (80%)	17 (20%)	1	6
14	CQ	87/88 (99%)	72 (83%)	15 (17%)	2	10
15	AR	120/127 (94%)	103 (86%)	17 (14%)	3	18
15	CR	120/127 (94%)	105 (88%)	15 (12%)	5	21
16	A1	93/94 (99%)	79 (85%)	14 (15%)	3	15
16	C1	93/94 (99%)	80 (86%)	13 (14%)	4	18
17	A2	82/82 (100%)	69 (84%)	13 (16%)	3	13
17	C2	82/82 (100%)	62 (76%)	20 (24%)	1	2
18	AS	92/92 (100%)	73 (79%)	19 (21%)	1	5
18	CS	92/92 (100%)	80 (87%)	12 (13%)	4	20
19	AT	74/78 (95%)	65 (88%)	9 (12%)	5	23
19	CT	74/78 (95%)	64 (86%)	10 (14%)	4	18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AU	85/91 (93%)	72 (85%)	13 (15%)	3	14
20	CU	85/91 (93%)	65 (76%)	20 (24%)	1	3
21	AV	154/179 (86%)	130 (84%)	24 (16%)	3	14
21	CV	158/179 (88%)	137 (87%)	21 (13%)	4	19
22	A3	61/67 (91%)	55 (90%)	6 (10%)	9	32
22	C3	62/67 (92%)	58 (94%)	4 (6%)	19	51
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	3	16
23	CZ	82/83 (99%)	73 (89%)	9 (11%)	7	27
24	AW	62/67 (92%)	49 (79%)	13 (21%)	1	5
24	CW	62/67 (92%)	52 (84%)	10 (16%)	2	12
25	AX	51/52 (98%)	43 (84%)	8 (16%)	3	14
25	CX	51/52 (98%)	46 (90%)	5 (10%)	9	32
26	A4	59/63 (94%)	52 (88%)	7 (12%)	6	23
26	C4	57/63 (90%)	45 (79%)	12 (21%)	1	5
27	A5	51/52 (98%)	41 (80%)	10 (20%)	1	6
27	C5	51/52 (98%)	44 (86%)	7 (14%)	4	18
28	A6	44/52 (85%)	30 (68%)	14 (32%)	0	1
28	C6	44/52 (85%)	38 (86%)	6 (14%)	4	18
29	A7	38/42 (90%)	33 (87%)	5 (13%)	4	19
29	C7	38/42 (90%)	31 (82%)	7 (18%)	2	8
30	A8	50/55 (91%)	39 (78%)	11 (22%)	1	4
30	C8	50/55 (91%)	37 (74%)	13 (26%)	0	2
32	BE	205/220 (93%)	172 (84%)	33 (16%)	2	12
32	DE	205/220 (93%)	177 (86%)	28 (14%)	4	18
33	BF	159/188 (85%)	134 (84%)	25 (16%)	3	14
33	DF	160/188 (85%)	141 (88%)	19 (12%)	6	23
34	BG	180/180 (100%)	158 (88%)	22 (12%)	5	23
34	DG	180/180 (100%)	156 (87%)	24 (13%)	4	19
35	BH	116/123 (94%)	100 (86%)	16 (14%)	4	18
35	DH	116/123 (94%)	95 (82%)	21 (18%)	2	9
36	BI	90/90 (100%)	82 (91%)	8 (9%)	11	36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DI	90/90 (100%)	80 (89%)	10 (11%)	7	26
37	BJ	126/127 (99%)	106 (84%)	20 (16%)	3	13
37	DJ	126/127 (99%)	109 (86%)	17 (14%)	4	18
38	BK	119/119 (100%)	99 (83%)	20 (17%)	2	11
38	DK	119/119 (100%)	105 (88%)	14 (12%)	6	24
39	BL	98/99 (99%)	85 (87%)	13 (13%)	4	19
39	DL	98/99 (99%)	82 (84%)	16 (16%)	2	12
40	BM	89/92 (97%)	76 (85%)	13 (15%)	3	16
40	DM	89/92 (97%)	80 (90%)	9 (10%)	8	30
41	BN	90/99 (91%)	78 (87%)	12 (13%)	4	19
41	DN	90/99 (91%)	83 (92%)	7 (8%)	14	42
42	BO	104/109 (95%)	92 (88%)	12 (12%)	6	25
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	8
43	BP	94/101 (93%)	80 (85%)	14 (15%)	3	15
43	DP	94/101 (93%)	82 (87%)	12 (13%)	5	20
44	BQ	48/50 (96%)	42 (88%)	6 (12%)	5	21
44	DQ	48/50 (96%)	44 (92%)	4 (8%)	12	40
45	BR	79/80 (99%)	74 (94%)	5 (6%)	20	52
45	DR	79/80 (99%)	72 (91%)	7 (9%)	11	36
46	BS	72/74 (97%)	60 (83%)	12 (17%)	2	11
46	DS	72/74 (97%)	66 (92%)	6 (8%)	12	40
47	BT	95/97 (98%)	84 (88%)	11 (12%)	6	25
47	DT	95/97 (98%)	88 (93%)	7 (7%)	15	44
48	BU	63/77 (82%)	61 (97%)	2 (3%)	42	72
48	DU	63/77 (82%)	54 (86%)	9 (14%)	3	17
49	BV	67/80 (84%)	55 (82%)	12 (18%)	2	9
49	DV	67/80 (84%)	55 (82%)	12 (18%)	2	9
50	BW	76/82 (93%)	68 (90%)	8 (10%)	7	28
50	DW	76/82 (93%)	68 (90%)	8 (10%)	7	28
51	BX	20/22 (91%)	19 (95%)	1 (5%)	27	60
51	DX	20/22 (91%)	19 (95%)	1 (5%)	27	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9565/9996 (96%)	8122 (85%)	1443 (15%)	<b>3</b> <b>15</b>

5 of 1443 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BN	93	GLN
4	CE	203	LYS
39	DL	79	LEU
43	BP	32	GLU
50	BW	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 281 such sidechains are listed below:

Mol	Chain	Res	Type
42	BO	6	GLN
5	CF	169	ASN
41	DN	93	GLN
43	BP	101	GLN
50	BW	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	616 (21%)	54 (1%)
1	CA	2905/2912 (99%)	632 (21%)	51 (1%)
2	AB	121/122 (99%)	16 (13%)	0
2	CB	121/122 (99%)	29 (23%)	2 (1%)
31	BA	1501/1506 (99%)	318 (21%)	42 (2%)
31	DA	1501/1506 (99%)	325 (21%)	46 (3%)
52	BB	83/85 (97%)	47 (56%)	10 (12%)
52	BD	83/85 (97%)	32 (38%)	5 (6%)
52	DB	83/85 (97%)	49 (59%)	9 (10%)
52	DD	83/85 (97%)	31 (37%)	5 (6%)
53	BC	76/77 (98%)	16 (21%)	2 (2%)
53	DC	76/77 (98%)	15 (19%)	2 (2%)
54	B1	15/16 (93%)	5 (33%)	3 (20%)
54	D1	15/16 (93%)	5 (33%)	3 (20%)
All	All	9574/9606 (99%)	2136 (22%)	234 (2%)

5 of 2136 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	17	G
1	AA	18	C
1	AA	27	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BB	78	C
1	CA	936	C
52	DB	6	G
52	BD	17	G
1	CA	126	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
52	MIA	BB	38	52	22,31,32	1.44	1 (4%)	26,44,47	2.22	9 (34%)
52	MIA	BD	38	52	22,31,32	1.42	1 (4%)	26,44,47	2.71	9 (34%)
52	MIA	DB	38	52	22,31,32	1.54	1 (4%)	26,44,47	2.54	9 (34%)
52	MIA	DD	38	52	22,31,32	1.45	1 (4%)	26,44,47	2.37	9 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MIA	BB	38	52	-	3/11/33/34	0/3/3/3
52	MIA	BD	38	52	-	8/11/33/34	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	MIA	DB	38	52	-	4/11/33/34	0/3/3/3
52	MIA	DD	38	52	-	8/11/33/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DB	38	MIA	C13-C14	6.19	1.50	1.32
52	BB	38	MIA	C13-C14	6.03	1.50	1.32
52	DD	38	MIA	C13-C14	5.99	1.50	1.32
52	BD	38	MIA	C13-C14	5.90	1.49	1.32

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BD	38	MIA	C11-S10-C2	9.63	109.41	102.29
52	DB	38	MIA	C11-S10-C2	9.14	109.06	102.29
52	DD	38	MIA	C11-S10-C2	7.45	107.80	102.29
52	BB	38	MIA	C11-S10-C2	6.27	106.93	102.29
52	BD	38	MIA	C12-C13-C14	-5.26	116.73	127.10

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	DB	38	MIA	N1-C2-S10-C11
52	DB	38	MIA	N3-C2-S10-C11
52	DB	38	MIA	C12-C13-C14-C15
52	DB	38	MIA	C12-C13-C14-C16
52	BB	38	MIA	N1-C2-S10-C11

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	BD	38	MIA	3	0
52	DB	38	MIA	2	0
52	DD	38	MIA	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1610 ligands modelled in this entry, 898 are monoatomic - leaving 712 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	$\# Z  > 2$
56	OHX	A1	202	-	0,6,6	0.00	-	-		
56	OHX	A1	203	-	0,6,6	0.00	-	-		
56	OHX	A3	102	-	0,6,6	0.00	-	-		
56	OHX	A6	101	-	0,6,6	0.00	-	-		
56	OHX	AA	3138	-	0,6,6	0.00	-	-		
56	OHX	AA	3147	-	0,6,6	0.00	-	-		
56	OHX	AA	3154	-	0,6,6	0.00	-	-		
56	OHX	AA	3160	-	0,6,6	0.00	-	-		
56	OHX	AA	3263	-	0,6,6	0.00	-	-		
56	OHX	AA	3287	-	0,6,6	0.00	-	-		
56	OHX	AA	3288	-	0,6,6	0.00	-	-		
56	OHX	AA	3289	-	0,6,6	0.00	-	-		
56	OHX	AA	3290	-	0,6,6	0.00	-	-		
56	OHX	AA	3291	-	0,6,6	0.00	-	-		
56	OHX	AA	3292	-	0,6,6	0.00	-	-		
56	OHX	AA	3293	-	0,6,6	0.00	-	-		
56	OHX	AA	3294	-	0,6,6	0.00	-	-		
56	OHX	AA	3295	-	0,6,6	0.00	-	-		
56	OHX	AA	3296	-	0,6,6	0.00	-	-		
56	OHX	AA	3297	-	0,6,6	0.00	-	-		
56	OHX	AA	3298	-	0,6,6	0.00	-	-		
56	OHX	AA	3299	-	0,6,6	0.00	-	-		
56	OHX	AA	3300	-	0,6,6	0.00	-	-		
56	OHX	AA	3301	-	0,6,6	0.00	-	-		
56	OHX	AA	3302	-	0,6,6	0.00	-	-		
56	OHX	AA	3303	-	0,6,6	0.00	-	-		
56	OHX	AA	3304	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3305	-	0,6,6	0.00	-	-		
56	OHX	AA	3306	-	0,6,6	0.00	-	-		
56	OHX	AA	3307	-	0,6,6	0.00	-	-		
56	OHX	AA	3308	-	0,6,6	0.00	-	-		
56	OHX	AA	3309	-	0,6,6	0.00	-	-		
56	OHX	AA	3310	-	0,6,6	0.00	-	-		
56	OHX	AA	3311	-	0,6,6	0.00	-	-		
56	OHX	AA	3312	-	0,6,6	0.00	-	-		
56	OHX	AA	3313	-	0,6,6	0.00	-	-		
56	OHX	AA	3314	-	0,6,6	0.00	-	-		
56	OHX	AA	3315	-	0,6,6	0.00	-	-		
56	OHX	AA	3316	-	0,6,6	0.00	-	-		
56	OHX	AA	3317	-	0,6,6	0.00	-	-		
56	OHX	AA	3318	-	0,6,6	0.00	-	-		
56	OHX	AA	3319	-	0,6,6	0.00	-	-		
56	OHX	AA	3320	-	0,6,6	0.00	-	-		
56	OHX	AA	3321	-	0,6,6	0.00	-	-		
56	OHX	AA	3322	-	0,6,6	0.00	-	-		
56	OHX	AA	3323	-	0,6,6	0.00	-	-		
56	OHX	AA	3324	-	0,6,6	0.00	-	-		
56	OHX	AA	3325	-	0,6,6	0.00	-	-		
56	OHX	AA	3326	-	0,6,6	0.00	-	-		
56	OHX	AA	3327	-	0,6,6	0.00	-	-		
56	OHX	AA	3328	-	0,6,6	0.00	-	-		
56	OHX	AA	3329	-	0,6,6	0.00	-	-		
56	OHX	AA	3330	-	0,6,6	0.00	-	-		
56	OHX	AA	3331	-	0,6,6	0.00	-	-		
56	OHX	AA	3332	-	0,6,6	0.00	-	-		
56	OHX	AA	3333	-	0,6,6	0.00	-	-		
56	OHX	AA	3334	-	0,6,6	0.00	-	-		
56	OHX	AA	3335	-	0,6,6	0.00	-	-		
56	OHX	AA	3336	-	0,6,6	0.00	-	-		
56	OHX	AA	3337	-	0,6,6	0.00	-	-		
56	OHX	AA	3338	-	0,6,6	0.00	-	-		
56	OHX	AA	3339	-	0,6,6	0.00	-	-		
56	OHX	AA	3340	-	0,6,6	0.00	-	-		
56	OHX	AA	3341	-	0,6,6	0.00	-	-		
56	OHX	AA	3342	-	0,6,6	0.00	-	-		
56	OHX	AA	3359	-	0,6,6	0.00	-	-		
56	OHX	AA	3360	-	0,6,6	0.00	-	-		
56	OHX	AA	3361	-	0,6,6	0.00	-	-		
56	OHX	AA	3362	-	0,6,6	0.00	-	-		
56	OHX	AA	3363	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3364	-	0,6,6	0.00	-	-		
56	OHX	AA	3365	-	0,6,6	0.00	-	-		
56	OHX	AA	3366	-	0,6,6	0.00	-	-		
56	OHX	AA	3367	-	0,6,6	0.00	-	-		
56	OHX	AA	3368	-	0,6,6	0.00	-	-		
56	OHX	AA	3369	-	0,6,6	0.00	-	-		
56	OHX	AA	3370	-	0,6,6	0.00	-	-		
56	OHX	AA	3371	-	0,6,6	0.00	-	-		
56	OHX	AA	3372	-	0,6,6	0.00	-	-		
56	OHX	AA	3373	-	0,6,6	0.00	-	-		
56	OHX	AA	3399	-	0,6,6	0.00	-	-		
56	OHX	AA	3400	-	0,6,6	0.00	-	-		
56	OHX	AA	3401	-	0,6,6	0.00	-	-		
56	OHX	AA	3402	-	0,6,6	0.00	-	-		
56	OHX	AA	3403	-	0,6,6	0.00	-	-		
56	OHX	AA	3404	-	0,6,6	0.00	-	-		
56	OHX	AA	3405	-	0,6,6	0.00	-	-		
56	OHX	AA	3406	-	0,6,6	0.00	-	-		
56	OHX	AA	3407	-	0,6,6	0.00	-	-		
56	OHX	AA	3417	-	0,6,6	0.00	-	-		
56	OHX	AA	3418	-	0,6,6	0.00	-	-		
56	OHX	AA	3419	-	0,6,6	0.00	-	-		
56	OHX	AA	3420	-	0,6,6	0.00	-	-		
56	OHX	AA	3421	-	0,6,6	0.00	-	-		
56	OHX	AA	3422	-	0,6,6	0.00	-	-		
56	OHX	AA	3423	-	0,6,6	0.00	-	-		
56	OHX	AA	3424	-	0,6,6	0.00	-	-		
56	OHX	AA	3425	-	0,6,6	0.00	-	-		
56	OHX	AA	3426	-	0,6,6	0.00	-	-		
56	OHX	AA	3427	-	0,6,6	0.00	-	-		
56	OHX	AA	3428	-	0,6,6	0.00	-	-		
56	OHX	AA	3429	-	0,6,6	0.00	-	-		
56	OHX	AA	3430	-	0,6,6	0.00	-	-		
56	OHX	AA	3431	-	0,6,6	0.00	-	-		
56	OHX	AA	3432	-	0,6,6	0.00	-	-		
56	OHX	AA	3433	-	0,6,6	0.00	-	-		
56	OHX	AA	3434	-	0,6,6	0.00	-	-		
56	OHX	AA	3435	-	0,6,6	0.00	-	-		
56	OHX	AA	3436	-	0,6,6	0.00	-	-		
56	OHX	AA	3437	-	0,6,6	0.00	-	-		
56	OHX	AA	3438	-	0,6,6	0.00	-	-		
56	OHX	AA	3439	-	0,6,6	0.00	-	-		
56	OHX	AA	3440	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3441	-	0,6,6	0.00	-	-		
56	OHX	AA	3442	-	0,6,6	0.00	-	-		
56	OHX	AA	3443	-	0,6,6	0.00	-	-		
56	OHX	AA	3444	-	0,6,6	0.00	-	-		
56	OHX	AA	3445	-	0,6,6	0.00	-	-		
56	OHX	AA	3446	-	0,6,6	0.00	-	-		
56	OHX	AA	3447	-	0,6,6	0.00	-	-		
56	OHX	AA	3448	-	0,6,6	0.00	-	-		
56	OHX	AA	3449	-	0,6,6	0.00	-	-		
56	OHX	AA	3450	-	0,6,6	0.00	-	-		
56	OHX	AA	3451	-	0,6,6	0.00	-	-		
56	OHX	AA	3452	-	0,6,6	0.00	-	-		
56	OHX	AA	3453	-	0,6,6	0.00	-	-		
56	OHX	AA	3454	-	0,6,6	0.00	-	-		
56	OHX	AA	3455	-	0,6,6	0.00	-	-		
56	OHX	AA	3456	-	0,6,6	0.00	-	-		
56	OHX	AA	3457	-	0,6,6	0.00	-	-		
56	OHX	AA	3458	-	0,6,6	0.00	-	-		
56	OHX	AA	3459	-	0,6,6	0.00	-	-		
56	OHX	AA	3460	-	0,6,6	0.00	-	-		
56	OHX	AA	3461	-	0,6,6	0.00	-	-		
56	OHX	AA	3462	-	0,6,6	0.00	-	-		
56	OHX	AA	3463	-	0,6,6	0.00	-	-		
56	OHX	AA	3464	-	0,6,6	0.00	-	-		
56	OHX	AA	3465	-	0,6,6	0.00	-	-		
56	OHX	AA	3466	-	0,6,6	0.00	-	-		
56	OHX	AA	3467	-	0,6,6	0.00	-	-		
56	OHX	AA	3468	-	0,6,6	0.00	-	-		
56	OHX	AA	3469	-	0,6,6	0.00	-	-		
56	OHX	AA	3470	-	0,6,6	0.00	-	-		
56	OHX	AA	3471	-	0,6,6	0.00	-	-		
56	OHX	AA	3472	-	0,6,6	0.00	-	-		
56	OHX	AA	3473	-	0,6,6	0.00	-	-		
56	OHX	AA	3474	-	0,6,6	0.00	-	-		
56	OHX	AA	3475	-	0,6,6	0.00	-	-		
56	OHX	AA	3476	-	0,6,6	0.00	-	-		
56	OHX	AA	3477	-	0,6,6	0.00	-	-		
56	OHX	AA	3478	-	0,6,6	0.00	-	-		
56	OHX	AA	3479	-	0,6,6	0.00	-	-		
56	OHX	AA	3480	-	0,6,6	0.00	-	-		
56	OHX	AA	3481	-	0,6,6	0.00	-	-		
56	OHX	AA	3482	-	0,6,6	0.00	-	-		
56	OHX	AA	3483	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3484	-	0,6,6	0.00	-	-		
56	OHX	AA	3485	-	0,6,6	0.00	-	-		
56	OHX	AA	3486	-	0,6,6	0.00	-	-		
56	OHX	AA	3487	-	0,6,6	0.00	-	-		
56	OHX	AA	3488	-	0,6,6	0.00	-	-		
56	OHX	AA	3489	-	0,6,6	0.00	-	-		
56	OHX	AA	3490	-	0,6,6	0.00	-	-		
56	OHX	AA	3491	-	0,6,6	0.00	-	-		
56	OHX	AA	3492	-	0,6,6	0.00	-	-		
56	OHX	AA	3493	-	0,6,6	0.00	-	-		
56	OHX	AA	3494	-	0,6,6	0.00	-	-		
56	OHX	AA	3495	-	0,6,6	0.00	-	-		
56	OHX	AA	3496	-	0,6,6	0.00	-	-		
56	OHX	AA	3497	-	0,6,6	0.00	-	-		
56	OHX	AA	3498	-	0,6,6	0.00	-	-		
56	OHX	AA	3499	-	0,6,6	0.00	-	-		
56	OHX	AA	3500	-	0,6,6	0.00	-	-		
56	OHX	AA	3501	-	0,6,6	0.00	-	-		
56	OHX	AA	3502	-	0,6,6	0.00	-	-		
56	OHX	AA	3503	-	0,6,6	0.00	-	-		
56	OHX	AA	3504	-	0,6,6	0.00	-	-		
56	OHX	AA	3505	-	0,6,6	0.00	-	-		
56	OHX	AA	3506	-	0,6,6	0.00	-	-		
56	OHX	AA	3507	-	0,6,6	0.00	-	-		
56	OHX	AA	3508	-	0,6,6	0.00	-	-		
56	OHX	AA	3509	-	0,6,6	0.00	-	-		
56	OHX	AA	3510	-	0,6,6	0.00	-	-		
56	OHX	AA	3511	-	0,6,6	0.00	-	-		
56	OHX	AA	3512	-	0,6,6	0.00	-	-		
56	OHX	AA	3513	-	0,6,6	0.00	-	-		
56	OHX	AA	3514	-	0,6,6	0.00	-	-		
56	OHX	AA	3515	-	0,6,6	0.00	-	-		
56	OHX	AA	3516	-	0,6,6	0.00	-	-		
56	OHX	AA	3517	-	0,6,6	0.00	-	-		
56	OHX	AA	3518	-	0,6,6	0.00	-	-		
56	OHX	AA	3519	-	0,6,6	0.00	-	-		
56	OHX	AA	3520	-	0,6,6	0.00	-	-		
56	OHX	AA	3521	-	0,6,6	0.00	-	-		
56	OHX	AA	3522	-	0,6,6	0.00	-	-		
56	OHX	AA	3523	-	0,6,6	0.00	-	-		
56	OHX	AA	3524	-	0,6,6	0.00	-	-		
56	OHX	AA	3525	-	0,6,6	0.00	-	-		
56	OHX	AA	3526	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AA	3527	-	0,6,6	0.00	-	-		
56	OHX	AA	3528	-	0,6,6	0.00	-	-		
56	OHX	AA	3529	-	0,6,6	0.00	-	-		
56	OHX	AA	3530	-	0,6,6	0.00	-	-		
56	OHX	AA	3531	-	0,6,6	0.00	-	-		
56	OHX	AA	3532	-	0,6,6	0.00	-	-		
56	OHX	AA	3533	-	0,6,6	0.00	-	-		
56	OHX	AA	3534	-	0,6,6	0.00	-	-		
56	OHX	AA	3535	-	0,6,6	0.00	-	-		
56	OHX	AA	3536	-	0,6,6	0.00	-	-		
56	OHX	AA	3537	-	0,6,6	0.00	-	-		
56	OHX	AA	3538	-	0,6,6	0.00	-	-		
56	OHX	AA	3539	-	0,6,6	0.00	-	-		
56	OHX	AA	3540	-	0,6,6	0.00	-	-		
56	OHX	AA	3541	-	0,6,6	0.00	-	-		
56	OHX	AA	3542	-	0,6,6	0.00	-	-		
56	OHX	AA	3543	-	0,6,6	0.00	-	-		
56	OHX	AA	3544	-	0,6,6	0.00	-	-		
56	OHX	AA	3545	-	0,6,6	0.00	-	-		
56	OHX	AA	3546	-	0,6,6	0.00	-	-		
56	OHX	AA	3547	-	0,6,6	0.00	-	-		
56	OHX	AA	3548	-	0,6,6	0.00	-	-		
56	OHX	AA	3549	-	0,6,6	0.00	-	-		
56	OHX	AA	3550	-	0,6,6	0.00	-	-		
56	OHX	AA	3551	-	0,6,6	0.00	-	-		
56	OHX	AA	3552	-	0,6,6	0.00	-	-		
56	OHX	AA	3553	-	0,6,6	0.00	-	-		
56	OHX	AA	3554	-	0,6,6	0.00	-	-		
56	OHX	AA	3555	-	0,6,6	0.00	-	-		
56	OHX	AA	3556	-	0,6,6	0.00	-	-		
56	OHX	AA	3557	-	0,6,6	0.00	-	-		
56	OHX	AA	3558	-	0,6,6	0.00	-	-		
56	OHX	AA	3559	-	0,6,6	0.00	-	-		
56	OHX	AA	3560	-	0,6,6	0.00	-	-		
56	OHX	AA	3561	-	0,6,6	0.00	-	-		
56	OHX	AA	3562	-	0,6,6	0.00	-	-		
56	OHX	AA	3563	-	0,6,6	0.00	-	-		
56	OHX	AA	3564	-	0,6,6	0.00	-	-		
56	OHX	AA	3565	-	0,6,6	0.00	-	-		
56	OHX	AA	3566	-	0,6,6	0.00	-	-		
56	OHX	AA	3567	-	0,6,6	0.00	-	-		
56	OHX	AA	3568	-	0,6,6	0.00	-	-		
56	OHX	AA	3569	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	AB	207	-	0,6,6	0.00	-	-		
56	OHX	AB	208	-	0,6,6	0.00	-	-		
56	OHX	AB	209	-	0,6,6	0.00	-	-		
56	OHX	AB	210	-	0,6,6	0.00	-	-		
56	OHX	AB	211	-	0,6,6	0.00	-	-		
56	OHX	AB	212	-	0,6,6	0.00	-	-		
56	OHX	AB	213	-	0,6,6	0.00	-	-		
56	OHX	AB	214	-	0,6,6	0.00	-	-		
56	OHX	AB	215	-	0,6,6	0.00	-	-		
56	OHX	AB	216	-	0,6,6	0.00	-	-		
56	OHX	AB	217	-	0,6,6	0.00	-	-		
56	OHX	AB	218	-	0,6,6	0.00	-	-		
56	OHX	AB	219	-	0,6,6	0.00	-	-		
56	OHX	AE	304	-	0,6,6	0.00	-	-		
56	OHX	AF	303	-	0,6,6	0.00	-	-		
56	OHX	AO	204	-	0,6,6	0.00	-	-		
56	OHX	AO	205	-	0,6,6	0.00	-	-		
56	OHX	AW	101	-	0,6,6	0.00	-	-		
56	OHX	BA	1656	-	0,6,6	0.00	-	-		
56	OHX	BA	1657	-	0,6,6	0.00	-	-		
56	OHX	BA	1659	-	0,6,6	0.00	-	-		
56	OHX	BA	1661	-	0,6,6	0.00	-	-		
56	OHX	BA	1662	-	0,6,6	0.00	-	-		
56	OHX	BA	1663	-	0,6,6	0.00	-	-		
56	OHX	BA	1664	-	0,6,6	0.00	-	-		
56	OHX	BA	1665	-	0,6,6	0.00	-	-		
56	OHX	BA	1666	-	0,6,6	0.00	-	-		
56	OHX	BA	1667	-	0,6,6	0.00	-	-		
56	OHX	BA	1668	-	0,6,6	0.00	-	-		
56	OHX	BA	1669	-	0,6,6	0.00	-	-		
56	OHX	BA	1670	-	0,6,6	0.00	-	-		
56	OHX	BA	1671	-	0,6,6	0.00	-	-		
56	OHX	BA	1672	-	0,6,6	0.00	-	-		
56	OHX	BA	1673	-	0,6,6	0.00	-	-		
56	OHX	BA	1674	-	0,6,6	0.00	-	-		
56	OHX	BA	1675	-	0,6,6	0.00	-	-		
56	OHX	BA	1676	-	0,6,6	0.00	-	-		
56	OHX	BA	1677	-	0,6,6	0.00	-	-		
56	OHX	BA	1678	-	0,6,6	0.00	-	-		
56	OHX	BA	1679	-	0,6,6	0.00	-	-		
56	OHX	BA	1680	-	0,6,6	0.00	-	-		
56	OHX	BA	1681	-	0,6,6	0.00	-	-		
56	OHX	BA	1682	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	BA	1683	-	0,6,6	0.00	-	-		
56	OHX	BA	1684	-	0,6,6	0.00	-	-		
56	OHX	BA	1685	-	0,6,6	0.00	-	-		
56	OHX	BA	1686	-	0,6,6	0.00	-	-		
56	OHX	BA	1687	-	0,6,6	0.00	-	-		
56	OHX	BA	1688	-	0,6,6	0.00	-	-		
56	OHX	BA	1689	-	0,6,6	0.00	-	-		
56	OHX	BA	1690	-	0,6,6	0.00	-	-		
56	OHX	BA	1691	-	0,6,6	0.00	-	-		
56	OHX	BA	1692	-	0,6,6	0.00	-	-		
56	OHX	BA	1693	-	0,6,6	0.00	-	-		
56	OHX	BA	1694	-	0,6,6	0.00	-	-		
56	OHX	BA	1695	-	0,6,6	0.00	-	-		
56	OHX	BA	1696	-	0,6,6	0.00	-	-		
56	OHX	BA	1755	-	0,6,6	0.00	-	-		
56	OHX	BA	1756	-	0,6,6	0.00	-	-		
56	OHX	BA	1757	-	0,6,6	0.00	-	-		
56	OHX	BA	1758	-	0,6,6	0.00	-	-		
56	OHX	BA	1759	-	0,6,6	0.00	-	-		
56	OHX	BA	1760	-	0,6,6	0.00	-	-		
56	OHX	BA	1761	-	0,6,6	0.00	-	-		
56	OHX	BA	1762	-	0,6,6	0.00	-	-		
56	OHX	BA	1763	-	0,6,6	0.00	-	-		
56	OHX	BA	1764	-	0,6,6	0.00	-	-		
56	OHX	BA	1765	-	0,6,6	0.00	-	-		
56	OHX	BA	1766	-	0,6,6	0.00	-	-		
56	OHX	BA	1767	-	0,6,6	0.00	-	-		
56	OHX	BA	1768	-	0,6,6	0.00	-	-		
56	OHX	BA	1769	-	0,6,6	0.00	-	-		
56	OHX	BA	1770	-	0,6,6	0.00	-	-		
56	OHX	BA	1771	-	0,6,6	0.00	-	-		
56	OHX	BA	1772	-	0,6,6	0.00	-	-		
56	OHX	BA	1773	-	0,6,6	0.00	-	-		
56	OHX	BA	1774	-	0,6,6	0.00	-	-		
56	OHX	BA	1775	-	0,6,6	0.00	-	-		
56	OHX	BA	1776	-	0,6,6	0.00	-	-		
56	OHX	BA	1777	-	0,6,6	0.00	-	-		
56	OHX	BA	1778	-	0,6,6	0.00	-	-		
56	OHX	BA	1779	-	0,6,6	0.00	-	-		
56	OHX	BA	1780	-	0,6,6	0.00	-	-		
56	OHX	BA	1781	-	0,6,6	0.00	-	-		
56	OHX	BA	1782	-	0,6,6	0.00	-	-		
56	OHX	BA	1783	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	BA	1784	-	0,6,6	0.00	-	-		
56	OHX	BA	1785	-	0,6,6	0.00	-	-		
56	OHX	BA	1786	-	0,6,6	0.00	-	-		
56	OHX	BA	1787	-	0,6,6	0.00	-	-		
56	OHX	BA	1788	-	0,6,6	0.00	-	-		
56	OHX	BA	1789	-	0,6,6	0.00	-	-		
56	OHX	BA	1790	-	0,6,6	0.00	-	-		
56	OHX	BA	1791	-	0,6,6	0.00	-	-		
56	OHX	BA	1792	-	0,6,6	0.00	-	-		
56	OHX	BA	1793	-	0,6,6	0.00	-	-		
56	OHX	BA	1794	-	0,6,6	0.00	-	-		
56	OHX	BA	1795	-	0,6,6	0.00	-	-		
56	OHX	BA	1796	-	0,6,6	0.00	-	-		
56	OHX	BA	1797	-	0,6,6	0.00	-	-		
56	OHX	BA	1798	-	0,6,6	0.00	-	-		
56	OHX	BA	1799	-	0,6,6	0.00	-	-		
56	OHX	BA	1800	-	0,6,6	0.00	-	-		
56	OHX	BA	1801	-	0,6,6	0.00	-	-		
56	OHX	BA	1802	-	0,6,6	0.00	-	-		
56	OHX	BA	1803	-	0,6,6	0.00	-	-		
56	OHX	BA	1804	-	0,6,6	0.00	-	-		
56	OHX	BA	1805	-	0,6,6	0.00	-	-		
56	OHX	BA	1806	-	0,6,6	0.00	-	-		
56	OHX	BA	1807	-	0,6,6	0.00	-	-		
56	OHX	BA	1808	-	0,6,6	0.00	-	-		
56	OHX	BA	1809	-	0,6,6	0.00	-	-		
56	OHX	BA	1810	-	0,6,6	0.00	-	-		
56	OHX	BA	1811	-	0,6,6	0.00	-	-		
56	OHX	BA	1812	-	0,6,6	0.00	-	-		
56	OHX	BA	1813	-	0,6,6	0.00	-	-		
56	OHX	BA	1814	-	0,6,6	0.00	-	-		
56	OHX	BA	1815	-	0,6,6	0.00	-	-		
56	OHX	BA	1816	-	0,6,6	0.00	-	-		
56	OHX	BB	106	-	0,6,6	0.00	-	-		
56	OHX	BB	107	-	0,6,6	0.00	-	-		
56	OHX	BC	106	-	0,6,6	0.00	-	-		
56	OHX	BC	107	-	0,6,6	0.00	-	-		
56	OHX	BD	102	-	0,6,6	0.00	-	-		
56	OHX	BD	103	-	0,6,6	0.00	-	-		
56	OHX	BD	104	-	0,6,6	0.00	-	-		
56	OHX	BG	302	-	0,6,6	0.00	-	-		
56	OHX	BR	101	-	0,6,6	0.00	-	-		
56	OHX	C1	201	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	C3	101	-	0,6,6	0.00	-	-		
56	OHX	C5	102	-	0,6,6	0.00	-	-		
56	OHX	C6	101	-	0,6,6	0.00	-	-		
56	OHX	CA	3232	-	0,6,6	0.00	-	-		
56	OHX	CA	3233	-	0,6,6	0.00	-	-		
56	OHX	CA	3234	-	0,6,6	0.00	-	-		
56	OHX	CA	3235	-	0,6,6	0.00	-	-		
56	OHX	CA	3236	-	0,6,6	0.00	-	-		
56	OHX	CA	3237	-	0,6,6	0.00	-	-		
56	OHX	CA	3238	-	0,6,6	0.00	-	-		
56	OHX	CA	3239	-	0,6,6	0.00	-	-		
56	OHX	CA	3240	-	0,6,6	0.00	-	-		
56	OHX	CA	3241	-	0,6,6	0.00	-	-		
56	OHX	CA	3242	-	0,6,6	0.00	-	-		
56	OHX	CA	3243	-	0,6,6	0.00	-	-		
56	OHX	CA	3244	-	0,6,6	0.00	-	-		
56	OHX	CA	3245	-	0,6,6	0.00	-	-		
56	OHX	CA	3246	-	0,6,6	0.00	-	-		
56	OHX	CA	3247	-	0,6,6	0.00	-	-		
56	OHX	CA	3248	-	0,6,6	0.00	-	-		
56	OHX	CA	3249	-	0,6,6	0.00	-	-		
56	OHX	CA	3250	-	0,6,6	0.00	-	-		
56	OHX	CA	3251	-	0,6,6	0.00	-	-		
56	OHX	CA	3252	-	0,6,6	0.00	-	-		
56	OHX	CA	3253	-	0,6,6	0.00	-	-		
56	OHX	CA	3254	-	0,6,6	0.00	-	-		
56	OHX	CA	3255	-	0,6,6	0.00	-	-		
56	OHX	CA	3256	-	0,6,6	0.00	-	-		
56	OHX	CA	3269	-	0,6,6	0.00	-	-		
56	OHX	CA	3270	-	0,6,6	0.00	-	-		
56	OHX	CA	3271	-	0,6,6	0.00	-	-		
56	OHX	CA	3272	-	0,6,6	0.00	-	-		
56	OHX	CA	3273	-	0,6,6	0.00	-	-		
56	OHX	CA	3274	-	0,6,6	0.00	-	-		
56	OHX	CA	3275	-	0,6,6	0.00	-	-		
56	OHX	CA	3276	-	0,6,6	0.00	-	-		
56	OHX	CA	3277	-	0,6,6	0.00	-	-		
56	OHX	CA	3278	-	0,6,6	0.00	-	-		
56	OHX	CA	3279	-	0,6,6	0.00	-	-		
56	OHX	CA	3280	-	0,6,6	0.00	-	-		
56	OHX	CA	3281	-	0,6,6	0.00	-	-		
56	OHX	CA	3282	-	0,6,6	0.00	-	-		
56	OHX	CA	3283	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3284	-	0,6,6	0.00	-	-		
56	OHX	CA	3285	-	0,6,6	0.00	-	-		
56	OHX	CA	3286	-	0,6,6	0.00	-	-		
56	OHX	CA	3287	-	0,6,6	0.00	-	-		
56	OHX	CA	3288	-	0,6,6	0.00	-	-		
56	OHX	CA	3289	-	0,6,6	0.00	-	-		
56	OHX	CA	3290	-	0,6,6	0.00	-	-		
56	OHX	CA	3291	-	0,6,6	0.00	-	-		
56	OHX	CA	3292	-	0,6,6	0.00	-	-		
56	OHX	CA	3293	-	0,6,6	0.00	-	-		
56	OHX	CA	3294	-	0,6,6	0.00	-	-		
56	OHX	CA	3295	-	0,6,6	0.00	-	-		
56	OHX	CA	3296	-	0,6,6	0.00	-	-		
56	OHX	CA	3297	-	0,6,6	0.00	-	-		
56	OHX	CA	3298	-	0,6,6	0.00	-	-		
56	OHX	CA	3299	-	0,6,6	0.00	-	-		
56	OHX	CA	3300	-	0,6,6	0.00	-	-		
56	OHX	CA	3301	-	0,6,6	0.00	-	-		
56	OHX	CA	3302	-	0,6,6	0.00	-	-		
56	OHX	CA	3303	-	0,6,6	0.00	-	-		
56	OHX	CA	3304	-	0,6,6	0.00	-	-		
56	OHX	CA	3305	-	0,6,6	0.00	-	-		
56	OHX	CA	3306	-	0,6,6	0.00	-	-		
56	OHX	CA	3307	-	0,6,6	0.00	-	-		
56	OHX	CA	3308	-	0,6,6	0.00	-	-		
56	OHX	CA	3309	-	0,6,6	0.00	-	-		
56	OHX	CA	3310	-	0,6,6	0.00	-	-		
56	OHX	CA	3311	-	0,6,6	0.00	-	-		
56	OHX	CA	3312	-	0,6,6	0.00	-	-		
56	OHX	CA	3313	-	0,6,6	0.00	-	-		
56	OHX	CA	3314	-	0,6,6	0.00	-	-		
56	OHX	CA	3315	-	0,6,6	0.00	-	-		
56	OHX	CA	3316	-	0,6,6	0.00	-	-		
56	OHX	CA	3317	-	0,6,6	0.00	-	-		
56	OHX	CA	3318	-	0,6,6	0.00	-	-		
56	OHX	CA	3319	-	0,6,6	0.00	-	-		
56	OHX	CA	3320	-	0,6,6	0.00	-	-		
56	OHX	CA	3321	-	0,6,6	0.00	-	-		
56	OHX	CA	3322	-	0,6,6	0.00	-	-		
56	OHX	CA	3323	-	0,6,6	0.00	-	-		
56	OHX	CA	3324	-	0,6,6	0.00	-	-		
56	OHX	CA	3325	-	0,6,6	0.00	-	-		
56	OHX	CA	3326	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3327	-	0,6,6	0.00	-	-		
56	OHX	CA	3328	-	0,6,6	0.00	-	-		
56	OHX	CA	3329	-	0,6,6	0.00	-	-		
56	OHX	CA	3330	-	0,6,6	0.00	-	-		
56	OHX	CA	3331	-	0,6,6	0.00	-	-		
56	OHX	CA	3332	-	0,6,6	0.00	-	-		
56	OHX	CA	3333	-	0,6,6	0.00	-	-		
56	OHX	CA	3334	-	0,6,6	0.00	-	-		
56	OHX	CA	3335	-	0,6,6	0.00	-	-		
56	OHX	CA	3336	-	0,6,6	0.00	-	-		
56	OHX	CA	3337	-	0,6,6	0.00	-	-		
56	OHX	CA	3338	-	0,6,6	0.00	-	-		
56	OHX	CA	3339	-	0,6,6	0.00	-	-		
56	OHX	CA	3340	-	0,6,6	0.00	-	-		
56	OHX	CA	3341	-	0,6,6	0.00	-	-		
56	OHX	CA	3342	-	0,6,6	0.00	-	-		
56	OHX	CA	3343	-	0,6,6	0.00	-	-		
56	OHX	CA	3344	-	0,6,6	0.00	-	-		
56	OHX	CA	3345	-	0,6,6	0.00	-	-		
56	OHX	CA	3346	-	0,6,6	0.00	-	-		
56	OHX	CA	3347	-	0,6,6	0.00	-	-		
56	OHX	CA	3348	-	0,6,6	0.00	-	-		
56	OHX	CA	3349	-	0,6,6	0.00	-	-		
56	OHX	CA	3350	-	0,6,6	0.00	-	-		
56	OHX	CA	3351	-	0,6,6	0.00	-	-		
56	OHX	CA	3352	-	0,6,6	0.00	-	-		
56	OHX	CA	3353	-	0,6,6	0.00	-	-		
56	OHX	CA	3354	-	0,6,6	0.00	-	-		
56	OHX	CA	3355	-	0,6,6	0.00	-	-		
56	OHX	CA	3356	-	0,6,6	0.00	-	-		
56	OHX	CA	3357	-	0,6,6	0.00	-	-		
56	OHX	CA	3358	-	0,6,6	0.00	-	-		
56	OHX	CA	3359	-	0,6,6	0.00	-	-		
56	OHX	CA	3360	-	0,6,6	0.00	-	-		
56	OHX	CA	3361	-	0,6,6	0.00	-	-		
56	OHX	CA	3362	-	0,6,6	0.00	-	-		
56	OHX	CA	3363	-	0,6,6	0.00	-	-		
56	OHX	CA	3364	-	0,6,6	0.00	-	-		
56	OHX	CA	3365	-	0,6,6	0.00	-	-		
56	OHX	CA	3366	-	0,6,6	0.00	-	-		
56	OHX	CA	3367	-	0,6,6	0.00	-	-		
56	OHX	CA	3368	-	0,6,6	0.00	-	-		
56	OHX	CA	3369	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3370	-	0,6,6	0.00	-	-		
56	OHX	CA	3371	-	0,6,6	0.00	-	-		
56	OHX	CA	3372	-	0,6,6	0.00	-	-		
56	OHX	CA	3373	-	0,6,6	0.00	-	-		
56	OHX	CA	3374	-	0,6,6	0.00	-	-		
56	OHX	CA	3375	-	0,6,6	0.00	-	-		
56	OHX	CA	3376	-	0,6,6	0.00	-	-		
56	OHX	CA	3377	-	0,6,6	0.00	-	-		
56	OHX	CA	3378	-	0,6,6	0.00	-	-		
56	OHX	CA	3379	-	0,6,6	0.00	-	-		
56	OHX	CA	3380	-	0,6,6	0.00	-	-		
56	OHX	CA	3381	-	0,6,6	0.00	-	-		
56	OHX	CA	3382	-	0,6,6	0.00	-	-		
56	OHX	CA	3383	-	0,6,6	0.00	-	-		
56	OHX	CA	3384	-	0,6,6	0.00	-	-		
56	OHX	CA	3385	-	0,6,6	0.00	-	-		
56	OHX	CA	3386	-	0,6,6	0.00	-	-		
56	OHX	CA	3387	-	0,6,6	0.00	-	-		
56	OHX	CA	3388	-	0,6,6	0.00	-	-		
56	OHX	CA	3389	-	0,6,6	0.00	-	-		
56	OHX	CA	3390	-	0,6,6	0.00	-	-		
56	OHX	CA	3391	-	0,6,6	0.00	-	-		
56	OHX	CA	3392	-	0,6,6	0.00	-	-		
56	OHX	CA	3393	-	0,6,6	0.00	-	-		
56	OHX	CA	3394	-	0,6,6	0.00	-	-		
56	OHX	CA	3395	-	0,6,6	0.00	-	-		
56	OHX	CA	3396	-	0,6,6	0.00	-	-		
56	OHX	CA	3397	-	0,6,6	0.00	-	-		
56	OHX	CA	3398	-	0,6,6	0.00	-	-		
56	OHX	CA	3399	-	0,6,6	0.00	-	-		
56	OHX	CA	3400	-	0,6,6	0.00	-	-		
56	OHX	CA	3401	-	0,6,6	0.00	-	-		
56	OHX	CA	3402	-	0,6,6	0.00	-	-		
56	OHX	CA	3403	-	0,6,6	0.00	-	-		
56	OHX	CA	3404	-	0,6,6	0.00	-	-		
56	OHX	CA	3405	-	0,6,6	0.00	-	-		
56	OHX	CA	3406	-	0,6,6	0.00	-	-		
56	OHX	CA	3407	-	0,6,6	0.00	-	-		
56	OHX	CA	3408	-	0,6,6	0.00	-	-		
56	OHX	CA	3409	-	0,6,6	0.00	-	-		
56	OHX	CA	3410	-	0,6,6	0.00	-	-		
56	OHX	CA	3411	-	0,6,6	0.00	-	-		
56	OHX	CA	3412	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3413	-	0,6,6	0.00	-	-		
56	OHX	CA	3414	-	0,6,6	0.00	-	-		
56	OHX	CA	3415	-	0,6,6	0.00	-	-		
56	OHX	CA	3416	-	0,6,6	0.00	-	-		
56	OHX	CA	3417	-	0,6,6	0.00	-	-		
56	OHX	CA	3418	-	0,6,6	0.00	-	-		
56	OHX	CA	3419	-	0,6,6	0.00	-	-		
56	OHX	CA	3420	-	0,6,6	0.00	-	-		
56	OHX	CA	3421	-	0,6,6	0.00	-	-		
56	OHX	CA	3422	-	0,6,6	0.00	-	-		
56	OHX	CA	3423	-	0,6,6	0.00	-	-		
56	OHX	CA	3424	-	0,6,6	0.00	-	-		
56	OHX	CA	3425	-	0,6,6	0.00	-	-		
56	OHX	CA	3426	-	0,6,6	0.00	-	-		
56	OHX	CA	3427	-	0,6,6	0.00	-	-		
56	OHX	CA	3428	-	0,6,6	0.00	-	-		
56	OHX	CA	3429	-	0,6,6	0.00	-	-		
56	OHX	CA	3430	-	0,6,6	0.00	-	-		
56	OHX	CA	3431	-	0,6,6	0.00	-	-		
56	OHX	CA	3432	-	0,6,6	0.00	-	-		
56	OHX	CA	3433	-	0,6,6	0.00	-	-		
56	OHX	CA	3434	-	0,6,6	0.00	-	-		
56	OHX	CA	3435	-	0,6,6	0.00	-	-		
56	OHX	CA	3436	-	0,6,6	0.00	-	-		
56	OHX	CA	3437	-	0,6,6	0.00	-	-		
56	OHX	CA	3438	-	0,6,6	0.00	-	-		
56	OHX	CA	3450	-	0,6,6	0.00	-	-		
56	OHX	CA	3461	-	0,6,6	0.00	-	-		
56	OHX	CA	3462	-	0,6,6	0.00	-	-		
56	OHX	CA	3463	-	0,6,6	0.00	-	-		
56	OHX	CA	3464	-	0,6,6	0.00	-	-		
56	OHX	CA	3465	-	0,6,6	0.00	-	-		
56	OHX	CA	3466	-	0,6,6	0.00	-	-		
56	OHX	CA	3467	-	0,6,6	0.00	-	-		
56	OHX	CA	3468	-	0,6,6	0.00	-	-		
56	OHX	CA	3469	-	0,6,6	0.00	-	-		
56	OHX	CA	3470	-	0,6,6	0.00	-	-		
56	OHX	CA	3481	-	0,6,6	0.00	-	-		
56	OHX	CA	3482	-	0,6,6	0.00	-	-		
56	OHX	CA	3483	-	0,6,6	0.00	-	-		
56	OHX	CA	3484	-	0,6,6	0.00	-	-		
56	OHX	CA	3485	-	0,6,6	0.00	-	-		
56	OHX	CA	3486	-	0,6,6	0.00	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	CA	3487	-	0,6,6	0.00	-	-		
56	OHX	CA	3488	-	0,6,6	0.00	-	-		
56	OHX	CA	3489	-	0,6,6	0.00	-	-		
56	OHX	CA	3490	-	0,6,6	0.00	-	-		
56	OHX	CA	3491	-	0,6,6	0.00	-	-		
56	OHX	CA	3492	-	0,6,6	0.00	-	-		
56	OHX	CB	208	-	0,6,6	0.00	-	-		
56	OHX	CB	209	-	0,6,6	0.00	-	-		
56	OHX	CB	210	-	0,6,6	0.00	-	-		
56	OHX	CB	211	-	0,6,6	0.00	-	-		
56	OHX	CB	212	-	0,6,6	0.00	-	-		
56	OHX	CB	213	-	0,6,6	0.00	-	-		
56	OHX	CB	214	-	0,6,6	0.00	-	-		
56	OHX	CB	215	-	0,6,6	0.00	-	-		
56	OHX	CB	216	-	0,6,6	0.00	-	-		
56	OHX	CB	217	-	0,6,6	0.00	-	-		
56	OHX	CB	218	-	0,6,6	0.00	-	-		
56	OHX	CB	219	-	0,6,6	0.00	-	-		
56	OHX	CB	220	-	0,6,6	0.00	-	-		
56	OHX	CF	301	-	0,6,6	0.00	-	-		
56	OHX	CO	201	-	0,6,6	0.00	-	-		
56	OHX	DA	1718	-	0,6,6	0.00	-	-		
56	OHX	DA	1719	-	0,6,6	0.00	-	-		
56	OHX	DA	1721	-	0,6,6	0.00	-	-		
56	OHX	DA	1722	-	0,6,6	0.00	-	-		
56	OHX	DA	1723	-	0,6,6	0.00	-	-		
56	OHX	DA	1724	-	0,6,6	0.00	-	-		
56	OHX	DA	1726	-	0,6,6	0.00	-	-		
56	OHX	DA	1727	-	0,6,6	0.00	-	-		
56	OHX	DA	1728	-	0,6,6	0.00	-	-		
56	OHX	DA	1729	-	0,6,6	0.00	-	-		
56	OHX	DA	1730	-	0,6,6	0.00	-	-		
56	OHX	DA	1731	-	0,6,6	0.00	-	-		
56	OHX	DA	1732	-	0,6,6	0.00	-	-		
56	OHX	DA	1733	-	0,6,6	0.00	-	-		
56	OHX	DA	1734	-	0,6,6	0.00	-	-		
56	OHX	DA	1735	-	0,6,6	0.00	-	-		
56	OHX	DA	1736	-	0,6,6	0.00	-	-		
56	OHX	DA	1737	-	0,6,6	0.00	-	-		
56	OHX	DA	1738	-	0,6,6	0.00	-	-		
56	OHX	DA	1739	-	0,6,6	0.00	-	-		
56	OHX	DA	1740	-	0,6,6	0.00	-	-		
56	OHX	DA	1741	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	DA	1742	-	0,6,6	0.00	-	-		
56	OHX	DA	1743	-	0,6,6	0.00	-	-		
56	OHX	DA	1744	-	0,6,6	0.00	-	-		
56	OHX	DA	1745	-	0,6,6	0.00	-	-		
56	OHX	DA	1746	-	0,6,6	0.00	-	-		
56	OHX	DA	1747	-	0,6,6	0.00	-	-		
56	OHX	DA	1748	-	0,6,6	0.00	-	-		
56	OHX	DA	1749	-	0,6,6	0.00	-	-		
56	OHX	DA	1750	-	0,6,6	0.00	-	-		
56	OHX	DA	1751	-	0,6,6	0.00	-	-		
56	OHX	DA	1752	-	0,6,6	0.00	-	-		
56	OHX	DA	1753	-	0,6,6	0.00	-	-		
56	OHX	DA	1754	-	0,6,6	0.00	-	-		
56	OHX	DA	1755	-	0,6,6	0.00	-	-		
56	OHX	DA	1756	-	0,6,6	0.00	-	-		
56	OHX	DA	1757	-	0,6,6	0.00	-	-		
56	OHX	DA	1758	-	0,6,6	0.00	-	-		
56	OHX	DA	1759	-	0,6,6	0.00	-	-		
56	OHX	DA	1760	-	0,6,6	0.00	-	-		
56	OHX	DA	1761	-	0,6,6	0.00	-	-		
56	OHX	DA	1762	-	0,6,6	0.00	-	-		
56	OHX	DA	1763	-	0,6,6	0.00	-	-		
56	OHX	DA	1764	-	0,6,6	0.00	-	-		
56	OHX	DA	1765	-	0,6,6	0.00	-	-		
56	OHX	DA	1766	-	0,6,6	0.00	-	-		
56	OHX	DA	1767	-	0,6,6	0.00	-	-		
56	OHX	DA	1768	-	0,6,6	0.00	-	-		
56	OHX	DA	1769	-	0,6,6	0.00	-	-		
56	OHX	DA	1770	-	0,6,6	0.00	-	-		
56	OHX	DA	1771	-	0,6,6	0.00	-	-		
56	OHX	DA	1772	-	0,6,6	0.00	-	-		
56	OHX	DA	1773	-	0,6,6	0.00	-	-		
56	OHX	DA	1774	-	0,6,6	0.00	-	-		
56	OHX	DA	1775	-	0,6,6	0.00	-	-		
56	OHX	DA	1776	-	0,6,6	0.00	-	-		
56	OHX	DA	1777	-	0,6,6	0.00	-	-		
56	OHX	DA	1778	-	0,6,6	0.00	-	-		
56	OHX	DA	1779	-	0,6,6	0.00	-	-		
56	OHX	DA	1780	-	0,6,6	0.00	-	-		
56	OHX	DA	1781	-	0,6,6	0.00	-	-		
56	OHX	DA	1782	-	0,6,6	0.00	-	-		
56	OHX	DA	1783	-	0,6,6	0.00	-	-		
56	OHX	DA	1784	-	0,6,6	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	OHX	DA	1785	-	0,6,6	0.00	-	-		
56	OHX	DA	1786	-	0,6,6	0.00	-	-		
56	OHX	DA	1787	-	0,6,6	0.00	-	-		
56	OHX	DA	1788	-	0,6,6	0.00	-	-		
56	OHX	DA	1789	-	0,6,6	0.00	-	-		
56	OHX	DA	1790	-	0,6,6	0.00	-	-		
56	OHX	DA	1791	-	0,6,6	0.00	-	-		
56	OHX	DA	1792	-	0,6,6	0.00	-	-		
56	OHX	DA	1793	-	0,6,6	0.00	-	-		
56	OHX	DA	1794	-	0,6,6	0.00	-	-		
56	OHX	DA	1795	-	0,6,6	0.00	-	-		
56	OHX	DA	1796	-	0,6,6	0.00	-	-		
56	OHX	DA	1797	-	0,6,6	0.00	-	-		
56	OHX	DA	1798	-	0,6,6	0.00	-	-		
56	OHX	DA	1799	-	0,6,6	0.00	-	-		
56	OHX	DA	1800	-	0,6,6	0.00	-	-		
56	OHX	DA	1801	-	0,6,6	0.00	-	-		
56	OHX	DA	1802	-	0,6,6	0.00	-	-		
56	OHX	DA	1803	-	0,6,6	0.00	-	-		
56	OHX	DA	1804	-	0,6,6	0.00	-	-		
56	OHX	DA	1805	-	0,6,6	0.00	-	-		
56	OHX	DA	1806	-	0,6,6	0.00	-	-		
56	OHX	DA	1807	-	0,6,6	0.00	-	-		
56	OHX	DA	1808	-	0,6,6	0.00	-	-		
56	OHX	DA	1809	-	0,6,6	0.00	-	-		
56	OHX	DA	1810	-	0,6,6	0.00	-	-		
56	OHX	DA	1811	-	0,6,6	0.00	-	-		
56	OHX	DA	1812	-	0,6,6	0.00	-	-		
56	OHX	DB	103	-	0,6,6	0.00	-	-		
56	OHX	DB	104	-	0,6,6	0.00	-	-		
56	OHX	DB	105	-	0,6,6	0.00	-	-		
56	OHX	DC	107	-	0,6,6	0.00	-	-		
56	OHX	DC	108	-	0,6,6	0.00	-	-		
56	OHX	DC	109	-	0,6,6	0.00	-	-		
56	OHX	DC	110	-	0,6,6	0.00	-	-		
56	OHX	DD	101	-	0,6,6	0.00	-	-		
56	OHX	DG	302	-	0,6,6	0.00	-	-		
56	OHX	DK	201	-	0,6,6	0.00	-	-		
56	OHX	DR	101	-	0,6,6	0.00	-	-		
56	OHX	DV	101	-	0,6,6	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	AA	2912/2912 (100%)	-0.21	50 (1%) 70 68	45, 76, 209, 243	0
1	CA	2907/2912 (99%)	-0.39	42 (1%) 75 74	58, 92, 230, 245	0
2	AB	122/122 (100%)	-0.35	2 (1%) 72 70	73, 95, 116, 177	0
2	CB	122/122 (100%)	-0.59	1 (0%) 86 86	92, 127, 146, 198	0
3	AD	272/276 (98%)	-0.02	2 (0%) 87 88	39, 66, 84, 105	0
3	CD	272/276 (98%)	0.16	5 (1%) 68 67	55, 78, 96, 128	0
4	AE	205/206 (99%)	0.74	29 (14%) 2 2	51, 86, 130, 142	0
4	CE	205/206 (99%)	0.51	18 (8%) 10 11	64, 100, 148, 165	0
5	AF	202/210 (96%)	0.08	6 (2%) 50 50	47, 81, 118, 130	0
5	CF	208/210 (99%)	0.41	18 (8%) 10 11	62, 106, 160, 184	0
6	AG	181/182 (99%)	0.63	17 (9%) 8 9	84, 107, 138, 149	0
6	CG	181/182 (99%)	0.67	21 (11%) 4 4	120, 141, 164, 171	0
7	AH	170/180 (94%)	0.32	7 (4%) 37 36	86, 112, 130, 157	0
7	CH	170/180 (94%)	3.33	117 (68%) 0 0	155, 198, 220, 229	0
8	AK	146/148 (98%)	0.56	17 (11%) 4 4	79, 131, 147, 150	0
8	CK	146/148 (98%)	0.60	17 (11%) 4 4	84, 130, 152, 158	0
9	AM	138/140 (98%)	0.47	8 (5%) 23 23	66, 87, 124, 136	0
9	CM	138/140 (98%)	1.15	28 (20%) 1 1	83, 114, 140, 156	0
10	AN	122/122 (100%)	0.21	2 (1%) 72 70	57, 78, 93, 101	0
10	CN	122/122 (100%)	0.32	4 (3%) 46 45	75, 95, 111, 124	0
11	AO	150/150 (100%)	0.00	6 (4%) 38 37	48, 88, 117, 160	0
11	CO	150/150 (100%)	1.15	37 (24%) 0 0	45, 108, 146, 178	0
12	AP	141/141 (100%)	0.39	6 (4%) 35 35	58, 83, 105, 127	0
12	CP	141/141 (100%)	0.65	19 (13%) 3 3	58, 109, 140, 159	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	A0	118/118 (100%)	0.42	2 (1%) 70 68	61, 81, 103, 113	0
13	C0	117/118 (99%)	0.03	0 100 100	69, 87, 106, 121	0
14	AQ	111/112 (99%)	0.36	4 (3%) 42 41	70, 92, 117, 131	0
14	CQ	111/112 (99%)	-0.15	3 (2%) 54 53	86, 123, 147, 162	0
15	AR	137/146 (93%)	0.78	14 (10%) 7 7	73, 93, 143, 170	0
15	CR	137/146 (93%)	0.27	11 (8%) 12 13	84, 104, 163, 183	0
16	A1	117/118 (99%)	0.07	2 (1%) 70 68	52, 75, 108, 139	0
16	C1	117/118 (99%)	0.81	20 (17%) 1 1	67, 106, 143, 162	0
17	A2	101/101 (100%)	0.95	16 (15%) 2 2	53, 98, 122, 141	0
17	C2	101/101 (100%)	1.58	32 (31%) 0 0	67, 129, 142, 151	0
18	AS	113/113 (100%)	0.46	5 (4%) 34 34	54, 73, 104, 156	0
18	CS	113/113 (100%)	0.02	2 (1%) 68 67	64, 80, 114, 158	0
19	AT	92/96 (95%)	0.15	4 (4%) 35 35	57, 71, 95, 107	0
19	CT	92/96 (95%)	0.19	3 (3%) 46 45	74, 88, 113, 127	0
20	AU	102/110 (92%)	0.81	17 (16%) 1 1	74, 101, 152, 162	0
20	CU	102/110 (92%)	0.64	15 (14%) 2 2	95, 118, 166, 181	0
21	AV	175/206 (84%)	1.67	51 (29%) 0 0	87, 126, 188, 191	0
21	CV	179/206 (86%)	1.77	69 (38%) 0 0	122, 160, 208, 216	0
22	A3	76/85 (89%)	0.04	1 (1%) 77 77	59, 77, 91, 132	0
22	C3	77/85 (90%)	-0.07	1 (1%) 77 77	83, 95, 117, 147	0
23	AZ	97/98 (98%)	0.17	7 (7%) 15 17	58, 78, 126, 156	0
23	CZ	97/98 (98%)	0.33	5 (5%) 27 26	68, 86, 132, 155	0
24	AW	66/72 (91%)	0.36	1 (1%) 73 71	63, 84, 98, 125	0
24	CW	66/72 (91%)	0.40	3 (4%) 33 33	84, 107, 130, 139	0
25	AX	59/60 (98%)	0.16	1 (1%) 70 68	63, 83, 112, 130	0
25	CX	59/60 (98%)	1.02	12 (20%) 1 1	80, 110, 141, 162	0
26	A4	66/71 (92%)	2.07	30 (45%) 0 0	120, 156, 173, 179	0
26	C4	63/71 (88%)	3.34	47 (74%) 0 0	146, 185, 194, 199	0
27	A5	59/60 (98%)	1.32	12 (20%) 1 1	49, 88, 168, 171	0
27	C5	59/60 (98%)	0.56	12 (20%) 1 1	65, 92, 173, 187	0
28	A6	45/54 (83%)	5.50	42 (93%) 0 0	124, 151, 168, 177	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C6	45/54 (83%)	2.85	25 (55%) 0 0	141, 169, 183, 186	0
29	A7	45/49 (91%)	-0.30	0 100 100	47, 55, 69, 78	0
29	C7	45/49 (91%)	-0.26	0 100 100	56, 66, 77, 100	0
30	A8	60/65 (92%)	0.25	1 (1%) 70 68	55, 73, 90, 114	0
30	C8	60/65 (92%)	0.51	1 (1%) 70 68	78, 90, 112, 137	0
31	BA	1502/1506 (99%)	-0.46	10 (0%) 87 88	58, 107, 187, 244	0
31	DA	1502/1506 (99%)	-0.56	11 (0%) 87 88	71, 119, 189, 244	0
32	BE	237/256 (92%)	0.64	20 (8%) 11 12	111, 144, 182, 193	0
32	DE	237/256 (92%)	0.64	29 (12%) 4 4	126, 161, 196, 211	0
33	BF	205/239 (85%)	0.57	16 (7%) 13 13	96, 119, 152, 160	0
33	DF	206/239 (86%)	1.16	47 (22%) 0 1	127, 147, 175, 180	0
34	BG	208/208 (100%)	-0.08	3 (1%) 75 74	92, 116, 136, 147	0
34	DG	208/208 (100%)	-0.04	5 (2%) 59 56	93, 111, 132, 145	0
35	BH	151/162 (93%)	0.19	4 (2%) 56 54	81, 105, 127, 161	0
35	DH	151/162 (93%)	-0.01	3 (1%) 65 64	104, 121, 142, 165	0
36	BI	101/101 (100%)	-0.10	1 (0%) 82 82	81, 108, 122, 145	0
36	DI	101/101 (100%)	0.30	0 100 100	81, 106, 124, 149	0
37	BJ	155/156 (99%)	0.67	19 (12%) 4 4	106, 121, 149, 158	0
37	DJ	155/156 (99%)	0.38	5 (3%) 47 46	113, 131, 153, 164	0
38	BK	138/138 (100%)	-0.10	1 (0%) 87 88	89, 110, 123, 129	0
38	DK	138/138 (100%)	-0.09	0 100 100	104, 125, 136, 146	0
39	BL	127/128 (99%)	0.47	12 (9%) 8 9	87, 142, 160, 169	0
39	DL	127/128 (99%)	0.11	4 (3%) 49 48	117, 155, 168, 174	0
40	BM	99/105 (94%)	0.45	6 (6%) 21 21	91, 142, 170, 174	0
40	DM	99/105 (94%)	0.44	10 (10%) 7 7	124, 159, 175, 179	0
41	BN	119/129 (92%)	0.89	14 (11%) 4 4	72, 104, 133, 161	0
41	DN	119/129 (92%)	0.70	14 (11%) 4 4	91, 112, 139, 167	0
42	BO	125/132 (94%)	0.34	6 (4%) 30 30	69, 83, 112, 158	0
42	DO	125/132 (94%)	0.66	12 (9%) 8 9	93, 110, 134, 166	0
43	BP	116/126 (92%)	0.15	3 (2%) 56 54	92, 128, 145, 153	0
43	DP	117/126 (92%)	0.25	4 (3%) 45 44	106, 156, 169, 171	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	58/61 (95%)	-0.07	0 <span>100</span> <span>100</span>	91, 108, 122, 129	0
44	DQ	58/61 (95%)	0.91	9 (15%) <span>2</span> <span>2</span>	126, 140, 157, 160	0
45	BR	88/89 (98%)	-0.31	0 <span>100</span> <span>100</span>	80, 100, 121, 125	0
45	DR	88/89 (98%)	-0.11	0 <span>100</span> <span>100</span>	85, 112, 133, 140	0
46	BS	84/88 (95%)	-0.14	1 (1%) <span>79</span> <span>78</span>	100, 118, 139, 175	0
46	DS	84/88 (95%)	-0.12	0 <span>100</span> <span>100</span>	96, 107, 127, 158	0
47	BT	100/105 (95%)	-0.24	1 (1%) <span>82</span> <span>82</span>	93, 112, 125, 133	0
47	DT	100/105 (95%)	0.07	3 (3%) <span>50</span> <span>50</span>	94, 114, 135, 143	0
48	BU	72/88 (81%)	0.14	4 (5%) <span>24</span> <span>23</span>	88, 106, 139, 164	0
48	DU	72/88 (81%)	0.39	7 (9%) <span>8</span> <span>8</span>	97, 114, 155, 169	0
49	BV	78/93 (83%)	0.31	4 (5%) <span>28</span> <span>27</span>	109, 130, 147, 152	0
49	DV	78/93 (83%)	0.33	5 (6%) <span>19</span> <span>20</span>	145, 163, 182, 185	0
50	BW	99/106 (93%)	0.34	8 (8%) <span>12</span> <span>12</span>	105, 124, 155, 160	0
50	DW	99/106 (93%)	0.21	4 (4%) <span>38</span> <span>37</span>	95, 117, 153, 163	0
51	BX	25/27 (92%)	-0.58	0 <span>100</span> <span>100</span>	102, 117, 137, 154	0
51	DX	25/27 (92%)	-0.45	0 <span>100</span> <span>100</span>	122, 143, 158, 168	0
52	BB	84/85 (98%)	0.58	11 (13%) <span>3</span> <span>3</span>	82, 123, 154, 169	0
52	BD	84/85 (98%)	-0.22	3 (3%) <span>42</span> <span>41</span>	75, 137, 217, 227	0
52	DB	84/85 (98%)	0.58	11 (13%) <span>3</span> <span>3</span>	93, 128, 156, 171	0
52	DD	84/85 (98%)	-0.47	2 (2%) <span>59</span> <span>56</span>	84, 137, 217, 225	0
53	BC	77/77 (100%)	-0.36	0 <span>100</span> <span>100</span>	77, 114, 139, 153	0
53	DC	77/77 (100%)	-0.74	0 <span>100</span> <span>100</span>	88, 122, 150, 157	0
54	B1	16/16 (100%)	0.05	1 (6%) <span>20</span> <span>20</span>	76, 104, 156, 163	0
54	D1	16/16 (100%)	-0.45	0 <span>100</span> <span>100</span>	85, 109, 157, 165	0
All	All	21100/21658 (97%)	0.12	1283 (6%) <span>21</span> <span>21</span>	39, 105, 182, 245	0

The worst 5 of 1283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CH	99	VAL	15.9
1	CA	690	A	14.9
1	CA	691	C	13.0
42	BO	126	ALA	12.9
1	CA	689	C	12.4



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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
52	MIA	BD	38	29/30	0.85	0.25	116,135,182,198	0
52	MIA	DD	38	29/30	0.88	0.20	120,140,186,205	0
52	MIA	DB	38	29/30	0.90	0.21	84,93,111,126	0
52	MIA	BB	38	29/30	0.95	0.18	68,83,97,106	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	MG	CA	3457	1/1	0.31	0.32	66,66,66,66	0
55	MG	DA	1720	1/1	0.31	0.48	105,105,105,105	0
55	MG	BA	1751	1/1	0.42	0.48	95,95,95,95	0
55	MG	BA	1648	1/1	0.43	0.49	99,99,99,99	0
55	MG	BC	102	1/1	0.49	0.21	68,68,68,68	0
55	MG	BA	1699	1/1	0.55	0.43	79,79,79,79	0
55	MG	DA	1708	1/1	0.55	0.46	87,87,87,87	0
55	MG	DA	1696	1/1	0.57	0.21	112,112,112,112	0
55	MG	CA	3034	1/1	0.59	0.36	91,91,91,91	0
55	MG	BA	1746	1/1	0.60	0.40	82,82,82,82	0
55	MG	AA	3165	1/1	0.60	0.57	84,84,84,84	0
55	MG	AA	3221	1/1	0.61	0.25	68,68,68,68	0
55	MG	DA	1628	1/1	0.61	0.47	78,78,78,78	0
55	MG	DA	1710	1/1	0.62	0.20	103,103,103,103	0
55	MG	CA	3136	1/1	0.62	0.42	91,91,91,91	0
55	MG	CA	3187	1/1	0.62	0.41	86,86,86,86	0
55	MG	DA	1617	1/1	0.63	0.23	115,115,115,115	0
55	MG	AA	3105	1/1	0.64	0.44	124,124,124,124	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3190	1/1	0.64	0.40	69,69,69,69	0
55	MG	DA	1715	1/1	0.64	0.28	89,89,89,89	0
55	MG	BA	1618	1/1	0.64	0.39	63,63,63,63	0
55	MG	CA	3027	1/1	0.64	0.35	81,81,81,81	0
55	MG	AA	3137	1/1	0.64	0.49	51,51,51,51	0
55	MG	DA	1725	1/1	0.65	0.41	87,87,87,87	0
55	MG	DC	103	1/1	0.65	0.29	96,96,96,96	0
55	MG	D1	101	1/1	0.66	0.36	78,78,78,78	0
55	MG	AA	3087	1/1	0.67	0.51	83,83,83,83	0
55	MG	CA	3046	1/1	0.67	0.26	76,76,76,76	0
55	MG	DA	1624	1/1	0.67	0.10	73,73,73,73	0
55	MG	CA	3088	1/1	0.68	0.39	86,86,86,86	0
55	MG	BA	1710	1/1	0.68	0.51	97,97,97,97	0
55	MG	CA	3110	1/1	0.68	0.39	85,85,85,85	0
55	MG	AA	3397	1/1	0.68	0.18	80,80,80,80	0
55	MG	DA	1698	1/1	0.68	0.50	95,95,95,95	0
55	MG	DA	1641	1/1	0.68	0.42	130,130,130,130	0
55	MG	CA	3213	1/1	0.69	0.23	121,121,121,121	0
55	MG	AA	3095	1/1	0.70	0.39	89,89,89,89	0
56	OHX	BA	1686	7/7	0.70	0.17	141,143,153,230	1
55	MG	AA	3015	1/1	0.70	0.43	76,76,76,76	0
55	MG	BA	1628	1/1	0.70	0.36	80,80,80,80	0
55	MG	AA	3248	1/1	0.70	0.39	86,86,86,86	0
55	MG	CA	3222	1/1	0.70	0.21	81,81,81,81	0
55	MG	AA	3009	1/1	0.71	0.42	89,89,89,89	0
55	MG	AA	3220	1/1	0.71	0.48	64,64,64,64	0
55	MG	CA	3085	1/1	0.72	0.32	102,102,102,102	0
55	MG	BA	1703	1/1	0.72	0.50	108,108,108,108	0
55	MG	DA	1701	1/1	0.72	0.41	90,90,90,90	0
55	MG	DA	1681	1/1	0.72	0.32	100,100,100,100	0
55	MG	DA	1643	1/1	0.72	0.34	136,136,136,136	0
55	MG	BA	1601	1/1	0.73	0.22	81,81,81,81	0
55	MG	CA	3164	1/1	0.73	0.47	97,97,97,97	0
55	MG	AA	3044	1/1	0.73	0.53	72,72,72,72	0
55	MG	CA	3215	1/1	0.73	0.30	137,137,137,137	0
55	MG	CA	3198	1/1	0.74	0.30	118,118,118,118	0
55	MG	BA	1730	1/1	0.74	0.55	73,73,73,73	0
56	OHX	DA	1812	7/7	0.74	0.13	149,158,168,252	1
55	MG	DA	1634	1/1	0.74	0.10	118,118,118,118	0
55	MG	BA	1744	1/1	0.74	0.19	90,90,90,90	0
55	MG	CA	3455	1/1	0.74	0.41	97,97,97,97	0
55	MG	BB	104	1/1	0.74	0.50	87,87,87,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3208	1/1	0.75	0.37	65,65,65,65	0
55	MG	CB	204	1/1	0.75	0.38	73,73,73,73	0
55	MG	DA	1706	1/1	0.75	0.17	100,100,100,100	0
55	MG	AA	3068	1/1	0.75	0.26	61,61,61,61	0
55	MG	DA	1632	1/1	0.76	0.27	83,83,83,83	0
55	MG	BA	1727	1/1	0.76	0.43	70,70,70,70	0
55	MG	AA	3354	1/1	0.76	0.39	57,57,57,57	0
55	MG	AA	3107	1/1	0.76	0.44	79,79,79,79	0
55	MG	AA	3100	1/1	0.76	0.38	108,108,108,108	0
55	MG	DA	1688	1/1	0.76	0.34	101,101,101,101	0
55	MG	CA	3042	1/1	0.76	0.27	67,67,67,67	0
55	MG	DA	1714	1/1	0.76	0.33	97,97,97,97	0
55	MG	AA	3132	1/1	0.76	0.51	81,81,81,81	0
55	MG	DA	1630	1/1	0.76	0.34	95,95,95,95	0
55	MG	BA	1631	1/1	0.76	0.30	78,78,78,78	0
55	MG	AA	3108	1/1	0.77	0.31	82,82,82,82	0
55	MG	DA	1621	1/1	0.77	0.32	98,98,98,98	0
55	MG	CA	3192	1/1	0.77	0.26	87,87,87,87	0
55	MG	CA	3038	1/1	0.77	0.17	74,74,74,74	0
55	MG	AA	3048	1/1	0.77	0.61	94,94,94,94	0
55	MG	AA	3024	1/1	0.77	0.38	63,63,63,63	0
55	MG	BA	1627	1/1	0.77	0.40	80,80,80,80	0
55	MG	AA	3052	1/1	0.77	0.47	85,85,85,85	0
55	MG	DA	1622	1/1	0.77	0.20	122,122,122,122	0
55	MG	CA	3220	1/1	0.77	0.30	85,85,85,85	0
55	MG	AA	3284	1/1	0.77	0.36	66,66,66,66	0
55	MG	BA	1646	1/1	0.77	0.40	95,95,95,95	0
55	MG	CA	3079	1/1	0.77	0.29	73,73,73,73	0
55	MG	DA	1661	1/1	0.77	0.41	76,76,76,76	0
55	MG	AA	3079	1/1	0.78	0.40	88,88,88,88	0
55	MG	DA	1695	1/1	0.78	0.51	76,76,76,76	0
55	MG	BA	1748	1/1	0.78	0.23	66,66,66,66	0
55	MG	DA	1631	1/1	0.78	0.47	111,111,111,111	0
55	MG	AA	3059	1/1	0.78	0.57	85,85,85,85	0
56	OHX	BA	1669	7/7	0.78	0.18	124,127,142,200	1
55	MG	CA	3477	1/1	0.78	0.42	60,60,60,60	0
55	MG	DA	1673	1/1	0.78	0.35	80,80,80,80	0
55	MG	CA	3441	1/1	0.78	0.34	99,99,99,99	0
55	MG	BA	1718	1/1	0.78	0.23	78,78,78,78	0
55	MG	CA	3057	1/1	0.78	0.36	95,95,95,95	0
55	MG	CA	3206	1/1	0.78	0.46	90,90,90,90	0
55	MG	BA	1711	1/1	0.78	0.50	94,94,94,94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3179	1/1	0.78	0.12	73,73,73,73	0
55	MG	DA	1660	1/1	0.79	0.48	88,88,88,88	0
55	MG	DB	101	1/1	0.79	0.42	78,78,78,78	0
55	MG	DA	1702	1/1	0.79	0.20	122,122,122,122	0
55	MG	DA	1629	1/1	0.79	0.22	93,93,93,93	0
55	MG	AA	3224	1/1	0.79	0.55	68,68,68,68	0
55	MG	BA	1720	1/1	0.79	0.51	58,58,58,58	0
55	MG	CA	3223	1/1	0.79	0.39	88,88,88,88	0
55	MG	CA	3202	1/1	0.79	0.49	79,79,79,79	0
55	MG	AA	3282	1/1	0.79	0.37	69,69,69,69	0
55	MG	DA	1642	1/1	0.79	0.45	112,112,112,112	0
55	MG	AA	3264	1/1	0.79	0.42	76,76,76,76	0
55	MG	CA	3037	1/1	0.79	0.35	89,89,89,89	0
55	MG	AA	3092	1/1	0.79	0.17	73,73,73,73	0
55	MG	AA	3199	1/1	0.79	0.64	76,76,76,76	0
55	MG	AA	3076	1/1	0.80	0.42	72,72,72,72	0
55	MG	DA	1717	1/1	0.80	0.26	100,100,100,100	0
55	MG	DA	1682	1/1	0.80	0.57	87,87,87,87	0
55	MG	AA	3035	1/1	0.80	0.57	64,64,64,64	0
55	MG	BA	1604	1/1	0.80	0.42	72,72,72,72	0
55	MG	BA	1611	1/1	0.80	0.35	84,84,84,84	0
55	MG	AA	3174	1/1	0.80	0.49	76,76,76,76	0
55	MG	BA	1705	1/1	0.80	0.29	63,63,63,63	0
55	MG	BC	105	1/1	0.80	0.47	87,87,87,87	0
55	MG	DA	1659	1/1	0.80	0.25	89,89,89,89	0
55	MG	AA	3135	1/1	0.80	0.30	67,67,67,67	0
55	MG	AA	3347	1/1	0.80	0.46	70,70,70,70	0
55	MG	AA	3026	1/1	0.81	0.44	92,92,92,92	0
55	MG	BA	1635	1/1	0.81	0.23	96,96,96,96	0
55	MG	AA	3150	1/1	0.81	0.41	68,68,68,68	0
55	MG	DA	1674	1/1	0.81	0.30	99,99,99,99	0
55	MG	CA	3201	1/1	0.81	0.51	79,79,79,79	0
55	MG	AA	3017	1/1	0.81	0.49	100,100,100,100	0
55	MG	DA	1623	1/1	0.81	0.47	124,124,124,124	0
55	MG	DA	1675	1/1	0.81	0.37	92,92,92,92	0
55	MG	AA	3091	1/1	0.81	0.19	77,77,77,77	0
55	MG	CA	3129	1/1	0.81	0.60	81,81,81,81	0
55	MG	AA	3275	1/1	0.81	0.42	64,64,64,64	0
55	MG	BA	1702	1/1	0.82	0.27	62,62,62,62	0
55	MG	AA	3231	1/1	0.82	0.48	66,66,66,66	0
55	MG	CA	3095	1/1	0.82	0.26	54,54,54,54	0
56	OHX	CB	218	7/7	0.82	0.12	141,159,166,235	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BS	101	1/1	0.82	0.32	93,93,93,93	0
55	MG	CA	3140	1/1	0.82	0.37	59,59,59,59	0
55	MG	CA	3178	1/1	0.82	0.28	52,52,52,52	0
55	MG	A1	201	1/1	0.82	0.28	71,71,71,71	0
55	MG	AA	3271	1/1	0.82	0.14	39,39,39,39	0
55	MG	CA	3196	1/1	0.82	0.52	92,92,92,92	0
55	MG	CA	3217	1/1	0.82	0.37	58,58,58,58	0
55	MG	AA	3260	1/1	0.82	0.52	58,58,58,58	0
55	MG	CA	3005	1/1	0.82	0.21	48,48,48,48	0
56	OHX	BA	1657	7/7	0.82	0.19	116,125,141,215	1
55	MG	AA	3121	1/1	0.82	0.42	53,53,53,53	0
55	MG	BA	1615	1/1	0.82	0.26	113,113,113,113	0
56	OHX	DB	104	7/7	0.82	0.16	129,133,143,205	2
55	MG	AA	3245	1/1	0.83	0.27	68,68,68,68	0
55	MG	DC	105	1/1	0.83	0.51	54,54,54,54	0
55	MG	AA	3234	1/1	0.83	0.14	56,56,56,56	0
55	MG	CA	3207	1/1	0.83	0.29	68,68,68,68	0
55	MG	DA	1667	1/1	0.83	0.42	68,68,68,68	0
55	MG	CA	3228	1/1	0.83	0.09	65,65,65,65	0
55	MG	CA	3033	1/1	0.83	0.26	71,71,71,71	0
55	MG	DA	1635	1/1	0.83	0.41	96,96,96,96	0
55	MG	DA	1694	1/1	0.83	0.38	104,104,104,104	0
55	MG	BA	1734	1/1	0.83	0.44	70,70,70,70	0
55	MG	AA	3077	1/1	0.83	0.29	73,73,73,73	0
55	MG	CA	3114	1/1	0.83	0.45	57,57,57,57	0
56	OHX	CA	3407	7/7	0.83	0.12	142,149,155,227	1
55	MG	BA	1712	1/1	0.83	0.56	95,95,95,95	0
56	OHX	DA	1786	7/7	0.83	0.14	143,151,161,223	1
55	MG	CA	3137	1/1	0.83	0.43	74,74,74,74	0
55	MG	CA	3107	1/1	0.83	0.24	82,82,82,82	0
55	MG	DA	1707	1/1	0.83	0.45	85,85,85,85	0
55	MG	BA	1704	1/1	0.83	0.24	88,88,88,88	0
55	MG	AA	3097	1/1	0.83	0.23	59,59,59,59	0
56	OHX	CA	3419	7/7	0.83	0.13	153,156,164,238	1
55	MG	CA	3119	1/1	0.83	0.28	61,61,61,61	0
56	OHX	DA	1794	7/7	0.84	0.14	124,130,139,205	1
55	MG	BA	1658	1/1	0.84	0.41	71,71,71,71	0
55	MG	CA	3478	1/1	0.84	0.47	82,82,82,82	0
55	MG	CA	3447	1/1	0.84	0.46	58,58,58,58	0
55	MG	CA	3031	1/1	0.84	0.10	53,53,53,53	0
55	MG	CA	3091	1/1	0.84	0.42	74,74,74,74	0
55	MG	AA	3216	1/1	0.84	0.44	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3166	1/1	0.84	0.48	66,66,66,66	0
56	OHX	AA	3522	7/7	0.84	0.17	118,131,145,201	1
56	OHX	CA	3420	7/7	0.84	0.14	131,141,152,216	1
56	OHX	AA	3536	7/7	0.84	0.25	116,124,157,192	1
55	MG	BA	1637	1/1	0.84	0.08	83,83,83,83	0
55	MG	CA	3060	1/1	0.84	0.23	75,75,75,75	0
55	MG	CA	3036	1/1	0.84	0.25	87,87,87,87	0
55	MG	CA	3039	1/1	0.84	0.36	65,65,65,65	0
55	MG	CA	3204	1/1	0.84	0.41	73,73,73,73	0
55	MG	AA	3149	1/1	0.84	0.31	74,74,74,74	0
55	MG	DA	1626	1/1	0.84	0.52	84,84,84,84	0
55	MG	BA	1650	1/1	0.84	0.55	72,72,72,72	0
55	MG	CA	3082	1/1	0.84	0.42	62,62,62,62	0
55	MG	BA	1602	1/1	0.84	0.44	75,75,75,75	0
55	MG	BA	1606	1/1	0.84	0.42	92,92,92,92	0
55	MG	CA	3076	1/1	0.84	0.40	64,64,64,64	0
55	MG	AA	3021	1/1	0.84	0.51	80,80,80,80	0
55	MG	CA	3142	1/1	0.84	0.33	71,71,71,71	0
55	MG	DA	1678	1/1	0.84	0.15	118,118,118,118	0
55	MG	CA	3456	1/1	0.84	0.21	66,66,66,66	0
55	MG	BA	1633	1/1	0.84	0.16	59,59,59,59	0
55	MG	AA	3285	1/1	0.84	0.50	80,80,80,80	0
55	MG	CA	3205	1/1	0.84	0.31	63,63,63,63	0
55	MG	CE	301	1/1	0.84	0.37	56,56,56,56	0
55	MG	BA	1713	1/1	0.84	0.27	59,59,59,59	0
56	OHX	CA	3435	7/7	0.84	0.18	105,108,131,192	1
55	MG	DA	1611	1/1	0.84	0.28	92,92,92,92	0
55	MG	DC	106	1/1	0.85	0.55	91,91,91,91	0
55	MG	CA	3040	1/1	0.85	0.44	70,70,70,70	0
55	MG	CA	3175	1/1	0.85	0.37	64,64,64,64	0
55	MG	CA	3062	1/1	0.85	0.14	78,78,78,78	0
55	MG	CA	3077	1/1	0.85	0.24	57,57,57,57	0
55	MG	CA	3218	1/1	0.85	0.26	83,83,83,83	0
55	MG	CA	3059	1/1	0.85	0.41	63,63,63,63	0
55	MG	CB	207	1/1	0.85	0.47	76,76,76,76	0
55	MG	CA	3184	1/1	0.85	0.41	60,60,60,60	0
55	MG	AA	3270	1/1	0.85	0.10	94,94,94,94	0
55	MG	DA	1665	1/1	0.85	0.48	70,70,70,70	0
56	OHX	BA	1656	7/7	0.85	0.10	160,162,176,267	0
55	MG	CA	3087	1/1	0.85	0.14	70,70,70,70	0
55	MG	DA	1670	1/1	0.85	0.40	64,64,64,64	0
55	MG	DA	1645	1/1	0.85	0.47	91,91,91,91	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1747	1/1	0.85	0.38	74,74,74,74	0
55	MG	AA	3218	1/1	0.85	0.39	82,82,82,82	0
55	MG	AA	3058	1/1	0.85	0.32	73,73,73,73	0
55	MG	CB	202	1/1	0.85	0.17	99,99,99,99	0
55	MG	AA	3206	1/1	0.86	0.52	64,64,64,64	0
55	MG	CA	3061	1/1	0.86	0.29	64,64,64,64	0
55	MG	DA	1716	1/1	0.86	0.33	85,85,85,85	0
55	MG	DA	1712	1/1	0.86	0.31	98,98,98,98	0
55	MG	AA	3236	1/1	0.86	0.40	40,40,40,40	0
55	MG	DA	1662	1/1	0.86	0.36	73,73,73,73	0
55	MG	BA	1723	1/1	0.86	0.30	82,82,82,82	0
56	OHX	AA	3526	7/7	0.86	0.15	120,129,136,176	1
55	MG	AA	3409	1/1	0.86	0.48	56,56,56,56	0
55	MG	DA	1649	1/1	0.86	0.28	87,87,87,87	0
55	MG	BA	1721	1/1	0.86	0.39	70,70,70,70	0
56	OHX	AA	3537	7/7	0.86	0.11	171,189,202,242	1
55	MG	BA	1610	1/1	0.86	0.31	92,92,92,92	0
55	MG	AA	3103	1/1	0.86	0.11	97,97,97,97	0
55	MG	AE	302	1/1	0.86	0.21	71,71,71,71	0
55	MG	AA	3162	1/1	0.86	0.55	38,38,38,38	0
55	MG	CA	3214	1/1	0.86	0.28	65,65,65,65	0
55	MG	CA	3229	1/1	0.86	0.39	80,80,80,80	0
55	MG	AB	202	1/1	0.86	0.22	72,72,72,72	0
56	OHX	DA	1783	7/7	0.86	0.12	123,123,145,185	1
55	MG	AA	3348	1/1	0.86	0.41	46,46,46,46	0
55	MG	AA	3119	1/1	0.86	0.37	64,64,64,64	0
56	OHX	AA	3554	7/7	0.86	0.13	116,128,150,205	1
55	MG	AA	3169	1/1	0.86	0.53	76,76,76,76	0
55	MG	BA	1728	1/1	0.86	0.46	90,90,90,90	0
55	MG	AA	3124	1/1	0.86	0.44	70,70,70,70	0
55	MG	AA	3279	1/1	0.86	0.39	81,81,81,81	0
55	MG	BQ	101	1/1	0.86	0.54	96,96,96,96	0
55	MG	AA	3136	1/1	0.86	0.27	57,57,57,57	0
56	OHX	DA	1774	7/7	0.86	0.15	131,135,155,208	1
55	MG	AA	3145	1/1	0.86	0.44	56,56,56,56	0
55	MG	AA	3227	1/1	0.86	0.40	63,63,63,63	0
55	MG	DA	1613	1/1	0.87	0.25	87,87,87,87	0
55	MG	BA	1614	1/1	0.87	0.36	73,73,73,73	0
55	MG	AA	3379	1/1	0.87	0.43	55,55,55,55	0
55	MG	AA	3127	1/1	0.87	0.37	57,57,57,57	0
55	MG	CA	3159	1/1	0.87	0.33	75,75,75,75	0
55	MG	DA	1705	1/1	0.87	0.47	108,108,108,108	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1644	1/1	0.87	0.51	94,94,94,94	0
55	MG	CB	205	1/1	0.87	0.42	74,74,74,74	0
56	OHX	CA	3252	7/7	0.87	0.18	108,118,136,203	1
55	MG	AA	3109	1/1	0.87	0.47	47,47,47,47	0
56	OHX	CA	3397	7/7	0.87	0.10	128,138,154,219	1
55	MG	CA	3185	1/1	0.87	0.46	75,75,75,75	0
56	OHX	BA	1685	7/7	0.87	0.12	198,199,207,267	1
55	MG	AA	3159	1/1	0.87	0.29	65,65,65,65	0
56	OHX	CA	3409	7/7	0.87	0.17	97,100,119,183	1
55	MG	CA	3226	1/1	0.87	0.45	65,65,65,65	0
56	OHX	BA	1695	7/7	0.87	0.10	129,147,158,217	1
55	MG	AA	3164	1/1	0.87	0.27	70,70,70,70	0
56	OHX	AA	3556	7/7	0.87	0.11	212,217,223,266	1
55	MG	CA	3043	1/1	0.87	0.11	82,82,82,82	0
56	OHX	CA	3429	7/7	0.87	0.16	127,129,142,209	1
55	MG	CA	3086	1/1	0.87	0.39	68,68,68,68	0
55	MG	CA	3183	1/1	0.87	0.38	93,93,93,93	0
55	MG	AA	3034	1/1	0.87	0.43	56,56,56,56	0
55	MG	DA	1676	1/1	0.87	0.41	83,83,83,83	0
55	MG	CA	3169	1/1	0.87	0.23	71,71,71,71	0
56	OHX	AA	3545	7/7	0.87	0.21	90,96,105,167	2
55	MG	CA	3200	1/1	0.87	0.36	56,56,56,56	0
56	OHX	BA	1666	7/7	0.87	0.15	117,122,134,158	2
55	MG	AA	3122	1/1	0.87	0.43	62,62,62,62	0
55	MG	CA	3230	1/1	0.87	0.49	79,79,79,79	0
55	MG	CA	3155	1/1	0.87	0.17	58,58,58,58	0
55	MG	BA	1641	1/1	0.87	0.35	85,85,85,85	0
55	MG	CA	3074	1/1	0.88	0.32	64,64,64,64	0
56	OHX	BA	1677	7/7	0.88	0.12	141,145,154,220	1
55	MG	AA	3180	1/1	0.88	0.31	65,65,65,65	0
55	MG	DA	1640	1/1	0.88	0.35	83,83,83,83	0
55	MG	AA	3116	1/1	0.88	0.31	45,45,45,45	0
56	OHX	DA	1765	7/7	0.88	0.23	117,133,141,227	1
55	MG	AA	3046	1/1	0.88	0.50	68,68,68,68	0
55	MG	AA	3286	1/1	0.88	0.53	68,68,68,68	0
55	MG	AA	3280	1/1	0.88	0.40	77,77,77,77	0
55	MG	CA	3053	1/1	0.88	0.16	99,99,99,99	0
55	MG	AA	3120	1/1	0.88	0.27	71,71,71,71	0
55	MG	BA	1708	1/1	0.88	0.42	77,77,77,77	0
55	MG	AA	3249	1/1	0.88	0.41	58,58,58,58	0
55	MG	CA	3141	1/1	0.88	0.46	77,77,77,77	0
55	MG	BC	101	1/1	0.88	0.52	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1645	1/1	0.88	0.38	51,51,51,51	0
55	MG	AA	3247	1/1	0.88	0.35	81,81,81,81	0
55	MG	DA	1713	1/1	0.88	0.41	79,79,79,79	0
56	OHX	CA	3348	7/7	0.88	0.23	104,111,132,178	1
55	MG	CA	3097	1/1	0.88	0.34	67,67,67,67	0
56	OHX	DA	1784	7/7	0.88	0.10	150,153,166,225	1
55	MG	DA	1686	1/1	0.88	0.28	73,73,73,73	0
55	MG	DA	1683	1/1	0.88	0.47	71,71,71,71	0
55	MG	CA	3168	1/1	0.88	0.40	72,72,72,72	0
55	MG	BA	1742	1/1	0.88	0.46	86,86,86,86	0
56	OHX	DD	101	7/7	0.88	0.14	155,165,187,227	0
56	OHX	DB	105	7/7	0.88	0.20	88,91,103,175	5
56	OHX	CA	3284	7/7	0.88	0.13	136,147,155,216	1
55	MG	CA	3268	1/1	0.88	0.12	52,52,52,52	0
55	MG	DA	1655	1/1	0.88	0.15	78,78,78,78	0
55	MG	CA	3180	1/1	0.88	0.32	75,75,75,75	0
56	OHX	BA	1674	7/7	0.88	0.17	117,122,137,199	1
55	MG	AA	3028	1/1	0.88	0.38	66,66,66,66	0
55	MG	AB	206	1/1	0.88	0.56	83,83,83,83	0
55	MG	CA	3028	1/1	0.88	0.14	73,73,73,73	0
55	MG	BA	1617	1/1	0.88	0.48	71,71,71,71	0
55	MG	AA	3038	1/1	0.88	0.25	46,46,46,46	0
55	MG	DA	1679	1/1	0.88	0.28	69,69,69,69	0
55	MG	AA	3356	1/1	0.88	0.56	58,58,58,58	0
56	OHX	CA	3421	7/7	0.88	0.14	113,126,135,198	1
55	MG	AA	3266	1/1	0.88	0.29	78,78,78,78	0
55	MG	BA	1707	1/1	0.88	0.31	70,70,70,70	0
56	OHX	AA	3491	7/7	0.88	0.15	162,182,190,220	1
55	MG	AA	3067	1/1	0.88	0.17	97,97,97,97	0
55	MG	BA	1603	1/1	0.88	0.32	63,63,63,63	0
56	OHX	BD	102	7/7	0.88	0.10	153,174,197,228	0
56	OHX	BA	1667	7/7	0.88	0.17	118,130,146,200	1
56	OHX	AA	3532	7/7	0.88	0.20	89,105,116,172	1
55	MG	DA	1614	1/1	0.88	0.24	91,91,91,91	0
55	MG	C7	101	1/1	0.89	0.39	54,54,54,54	0
56	OHX	DA	1775	7/7	0.89	0.11	133,145,148,215	1
55	MG	DA	1672	1/1	0.89	0.31	83,83,83,83	0
56	OHX	DA	1805	7/7	0.89	0.09	155,158,165,245	1
56	OHX	CB	215	7/7	0.89	0.14	108,133,144,220	1
55	MG	CA	3156	1/1	0.89	0.37	84,84,84,84	0
55	MG	AA	3128	1/1	0.89	0.38	54,54,54,54	0
55	MG	AA	3215	1/1	0.89	0.52	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3130	1/1	0.89	0.33	75,75,75,75	0
56	OHX	C3	101	7/7	0.89	0.16	119,129,151,179	2
55	MG	CA	3448	1/1	0.89	0.17	63,63,63,63	0
55	MG	CA	3267	1/1	0.89	0.15	65,65,65,65	0
56	OHX	BA	1692	7/7	0.89	0.12	126,131,140,209	1
55	MG	AA	3350	1/1	0.89	0.43	80,80,80,80	0
55	MG	CA	3020	1/1	0.89	0.29	70,70,70,70	0
55	MG	BA	1639	1/1	0.89	0.10	102,102,102,102	0
55	MG	AA	3084	1/1	0.89	0.33	58,58,58,58	0
55	MG	AA	3244	1/1	0.89	0.22	49,49,49,49	0
56	OHX	A1	203	7/7	0.89	0.19	100,107,140,182	3
55	MG	CA	3260	1/1	0.89	0.24	71,71,71,71	0
55	MG	BA	1750	1/1	0.89	0.42	72,72,72,72	0
55	MG	AA	3209	1/1	0.89	0.35	57,57,57,57	0
56	OHX	BA	1806	7/7	0.89	0.19	97,127,142,180	2
56	OHX	CB	216	7/7	0.89	0.13	117,132,146,206	1
56	OHX	AA	3523	7/7	0.89	0.17	109,114,123,180	1
55	MG	CA	3117	1/1	0.89	0.23	69,69,69,69	0
55	MG	CA	3197	1/1	0.89	0.40	79,79,79,79	0
55	MG	CA	3104	1/1	0.89	0.42	41,41,41,41	0
56	OHX	CA	3399	7/7	0.89	0.18	97,104,115,165	2
56	OHX	DA	1753	7/7	0.89	0.18	120,124,134,196	1
55	MG	AA	3104	1/1	0.89	0.53	68,68,68,68	0
55	MG	AA	3193	1/1	0.89	0.19	58,58,58,58	0
55	MG	AA	3222	1/1	0.89	0.52	64,64,64,64	0
55	MG	DA	1636	1/1	0.89	0.32	75,75,75,75	0
55	MG	BA	1632	1/1	0.89	0.29	108,108,108,108	0
56	OHX	CB	219	7/7	0.89	0.10	145,151,161,232	1
56	OHX	CA	3269	7/7	0.89	0.17	98,100,123,153	2
55	MG	AA	3064	1/1	0.89	0.21	66,66,66,66	0
55	MG	BA	1636	1/1	0.89	0.27	61,61,61,61	0
56	OHX	BA	1804	7/7	0.89	0.17	134,142,150,227	1
55	MG	AA	3082	1/1	0.89	0.20	50,50,50,50	0
55	MG	CA	3019	1/1	0.89	0.19	46,46,46,46	0
55	MG	DA	1650	1/1	0.89	0.20	67,67,67,67	0
56	OHX	BA	1672	7/7	0.89	0.11	156,159,170,224	1
55	MG	AA	3089	1/1	0.89	0.55	84,84,84,84	0
55	MG	CA	3193	1/1	0.89	0.33	80,80,80,80	0
55	MG	BA	1629	1/1	0.89	0.23	112,112,112,112	0
56	OHX	AA	3510	7/7	0.89	0.18	92,103,113,152	2
56	OHX	BA	1691	7/7	0.89	0.11	148,150,156,215	1
55	MG	DA	1604	1/1	0.90	0.44	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3261	1/1	0.90	0.38	64,64,64,64	0
55	MG	BB	103	1/1	0.90	0.35	91,91,91,91	0
56	OHX	DC	107	7/7	0.90	0.11	131,132,141,177	1
55	MG	AA	3389	1/1	0.90	0.36	44,44,44,44	0
55	MG	BA	1625	1/1	0.90	0.46	65,65,65,65	0
56	OHX	AA	3484	7/7	0.90	0.20	76,100,111,147	2
55	MG	CA	3188	1/1	0.90	0.45	60,60,60,60	0
56	OHX	AA	3535	7/7	0.90	0.13	104,112,123,191	1
55	MG	AA	3281	1/1	0.90	0.52	70,70,70,70	0
55	MG	CA	3044	1/1	0.90	0.16	74,74,74,74	0
56	OHX	BA	1690	7/7	0.90	0.13	118,127,134,188	1
55	MG	AA	3378	1/1	0.90	0.34	47,47,47,47	0
55	MG	CA	3451	1/1	0.90	0.33	46,46,46,46	0
56	OHX	AA	3483	7/7	0.90	0.15	124,141,146,196	1
55	MG	AO	201	1/1	0.90	0.40	80,80,80,80	0
55	MG	AA	3191	1/1	0.90	0.30	45,45,45,45	0
55	MG	CA	3157	1/1	0.90	0.31	76,76,76,76	0
55	MG	BA	1716	1/1	0.90	0.36	55,55,55,55	0
56	OHX	AA	3562	7/7	0.90	0.16	98,105,127,189	1
55	MG	AA	3257	1/1	0.90	0.41	57,57,57,57	0
55	MG	AA	3229	1/1	0.90	0.50	59,59,59,59	0
55	MG	CA	3008	1/1	0.90	0.23	52,52,52,52	0
55	MG	DA	1684	1/1	0.90	0.52	79,79,79,79	0
55	MG	CA	3225	1/1	0.90	0.28	48,48,48,48	0
56	OHX	CA	3470	7/7	0.90	0.13	113,126,137,181	1
55	MG	AF	302	1/1	0.90	0.30	81,81,81,81	0
55	MG	BC	104	1/1	0.90	0.53	57,57,57,57	0
55	MG	CA	3135	1/1	0.90	0.44	45,45,45,45	0
55	MG	AA	3392	1/1	0.90	0.62	64,64,64,64	0
55	MG	AA	3037	1/1	0.90	0.48	63,63,63,63	0
56	OHX	AA	3306	7/7	0.90	0.12	134,139,151,214	1
56	OHX	AA	3569	7/7	0.90	0.15	116,117,125,191	1
55	MG	AA	3050	1/1	0.90	0.32	60,60,60,60	0
56	OHX	BA	1790	7/7	0.90	0.21	96,123,133,185	1
55	MG	DC	102	1/1	0.90	0.41	69,69,69,69	0
55	MG	AA	3391	1/1	0.90	0.28	59,59,59,59	0
55	MG	CA	3186	1/1	0.90	0.23	75,75,75,75	0
55	MG	BA	1609	1/1	0.90	0.32	73,73,73,73	0
55	MG	AA	3125	1/1	0.90	0.34	92,92,92,92	0
55	MG	BA	1700	1/1	0.90	0.42	61,61,61,61	0
55	MG	CA	3096	1/1	0.90	0.36	64,64,64,64	0
55	MG	CA	3101	1/1	0.90	0.38	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3255	1/1	0.90	0.20	64,64,64,64	0
55	MG	DA	1690	1/1	0.90	0.43	63,63,63,63	0
56	OHX	AA	3566	7/7	0.90	0.19	92,97,126,175	2
55	MG	CA	3216	1/1	0.90	0.39	91,91,91,91	0
56	OHX	AA	3331	7/7	0.90	0.27	72,87,130,163	3
55	MG	BA	1626	1/1	0.90	0.13	81,81,81,81	0
56	OHX	CA	3371	7/7	0.90	0.15	67,90,123,162	1
56	OHX	DA	1782	7/7	0.90	0.16	117,128,138,207	1
55	MG	AA	3383	1/1	0.90	0.32	46,46,46,46	0
55	MG	BA	1737	1/1	0.90	0.26	46,46,46,46	0
56	OHX	AA	3530	7/7	0.90	0.17	101,121,143,206	1
55	MG	CA	3479	1/1	0.90	0.47	64,64,64,64	0
55	MG	AA	3268	1/1	0.90	0.45	73,73,73,73	0
55	MG	AA	3139	1/1	0.90	0.37	48,48,48,48	0
55	MG	DA	1633	1/1	0.90	0.51	74,74,74,74	0
55	MG	AA	3223	1/1	0.90	0.37	56,56,56,56	0
55	MG	AA	3099	1/1	0.90	0.30	65,65,65,65	0
55	MG	DA	1654	1/1	0.90	0.36	61,61,61,61	0
55	MG	AA	3232	1/1	0.90	0.42	75,75,75,75	0
55	MG	DA	1680	1/1	0.90	0.27	72,72,72,72	0
55	MG	AA	3187	1/1	0.90	0.54	86,86,86,86	0
56	OHX	AA	3552	7/7	0.90	0.18	105,122,135,199	1
56	OHX	CA	3425	7/7	0.90	0.13	101,110,125,187	1
55	MG	BA	1749	1/1	0.90	0.49	88,88,88,88	0
55	MG	DA	1653	1/1	0.90	0.50	73,73,73,73	0
55	MG	AA	3238	1/1	0.90	0.55	50,50,50,50	0
56	OHX	AA	3365	7/7	0.90	0.22	90,106,114,161	2
55	MG	CA	3264	1/1	0.91	0.36	49,49,49,49	0
55	MG	CB	206	1/1	0.91	0.32	83,83,83,83	0
55	MG	CA	3134	1/1	0.91	0.34	65,65,65,65	0
56	OHX	AA	3312	7/7	0.91	0.17	64,87,123,173	1
55	MG	DN	201	1/1	0.91	0.12	80,80,80,80	0
55	MG	AB	201	1/1	0.91	0.39	73,73,73,73	0
55	MG	CA	3458	1/1	0.91	0.23	82,82,82,82	0
55	MG	AA	3353	1/1	0.91	0.25	39,39,39,39	0
55	MG	BA	1724	1/1	0.91	0.38	59,59,59,59	0
55	MG	CA	3191	1/1	0.91	0.46	72,72,72,72	0
56	OHX	AA	3333	7/7	0.91	0.19	91,114,128,179	2
56	OHX	AA	3567	7/7	0.91	0.14	103,106,118,172	1
55	MG	AA	3061	1/1	0.91	0.42	49,49,49,49	0
55	MG	DA	1697	1/1	0.91	0.40	72,72,72,72	0
55	MG	DA	1648	1/1	0.91	0.10	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3105	1/1	0.91	0.47	68,68,68,68	0
55	MG	AA	3056	1/1	0.91	0.21	36,36,36,36	0
55	MG	AA	3251	1/1	0.91	0.36	49,49,49,49	0
55	MG	AA	3144	1/1	0.91	0.55	71,71,71,71	0
55	MG	BB	105	1/1	0.91	0.51	63,63,63,63	0
55	MG	BA	1647	1/1	0.91	0.18	112,112,112,112	0
55	MG	AA	3045	1/1	0.91	0.41	65,65,65,65	0
56	OHX	CA	3422	7/7	0.91	0.11	126,137,143,193	1
56	OHX	DA	1778	7/7	0.91	0.15	142,148,154,267	0
55	MG	AA	3256	1/1	0.91	0.54	53,53,53,53	0
56	OHX	CA	3359	7/7	0.91	0.14	115,123,136,171	2
56	OHX	AA	3539	7/7	0.91	0.13	116,125,136,193	1
56	OHX	BB	107	7/7	0.91	0.23	71,92,103,147	3
55	MG	AA	3155	1/1	0.91	0.13	85,85,85,85	0
56	OHX	AA	3138	7/7	0.91	0.15	88,92,127,173	1
55	MG	DA	1677	1/1	0.91	0.34	76,76,76,76	0
55	MG	AA	3230	1/1	0.91	0.23	66,66,66,66	0
55	MG	BA	1652	1/1	0.91	0.33	63,63,63,63	0
56	OHX	BA	1673	7/7	0.91	0.13	117,123,127,191	1
56	OHX	BA	1812	7/7	0.91	0.13	151,164,170,231	1
56	OHX	DA	1808	7/7	0.91	0.14	119,124,131,178	1
56	OHX	CA	3328	7/7	0.91	0.16	50,117,131,206	0
56	OHX	CA	3413	7/7	0.91	0.15	121,130,144,215	1
55	MG	BA	1622	1/1	0.91	0.13	123,123,123,123	0
55	MG	CA	3017	1/1	0.91	0.21	92,92,92,92	0
55	MG	DA	1619	1/1	0.91	0.37	98,98,98,98	0
56	OHX	DA	1787	7/7	0.91	0.13	95,113,121,162	2
55	MG	BA	1643	1/1	0.91	0.11	78,78,78,78	0
55	MG	CA	3231	1/1	0.91	0.34	89,89,89,89	0
56	OHX	CA	3318	7/7	0.91	0.18	34,112,130,183	1
55	MG	BA	1634	1/1	0.91	0.20	74,74,74,74	0
55	MG	BA	1722	1/1	0.91	0.52	91,91,91,91	0
55	MG	CA	3084	1/1	0.91	0.38	60,60,60,60	0
55	MG	AA	3259	1/1	0.91	0.35	35,35,35,35	0
55	MG	C5	101	1/1	0.91	0.22	50,50,50,50	0
56	OHX	AA	3544	7/7	0.91	0.17	103,105,124,176	1
55	MG	BA	1660	1/1	0.91	0.25	97,97,97,97	0
55	MG	AO	203	1/1	0.91	0.28	56,56,56,56	0
55	MG	AA	3396	1/1	0.91	0.47	71,71,71,71	0
55	MG	CA	3480	1/1	0.91	0.23	72,72,72,72	0
56	OHX	BA	1694	7/7	0.91	0.08	159,161,173,226	1
55	MG	CA	3115	1/1	0.91	0.37	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3098	1/1	0.91	0.30	77,77,77,77	0
56	OHX	CA	3491	7/7	0.91	0.13	92,108,117,175	1
55	MG	AA	3074	1/1	0.91	0.36	73,73,73,73	0
56	OHX	CA	3433	7/7	0.91	0.17	121,129,144,183	1
56	OHX	CA	3402	7/7	0.91	0.11	159,162,170,218	1
56	OHX	AA	3559	7/7	0.91	0.10	124,133,143,186	1
55	MG	CA	3072	1/1	0.91	0.33	43,43,43,43	0
55	MG	AB	203	1/1	0.91	0.46	71,71,71,71	0
55	MG	CA	3121	1/1	0.91	0.35	55,55,55,55	0
55	MG	AA	3186	1/1	0.91	0.37	49,49,49,49	0
55	MG	AA	3381	1/1	0.91	0.30	59,59,59,59	0
56	OHX	AA	3547	7/7	0.91	0.17	69,84,101,157	2
55	MG	CA	3013	1/1	0.91	0.20	47,47,47,47	0
55	MG	BC	103	1/1	0.91	0.43	62,62,62,62	0
55	MG	CA	3093	1/1	0.91	0.32	81,81,81,81	0
56	OHX	CA	3431	7/7	0.91	0.13	105,117,132,179	1
55	MG	AA	3273	1/1	0.91	0.57	66,66,66,66	0
55	MG	BD	101	1/1	0.91	0.30	93,93,93,93	0
55	MG	AA	3201	1/1	0.91	0.34	45,45,45,45	0
55	MG	CA	3211	1/1	0.91	0.15	116,116,116,116	0
56	OHX	CA	3432	7/7	0.91	0.13	119,135,143,173	1
55	MG	DA	1669	1/1	0.91	0.36	64,64,64,64	0
56	OHX	AA	3564	7/7	0.91	0.17	102,105,128,167	1
55	MG	AB	205	1/1	0.91	0.33	50,50,50,50	0
56	OHX	AA	3370	7/7	0.91	0.21	115,126,140,200	1
56	OHX	AA	3512	7/7	0.91	0.18	99,114,126,166	2
55	MG	CA	3265	1/1	0.92	0.22	55,55,55,55	0
55	MG	DA	1620	1/1	0.92	0.50	79,79,79,79	0
56	OHX	CA	3390	7/7	0.92	0.10	117,128,152,209	1
55	MG	BA	1698	1/1	0.92	0.50	62,62,62,62	0
56	OHX	AA	3147	7/7	0.92	0.19	89,98,103,163	1
56	OHX	CA	3387	7/7	0.92	0.16	111,127,150,170	2
55	MG	CA	3029	1/1	0.92	0.28	76,76,76,76	0
55	MG	CA	3452	1/1	0.92	0.18	51,51,51,51	0
55	MG	AA	3141	1/1	0.92	0.55	44,44,44,44	0
55	MG	CA	3460	1/1	0.92	0.27	72,72,72,72	0
55	MG	BA	1621	1/1	0.92	0.45	55,55,55,55	0
55	MG	DA	1657	1/1	0.92	0.42	70,70,70,70	0
55	MG	CA	3099	1/1	0.92	0.34	51,51,51,51	0
56	OHX	CA	3434	7/7	0.92	0.14	96,110,126,177	1
55	MG	AA	3157	1/1	0.92	0.47	49,49,49,49	0
56	OHX	AA	3541	7/7	0.92	0.21	102,114,134,158	2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3396	7/7	0.92	0.13	135,136,150,198	1
56	OHX	AA	3534	7/7	0.92	0.12	136,141,145,222	1
55	MG	CA	3094	1/1	0.92	0.54	79,79,79,79	0
55	MG	CA	3439	1/1	0.92	0.33	63,63,63,63	0
55	MG	DL	201	1/1	0.92	0.48	92,92,92,92	0
56	OHX	BA	1681	7/7	0.92	0.11	153,163,173,229	1
55	MG	AE	303	1/1	0.92	0.28	32,32,32,32	0
55	MG	CA	3171	1/1	0.92	0.36	82,82,82,82	0
55	MG	AA	3102	1/1	0.92	0.40	79,79,79,79	0
55	MG	DB	102	1/1	0.92	0.25	102,102,102,102	0
55	MG	CA	3023	1/1	0.92	0.23	85,85,85,85	0
56	OHX	DA	1781	7/7	0.92	0.12	107,126,135,195	1
56	OHX	CA	3427	7/7	0.92	0.10	114,126,136,203	1
55	MG	DA	1637	1/1	0.92	0.54	106,106,106,106	0
55	MG	CA	3154	1/1	0.92	0.32	46,46,46,46	0
55	MG	CA	3210	1/1	0.92	0.56	74,74,74,74	0
55	MG	BA	1608	1/1	0.92	0.26	55,55,55,55	0
55	MG	AA	3374	1/1	0.92	0.34	29,29,29,29	0
56	OHX	CA	3486	7/7	0.92	0.17	87,109,129,181	2
56	OHX	AA	3488	7/7	0.92	0.19	86,101,105,150	1
55	MG	AA	3081	1/1	0.92	0.39	56,56,56,56	0
56	OHX	AA	3369	7/7	0.92	0.18	80,102,119,165	1
55	MG	BA	1741	1/1	0.92	0.48	73,73,73,73	0
55	MG	AA	3117	1/1	0.92	0.33	48,48,48,48	0
55	MG	BA	1739	1/1	0.92	0.44	70,70,70,70	0
55	MG	AA	3217	1/1	0.92	0.45	60,60,60,60	0
56	OHX	CA	3373	7/7	0.92	0.16	113,122,129,160	1
56	OHX	BA	1680	7/7	0.92	0.11	120,125,145,238	1
55	MG	AA	3254	1/1	0.92	0.33	42,42,42,42	0
55	MG	AA	3093	1/1	0.92	0.47	91,91,91,91	0
56	OHX	AA	3565	7/7	0.92	0.19	117,122,134,195	1
55	MG	DA	1663	1/1	0.92	0.27	66,66,66,66	0
55	MG	AA	3070	1/1	0.92	0.21	52,52,52,52	0
55	MG	BA	1729	1/1	0.92	0.53	73,73,73,73	0
55	MG	CA	3103	1/1	0.92	0.24	70,70,70,70	0
56	OHX	DA	1763	7/7	0.92	0.10	154,159,173,250	0
56	OHX	BA	1796	7/7	0.92	0.12	143,156,164,225	0
56	OHX	AB	210	7/7	0.92	0.21	83,107,129,146	3
55	MG	AA	3013	1/1	0.92	0.42	41,41,41,41	0
55	MG	CA	3203	1/1	0.92	0.40	47,47,47,47	0
55	MG	AA	3267	1/1	0.92	0.41	80,80,80,80	0
55	MG	CA	3148	1/1	0.92	0.28	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1613	1/1	0.92	0.30	65,65,65,65	0
55	MG	BA	1607	1/1	0.92	0.39	93,93,93,93	0
55	MG	CA	3199	1/1	0.92	0.34	62,62,62,62	0
55	MG	AA	3106	1/1	0.92	0.44	70,70,70,70	0
56	OHX	CA	3436	7/7	0.92	0.14	115,121,137,192	1
55	MG	AA	3163	1/1	0.92	0.35	61,61,61,61	0
56	OHX	CB	220	7/7	0.92	0.13	133,142,154,201	0
56	OHX	AA	3403	7/7	0.92	0.19	109,110,128,178	1
55	MG	AA	3170	1/1	0.92	0.20	50,50,50,50	0
55	MG	AA	3057	1/1	0.92	0.41	72,72,72,72	0
55	MG	DA	1656	1/1	0.92	0.36	68,68,68,68	0
55	MG	AA	3181	1/1	0.92	0.45	61,61,61,61	0
55	MG	AA	3250	1/1	0.92	0.35	56,56,56,56	0
56	OHX	AA	3490	7/7	0.92	0.16	94,113,129,158	1
55	MG	AA	3380	1/1	0.92	0.28	66,66,66,66	0
55	MG	CA	3123	1/1	0.92	0.28	36,36,36,36	0
55	MG	CA	3443	1/1	0.92	0.42	49,49,49,49	0
56	OHX	BA	1689	7/7	0.92	0.13	113,130,139,190	1
55	MG	AA	3133	1/1	0.92	0.22	54,54,54,54	0
56	OHX	DA	1745	7/7	0.92	0.14	115,123,143,223	0
55	MG	AF	301	1/1	0.92	0.28	83,83,83,83	0
55	MG	BA	1735	1/1	0.93	0.21	48,48,48,48	0
55	MG	AA	3414	1/1	0.93	0.29	57,57,57,57	0
55	MG	AA	3274	1/1	0.93	0.59	89,89,89,89	0
56	OHX	CB	217	7/7	0.93	0.22	128,135,146,182	1
55	MG	DA	1652	1/1	0.93	0.42	52,52,52,52	0
56	OHX	AA	3519	7/7	0.93	0.10	140,146,150,214	1
55	MG	CA	3152	1/1	0.93	0.37	54,54,54,54	0
56	OHX	DA	1773	7/7	0.93	0.10	122,126,137,197	1
55	MG	AA	3253	1/1	0.93	0.39	53,53,53,53	0
56	OHX	AA	3540	7/7	0.93	0.14	109,134,164,188	2
55	MG	BA	1726	1/1	0.93	0.33	61,61,61,61	0
55	MG	AA	3183	1/1	0.93	0.43	88,88,88,88	0
55	MG	BA	1754	1/1	0.93	0.38	61,61,61,61	0
55	MG	AA	3131	1/1	0.93	0.32	94,94,94,94	0
55	MG	CA	3146	1/1	0.93	0.38	77,77,77,77	0
55	MG	BB	101	1/1	0.93	0.49	70,70,70,70	0
55	MG	AA	3134	1/1	0.93	0.21	82,82,82,82	0
55	MG	CB	201	1/1	0.93	0.24	77,77,77,77	0
56	OHX	AB	217	7/7	0.93	0.17	85,105,116,146	1
56	OHX	CA	3428	7/7	0.93	0.13	123,134,138,182	1
55	MG	CA	3002	1/1	0.93	0.33	50,50,50,50	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	1671	1/1	0.93	0.22	64,64,64,64	0
55	MG	CA	3266	1/1	0.93	0.33	64,64,64,64	0
55	MG	AA	3188	1/1	0.93	0.30	40,40,40,40	0
56	OHX	AA	3542	7/7	0.93	0.13	118,127,135,189	1
55	MG	CA	3151	1/1	0.93	0.37	76,76,76,76	0
55	MG	BA	1620	1/1	0.93	0.44	70,70,70,70	0
56	OHX	CA	3350	7/7	0.93	0.15	112,134,144,175	1
55	MG	CA	3160	1/1	0.93	0.39	49,49,49,49	0
55	MG	CA	3149	1/1	0.93	0.39	55,55,55,55	0
55	MG	DA	1709	1/1	0.93	0.50	80,80,80,80	0
56	OHX	CB	213	7/7	0.93	0.12	131,144,166,188	1
56	OHX	CA	3304	7/7	0.93	0.13	113,122,141,181	2
55	MG	DA	1606	1/1	0.93	0.19	84,84,84,84	0
56	OHX	DV	101	7/7	0.93	0.09	162,169,185,231	1
56	OHX	CA	3379	7/7	0.93	0.11	134,137,155,207	1
56	OHX	CA	3404	7/7	0.93	0.10	149,155,166,217	1
56	OHX	BA	1816	7/7	0.93	0.14	127,130,142,194	1
55	MG	CA	3109	1/1	0.93	0.29	56,56,56,56	0
56	OHX	BA	1805	7/7	0.93	0.17	90,105,122,143	3
55	MG	DA	1691	1/1	0.93	0.38	54,54,54,54	0
56	OHX	CA	3358	7/7	0.93	0.11	128,130,147,230	1
55	MG	AA	3085	1/1	0.93	0.11	58,58,58,58	0
55	MG	AA	3129	1/1	0.93	0.32	83,83,83,83	0
55	MG	DA	1644	1/1	0.93	0.14	149,149,149,149	0
55	MG	CA	3170	1/1	0.93	0.20	65,65,65,65	0
55	MG	CA	3209	1/1	0.93	0.35	85,85,85,85	0
56	OHX	BA	1803	7/7	0.93	0.15	101,126,136,190	1
55	MG	AA	3086	1/1	0.93	0.38	95,95,95,95	0
56	OHX	AB	216	7/7	0.93	0.19	88,124,141,184	1
56	OHX	CA	3426	7/7	0.93	0.09	142,146,155,215	1
55	MG	CA	3227	1/1	0.93	0.34	79,79,79,79	0
56	OHX	CB	212	7/7	0.93	0.15	101,120,135,155	1
55	MG	CA	3221	1/1	0.93	0.43	69,69,69,69	0
55	MG	AA	3151	1/1	0.93	0.35	62,62,62,62	0
55	MG	AA	3023	1/1	0.93	0.50	52,52,52,52	0
55	MG	BA	1640	1/1	0.93	0.35	73,73,73,73	0
56	OHX	DA	1777	7/7	0.93	0.09	150,152,155,232	1
55	MG	AA	3156	1/1	0.93	0.46	45,45,45,45	0
55	MG	DA	1616	1/1	0.93	0.39	88,88,88,88	0
55	MG	CA	3056	1/1	0.93	0.49	79,79,79,79	0
55	MG	CA	3083	1/1	0.93	0.35	44,44,44,44	0
55	MG	BB	102	1/1	0.93	0.27	85,85,85,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3489	7/7	0.93	0.14	91,101,112,140	1
55	MG	AA	3055	1/1	0.93	0.39	65,65,65,65	0
55	MG	AA	3152	1/1	0.93	0.35	56,56,56,56	0
55	MG	CA	3070	1/1	0.93	0.24	44,44,44,44	0
56	OHX	AA	3528	7/7	0.93	0.14	112,118,137,160	2
56	OHX	DA	1755	7/7	0.93	0.16	103,120,143,191	1
55	MG	AA	3386	1/1	0.93	0.23	42,42,42,42	0
55	MG	AA	3192	1/1	0.93	0.39	48,48,48,48	0
55	MG	BA	1753	1/1	0.93	0.46	67,67,67,67	0
55	MG	CA	3035	1/1	0.93	0.24	92,92,92,92	0
55	MG	DA	1711	1/1	0.93	0.23	107,107,107,107	0
56	OHX	CA	3302	7/7	0.93	0.19	79,86,104,139	1
55	MG	CA	3143	1/1	0.93	0.37	60,60,60,60	0
56	OHX	AA	3509	7/7	0.93	0.14	92,96,122,175	1
56	OHX	CA	3467	7/7	0.93	0.12	131,146,152,199	1
55	MG	CA	3073	1/1	0.93	0.18	54,54,54,54	0
55	MG	AA	3075	1/1	0.93	0.52	44,44,44,44	0
56	OHX	BD	104	7/7	0.93	0.24	82,85,90,147	2
56	OHX	DA	1799	7/7	0.93	0.13	122,127,139,209	1
55	MG	AA	3246	1/1	0.93	0.39	36,36,36,36	0
55	MG	CA	3442	1/1	0.93	0.21	61,61,61,61	0
56	OHX	CA	3376	7/7	0.93	0.14	113,130,136,172	1
55	MG	DA	1689	1/1	0.93	0.39	87,87,87,87	0
55	MG	AA	3202	1/1	0.93	0.38	45,45,45,45	0
55	MG	DA	1618	1/1	0.93	0.26	105,105,105,105	0
55	MG	CA	3258	1/1	0.93	0.35	56,56,56,56	0
55	MG	CA	3212	1/1	0.93	0.46	75,75,75,75	0
55	MG	CA	3459	1/1	0.93	0.29	56,56,56,56	0
55	MG	CA	3132	1/1	0.93	0.25	80,80,80,80	0
55	MG	AA	3179	1/1	0.93	0.52	60,60,60,60	0
56	OHX	CA	3417	7/7	0.93	0.10	151,167,187,222	1
55	MG	AA	3416	1/1	0.93	0.40	74,74,74,74	0
56	OHX	AA	3493	7/7	0.93	0.14	109,111,123,166	1
55	MG	AA	3262	1/1	0.93	0.38	52,52,52,52	0
56	OHX	DC	108	7/7	0.93	0.10	120,132,142,180	1
56	OHX	CA	3250	7/7	0.94	0.14	106,109,126,164	1
56	OHX	BA	1797	7/7	0.94	0.22	71,104,132,136	3
55	MG	CA	3176	1/1	0.94	0.33	67,67,67,67	0
55	MG	CA	3208	1/1	0.94	0.35	70,70,70,70	0
55	MG	AA	3228	1/1	0.94	0.27	67,67,67,67	0
55	MG	BA	1715	1/1	0.94	0.36	74,74,74,74	0
56	OHX	CB	214	7/7	0.94	0.12	129,139,146,186	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3252	1/1	0.94	0.38	47,47,47,47	0
55	MG	AA	3118	1/1	0.94	0.29	53,53,53,53	0
55	MG	CA	3147	1/1	0.94	0.35	51,51,51,51	0
55	MG	CA	3263	1/1	0.94	0.28	69,69,69,69	0
56	OHX	AA	3304	7/7	0.94	0.13	109,115,135,200	1
56	OHX	DA	1757	7/7	0.94	0.12	123,127,134,157	1
55	MG	CA	3113	1/1	0.94	0.32	61,61,61,61	0
55	MG	AA	3010	1/1	0.94	0.26	40,40,40,40	0
55	MG	AA	3235	1/1	0.94	0.34	50,50,50,50	0
56	OHX	DA	1806	7/7	0.94	0.07	142,150,160,228	1
55	MG	BA	1717	1/1	0.94	0.45	51,51,51,51	0
56	OHX	DA	1732	7/7	0.94	0.17	134,143,157,195	0
55	MG	AA	3276	1/1	0.94	0.41	69,69,69,69	0
55	MG	AA	3065	1/1	0.94	0.38	49,49,49,49	0
55	MG	BA	1642	1/1	0.94	0.23	102,102,102,102	0
55	MG	AA	3140	1/1	0.94	0.24	41,41,41,41	0
55	MG	CA	3174	1/1	0.94	0.48	52,52,52,52	0
55	MG	AA	3207	1/1	0.94	0.47	57,57,57,57	0
56	OHX	DG	302	7/7	0.94	0.09	133,142,147,197	1
56	OHX	CA	3367	7/7	0.94	0.09	129,137,147,194	1
56	OHX	AB	218	7/7	0.94	0.17	128,132,146,199	1
56	OHX	CA	3383	7/7	0.94	0.14	111,116,132,194	1
55	MG	AA	3002	1/1	0.94	0.44	41,41,41,41	0
55	MG	AA	3078	1/1	0.94	0.32	59,59,59,59	0
56	OHX	AA	3529	7/7	0.94	0.17	90,106,115,167	1
55	MG	CA	3195	1/1	0.94	0.24	68,68,68,68	0
56	OHX	CA	3374	7/7	0.94	0.12	106,124,128,169	1
56	OHX	C6	101	7/7	0.94	0.11	132,145,157,184	1
56	OHX	DA	1779	7/7	0.94	0.09	144,146,155,215	1
56	OHX	AA	3550	7/7	0.94	0.16	111,121,131,187	1
55	MG	AA	3204	1/1	0.94	0.16	61,61,61,61	0
56	OHX	CA	3395	7/7	0.94	0.17	106,111,125,156	1
56	OHX	DA	1810	7/7	0.94	0.14	134,135,143,197	1
55	MG	CA	3177	1/1	0.94	0.32	57,57,57,57	0
55	MG	CA	3153	1/1	0.94	0.23	56,56,56,56	0
55	MG	DA	1638	1/1	0.94	0.18	89,89,89,89	0
56	OHX	DA	1798	7/7	0.94	0.09	128,133,140,212	1
55	MG	BA	1653	1/1	0.94	0.35	63,63,63,63	0
56	OHX	AA	3366	7/7	0.94	0.20	85,90,106,173	1
55	MG	AA	3019	1/1	0.94	0.48	72,72,72,72	0
55	MG	AA	3123	1/1	0.94	0.24	72,72,72,72	0
56	OHX	AA	3458	7/7	0.94	0.23	34,48,113,148	3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3553	7/7	0.94	0.12	113,118,133,183	1
56	OHX	DA	1785	7/7	0.94	0.13	110,114,129,164	1
56	OHX	CA	3466	7/7	0.94	0.15	96,98,116,157	1
55	MG	AA	3126	1/1	0.94	0.34	85,85,85,85	0
56	OHX	AA	3551	7/7	0.94	0.10	141,143,149,194	1
55	MG	AA	3237	1/1	0.94	0.34	45,45,45,45	0
56	OHX	AA	3555	7/7	0.94	0.16	112,114,124,192	1
55	MG	DC	104	1/1	0.94	0.40	77,77,77,77	0
55	MG	CA	3063	1/1	0.94	0.24	70,70,70,70	0
55	MG	AA	3398	1/1	0.94	0.40	51,51,51,51	0
56	OHX	AA	3527	7/7	0.94	0.10	130,134,147,188	1
56	OHX	BA	1794	7/7	0.94	0.11	118,138,149,184	1
55	MG	BA	1655	1/1	0.94	0.23	60,60,60,60	0
56	OHX	CA	3245	7/7	0.94	0.12	99,120,129,189	1
55	MG	AA	3032	1/1	0.94	0.30	41,41,41,41	0
56	OHX	AA	3560	7/7	0.94	0.14	102,104,127,184	1
56	OHX	A6	101	7/7	0.94	0.14	113,122,137,155	1
55	MG	CA	3012	1/1	0.94	0.27	53,53,53,53	0
56	OHX	AA	3524	7/7	0.94	0.13	111,120,128,172	1
55	MG	A3	101	1/1	0.94	0.44	60,60,60,60	0
55	MG	DA	1704	1/1	0.94	0.44	73,73,73,73	0
56	OHX	DA	1752	7/7	0.94	0.12	107,121,128,186	1
56	OHX	CA	3410	7/7	0.94	0.11	114,125,132,190	1
56	OHX	DA	1769	7/7	0.94	0.11	133,140,147,188	1
55	MG	CA	3162	1/1	0.94	0.48	65,65,65,65	0
56	OHX	AA	3533	7/7	0.94	0.15	98,103,114,150	2
56	OHX	CA	3411	7/7	0.94	0.11	117,123,138,184	1
55	MG	CA	3089	1/1	0.94	0.27	60,60,60,60	0
55	MG	DA	1612	1/1	0.94	0.40	86,86,86,86	0
55	MG	DA	1627	1/1	0.94	0.51	77,77,77,77	0
56	OHX	CA	3464	7/7	0.94	0.16	78,109,122,137	3
55	MG	CA	3058	1/1	0.94	0.39	50,50,50,50	0
55	MG	AA	3005	1/1	0.94	0.41	43,43,43,43	0
55	MG	AA	3090	1/1	0.94	0.17	85,85,85,85	0
56	OHX	AA	3407	7/7	0.94	0.15	108,117,126,165	1
55	MG	AA	3153	1/1	0.94	0.67	64,64,64,64	0
55	MG	AA	3114	1/1	0.94	0.37	47,47,47,47	0
55	MG	CA	3010	1/1	0.94	0.21	47,47,47,47	0
56	OHX	AA	3373	7/7	0.94	0.17	75,103,110,155	1
56	OHX	AO	205	7/7	0.94	0.18	83,89,107,180	1
56	OHX	CA	3437	7/7	0.94	0.13	98,105,117,166	2
56	OHX	BA	1664	7/7	0.94	0.15	108,126,142,197	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	1649	1/1	0.94	0.28	74,74,74,74	0
56	OHX	CA	3377	7/7	0.94	0.14	90,95,111,135	2
56	OHX	CA	3403	7/7	0.94	0.14	88,108,114,167	1
56	OHX	CA	3416	7/7	0.94	0.16	114,117,128,182	1
56	OHX	BA	1662	7/7	0.94	0.14	105,117,141,193	1
55	MG	BA	1736	1/1	0.94	0.51	64,64,64,64	0
55	MG	AA	3112	1/1	0.94	0.26	47,47,47,47	0
55	MG	DA	1692	1/1	0.94	0.50	70,70,70,70	0
55	MG	DA	1608	1/1	0.94	0.21	78,78,78,78	0
56	OHX	CA	3306	7/7	0.94	0.12	98,106,119,148	1
55	MG	AA	3049	1/1	0.94	0.35	64,64,64,64	0
55	MG	AA	3241	1/1	0.94	0.32	60,60,60,60	0
56	OHX	CA	3244	7/7	0.94	0.17	94,113,121,172	1
55	MG	AA	3101	1/1	0.94	0.44	63,63,63,63	0
56	OHX	AA	3546	7/7	0.94	0.16	98,103,119,179	1
55	MG	DA	1609	1/1	0.94	0.37	91,91,91,91	0
56	OHX	AB	215	7/7	0.94	0.18	105,114,120,153	1
55	MG	CA	3172	1/1	0.94	0.33	86,86,86,86	0
55	MG	BA	1630	1/1	0.94	0.12	90,90,90,90	0
55	MG	CA	3219	1/1	0.94	0.53	79,79,79,79	0
56	OHX	CA	3415	7/7	0.94	0.13	134,135,143,187	1
56	OHX	CA	3370	7/7	0.94	0.13	116,120,142,180	1
56	OHX	CA	3340	7/7	0.94	0.13	115,122,140,168	1
55	MG	AA	3083	1/1	0.94	0.29	88,88,88,88	0
55	MG	CA	3112	1/1	0.94	0.35	41,41,41,41	0
55	MG	DA	1666	1/1	0.94	0.44	62,62,62,62	0
56	OHX	AA	3506	7/7	0.94	0.14	97,110,123,157	1
55	MG	AA	3096	1/1	0.94	0.32	71,71,71,71	0
55	MG	CA	3150	1/1	0.94	0.35	55,55,55,55	0
55	MG	CA	3064	1/1	0.94	0.22	89,89,89,89	0
56	OHX	DA	1749	7/7	0.94	0.18	91,120,126,173	1
56	OHX	CA	3366	7/7	0.94	0.10	140,148,168,207	0
56	OHX	BA	1659	7/7	0.94	0.16	114,130,135,179	1
56	OHX	DA	1801	7/7	0.94	0.11	141,143,154,216	1
55	MG	CA	3444	1/1	0.94	0.27	52,52,52,52	0
56	OHX	CA	3393	7/7	0.94	0.12	93,114,121,181	1
55	MG	AA	3200	1/1	0.94	0.44	45,45,45,45	0
56	OHX	DA	1790	7/7	0.94	0.11	135,136,148,199	1
55	MG	BA	1612	1/1	0.94	0.39	81,81,81,81	0
55	MG	CA	3045	1/1	0.94	0.62	91,91,91,91	0
56	OHX	AA	3402	7/7	0.94	0.21	87,110,129,141	3
55	MG	AA	3384	1/1	0.95	0.42	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1678	7/7	0.95	0.15	115,118,134,165	1
56	OHX	AA	3515	7/7	0.95	0.14	100,121,139,211	1
56	OHX	AA	3479	7/7	0.95	0.15	106,122,142,174	1
55	MG	CA	3181	1/1	0.95	0.33	62,62,62,62	0
55	MG	DA	1664	1/1	0.95	0.47	31,31,31,31	0
55	MG	CA	3071	1/1	0.95	0.25	51,51,51,51	0
56	OHX	AA	3505	7/7	0.95	0.19	86,108,110,156	1
56	OHX	DA	1796	7/7	0.95	0.11	134,139,149,195	1
56	OHX	CA	3385	7/7	0.95	0.11	115,124,135,193	1
55	MG	AA	3265	1/1	0.95	0.27	85,85,85,85	0
56	OHX	CA	3392	7/7	0.95	0.11	126,132,142,192	1
56	OHX	DA	1747	7/7	0.95	0.15	109,122,155,200	1
56	OHX	AA	3513	7/7	0.95	0.15	80,88,116,153	1
55	MG	BA	1709	1/1	0.95	0.31	100,100,100,100	0
55	MG	AA	3233	1/1	0.95	0.13	59,59,59,59	0
55	MG	CA	3078	1/1	0.95	0.35	76,76,76,76	0
55	MG	BA	1697	1/1	0.95	0.40	37,37,37,37	0
56	OHX	AB	219	7/7	0.95	0.15	104,111,125,162	1
56	OHX	BA	1815	7/7	0.95	0.15	110,125,133,172	1
55	MG	CB	203	1/1	0.95	0.14	111,111,111,111	0
56	OHX	AA	3154	7/7	0.95	0.17	76,89,110,133	1
56	OHX	CA	3408	7/7	0.95	0.09	136,139,143,209	1
55	MG	CA	3189	1/1	0.95	0.41	67,67,67,67	0
55	MG	AA	3173	1/1	0.95	0.32	52,52,52,52	0
55	MG	CA	3130	1/1	0.95	0.43	58,58,58,58	0
56	OHX	DK	201	7/7	0.95	0.09	137,138,149,200	1
56	OHX	AA	3474	7/7	0.95	0.18	51,85,127,151	2
55	MG	AA	3072	1/1	0.95	0.28	65,65,65,65	0
55	MG	CA	3440	1/1	0.95	0.36	54,54,54,54	0
55	MG	AA	3413	1/1	0.95	0.30	57,57,57,57	0
56	OHX	AA	3531	7/7	0.95	0.11	119,124,135,185	1
56	OHX	AA	3516	7/7	0.95	0.14	101,109,121,183	1
56	OHX	BA	1679	7/7	0.95	0.12	116,125,129,189	1
55	MG	CA	3182	1/1	0.95	0.46	59,59,59,59	0
56	OHX	DA	1793	7/7	0.95	0.10	146,150,161,207	1
55	MG	AA	3415	1/1	0.95	0.26	52,52,52,52	0
56	OHX	DA	1736	7/7	0.95	0.13	130,135,157,193	0
56	OHX	DA	1800	7/7	0.95	0.08	137,140,150,220	1
55	MG	BA	1616	1/1	0.95	0.29	61,61,61,61	0
55	MG	CA	3021	1/1	0.95	0.17	60,60,60,60	0
56	OHX	BA	1809	7/7	0.95	0.10	141,153,160,232	0
55	MG	BA	1745	1/1	0.95	0.54	83,83,83,83	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3125	1/1	0.95	0.20	52,52,52,52	0
56	OHX	CA	3400	7/7	0.95	0.13	116,133,145,220	1
55	MG	CA	3158	1/1	0.95	0.41	56,56,56,56	0
56	OHX	AA	3313	7/7	0.95	0.16	96,112,122,174	0
56	OHX	CA	3375	7/7	0.95	0.15	103,118,131,145	1
55	MG	AA	3088	1/1	0.95	0.17	60,60,60,60	0
56	OHX	CA	3412	7/7	0.95	0.14	99,116,129,164	2
56	OHX	BR	101	7/7	0.95	0.10	117,129,143,169	1
55	MG	AA	3269	1/1	0.95	0.41	72,72,72,72	0
55	MG	CA	3194	1/1	0.95	0.25	63,63,63,63	0
55	MG	CA	3224	1/1	0.95	0.29	77,77,77,77	0
56	OHX	DA	1809	7/7	0.95	0.09	124,126,139,221	1
55	MG	CA	3165	1/1	0.95	0.45	57,57,57,57	0
56	OHX	DA	1807	7/7	0.95	0.10	117,126,135,195	1
56	OHX	C1	201	7/7	0.95	0.14	102,111,123,165	1
56	OHX	DA	1751	7/7	0.95	0.19	66,109,137,183	2
55	MG	AA	3411	1/1	0.95	0.32	63,63,63,63	0
56	OHX	BA	1670	7/7	0.95	0.10	135,143,147,201	1
55	MG	CA	3065	1/1	0.95	0.36	55,55,55,55	0
55	MG	AA	3054	1/1	0.95	0.33	49,49,49,49	0
56	OHX	AA	3543	7/7	0.95	0.10	113,117,131,189	1
55	MG	AA	3184	1/1	0.95	0.34	38,38,38,38	0
55	MG	DA	1646	1/1	0.95	0.23	64,64,64,64	0
56	OHX	BA	1792	7/7	0.95	0.09	150,163,168,209	1
56	OHX	AA	3476	7/7	0.95	0.14	102,122,137,175	1
56	OHX	AA	3336	7/7	0.95	0.11	146,153,168,218	0
56	OHX	BA	1772	7/7	0.95	0.14	106,118,144,175	0
56	OHX	AA	3568	7/7	0.95	0.13	78,93,100,118	1
55	MG	AA	3175	1/1	0.95	0.37	39,39,39,39	0
56	OHX	AA	3561	7/7	0.95	0.10	152,158,173,226	1
56	OHX	DA	1811	7/7	0.95	0.06	137,141,149,222	1
55	MG	A5	101	1/1	0.95	0.24	41,41,41,41	0
56	OHX	DA	1791	7/7	0.95	0.15	103,104,121,153	1
56	OHX	BA	1783	7/7	0.95	0.20	77,87,125,141	2
56	OHX	AA	3508	7/7	0.95	0.11	122,129,136,204	1
55	MG	AA	3063	1/1	0.95	0.34	76,76,76,76	0
56	OHX	CB	209	7/7	0.95	0.17	117,133,147,190	1
55	MG	BA	1733	1/1	0.95	0.51	60,60,60,60	0
56	OHX	AA	3492	7/7	0.95	0.17	79,89,95,107	3
56	OHX	DA	1770	7/7	0.95	0.12	136,142,156,217	1
55	MG	DA	1601	1/1	0.95	0.23	87,87,87,87	0
56	OHX	AA	3485	7/7	0.95	0.14	104,114,127,171	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3053	1/1	0.95	0.46	60,60,60,60	0
55	MG	AA	3003	1/1	0.95	0.34	39,39,39,39	0
55	MG	CA	3030	1/1	0.95	0.30	89,89,89,89	0
56	OHX	CA	3368	7/7	0.95	0.14	108,126,135,177	1
56	OHX	CA	3414	7/7	0.95	0.09	155,156,163,215	1
56	OHX	BA	1675	7/7	0.95	0.08	120,128,140,197	1
56	OHX	BA	1676	7/7	0.95	0.11	143,151,156,210	1
55	MG	CA	3066	1/1	0.95	0.38	56,56,56,56	0
55	MG	AA	3168	1/1	0.95	0.30	89,89,89,89	0
55	MG	BA	1651	1/1	0.95	0.09	90,90,90,90	0
55	MG	CA	3126	1/1	0.95	0.30	54,54,54,54	0
55	MG	AA	3239	1/1	0.95	0.28	44,44,44,44	0
55	MG	AA	3390	1/1	0.95	0.20	46,46,46,46	0
55	MG	AB	204	1/1	0.95	0.61	68,68,68,68	0
55	MG	AA	3008	1/1	0.95	0.39	42,42,42,42	0
56	OHX	CA	3378	7/7	0.95	0.12	128,141,148,178	1
55	MG	DA	1687	1/1	0.95	0.15	63,63,63,63	0
56	OHX	BA	1801	7/7	0.95	0.08	118,138,142,207	1
55	MG	CA	3041	1/1	0.95	0.25	73,73,73,73	0
56	OHX	DA	1768	7/7	0.95	0.10	121,132,163,218	0
56	OHX	CA	3468	7/7	0.95	0.11	115,126,133,180	1
56	OHX	AA	3514	7/7	0.95	0.18	84,93,104,149	1
56	OHX	AB	212	7/7	0.95	0.17	81,99,131,153	1
55	MG	AA	3012	1/1	0.95	0.32	46,46,46,46	0
56	OHX	DB	103	7/7	0.95	0.10	166,171,179,191	1
56	OHX	CA	3344	7/7	0.95	0.17	96,110,117,162	1
55	MG	CA	3081	1/1	0.95	0.31	63,63,63,63	0
56	OHX	AB	214	7/7	0.95	0.16	110,118,132,162	1
56	OHX	DA	1728	7/7	0.95	0.18	78,116,123,162	0
55	MG	DA	1615	1/1	0.95	0.28	98,98,98,98	0
55	MG	CA	3446	1/1	0.95	0.30	47,47,47,47	0
55	MG	AA	3041	1/1	0.95	0.24	49,49,49,49	0
56	OHX	DA	1756	7/7	0.95	0.10	145,145,160,212	1
55	MG	AA	3377	1/1	0.95	0.33	51,51,51,51	0
55	MG	AA	3069	1/1	0.95	0.44	62,62,62,62	0
55	MG	AA	3031	1/1	0.95	0.25	35,35,35,35	0
56	OHX	CA	3360	7/7	0.95	0.10	116,124,135,193	1
56	OHX	CA	3386	7/7	0.95	0.15	110,116,134,181	1
56	OHX	BA	1661	7/7	0.95	0.12	108,124,128,170	1
55	MG	AA	3020	1/1	0.95	0.38	44,44,44,44	0
56	OHX	AA	3160	7/7	0.96	0.11	116,121,130,182	1
55	MG	AA	3195	1/1	0.96	0.38	43,43,43,43	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3548	7/7	0.96	0.11	113,118,133,172	1
55	MG	CA	3102	1/1	0.96	0.46	67,67,67,67	0
55	MG	CA	3453	1/1	0.96	0.29	58,58,58,58	0
55	MG	CA	3445	1/1	0.96	0.23	38,38,38,38	0
56	OHX	CA	3484	7/7	0.96	0.12	104,113,129,146	1
56	OHX	AA	3563	7/7	0.96	0.10	124,125,134,183	1
55	MG	DA	1658	1/1	0.96	0.46	64,64,64,64	0
55	MG	CA	3025	1/1	0.96	0.18	83,83,83,83	0
55	MG	CA	3167	1/1	0.96	0.48	75,75,75,75	0
55	MG	CA	3128	1/1	0.96	0.16	72,72,72,72	0
56	OHX	AA	3404	7/7	0.96	0.23	74,98,116,164	1
56	OHX	AA	3486	7/7	0.96	0.17	127,135,138,199	1
56	OHX	CA	3253	7/7	0.96	0.15	107,120,133,155	1
55	MG	CA	3054	1/1	0.96	0.30	54,54,54,54	0
56	OHX	CA	3333	7/7	0.96	0.11	104,127,133,184	1
56	OHX	AA	3324	7/7	0.96	0.15	92,110,118,165	1
55	MG	AA	3357	1/1	0.96	0.40	73,73,73,73	0
55	MG	CA	3145	1/1	0.96	0.43	74,74,74,74	0
56	OHX	AA	3494	7/7	0.96	0.15	59,86,128,185	1
56	OHX	CA	3487	7/7	0.96	0.08	135,139,147,210	1
56	OHX	CA	3418	7/7	0.96	0.12	115,119,129,166	1
56	OHX	DA	1788	7/7	0.96	0.12	96,113,128,168	1
56	OHX	CA	3430	7/7	0.96	0.11	96,106,114,197	1
55	MG	CA	3022	1/1	0.96	0.17	55,55,55,55	0
56	OHX	AA	3464	7/7	0.96	0.14	117,125,139,188	0
56	OHX	CA	3401	7/7	0.96	0.09	136,149,158,185	1
56	OHX	AA	3401	7/7	0.96	0.12	93,112,116,173	1
56	OHX	DA	1792	7/7	0.96	0.11	110,118,129,172	1
55	MG	AA	3039	1/1	0.96	0.33	40,40,40,40	0
55	MG	CA	3163	1/1	0.96	0.40	80,80,80,80	0
55	MG	AA	3243	1/1	0.96	0.39	51,51,51,51	0
56	OHX	AA	3339	7/7	0.96	0.11	151,155,164,211	1
55	MG	AA	3395	1/1	0.96	0.20	40,40,40,40	0
56	OHX	CA	3380	7/7	0.96	0.09	106,119,130,170	1
55	MG	BA	1605	1/1	0.96	0.19	104,104,104,104	0
56	OHX	AA	3473	7/7	0.96	0.17	66,95,102,124	1
55	MG	AA	3277	1/1	0.96	0.47	46,46,46,46	0
56	OHX	DA	1804	7/7	0.96	0.16	107,115,128,173	1
56	OHX	BA	1784	7/7	0.96	0.14	122,129,148,203	0
55	MG	CA	3009	1/1	0.96	0.31	39,39,39,39	0
56	OHX	CA	3381	7/7	0.96	0.10	102,112,121,159	1
55	MG	CA	3049	1/1	0.96	0.31	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BA	1778	7/7	0.96	0.14	99,120,131,182	0
56	OHX	BA	1793	7/7	0.96	0.10	95,105,117,163	1
55	MG	AA	3161	1/1	0.96	0.32	50,50,50,50	0
56	OHX	DA	1760	7/7	0.96	0.11	142,145,152,204	1
56	OHX	CA	3248	7/7	0.96	0.10	116,128,134,203	1
56	OHX	CA	3343	7/7	0.96	0.16	109,118,132,184	1
55	MG	AA	3376	1/1	0.96	0.34	33,33,33,33	0
56	OHX	CA	3382	7/7	0.96	0.10	129,131,148,199	1
56	OHX	DA	1789	7/7	0.96	0.06	176,179,184,242	1
55	MG	CA	3024	1/1	0.96	0.18	48,48,48,48	0
56	OHX	CA	3342	7/7	0.96	0.14	116,123,130,201	1
55	MG	CA	3001	1/1	0.96	0.26	46,46,46,46	0
55	MG	AA	3225	1/1	0.96	0.30	63,63,63,63	0
56	OHX	BA	1684	7/7	0.96	0.11	109,118,126,149	1
55	MG	CA	3026	1/1	0.96	0.10	58,58,58,58	0
56	OHX	AA	3487	7/7	0.96	0.13	95,110,116,167	1
55	MG	CA	3116	1/1	0.96	0.39	69,69,69,69	0
55	MG	DA	1603	1/1	0.96	0.40	71,71,71,71	0
56	OHX	AB	208	7/7	0.96	0.16	113,119,131,170	1
55	MG	AA	3146	1/1	0.96	0.32	41,41,41,41	0
55	MG	AA	3178	1/1	0.96	0.44	39,39,39,39	0
56	OHX	C5	102	7/7	0.96	0.14	114,118,133,165	1
56	OHX	CA	3309	7/7	0.96	0.17	92,108,125,150	1
55	MG	CA	3075	1/1	0.96	0.20	45,45,45,45	0
56	OHX	DA	1803	7/7	0.96	0.10	135,141,144,207	1
56	OHX	CA	3363	7/7	0.96	0.12	94,99,114,167	1
56	OHX	CA	3365	7/7	0.96	0.08	164,171,176,213	1
56	OHX	BD	103	7/7	0.96	0.14	86,95,103,174	1
56	OHX	AA	3302	7/7	0.96	0.14	88,114,124,193	1
56	OHX	BA	1787	7/7	0.96	0.13	107,117,138,149	2
56	OHX	AA	3337	7/7	0.96	0.14	97,106,127,177	1
56	OHX	AA	3525	7/7	0.96	0.13	100,109,122,187	1
55	MG	AA	3198	1/1	0.96	0.30	54,54,54,54	0
55	MG	BA	1619	1/1	0.96	0.27	50,50,50,50	0
55	MG	AA	3022	1/1	0.96	0.34	15,15,15,15	0
56	OHX	DC	109	7/7	0.96	0.15	88,92,104,159	3
56	OHX	BB	106	7/7	0.96	0.13	164,167,173,198	1
56	OHX	AA	3475	7/7	0.96	0.17	67,93,111,167	1
56	OHX	AA	3300	7/7	0.96	0.15	67,91,120,167	1
55	MG	CA	3476	1/1	0.96	0.35	52,52,52,52	0
56	OHX	CA	3482	7/7	0.96	0.12	84,120,131,181	0
56	OHX	BA	1693	7/7	0.96	0.15	112,112,134,152	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	3111	1/1	0.96	0.37	35,35,35,35	0
55	MG	BN	201	1/1	0.96	0.12	80,80,80,80	0
56	OHX	AA	3305	7/7	0.96	0.17	83,97,103,135	1
55	MG	CA	3259	1/1	0.96	0.24	65,65,65,65	0
55	MG	CA	3471	1/1	0.96	0.32	57,57,57,57	0
56	OHX	CB	210	7/7	0.96	0.15	104,124,140,171	1
56	OHX	BA	1777	7/7	0.96	0.14	114,118,140,171	1
56	OHX	BA	1668	7/7	0.96	0.10	116,121,137,182	1
56	OHX	BA	1798	7/7	0.96	0.12	140,143,151,221	1
55	MG	AA	3177	1/1	0.96	0.44	37,37,37,37	0
56	OHX	CA	3335	7/7	0.96	0.15	96,110,125,200	0
55	MG	CA	3016	1/1	0.96	0.23	55,55,55,55	0
56	OHX	AA	3507	7/7	0.96	0.12	101,111,128,158	1
56	OHX	AA	3496	7/7	0.96	0.17	117,124,142,215	0
56	OHX	CA	3341	7/7	0.96	0.14	74,100,107,145	2
56	OHX	DR	101	7/7	0.96	0.11	135,141,146,189	1
55	MG	AA	3205	1/1	0.96	0.17	40,40,40,40	0
56	OHX	CA	3438	7/7	0.96	0.10	97,104,116,167	1
55	MG	CA	3092	1/1	0.96	0.54	52,52,52,52	0
56	OHX	AA	3504	7/7	0.96	0.12	112,118,129,179	1
56	OHX	AA	3368	7/7	0.96	0.18	76,83,98,126	1
56	OHX	CA	3293	7/7	0.96	0.16	100,117,128,163	0
55	MG	CA	3032	1/1	0.96	0.29	70,70,70,70	0
55	MG	CA	3190	1/1	0.96	0.14	60,60,60,60	0
56	OHX	CA	3247	7/7	0.96	0.17	95,104,117,152	1
55	MG	AA	3073	1/1	0.96	0.33	69,69,69,69	0
56	OHX	CA	3391	7/7	0.96	0.10	140,144,157,182	1
56	OHX	DA	1750	7/7	0.96	0.13	127,137,146,202	1
55	MG	AA	3080	1/1	0.96	0.42	55,55,55,55	0
55	MG	CA	3048	1/1	0.96	0.34	44,44,44,44	0
56	OHX	AA	3371	7/7	0.96	0.14	93,107,117,177	1
55	MG	CA	3051	1/1	0.96	0.33	69,69,69,69	0
56	OHX	AA	3481	7/7	0.96	0.16	95,108,126,156	2
55	MG	CA	3161	1/1	0.96	0.28	71,71,71,71	0
56	OHX	CA	3364	7/7	0.96	0.10	117,120,133,182	1
55	MG	CA	3472	1/1	0.96	0.20	59,59,59,59	0
55	MG	AA	3358	1/1	0.96	0.29	51,51,51,51	0
55	MG	DA	1693	1/1	0.96	0.51	54,54,54,54	0
56	OHX	AB	209	7/7	0.96	0.18	63,88,125,152	2
55	MG	AA	3171	1/1	0.96	0.23	48,48,48,48	0
55	MG	AA	3278	1/1	0.96	0.43	35,35,35,35	0
56	OHX	BA	1771	7/7	0.96	0.20	77,100,122,150	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3477	7/7	0.96	0.14	108,119,125,208	1
56	OHX	CA	3384	7/7	0.96	0.12	118,124,135,184	1
55	MG	DA	1639	1/1	0.96	0.44	70,70,70,70	0
56	OHX	CA	3465	7/7	0.96	0.11	131,136,147,181	1
55	MG	CA	3262	1/1	0.96	0.46	74,74,74,74	0
55	MG	AA	3213	1/1	0.96	0.23	49,49,49,49	0
56	OHX	AA	3499	7/7	0.96	0.14	101,113,131,183	1
55	MG	AA	3001	1/1	0.96	0.41	28,28,28,28	0
56	OHX	CA	3337	7/7	0.96	0.13	109,124,136,185	0
55	MG	CA	3474	1/1	0.96	0.12	70,70,70,70	0
56	OHX	CA	3398	7/7	0.96	0.10	129,132,142,192	1
56	OHX	DA	1762	7/7	0.96	0.16	107,112,122,180	1
55	MG	AA	3011	1/1	0.96	0.36	49,49,49,49	0
56	OHX	CA	3246	7/7	0.96	0.16	113,116,120,151	1
56	OHX	AA	3367	7/7	0.96	0.14	121,129,147,173	1
56	OHX	CA	3388	7/7	0.96	0.12	112,116,127,180	1
56	OHX	AA	3452	7/7	0.96	0.22	61,75,91,137	2
56	OHX	DA	1772	7/7	0.96	0.09	131,135,143,214	1
55	MG	AA	3167	1/1	0.96	0.53	53,53,53,53	0
56	OHX	BA	1813	7/7	0.96	0.13	128,130,137,174	1
55	MG	AA	3272	1/1	0.97	0.50	50,50,50,50	0
56	OHX	AA	3480	7/7	0.97	0.18	90,100,124,135	1
55	MG	AA	3351	1/1	0.97	0.38	53,53,53,53	0
55	MG	BA	1624	1/1	0.97	0.29	70,70,70,70	0
55	MG	CA	3120	1/1	0.97	0.36	48,48,48,48	0
56	OHX	AA	3558	7/7	0.97	0.11	95,121,125,156	1
56	OHX	CA	3346	7/7	0.97	0.15	99,104,119,151	1
56	OHX	DA	1740	7/7	0.97	0.12	139,153,162,184	0
56	OHX	CB	211	7/7	0.97	0.10	122,128,152,168	1
56	OHX	BA	1799	7/7	0.97	0.11	158,163,176,213	1
55	MG	AA	3240	1/1	0.97	0.33	43,43,43,43	0
55	MG	DA	1610	1/1	0.97	0.24	96,96,96,96	0
55	MG	AA	3148	1/1	0.97	0.36	65,65,65,65	0
56	OHX	DA	1771	7/7	0.97	0.11	97,105,129,152	1
55	MG	DA	1602	1/1	0.97	0.41	68,68,68,68	0
56	OHX	DA	1730	7/7	0.97	0.15	102,111,123,157	0
57	ZN	BG	301	1/1	0.97	0.30	79,79,79,79	0
56	OHX	CA	3349	7/7	0.97	0.12	115,117,131,178	1
56	OHX	BC	106	7/7	0.97	0.15	110,133,144,147	1
55	MG	DC	101	1/1	0.97	0.31	85,85,85,85	0
56	OHX	DA	1743	7/7	0.97	0.14	109,113,118,148	1
56	OHX	AA	3497	7/7	0.97	0.15	94,106,111,138	2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1759	7/7	0.97	0.11	120,137,147,190	0
55	MG	AA	3029	1/1	0.97	0.30	38,38,38,38	0
56	OHX	CA	3355	7/7	0.97	0.12	108,110,119,149	1
56	OHX	BA	1788	7/7	0.97	0.14	118,118,132,157	1
56	OHX	DA	1797	7/7	0.97	0.06	149,152,159,218	1
56	OHX	CA	3362	7/7	0.97	0.08	129,136,141,186	1
56	OHX	BA	1770	7/7	0.97	0.16	102,113,126,149	1
56	OHX	AA	3468	7/7	0.97	0.14	99,111,119,167	1
56	OHX	BA	1781	7/7	0.97	0.13	91,111,121,156	1
56	OHX	CA	3462	7/7	0.97	0.16	71,82,94,110	1
56	OHX	AA	3322	7/7	0.97	0.12	89,98,107,146	1
56	OHX	CA	3490	7/7	0.97	0.14	102,105,118,156	1
56	OHX	CA	3353	7/7	0.97	0.15	81,96,110,140	1
55	MG	AA	3042	1/1	0.97	0.29	43,43,43,43	0
55	MG	CA	3080	1/1	0.97	0.09	57,57,57,57	0
55	MG	BA	1732	1/1	0.97	0.47	52,52,52,52	0
56	OHX	DA	1737	7/7	0.97	0.14	87,110,131,158	1
56	OHX	CA	3317	7/7	0.97	0.10	116,126,142,180	1
55	MG	BA	1714	1/1	0.97	0.29	56,56,56,56	0
56	OHX	AA	3482	7/7	0.97	0.12	105,118,127,177	1
55	MG	AA	3007	1/1	0.97	0.25	31,31,31,31	0
56	OHX	BC	107	7/7	0.97	0.16	105,124,134,145	1
56	OHX	DA	1731	7/7	0.97	0.10	129,139,145,172	1
55	MG	AA	3212	1/1	0.97	0.41	35,35,35,35	0
56	OHX	CA	3338	7/7	0.97	0.18	95,103,117,121	1
56	OHX	AA	3330	7/7	0.97	0.13	102,112,122,166	1
56	OHX	BA	1785	7/7	0.97	0.14	109,122,129,170	1
56	OHX	AW	101	7/7	0.97	0.15	103,112,128,156	1
55	MG	AA	3344	1/1	0.97	0.39	48,48,48,48	0
55	MG	AA	3349	1/1	0.97	0.44	61,61,61,61	0
56	OHX	AA	3503	7/7	0.97	0.12	99,121,138,179	1
56	OHX	AA	3471	7/7	0.97	0.16	98,107,114,163	1
56	OHX	CA	3298	7/7	0.97	0.14	90,98,134,148	0
55	MG	AA	3004	1/1	0.97	0.45	37,37,37,37	0
56	OHX	A3	102	7/7	0.97	0.14	90,98,113,134	2
56	OHX	CA	3347	7/7	0.97	0.13	86,102,110,148	1
56	OHX	AA	3340	7/7	0.97	0.10	159,167,171,209	0
56	OHX	CA	3345	7/7	0.97	0.13	91,108,114,146	1
55	MG	BA	1706	1/1	0.97	0.42	79,79,79,79	0
55	MG	CA	3018	1/1	0.97	0.33	55,55,55,55	0
56	OHX	CA	3308	7/7	0.97	0.17	88,90,121,161	0
55	MG	AA	3346	1/1	0.97	0.26	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3469	7/7	0.97	0.12	79,91,98,161	1
56	OHX	AA	3450	7/7	0.97	0.18	65,94,112,113	3
55	MG	CA	3139	1/1	0.97	0.29	56,56,56,56	0
55	MG	AA	3094	1/1	0.97	0.55	39,39,39,39	0
56	OHX	AA	3406	7/7	0.97	0.24	84,92,109,162	1
55	MG	CA	3257	1/1	0.97	0.30	60,60,60,60	0
56	OHX	AA	3517	7/7	0.97	0.17	88,111,115,145	1
55	MG	AA	3016	1/1	0.97	0.36	39,39,39,39	0
56	OHX	AA	3465	7/7	0.97	0.12	85,99,124,159	1
56	OHX	CA	3463	7/7	0.97	0.15	107,129,139,156	1
56	OHX	CA	3394	7/7	0.97	0.13	97,100,116,155	1
56	OHX	DA	1776	7/7	0.97	0.10	114,116,125,160	1
56	OHX	BA	1782	7/7	0.97	0.14	133,144,159,198	0
55	MG	AA	3352	1/1	0.97	0.21	41,41,41,41	0
56	OHX	CA	3481	7/7	0.97	0.15	35,87,114,138	2
56	OHX	CA	3492	7/7	0.97	0.15	97,102,115,126	1
56	OHX	AA	3495	7/7	0.97	0.17	86,93,120,158	1
55	MG	CA	3473	1/1	0.97	0.29	50,50,50,50	0
56	OHX	CA	3334	7/7	0.97	0.11	110,115,136,183	0
55	MG	AA	3027	1/1	0.97	0.37	42,42,42,42	0
56	OHX	AB	213	7/7	0.97	0.18	85,93,130,132	3
55	MG	CA	3069	1/1	0.97	0.23	69,69,69,69	0
55	MG	C0	201	1/1	0.97	0.16	61,61,61,61	0
56	OHX	AA	3478	7/7	0.97	0.16	77,90,100,131	1
56	OHX	BA	1811	7/7	0.97	0.13	88,104,115,154	1
55	MG	DA	1703	1/1	0.97	0.46	73,73,73,73	0
55	MG	AA	3071	1/1	0.97	0.60	68,68,68,68	0
56	OHX	BA	1767	7/7	0.97	0.17	92,119,140,142	0
55	MG	AA	3014	1/1	0.97	0.45	44,44,44,44	0
55	MG	AA	3385	1/1	0.97	0.46	34,34,34,34	0
56	OHX	AA	3500	7/7	0.97	0.13	94,114,122,159	1
56	OHX	BA	1802	7/7	0.97	0.15	107,121,133,185	1
56	OHX	CA	3351	7/7	0.97	0.14	102,107,134,173	1
56	OHX	AA	3498	7/7	0.97	0.16	92,94,127,136	1
56	OHX	AA	3372	7/7	0.97	0.14	93,103,121,167	1
55	MG	AA	3408	1/1	0.97	0.44	47,47,47,47	0
56	OHX	DA	1802	7/7	0.97	0.12	120,122,140,196	1
55	MG	DA	1607	1/1	0.97	0.35	82,82,82,82	0
55	MG	CA	3100	1/1	0.97	0.43	63,63,63,63	0
55	MG	CA	3173	1/1	0.97	0.33	53,53,53,53	0
55	MG	AO	202	1/1	0.97	0.30	55,55,55,55	0
56	OHX	BA	1663	7/7	0.97	0.10	132,137,143,190	1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3469	7/7	0.97	0.09	89,110,121,162	1
56	OHX	BA	1774	7/7	0.97	0.16	80,98,111,147	1
55	MG	BA	1719	1/1	0.97	0.43	51,51,51,51	0
56	OHX	CA	3356	7/7	0.97	0.14	96,109,118,157	1
56	OHX	CA	3325	7/7	0.97	0.14	108,122,148,156	1
55	MG	AA	3194	1/1	0.97	0.12	26,26,26,26	0
56	OHX	DA	1748	7/7	0.97	0.11	95,111,122,149	1
55	MG	AA	3158	1/1	0.97	0.42	50,50,50,50	0
55	MG	CA	3127	1/1	0.97	0.27	53,53,53,53	0
56	OHX	AA	3447	7/7	0.97	0.15	91,102,120,163	1
55	MG	AA	3066	1/1	0.97	0.36	83,83,83,83	0
56	OHX	AA	3317	7/7	0.97	0.16	79,88,118,156	1
55	MG	AA	3182	1/1	0.97	0.55	45,45,45,45	0
56	OHX	BA	1682	7/7	0.97	0.12	119,124,130,186	1
55	MG	CA	3015	1/1	0.97	0.27	54,54,54,54	0
56	OHX	DA	1795	7/7	0.97	0.11	112,118,132,167	1
55	MG	AA	3211	1/1	0.97	0.52	62,62,62,62	0
56	OHX	BA	1791	7/7	0.97	0.17	82,106,122,150	2
56	OHX	AA	3325	7/7	0.97	0.11	91,103,115,154	1
55	MG	CA	3106	1/1	0.97	0.27	61,61,61,61	0
56	OHX	AA	3511	7/7	0.97	0.12	133,145,154,207	0
55	MG	CA	3108	1/1	0.97	0.31	52,52,52,52	0
56	OHX	AA	3405	7/7	0.97	0.12	103,111,138,161	1
55	MG	CA	3475	1/1	0.97	0.20	55,55,55,55	0
55	MG	AA	3382	1/1	0.97	0.43	36,36,36,36	0
56	OHX	DA	1735	7/7	0.97	0.11	110,115,118,170	1
56	OHX	BA	1789	7/7	0.97	0.17	108,112,133,182	1
55	MG	AA	3387	1/1	0.97	0.35	42,42,42,42	0
56	OHX	BA	1795	7/7	0.97	0.12	109,127,134,173	1
55	MG	CA	3098	1/1	0.97	0.16	63,63,63,63	0
56	OHX	BA	1671	7/7	0.97	0.08	127,131,133,210	1
56	OHX	BA	1764	7/7	0.97	0.17	88,94,120,157	0
56	OHX	CA	3423	7/7	0.97	0.08	123,126,136,189	1
55	MG	CA	3047	1/1	0.97	0.38	41,41,41,41	0
55	MG	DA	1668	1/1	0.97	0.23	86,86,86,86	0
56	OHX	DA	1761	7/7	0.97	0.11	130,132,145,205	0
55	MG	DA	1685	1/1	0.97	0.17	59,59,59,59	0
56	OHX	BA	1814	7/7	0.97	0.11	101,109,125,174	1
56	OHX	CA	3406	7/7	0.97	0.08	151,161,169,211	1
55	MG	CA	3166	1/1	0.97	0.51	58,58,58,58	0
56	OHX	CA	3307	7/7	0.97	0.12	92,104,131,164	0
56	OHX	CA	3331	7/7	0.97	0.14	101,112,120,147	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3003	1/1	0.97	0.37	51,51,51,51	0
55	MG	AA	3172	1/1	0.97	0.43	38,38,38,38	0
55	MG	CA	3067	1/1	0.97	0.28	49,49,49,49	0
56	OHX	CA	3424	7/7	0.97	0.08	141,145,151,214	1
56	OHX	CA	3405	7/7	0.97	0.10	112,116,119,187	1
55	MG	CA	3131	1/1	0.97	0.34	65,65,65,65	0
55	MG	BA	1740	1/1	0.97	0.44	61,61,61,61	0
56	OHX	AA	3538	7/7	0.97	0.12	88,94,114,159	1
56	OHX	DA	1741	7/7	0.97	0.14	97,116,128,170	1
56	OHX	CA	3352	7/7	0.97	0.09	133,145,147,191	1
56	OHX	BA	1808	7/7	0.97	0.17	84,90,96,110	2
56	OHX	DA	1739	7/7	0.98	0.12	98,110,124,155	1
56	OHX	CA	3357	7/7	0.98	0.15	86,98,106,151	1
56	OHX	CA	3321	7/7	0.98	0.13	111,119,144,156	0
56	OHX	CA	3235	7/7	0.98	0.16	43,79,99,118	0
55	MG	AA	3219	1/1	0.98	0.34	48,48,48,48	0
56	OHX	AA	3318	7/7	0.98	0.16	92,102,113,133	1
56	OHX	CA	3319	7/7	0.98	0.15	87,97,106,138	1
56	OHX	AA	3521	7/7	0.98	0.13	87,94,107,160	1
56	OHX	CA	3251	7/7	0.98	0.13	88,107,125,141	1
56	OHX	AA	3287	7/7	0.98	0.15	75,88,103,129	2
56	OHX	AA	3461	7/7	0.98	0.18	60,78,98,143	1
56	OHX	CA	3278	7/7	0.98	0.15	81,96,114,120	0
56	OHX	BA	1688	7/7	0.98	0.13	107,112,123,154	1
56	OHX	AA	3303	7/7	0.98	0.13	93,102,117,145	1
55	MG	BA	1743	1/1	0.98	0.38	69,69,69,69	0
56	OHX	CA	3315	7/7	0.98	0.15	90,101,110,160	1
56	OHX	AA	3299	7/7	0.98	0.17	54,81,94,118	1
56	OHX	AA	3307	7/7	0.98	0.15	85,90,103,127	1
56	OHX	CA	3389	7/7	0.98	0.11	101,110,123,155	1
55	MG	CA	3144	1/1	0.98	0.34	54,54,54,54	0
56	OHX	AA	3472	7/7	0.98	0.12	120,126,137,153	1
56	OHX	AA	3520	7/7	0.98	0.11	127,132,145,185	1
56	OHX	CA	3372	7/7	0.98	0.14	112,137,145,182	0
57	ZN	DQ	101	1/1	0.98	0.14	123,123,123,123	0
56	OHX	BA	1786	7/7	0.98	0.11	93,97,101,149	1
55	MG	AA	3242	1/1	0.98	0.36	37,37,37,37	0
55	MG	AA	3226	1/1	0.98	0.48	42,42,42,42	0
56	OHX	AA	3467	7/7	0.98	0.12	100,105,117,133	1
55	MG	AA	3345	1/1	0.98	0.41	47,47,47,47	0
56	OHX	BA	1807	7/7	0.98	0.09	135,141,150,224	0
55	MG	DA	1605	1/1	0.98	0.26	63,63,63,63	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3364	7/7	0.98	0.16	92,103,108,119	1
56	OHX	DA	1733	7/7	0.98	0.15	146,151,163,202	0
56	OHX	AA	3456	7/7	0.98	0.20	59,75,90,132	2
56	OHX	AA	3441	7/7	0.98	0.17	84,93,115,140	0
56	OHX	AA	3502	7/7	0.98	0.11	97,102,112,146	1
56	OHX	CA	3339	7/7	0.98	0.12	100,105,127,171	1
56	OHX	DA	1744	7/7	0.98	0.14	103,108,120,148	1
56	OHX	DA	1726	7/7	0.98	0.17	87,101,123,159	0
55	MG	CA	3261	1/1	0.98	0.41	48,48,48,48	0
56	OHX	DA	1780	7/7	0.98	0.09	127,131,138,167	1
56	OHX	AA	3454	7/7	0.98	0.16	68,93,112,112	1
56	OHX	BA	1810	7/7	0.98	0.13	106,108,121,152	1
55	MG	BA	1638	1/1	0.98	0.33	57,57,57,57	0
56	OHX	CA	3240	7/7	0.98	0.12	96,99,103,148	1
56	OHX	CA	3295	7/7	0.98	0.15	102,105,117,137	1
56	OHX	A1	202	7/7	0.98	0.17	85,95,114,146	1
55	MG	DA	1647	1/1	0.98	0.40	90,90,90,90	0
55	MG	AA	3176	1/1	0.98	0.20	60,60,60,60	0
56	OHX	CA	3320	7/7	0.98	0.13	140,142,153,174	0
55	MG	AA	3062	1/1	0.98	0.37	73,73,73,73	0
55	MG	DA	1651	1/1	0.98	0.45	62,62,62,62	0
56	OHX	AA	3400	7/7	0.98	0.19	69,80,83,116	1
56	OHX	AA	3323	7/7	0.98	0.15	72,87,96,117	1
56	OHX	CA	3237	7/7	0.98	0.15	109,109,122,166	0
55	MG	AA	3143	1/1	0.98	0.42	46,46,46,46	0
56	OHX	CA	3330	7/7	0.98	0.10	102,106,115,169	0
56	OHX	CO	201	7/7	0.98	0.13	104,109,121,141	1
56	OHX	AA	3362	7/7	0.98	0.20	40,81,119,136	1
56	OHX	AA	3549	7/7	0.98	0.12	97,102,111,165	1
56	OHX	CA	3361	7/7	0.98	0.10	113,119,132,166	1
56	OHX	CA	3450	7/7	0.98	0.12	112,125,137,206	0
56	OHX	DA	1754	7/7	0.98	0.12	98,102,118,156	1
56	OHX	BA	1773	7/7	0.98	0.10	101,102,110,142	1
56	OHX	AA	3449	7/7	0.98	0.17	64,74,89,112	2
55	MG	AA	3258	1/1	0.98	0.46	65,65,65,65	0
55	MG	CA	3118	1/1	0.98	0.40	69,69,69,69	0
55	MG	AA	3412	1/1	0.98	0.41	39,39,39,39	0
56	OHX	AA	3470	7/7	0.98	0.15	107,109,130,160	1
55	MG	BA	1738	1/1	0.98	0.17	41,41,41,41	0
56	OHX	BA	1759	7/7	0.98	0.19	78,93,120,156	0
56	OHX	AA	3518	7/7	0.98	0.16	67,73,103,130	1
55	MG	AA	3033	1/1	0.98	0.37	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3328	7/7	0.98	0.11	89,97,114,142	1
56	OHX	CA	3243	7/7	0.98	0.12	121,128,140,172	0
56	OHX	AA	3326	7/7	0.98	0.15	83,94,100,118	1
56	OHX	BA	1665	7/7	0.98	0.14	82,92,111,128	1
55	MG	CA	3090	1/1	0.98	0.32	55,55,55,55	0
56	OHX	AA	3298	7/7	0.98	0.21	71,88,99,110	1
56	OHX	AA	3451	7/7	0.98	0.18	75,85,92,125	1
55	MG	AA	3283	1/1	0.98	0.33	55,55,55,55	0
56	OHX	AA	3295	7/7	0.98	0.15	84,98,116,152	0
56	OHX	DA	1724	7/7	0.98	0.14	84,106,133,148	1
55	MG	AA	3043	1/1	0.98	0.38	46,46,46,46	0
56	OHX	CA	3323	7/7	0.98	0.13	107,111,118,169	0
56	OHX	AA	3316	7/7	0.98	0.14	80,95,97,136	0
56	OHX	AA	3311	7/7	0.98	0.15	97,106,117,155	1
56	OHX	BA	1683	7/7	0.98	0.09	124,130,146,183	1
56	OHX	CA	3285	7/7	0.98	0.12	94,107,126,147	1
56	OHX	CA	3369	7/7	0.98	0.15	97,113,121,158	1
56	OHX	CA	3254	7/7	0.98	0.08	167,174,181,211	0
56	OHX	BA	1800	7/7	0.98	0.13	106,107,118,143	1
55	MG	AA	3018	1/1	0.98	0.40	43,43,43,43	0
55	MG	AA	3030	1/1	0.98	0.34	44,44,44,44	0
55	MG	BA	1701	1/1	0.98	0.31	57,57,57,57	0
55	MG	AA	3410	1/1	0.98	0.46	61,61,61,61	0
55	MG	CA	3133	1/1	0.98	0.35	48,48,48,48	0
56	OHX	DA	1764	7/7	0.98	0.09	115,121,127,171	1
56	OHX	CA	3238	7/7	0.98	0.17	80,102,103,125	1
56	OHX	AA	3342	7/7	0.98	0.18	78,85,104,123	1
55	MG	AA	3203	1/1	0.98	0.32	50,50,50,50	0
56	OHX	DA	1729	7/7	0.98	0.14	104,108,118,152	1
55	MG	CA	3068	1/1	0.98	0.35	44,44,44,44	0
56	OHX	AA	3338	7/7	0.98	0.14	82,93,108,126	1
56	OHX	AA	3489	7/7	0.98	0.14	72,78,92,128	1
55	MG	AA	3185	1/1	0.98	0.45	36,36,36,36	0
56	OHX	AA	3319	7/7	0.98	0.16	87,95,122,151	1
55	MG	AA	3040	1/1	0.98	0.46	47,47,47,47	0
56	OHX	CA	3488	7/7	0.98	0.08	113,123,127,179	1
56	OHX	AA	3448	7/7	0.98	0.14	87,90,112,131	1
55	MG	BA	1731	1/1	0.98	0.40	57,57,57,57	0
55	MG	AA	3214	1/1	0.98	0.32	46,46,46,46	0
56	OHX	CA	3483	7/7	0.98	0.14	84,93,103,136	1
55	MG	CA	3111	1/1	0.98	0.41	30,30,30,30	0
55	MG	CA	3124	1/1	0.98	0.31	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	DA	1758	7/7	0.98	0.08	132,137,143,204	0
56	OHX	BA	1768	7/7	0.98	0.12	128,139,147,175	0
56	OHX	CA	3296	7/7	0.98	0.14	65,90,108,135	2
55	MG	AA	3142	1/1	0.98	0.56	45,45,45,45	0
56	OHX	AA	3557	7/7	0.98	0.16	75,87,101,114	1
55	MG	AA	3110	1/1	0.98	0.50	48,48,48,48	0
56	OHX	AA	3290	7/7	0.98	0.18	10,72,91,128	0
56	OHX	CA	3485	7/7	0.98	0.15	88,102,109,144	1
55	MG	DA	1699	1/1	0.98	0.35	78,78,78,78	0
55	MG	AA	3047	1/1	0.98	0.37	54,54,54,54	0
56	OHX	DC	110	7/7	0.98	0.14	78,91,106,144	4
55	MG	AA	3355	1/1	0.98	0.48	36,36,36,36	0
56	OHX	BA	1769	7/7	0.98	0.15	102,107,127,145	0
57	ZN	DG	301	1/1	0.98	0.28	122,122,122,122	0
56	OHX	AA	3314	7/7	0.98	0.14	81,93,123,149	1
56	OHX	CA	3311	7/7	0.98	0.16	79,95,105,127	1
55	MG	CA	3004	1/1	0.98	0.28	49,49,49,49	0
56	OHX	AA	3263	7/7	0.98	0.16	76,102,114,143	1
56	OHX	CA	3300	7/7	0.98	0.16	66,75,91,101	1
56	OHX	CA	3249	7/7	0.98	0.17	86,90,104,128	1
55	MG	AA	3393	1/1	0.98	0.20	56,56,56,56	0
55	MG	AA	3060	1/1	0.98	0.24	70,70,70,70	0
55	MG	DA	1700	1/1	0.98	0.47	70,70,70,70	0
56	OHX	AA	3329	7/7	0.98	0.12	85,90,103,133	1
56	OHX	BA	1687	7/7	0.98	0.16	94,99,108,140	1
56	OHX	CA	3301	7/7	0.98	0.15	55,85,123,136	3
56	OHX	AA	3361	7/7	0.98	0.20	51,71,83,107	0
55	MG	BA	1752	1/1	0.98	0.47	53,53,53,53	0
56	OHX	DA	1766	7/7	0.98	0.10	118,124,133,175	1
56	OHX	AA	3327	7/7	0.98	0.13	107,115,135,188	1
56	OHX	CA	3322	7/7	0.98	0.13	104,117,127,154	1
56	OHX	AA	3321	7/7	0.98	0.11	97,109,121,173	1
56	OHX	AA	3308	7/7	0.98	0.17	66,73,104,120	2
56	OHX	CA	3233	7/7	0.98	0.16	74,85,95,121	0
56	OHX	CA	3336	7/7	0.98	0.13	114,127,138,191	0
55	MG	BA	1725	1/1	0.98	0.46	69,69,69,69	0
56	OHX	BA	1766	7/7	0.98	0.17	89,96,106,129	1
56	OHX	CA	3324	7/7	0.98	0.19	65,83,94,110	2
56	OHX	DA	1767	7/7	0.98	0.09	120,124,135,184	1
56	OHX	AB	207	7/7	0.98	0.15	89,99,126,152	1
55	MG	CA	3055	1/1	0.98	0.28	66,66,66,66	0
55	MG	CA	3052	1/1	0.98	0.39	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3334	7/7	0.98	0.17	66,79,94,105	1
55	MG	AA	3113	1/1	0.98	0.39	32,32,32,32	0
56	OHX	AA	3332	7/7	0.98	0.15	77,106,123,134	1
55	MG	BA	1623	1/1	0.98	0.30	67,67,67,67	0
56	OHX	CA	3314	7/7	0.98	0.16	84,93,97,114	1
56	OHX	CA	3294	7/7	0.98	0.14	91,93,107,125	1
56	OHX	CA	3299	7/7	0.98	0.15	99,105,124,141	1
55	MG	AA	3189	1/1	0.98	0.39	42,42,42,42	0
56	OHX	CA	3292	7/7	0.98	0.20	69,105,113,146	0
55	MG	CA	3014	1/1	0.98	0.30	76,76,76,76	0
56	OHX	CA	3287	7/7	0.98	0.17	69,74,104,109	3
56	OHX	AA	3501	7/7	0.98	0.16	101,109,129,149	1
56	OHX	CA	3288	7/7	0.98	0.16	87,95,104,133	0
56	OHX	DA	1738	7/7	0.98	0.09	115,122,137,171	1
55	MG	CA	3007	1/1	0.98	0.25	45,45,45,45	0
55	MG	CA	3011	1/1	0.98	0.35	46,46,46,46	0
55	MG	AA	3394	1/1	0.98	0.47	43,43,43,43	0
56	OHX	CA	3234	7/7	0.98	0.15	77,91,119,122	2
55	MG	CA	3006	1/1	0.98	0.20	47,47,47,47	0
56	OHX	CA	3273	7/7	0.99	0.20	58,69,86,110	0
56	OHX	AA	3427	7/7	0.99	0.19	29,70,88,108	0
55	MG	CA	3449	1/1	0.99	0.46	54,54,54,54	0
56	OHX	AA	3435	7/7	0.99	0.18	61,70,93,100	3
55	MG	CA	3138	1/1	0.99	0.45	53,53,53,53	0
56	OHX	DA	1722	7/7	0.99	0.15	84,90,106,116	0
56	OHX	AA	3455	7/7	0.99	0.17	56,75,100,119	2
56	OHX	AA	3439	7/7	0.99	0.15	69,82,92,115	1
56	OHX	AA	3428	7/7	0.99	0.19	67,79,86,113	0
56	OHX	CA	3271	7/7	0.99	0.23	67,82,101,115	0
56	OHX	BA	1763	7/7	0.99	0.15	94,115,123,136	0
56	OHX	AA	3445	7/7	0.99	0.15	75,87,109,120	1
55	MG	AA	3197	1/1	0.99	0.35	50,50,50,50	0
55	MG	DA	1625	1/1	0.99	0.13	97,97,97,97	0
56	OHX	AA	3320	7/7	0.99	0.18	69,81,96,121	1
56	OHX	DA	1721	7/7	0.99	0.14	94,108,116,135	0
56	OHX	CA	3236	7/7	0.99	0.20	81,104,120,146	0
56	OHX	AB	211	7/7	0.99	0.14	74,85,113,121	0
56	OHX	CA	3280	7/7	0.99	0.18	82,87,100,129	0
56	OHX	CA	3316	7/7	0.99	0.10	119,122,129,158	0
56	OHX	CA	3312	7/7	0.99	0.15	85,101,114,134	1
56	OHX	CB	208	7/7	0.99	0.13	105,109,142,147	0
56	OHX	AA	3424	7/7	0.99	0.18	92,97,108,112	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3313	7/7	0.99	0.12	103,112,124,157	0
56	OHX	AA	3301	7/7	0.99	0.15	88,89,93,110	1
56	OHX	BA	1775	7/7	0.99	0.10	111,114,129,169	1
56	OHX	AA	3292	7/7	0.99	0.17	50,75,88,112	0
56	OHX	CA	3281	7/7	0.99	0.19	101,105,126,132	0
56	OHX	AA	3418	7/7	0.99	0.20	39,61,82,95	0
55	MG	AA	3388	1/1	0.99	0.43	41,41,41,41	0
56	OHX	AA	3432	7/7	0.99	0.15	72,98,103,107	0
56	OHX	AA	3466	7/7	0.99	0.14	89,94,108,128	1
56	OHX	AA	3444	7/7	0.99	0.15	80,103,116,131	1
56	OHX	DA	1718	7/7	0.99	0.19	73,98,100,135	0
56	OHX	CA	3277	7/7	0.99	0.17	73,81,99,107	1
56	OHX	AA	3460	7/7	0.99	0.15	87,98,107,140	0
56	OHX	BA	1779	7/7	0.99	0.13	102,112,125,152	1
56	OHX	CA	3354	7/7	0.99	0.15	78,88,98,105	1
56	OHX	CA	3286	7/7	0.99	0.15	87,94,108,115	0
56	OHX	AA	3431	7/7	0.99	0.16	74,81,100,115	0
56	OHX	CA	3303	7/7	0.99	0.11	92,96,123,138	0
56	OHX	AA	3434	7/7	0.99	0.17	62,71,94,101	1
56	OHX	AA	3422	7/7	0.99	0.18	74,81,107,116	0
56	OHX	DA	1734	7/7	0.99	0.10	102,105,122,149	1
56	OHX	CA	3255	7/7	0.99	0.13	103,107,122,145	1
56	OHX	AA	3426	7/7	0.99	0.21	70,84,89,118	0
56	OHX	BA	1776	7/7	0.99	0.13	102,114,119,153	1
56	OHX	CA	3241	7/7	0.99	0.14	90,96,101,122	1
56	OHX	AA	3341	7/7	0.99	0.13	75,103,114,126	1
56	OHX	BA	1696	7/7	0.99	0.15	47,75,99,113	0
55	MG	A0	201	1/1	0.99	0.21	48,48,48,48	0
56	OHX	AA	3423	7/7	0.99	0.21	44,66,84,86	1
56	OHX	CA	3274	7/7	0.99	0.16	67,83,114,118	0
56	OHX	AA	3296	7/7	0.99	0.12	115,120,123,158	0
56	OHX	AA	3429	7/7	0.99	0.14	69,73,84,102	1
56	OHX	AO	204	7/7	0.99	0.14	83,94,106,121	1
56	OHX	CA	3275	7/7	0.99	0.15	56,80,112,114	1
56	OHX	CA	3327	7/7	0.99	0.14	76,83,103,129	1
56	OHX	CA	3329	7/7	0.99	0.11	102,103,123,146	1
56	OHX	AA	3293	7/7	0.99	0.16	54,82,88,102	2
56	OHX	BA	1755	7/7	0.99	0.19	72,74,97,109	0
56	OHX	AA	3430	7/7	0.99	0.17	63,78,92,111	1
56	OHX	CA	3256	7/7	0.99	0.16	88,101,112,126	1
56	OHX	AA	3288	7/7	0.99	0.20	76,85,101,127	1
56	OHX	CA	3283	7/7	0.99	0.16	81,83,86,120	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	CA	3305	7/7	0.99	0.16	70,83,99,129	1
56	OHX	CA	3310	7/7	0.99	0.14	74,88,107,129	1
56	OHX	AA	3436	7/7	0.99	0.11	78,91,117,117	0
56	OHX	AA	3457	7/7	0.99	0.15	73,83,101,131	1
56	OHX	AA	3335	7/7	0.99	0.12	94,101,113,136	1
56	OHX	AA	3462	7/7	0.99	0.15	75,85,103,106	1
56	OHX	BA	1756	7/7	0.99	0.20	59,79,107,108	0
56	OHX	BA	1758	7/7	0.99	0.17	69,88,100,119	0
55	MG	AA	3025	1/1	0.99	0.30	59,59,59,59	0
55	MG	AA	3375	1/1	0.99	0.37	31,31,31,31	0
55	MG	AA	3196	1/1	0.99	0.38	36,36,36,36	0
56	OHX	CA	3279	7/7	0.99	0.13	80,89,109,118	0
56	OHX	CA	3282	7/7	0.99	0.15	79,83,97,109	0
56	OHX	AA	3310	7/7	0.99	0.12	94,104,125,156	0
55	MG	CA	3050	1/1	0.99	0.27	65,65,65,65	0
56	OHX	AA	3360	7/7	0.99	0.16	58,67,70,97	1
56	OHX	AA	3291	7/7	0.99	0.17	68,75,102,108	3
56	OHX	AA	3446	7/7	0.99	0.15	68,90,101,115	2
55	MG	CA	3454	1/1	0.99	0.29	51,51,51,51	0
55	MG	BA	1654	1/1	0.99	0.35	47,47,47,47	0
55	MG	AA	3006	1/1	0.99	0.49	45,45,45,45	0
55	MG	AA	3210	1/1	0.99	0.49	41,41,41,41	0
55	MG	CA	3122	1/1	0.99	0.33	40,40,40,40	0
55	MG	AA	3115	1/1	0.99	0.32	51,51,51,51	0
56	OHX	CA	3239	7/7	0.99	0.16	66,92,107,113	1
56	OHX	BA	1780	7/7	0.99	0.16	94,102,115,117	1
56	OHX	AA	3437	7/7	0.99	0.14	81,95,107,131	0
56	OHX	BA	1765	7/7	0.99	0.12	111,119,130,164	0
56	OHX	DA	1742	7/7	0.99	0.10	117,127,141,176	1
56	OHX	CA	3461	7/7	0.99	0.20	38,55,94,109	0
56	OHX	AA	3433	7/7	0.99	0.17	63,65,104,122	1
56	OHX	CA	3291	7/7	0.99	0.13	86,105,118,139	0
56	OHX	AA	3363	7/7	0.99	0.14	90,99,133,145	1
56	OHX	CA	3289	7/7	0.99	0.14	69,83,106,125	0
56	OHX	AA	3459	7/7	0.99	0.14	71,92,105,129	1
56	OHX	AA	3463	7/7	0.99	0.15	77,89,96,134	1
56	OHX	AA	3443	7/7	0.99	0.16	69,76,84,127	1
56	OHX	DA	1723	7/7	0.99	0.15	107,111,116,151	0
56	OHX	AA	3419	7/7	0.99	0.18	67,75,91,95	0
55	MG	B1	101	1/1	0.99	0.50	26,26,26,26	0
56	OHX	AA	3309	7/7	0.99	0.17	64,84,90,112	1
55	MG	AA	3036	1/1	0.99	0.38	36,36,36,36	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	BG	302	7/7	0.99	0.09	128,137,145,186	1
55	MG	AA	3051	1/1	0.99	0.35	49,49,49,49	0
56	OHX	CA	3242	7/7	0.99	0.14	95,107,117,129	1
56	OHX	CA	3232	7/7	0.99	0.21	72,77,83,137	0
56	OHX	AA	3442	7/7	0.99	0.17	70,87,119,140	0
56	OHX	BA	1761	7/7	0.99	0.15	102,104,115,161	0
56	OHX	BA	1757	7/7	0.99	0.18	57,66,87,98	2
56	OHX	CA	3270	7/7	0.99	0.16	73,87,105,117	0
57	ZN	BQ	102	1/1	0.99	0.09	130,130,130,130	0
56	OHX	DA	1746	7/7	0.99	0.09	126,134,146,189	1
56	OHX	AA	3294	7/7	0.99	0.12	94,100,117,120	0
56	OHX	CA	3326	7/7	0.99	0.12	97,110,130,136	2
56	OHX	AA	3438	7/7	0.99	0.17	51,64,72,96	2
56	OHX	CA	3290	7/7	0.99	0.13	94,101,123,130	0
56	OHX	CA	3276	7/7	0.99	0.17	81,100,117,133	0
56	OHX	DA	1719	7/7	0.99	0.16	79,99,112,124	0
56	OHX	BA	1762	7/7	0.99	0.17	72,94,107,136	0
56	OHX	AA	3440	7/7	0.99	0.17	59,88,102,124	0
56	OHX	AA	3315	7/7	0.99	0.13	89,99,111,137	1
55	MG	AA	3343	1/1	0.99	0.43	34,34,34,34	0
56	OHX	DA	1727	7/7	0.99	0.14	114,126,131,160	0
56	OHX	AA	3297	7/7	0.99	0.15	87,98,102,106	1
56	OHX	AA	3453	7/7	0.99	0.12	95,106,114,148	0
56	OHX	CA	3297	7/7	0.99	0.14	84,94,129,142	1
55	MG	AE	301	1/1	0.99	0.31	52,52,52,52	0
56	OHX	AA	3420	7/7	0.99	0.22	63,69,102,115	0
56	OHX	CA	3332	7/7	0.99	0.15	70,82,93,103	1
56	OHX	BA	1760	7/7	0.99	0.15	71,106,126,148	0
56	OHX	AA	3289	7/7	1.00	0.19	53,58,81,93	0
56	OHX	AF	303	7/7	1.00	0.21	45,52,58,77	0
56	OHX	AE	304	7/7	1.00	0.16	74,87,107,110	1
56	OHX	AA	3421	7/7	1.00	0.20	50,71,87,114	0
56	OHX	CA	3272	7/7	1.00	0.20	54,70,84,85	1
56	OHX	AA	3417	7/7	1.00	0.21	68,72,82,103	0
56	OHX	AA	3399	7/7	1.00	0.20	42,51,73,98	0
56	OHX	AA	3359	7/7	1.00	0.18	61,75,93,113	0
56	OHX	CF	301	7/7	1.00	0.18	54,58,79,92	0
56	OHX	AA	3425	7/7	1.00	0.19	45,61,75,79	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.