



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 02:11 PM EDT

PDB ID : 4V8F  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-ttyr complex with paromomycin).  
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  
buster-report : 1.1.7 (2018)  
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

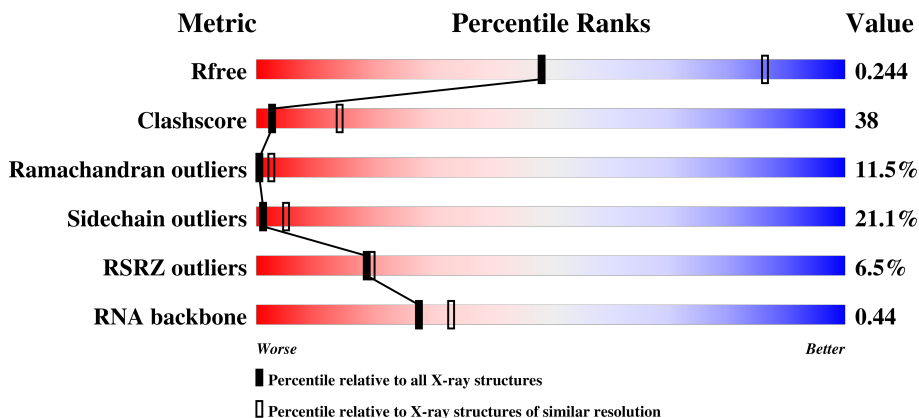
# 1 Overall quality at a glance

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></div> <div>28% 49% 21% .</div> </div>
1	DA	2912	<div> <div>2%</div> <div>27% 50% 21% .</div> </div>
2	AB	122	<div> <div></div> <div>24% 55% 19% .</div> </div>
2	DB	122	<div> <div></div> <div>23% 55% 21% .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AD	276	
3	DD	276	
4	AE	206	
4	DE	206	
5	AF	210	
5	DF	210	
6	AG	182	
6	DG	182	
7	AH	180	
7	DH	180	
8	AK	148	
8	DK	148	
9	AM	140	
9	DM	140	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
13	D0	118	
14	AQ	112	
14	DQ	112	
15	AR	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	DR	146	
16	A1	118	
16	D1	118	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	96	
19	DT	96	
20	AU	110	
20	DU	110	
21	AV	206	
21	DV	206	
22	A3	85	
22	D3	85	
23	AZ	98	
23	DZ	98	
24	AW	72	
24	DW	72	
25	AX	60	
25	DX	60	
26	A4	71	
26	D4	71	
27	A5	60	
27	D5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A6	54	
28	D6	54	
29	A7	49	
29	D7	49	
30	A8	65	
30	D8	65	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	85	
52	BD	85	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	CB	85	
52	CD	85	
53	BC	77	
53	CC	77	
54	B1	16	
54	C1	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	A3	101	-	-	-	X
55	MG	AA	3096	-	-	-	X
55	MG	AA	3142	-	-	-	X
55	MG	AA	3215	-	-	-	X
55	MG	AA	3222	-	-	-	X
55	MG	AA	3236	-	-	-	X
55	MG	AA	3245	-	-	-	X
55	MG	AA	3277	-	-	-	X
55	MG	AA	3279	-	-	-	X
55	MG	AA	3291	-	-	-	X
55	MG	AA	3305	-	-	-	X
55	MG	AA	3337	-	-	-	X
55	MG	BA	1615	-	-	-	X
55	MG	BA	1624	-	-	-	X
55	MG	BA	1675	-	-	-	X
55	MG	BA	1699	-	-	-	X
55	MG	BA	1714	-	-	-	X
55	MG	BB	104	-	-	-	X
55	MG	BB	106	-	-	-	X
55	MG	CA	1629	-	-	-	X
55	MG	CA	1641	-	-	-	X
55	MG	CA	1668	-	-	-	X
55	MG	CA	1672	-	-	-	X
55	MG	CA	1674	-	-	-	X
55	MG	CA	1685	-	-	-	X
55	MG	CA	1686	-	-	-	X
55	MG	CA	1699	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	1720	-	-	-	X
55	MG	CB	101	-	-	-	X
55	MG	CC	103	-	-	-	X
55	MG	CC	104	-	-	-	X
55	MG	DA	3048	-	-	-	X
55	MG	DA	3053	-	-	-	X
55	MG	DA	3112	-	-	-	X
55	MG	DA	3145	-	-	-	X
55	MG	DA	3158	-	-	-	X
55	MG	DA	3196	-	-	-	X
55	MG	DA	3201	-	-	-	X
55	MG	DA	3203	-	-	-	X
55	MG	DA	3252	-	-	-	X
55	MG	DA	3295	-	-	-	X
55	MG	DA	3307	-	-	-	X
55	MG	DA	3311	-	-	-	X
55	MG	DA	3320	-	-	-	X
55	MG	DA	3330	-	-	-	X
55	MG	DA	3331	-	-	-	X
55	MG	DB	206	-	-	-	X
56	OHX	AA	3330	-	-	X	-
56	OHX	AA	3365	-	-	X	-
56	OHX	AA	3504	-	-	X	-
56	OHX	AA	3547	-	-	X	-
56	OHX	BA	1785	-	-	X	-
56	OHX	BA	1802	-	-	X	-
56	OHX	CA	1762	-	-	X	-
56	OHX	CA	1798	-	-	X	-
56	OHX	CC	108	-	-	X	-
56	OHX	D8	101	-	-	X	-



## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 304031 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	DA	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
DA	168	U	-	insertion	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	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	DB	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	DD	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	DE	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	DF	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	DG	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	DH	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	DK	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	DM	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	DN	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	DO	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	DP	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	D0	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	DQ	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	DR	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	D1	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	D2	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	DS	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	DT	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	DU	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	DV	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	D3	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	DZ	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	DW	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	DX	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	D4	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	D5	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	D6	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	D7	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	D8	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	CA	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	CE	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	CF	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	CG	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	CH	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	CI	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	CJ	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	CK	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	CL	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	CM	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	CN	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	CO	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	CP	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	CQ	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	CR	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	CS	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	CT	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	CU	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	CV	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	CW	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	CX	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	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
52	CD	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	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

- 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	C1	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	114	Total	Mg	0	0
			114	114		
55	CA	121	Total	Mg	0	0
			121	121		
55	AB	6	Total	Mg	0	0
			6	6		

*Continued on next page...*

*Continued from previous page...*

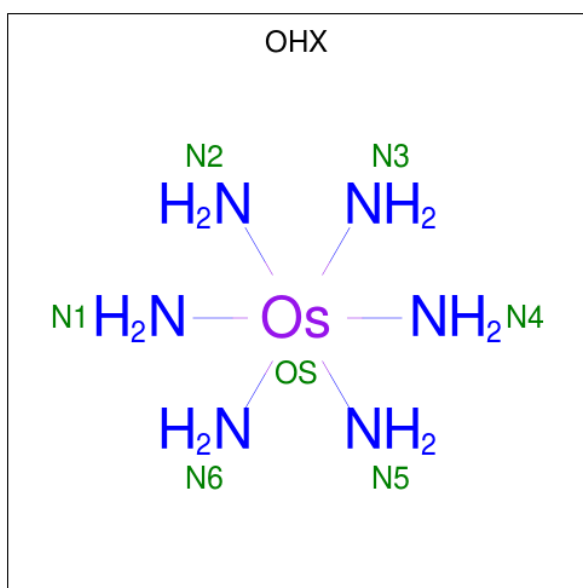
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B1	1	Total 1	Mg 1	0	0
55	C1	2	Total 2	Mg 2	0	0
55	BB	13	Total 13	Mg 13	0	0
55	AE	3	Total 3	Mg 3	0	0
55	BF	1	Total 1	Mg 1	0	0
55	AA	332	Total 332	Mg 332	0	0
55	A5	1	Total 1	Mg 1	0	0
55	D7	1	Total 1	Mg 1	0	0
55	BC	4	Total 4	Mg 4	0	0
55	A1	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	7	Total 7	Mg 7	0	0
55	DA	272	Total 272	Mg 272	0	0
55	A0	1	Total 1	Mg 1	0	0
55	DE	1	Total 1	Mg 1	0	0
55	CB	3	Total 3	Mg 3	0	0
55	BS	1	Total 1	Mg 1	0	0
55	A7	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AO	1	Total	Mg	0	0
			1	1		
55	BW	1	Total	Mg	0	0
			1	1		
55	A3	1	Total	Mg	0	0
			1	1		
55	AF	2	Total	Mg	0	0
			2	2		
55	DB	7	Total	Mg	0	0
			7	7		

- 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	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		
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		

*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	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		
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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	BC	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	1	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	CK	1	Total	N	Os	0	0
			7	6	1		
56	CR	1	Total	N	Os	0	0
			7	6	1		
56	CV	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	CC	1	Total	N	Os	0	0
			7	6	1		
56	CC	1	Total	N	Os	0	0
			7	6	1		
56	CC	1	Total	N	Os	0	0
			7	6	1		
56	CD	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		

*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		

*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		

*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	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...*

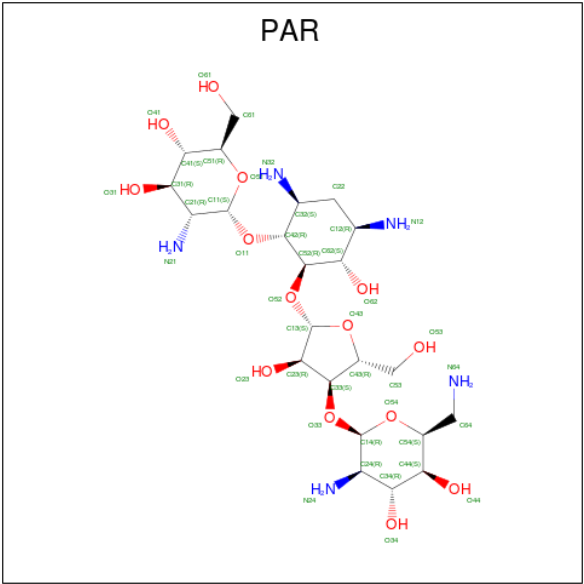
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0	0
			7	6	1		
56	DA	1	Total	N	Os	0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

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	DB	1	Total	N	Os	0	0
			7	6	1		
56	DB	1	Total	N	Os	0	0
			7	6	1		
56	DF	1	Total	N	Os	0	0
			7	6	1		
56	DO	1	Total	N	Os	0	0
			7	6	1		
56	D1	1	Total	N	Os	0	0
			7	6	1		
56	D3	1	Total	N	Os	0	0
			7	6	1		
56	D5	1	Total	N	Os	0	0
			7	6	1		
56	D8	1	Total	N	Os	0	0
			7	6	1		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	5	14		
57	CA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

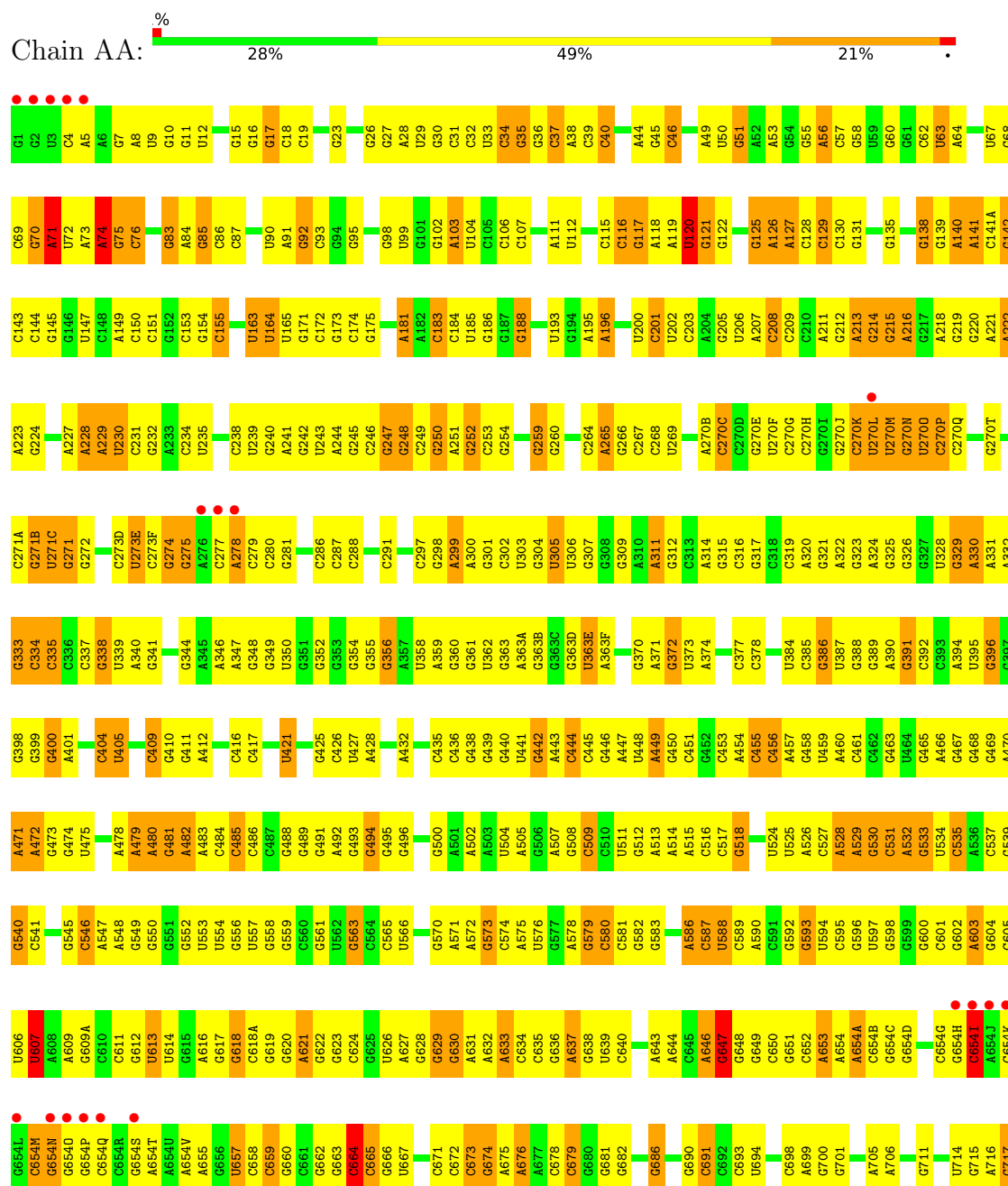
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BG	1	Total	Zn	0	0
			1	1		
58	BQ	1	Total	Zn	0	0
			1	1		
58	CQ	1	Total	Zn	0	0
			1	1		
58	CG	1	Total	Zn	0	0
			1	1		



### 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)

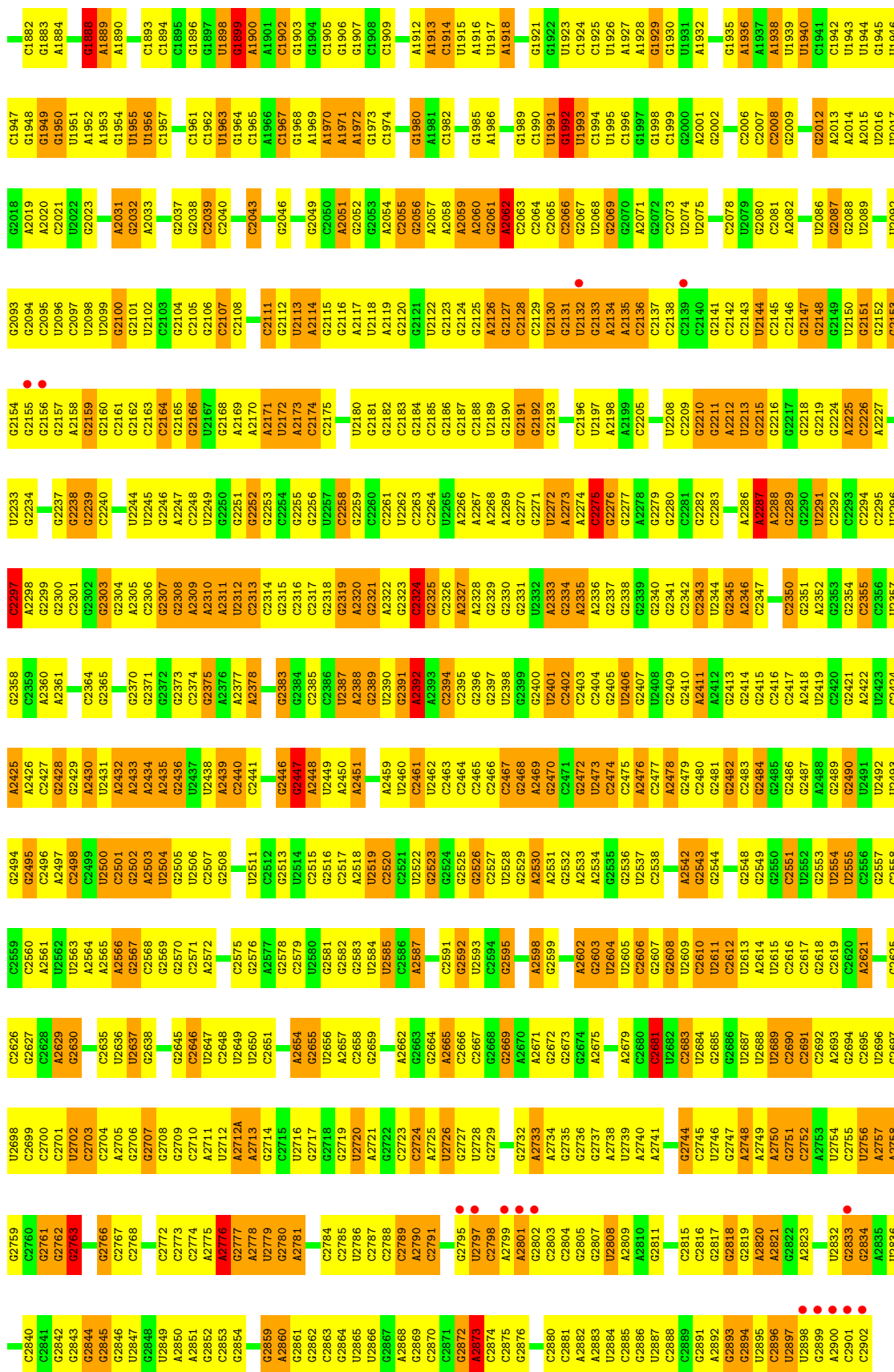


G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733																																																										
C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649																																																																				
G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575												
C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575												
G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475																																																			
C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475																																																			
A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315																																																																																
C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315																																																																																
G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253
C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253
A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111																																																																																		
C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111																																																																																		
G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051																																																																												
C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051																																																																												
C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985																																																																							
G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893																																																																																																							

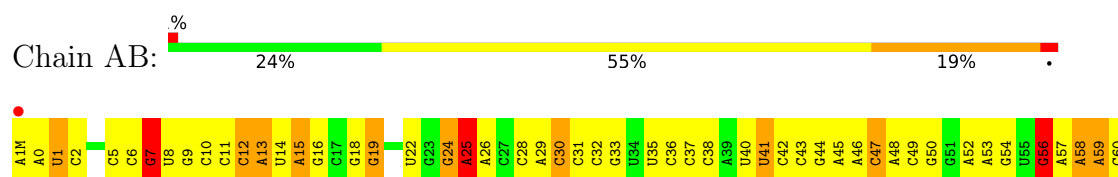
A2734	C2666	A2598	A2531	C2452	G2391	G2356	A2173	C2111	A2030	A1953	G1888	G1734
C2667	C2667	G2599	G2532	A2453	A2892	U2257	C2174	G2112	A2031	G1954	A1889	C1735
G2668	G2668	A2800	A2533	G2454	A2993	C2258		G2113	G2032	A1955	A1890	C1741
A2741	G2669	C2601	G2536	U2457	C2394	G2259	G2181	A2114	A2033	U1956		C1742
C2742	A2670	G2602	G2537	C2458	C2395	U2262	C2182	G2115	G2034	C1957	C1893	G1743
G2743	A2671	G2603	U2537		C2396	C2263	C2183	G2116	G2035		C1894	G1746
G2744	G2672	U2604	C2538		G2397		G2184	A2117	C2036	U1962	G1895	
G2745	G2673	U2605	G2539	C2461	U2398	A2267	C2186	U2118	G2037	U1963	G1896	A1749
		G2606	C2540	U2462	G2400	A2268	G2187	U2119	G2038	G1964		G1750
		G2607	A2541		U2401	A2269		A2120	C2039	U1965	G1816	G1751
		G2608	A2542	C2467	C2402	A2270	G2190	G2121		A1966	G1817	C1752
		U2609	G2543	C2468	C2403	G2270	G2191	U2122		G1967	A1901	C1753
		G2610	G2544	A2469	C2404	G2271	G2192	G2123		G1968	A1819	G1754
		U2611	G2545	G2470	C2405	U2272	G2193	G2124		A1969	U1820	A1755
		G2612	C2546		G2406	U2273	G2194	G2125	G2048	A1970	G1824	
		U2613	U2547	C2471	U2407	A2274	G2195	G2126	G2049	A1971	A1825	G1756
		A2614	G2548	U2472	C2408	C2275	G2196	U2127	C2050	A1972	G1826	U1757
		G2615	G2549	C2473	G2409	G2276	G2197	G2128	A2054	G1973	G1827	G1758
		U2616		C2474	C2410	G2277	A2198	U2129	C2055		C1908	A1760
		C2617	G2553	A2475		A2278	C2206	U2130	G2056	G1980	A1828	C1761
		U2618	U2554		G2413	C2281	C2207	G2131	A2057	A1981	A1829	
		G2619	C2555	A2476	G2414	C2282		U2132	A2058	A1982	C1830	A1762
		C2620	C2556		G2415	U2283	G2198	G2133	A2059	C1983	G1831	G1763
			G2557	G2481	G2416	C2284	A2199	A2134	A2060	G1984	U1833	C1765
			C2558	G2482	G2417	C2285	C2208	U2135	G2061	G1985	U1834	U1766
			C2559		G2418	C2286	G2209	G2136	A2062		G1835	
			C2560	G2486	A2419	A2287	U2210	C2137	C2063	G1989	A1916	G1769
			A2561	G2487	U2420	C2288	U2211	C2138	C2064	C1990	U1917	G1770
			U2562	A2488	G2421	A2289	U2212	G2139	C2065	A1991	G1839	C1771
			G2563	G2489	G2422	G2290	G2213	C2140		G1992	A1918	G1772
			A2564	G2490	U2423	U2291	G2214	G2141	U2068	U1993	C1920	A1773
			A2565		C2424		G2215	C2142	G2069	C1994	G1921	C1774
			A2566		A2425	C2294	G2216	C2143	G2070	U1995	G1922	U1775
			C2567	G2494	A2426	C2295	G2217	U2144		G1997	U1923	G1776
			C2568		A2427			A2225		A2001	C1924	U1777
				C2498	A2428			G2145	C2078		C1925	U1778
				U2499	G2429	A2298		G2146	G2080	U1926	U1926	U1779
				U2500	C2430	G2299	U2233	G2147	C2081	A1927	A1853	A1780
				C2501	A2431	G2300	G2234	G2148	A2082	A1928	A1854	C1781
				G2502	U2432	C2301	G2235	U2150	G2083	G1929		G1782
				U2503	A2433	G2302	C2236	G2151		U1930	G1858	A1783
				G2504	A2434	G2303	G2237	G2152	U2086	U1931	A1859	A1784
				U2505	A2435	G2304	G2238	G2153	U2087	G1932	G1860	A1785
				G2506	A2436	A2305	G2239	G2154		G1933		A1786
				C2507	A2437	C2306	C2240	G2155	U2092	A2013	G1863	A1787
				G2508	U2438	G2307	A2241	G2156	G2093	A2014	U1864	C1788
					A2439	G2308	G2242	G2157	G2094	A2015	G1869	U1798
					C2440	A2309	U2243	G2160	U2095	A1936	C1870	G1799
					G2441	A2310	U2244	U2167	G2096	U2017	A1871	C1790
					C2442	A2311	U2245	G2168	G2097	G2018	A1938	A1791
					G2443	C2312	G2246	G2169	U2098	A2019	A1872	
					C2444	C2313	U2247	C2163	U2099	A2020	G1878	U1796
					G2445	C2314	A2248	C2164	G2100	C1941	C1879	C1797
					G2446	G2315	U2249	G2165	G2101	C2021	C1880	U1798
					G2447	C2316	G2250	G2166	U2102	G1942	G1799	U1799
					A2448	C2317	G2251	G2167	G2023	G1945	C1882	C1800
					U2449	C2318	G2252	A2169	G2024	U1946	G1883	G1801
					A2450	C2319	G2253	A2170	C2103		A1884	A1802
					U2451	A2320	C2254	A2171	C2108	G1950	A1885	A1803
					A2452	U2321	G2255	U2172	G2109	U1951	C1886	C1804
					U2390				G2110	G1952	C1887	U1805



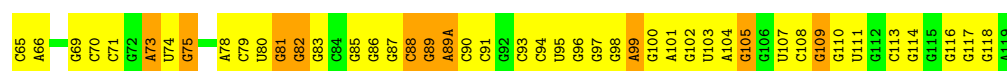
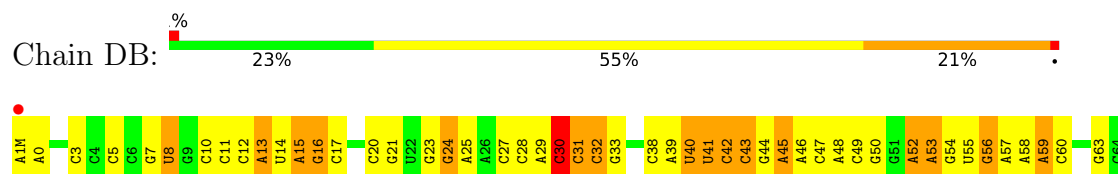
G1795	G1717	G1643	G1573	G1504	C1437	A1365	C1297	A1220	C1158	C1092	A1029	G988	G906	G845
U1796	G1718	G1644	G1574	C1505	U1438	G1368	C1298	C1223	U1159	G1093	G1030	U969	U907	C846
C1797	G1725	C1644	C1575	C1506	A1439	G1369	C1299	G1224	C1160	U1094	G1031	C970	C908	U847
C1800	U1727	G1647	C1576	A1507	G1440	G1370	U1300	C1225	C1161	A1095	A1032	C971	A909	G848
C1801	U1728	G1648	C1577	A1508	G1441	G1371	U1301	G1226	G1163	U1096	U1033	G972	A910	C849
A1802	U1729	G1649	C1578	C1509	G1442	U1372	A1302	A1227	G1164	U1097	G1034	A973	A911	C850
					G1443				U1165	A1098	U1035	G974	C912	U851
					G1444				U1166	G1099	G1036	G974A	U913	U852
					A1444A				C1167	C1100		G975	C914	G853
					A1445				U1167	G1099		G976	C915	G854
					C1446				G1168	C1040		G977	C916	G855
					G1447				C1169	G1041		G978	A917	C856
					G1448				G1170	U1105		G979	A918	C857
					A1449				G1171	G1042		A980	A919	U858
					G1449A				G1172	G1043		A981	G920	G859
					C1450				A1173	A1044		C982	G921	U860
					A1451				U1174	U1045		A983	U922	A861
					A1453				G1175	A1046		A984	C923	G862
									U1176	G1047		A985	G924	A863
									A1177	A1048		C986	C925	G864
									C1178	C1049		C987	A926	C865
									C1179	A1050		A988	C928	A866
									C1180	G1051		G989	G929	C867
									C1181	C1052		A990	U930	U868
									A1182	C1053		C991	G931	G869
									G1183	A1054		C992	G932	A870
									G1184	G1055		G993	A934	U871
									C1187	A1056		C994	A935	A872
									U1188	U1058		C995	C935	G873
									A1189	A1059		A996	G936	G874
									G1190	U1060		G997	U937	G875
									C1191	U1061		C998	U938	C876
									G1192	G1062		U999	U877	U877
									C1193	G1063		A1000	G940	A878
									A1194	C1064		A1001	G941	G879
									G1195	U1065		G1002	G942	G880
									C1196	U1066		G1003	U943	G881
									G1197	A1067		C1004	G944	G882
									U1198	G1068		C1005	A945	G883
									C1199	A1069		C1006	G946	C884
									C1200	G1070		C1007	G947	C885
									C1201	A1071			G948	C886
									G1202	C1072			G949	A887
									U1141	A1073			G950	C888
									A1142	G1074			C951	C889
									A1143	C1075			G952	A890
									C1144	G1076			A953	G892
									C1145	A1077			G954	C893
									G1146	U1078			G955	C894
									C1147	C1079			G956	U895
									U1148	A1080			A957	A896
									C1149	U1081			U958	C897
									G1150				A959	C898
									A1151	A1085			A960	A899
									C1152	G1086			G961	A900
									G1153	G1087			A901	C902
									C1154	A1088			G962	A901
									G1155	G1089			U963	C902
									A1156	U1090			G966	C903
									C1157	G1091			C967	U905



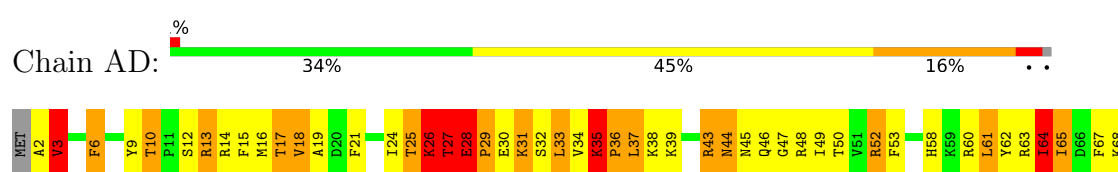
- Molecule 2: 5S RIBOSOMAL RNA



• Molecule 2: 5S RIBOSOMAL RNA

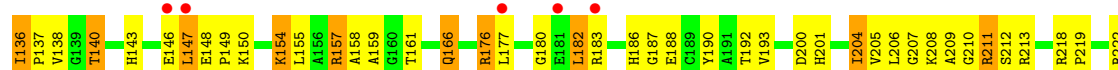
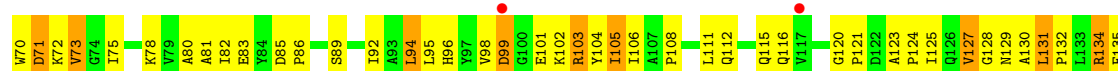
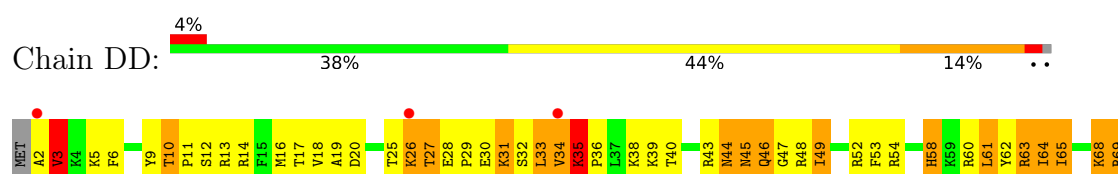


• Molecule 3: 50S ribosomal protein L2



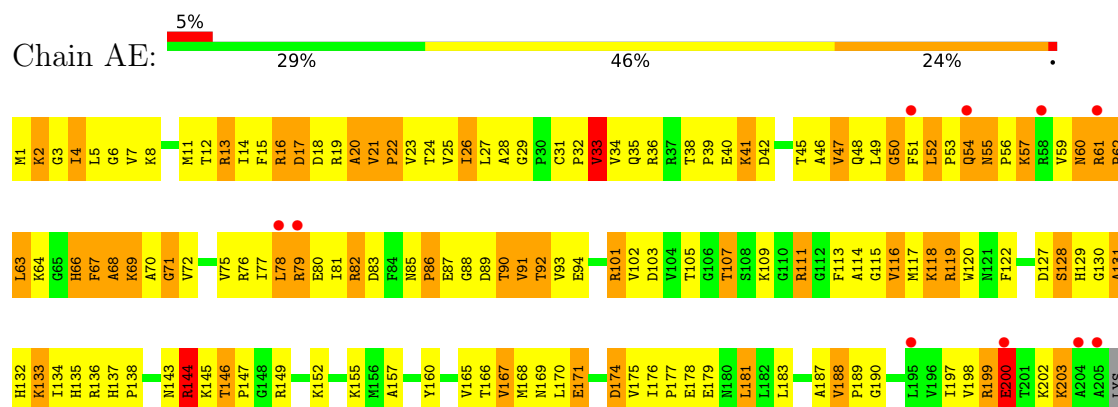
LYS

• Molecule 3: 50S ribosomal protein L2

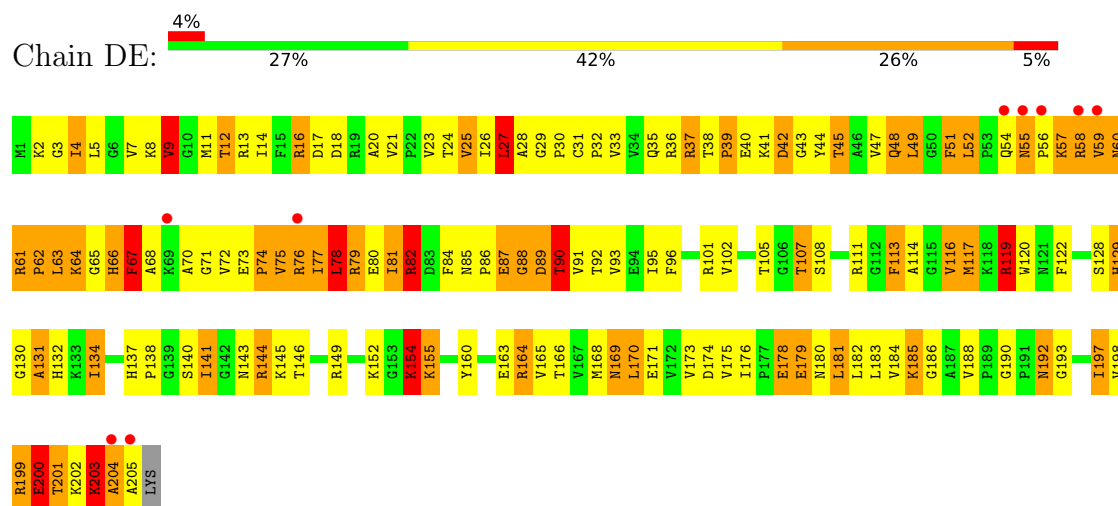




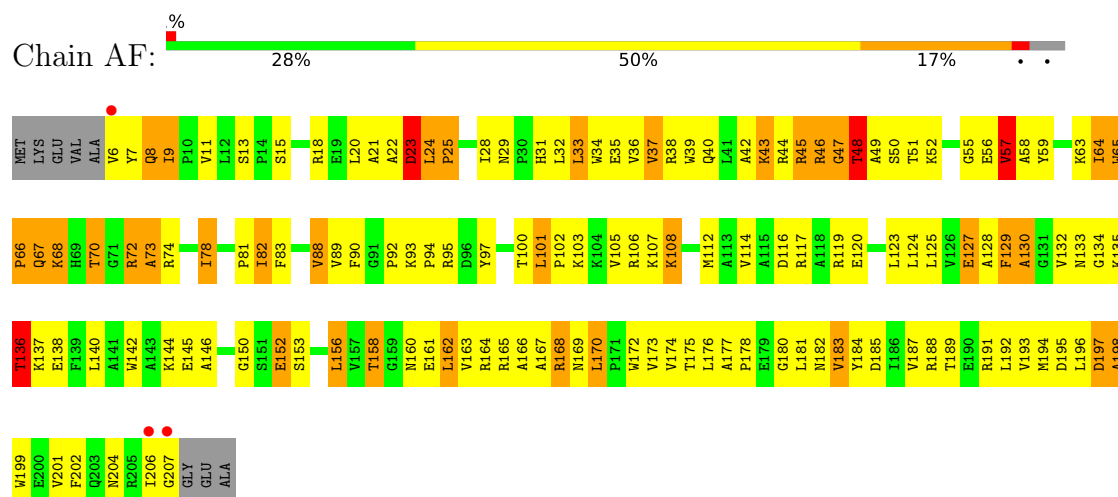
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

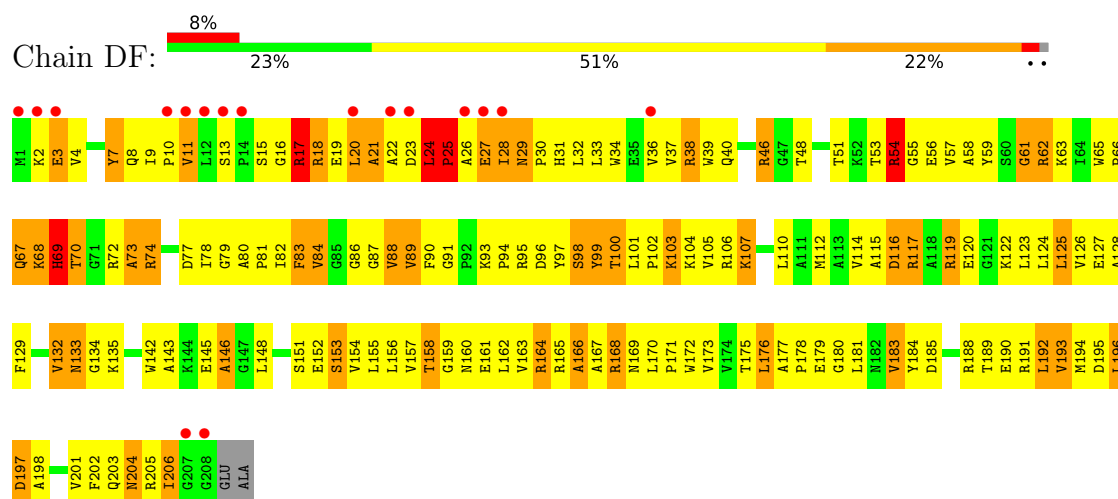


• Molecule 5: 50S ribosomal protein L4

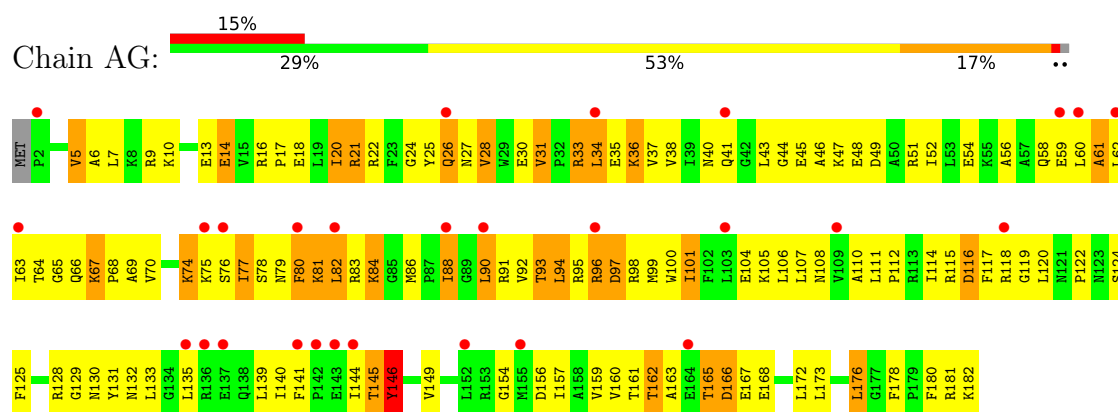




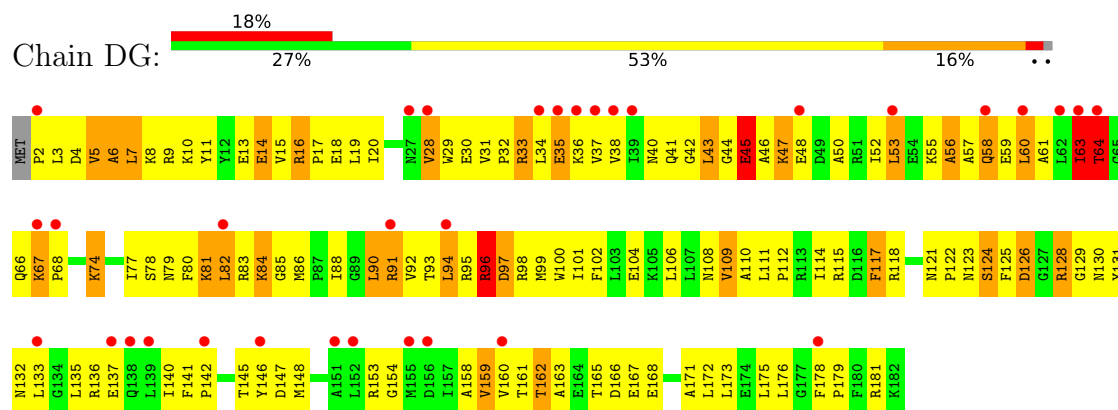
- Molecule 5: 50S ribosomal protein L4



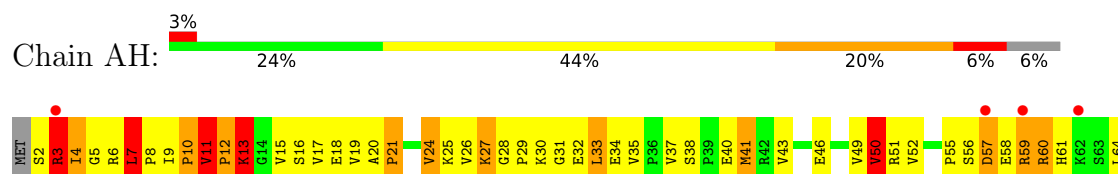
- Molecule 6: 50S ribosomal protein L5

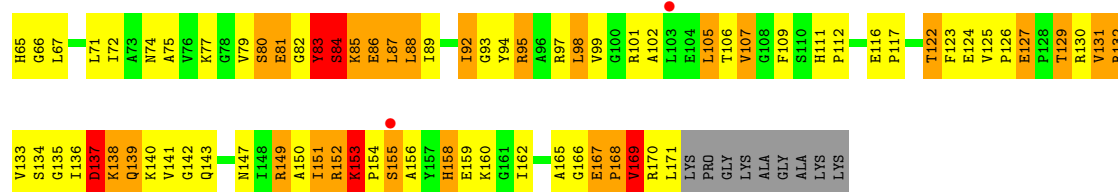


- Molecule 6: 50S ribosomal protein L5

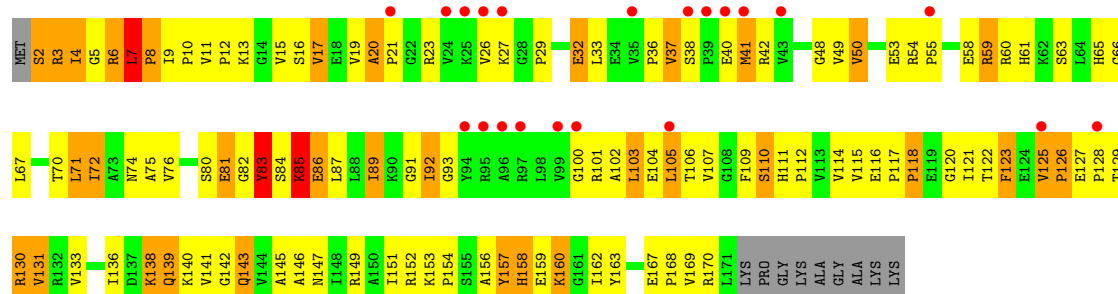


- Molecule 7: 50S ribosomal protein L6

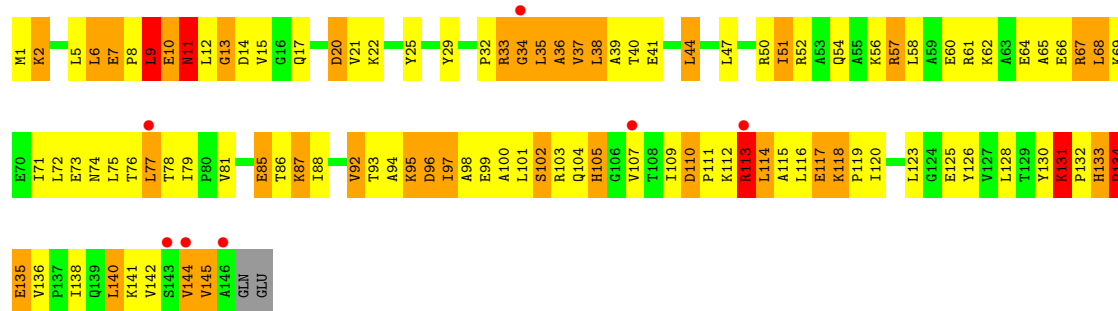




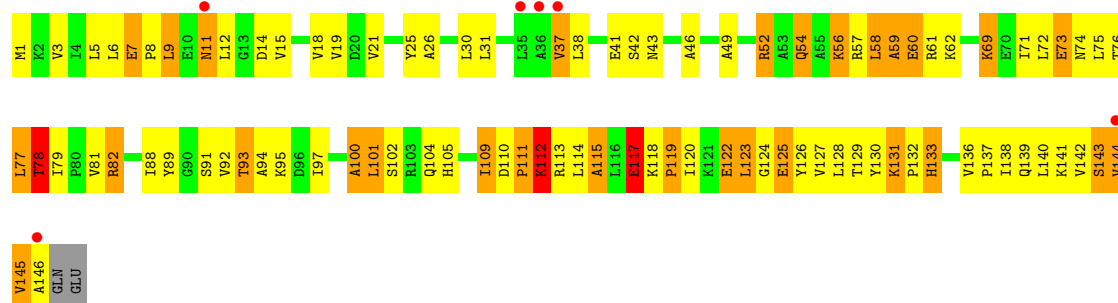
• Molecule 7: 50S ribosomal protein L6



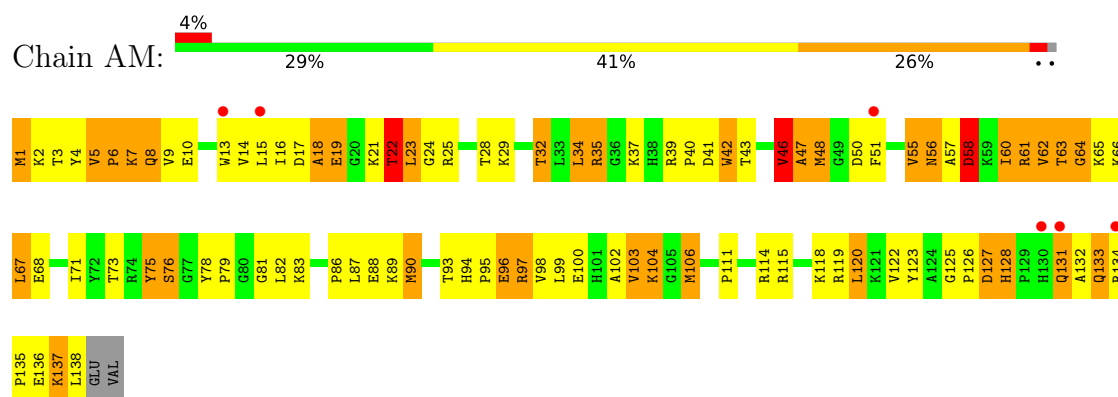
• Molecule 8: 50S ribosomal protein L9



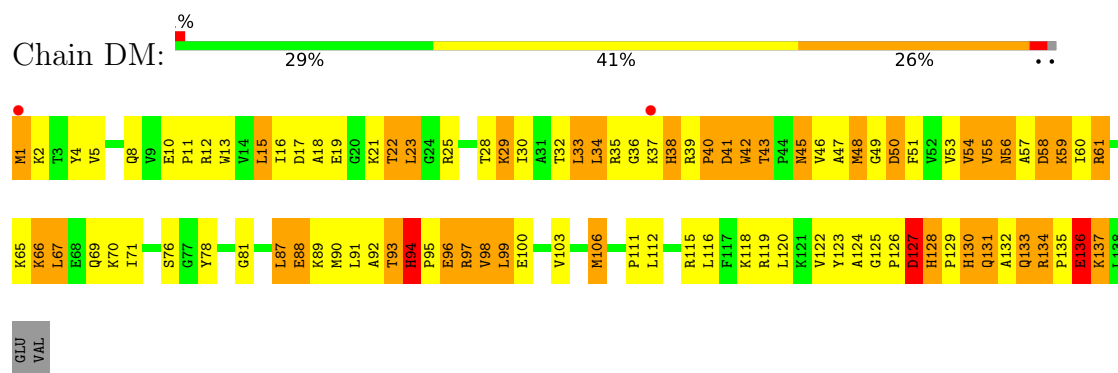
• Molecule 8: 50S ribosomal protein L9



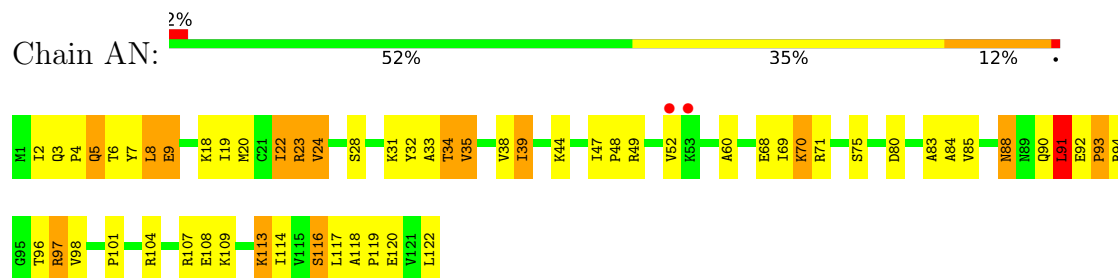
• Molecule 9: 50S ribosomal protein L13



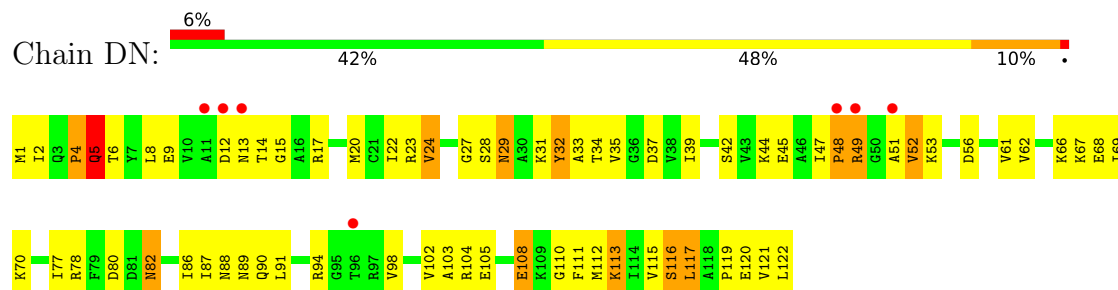
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

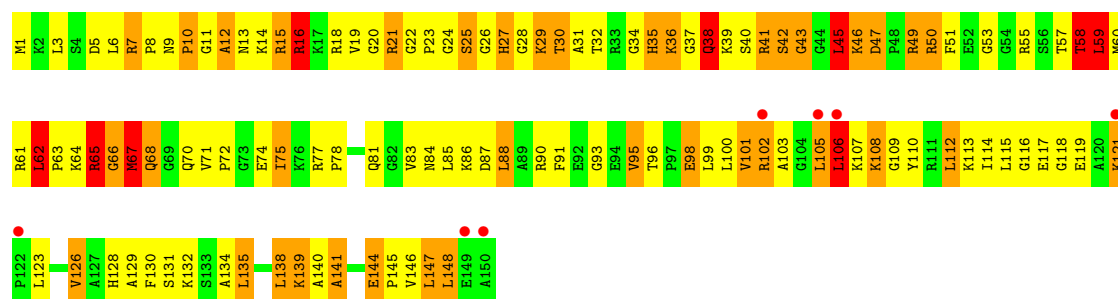


• Molecule 10: 50S ribosomal protein L14

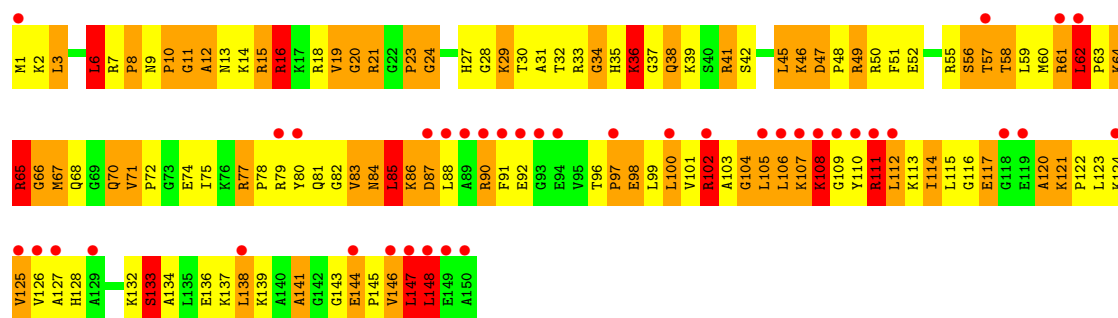
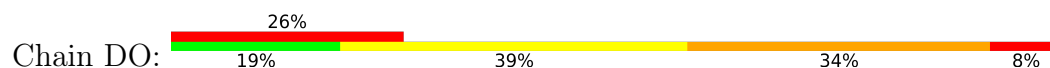


• Molecule 11: 50S ribosomal protein L15

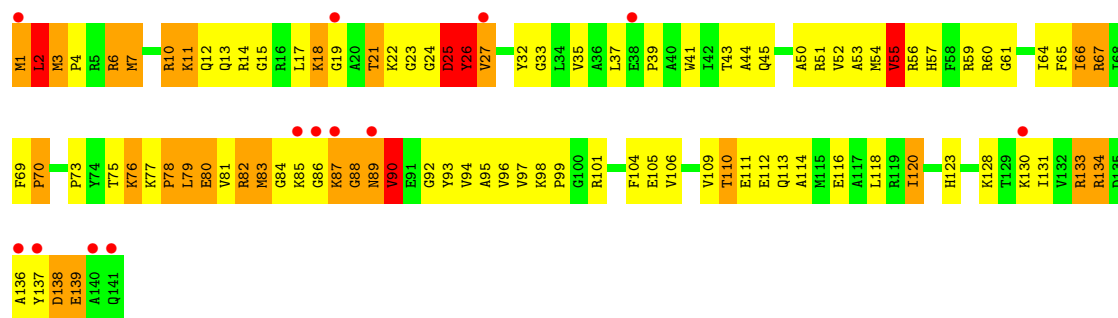




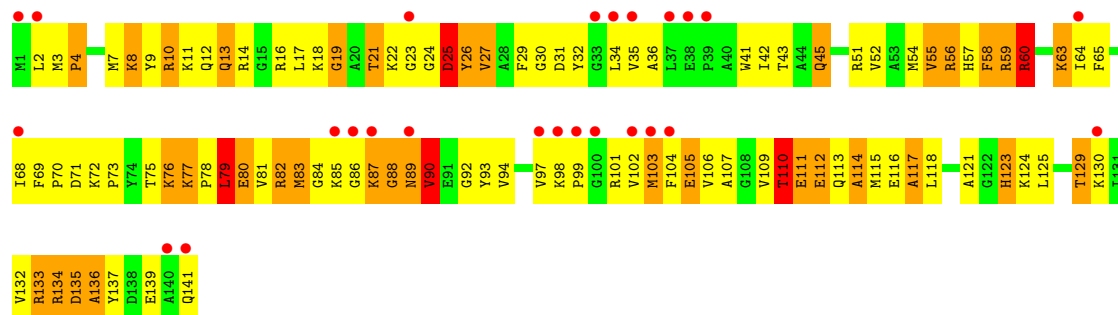
• Molecule 11: 50S ribosomal protein L15



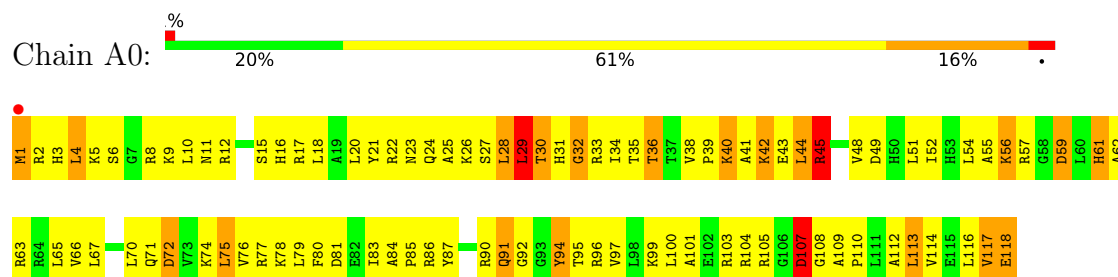
• Molecule 12: 50S ribosomal protein L16



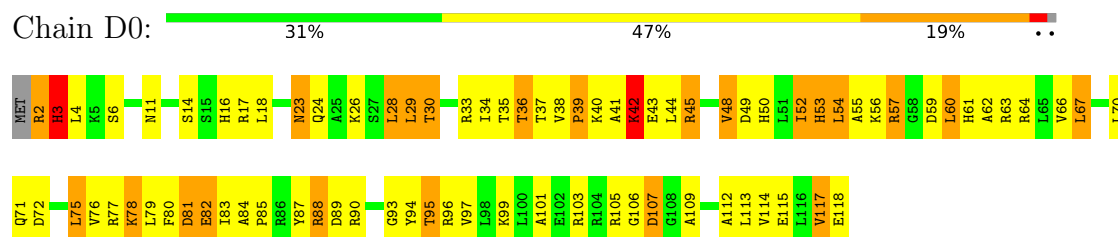
• Molecule 12: 50S ribosomal protein L16



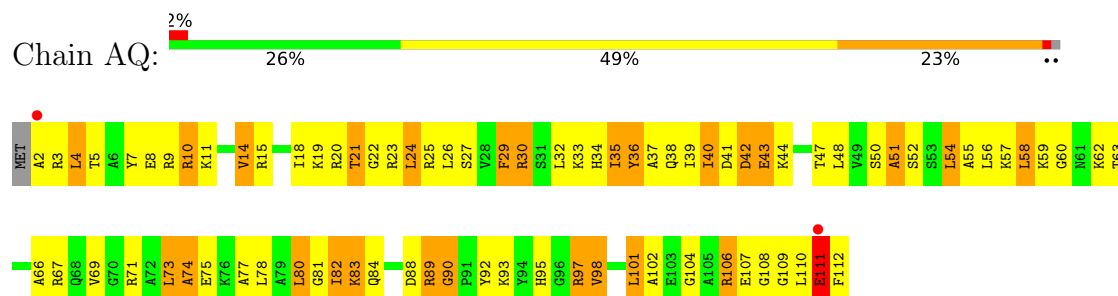
- Molecule 13: 50S ribosomal protein L17



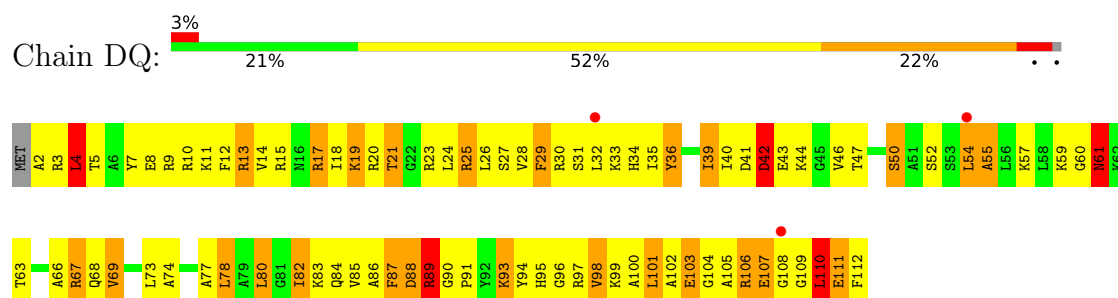
- Molecule 13: 50S ribosomal protein L17



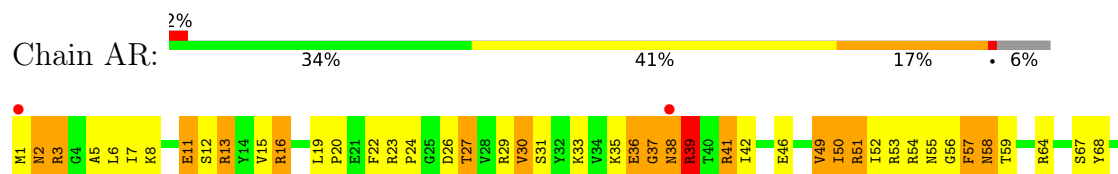
- Molecule 14: 50S ribosomal protein L18

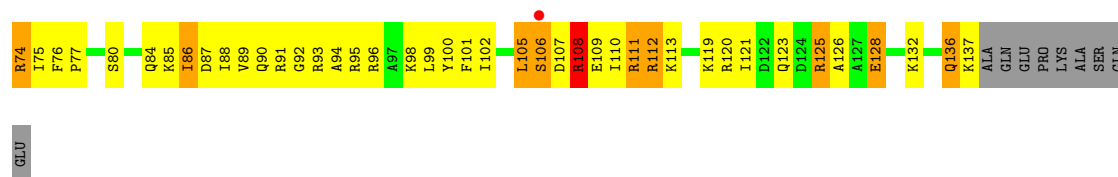


- Molecule 14: 50S ribosomal protein L18

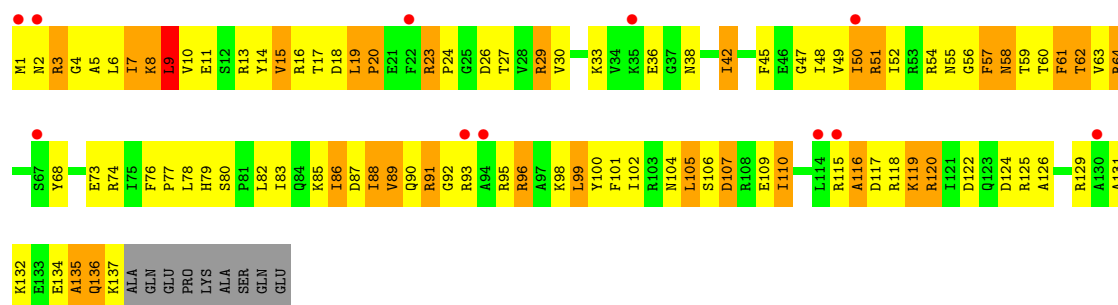


- Molecule 15: 50S ribosomal protein L19

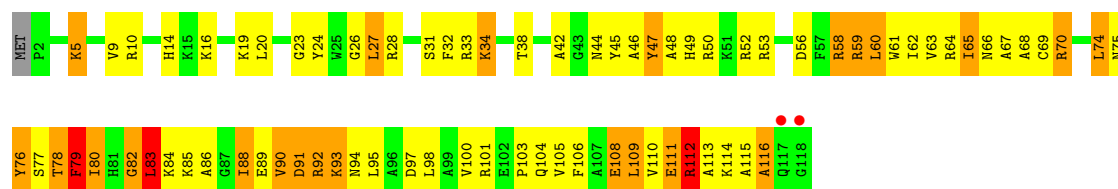




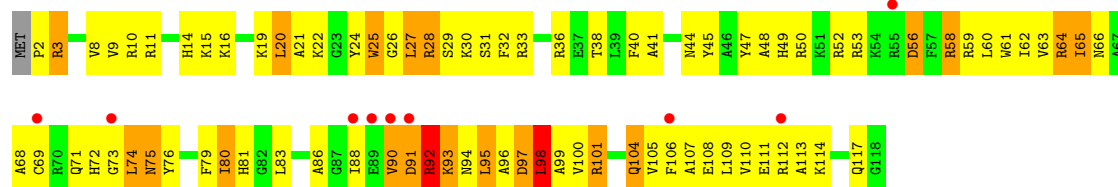
• Molecule 15: 50S ribosomal protein L19



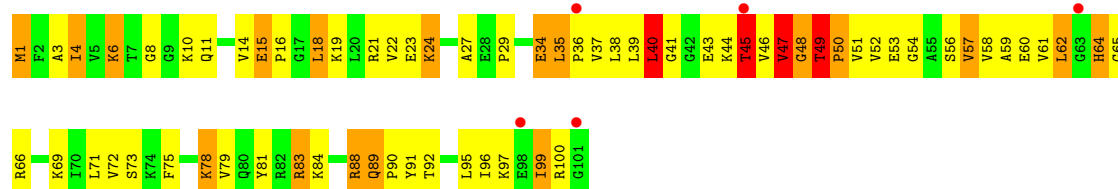
• Molecule 16: 50S ribosomal protein L20



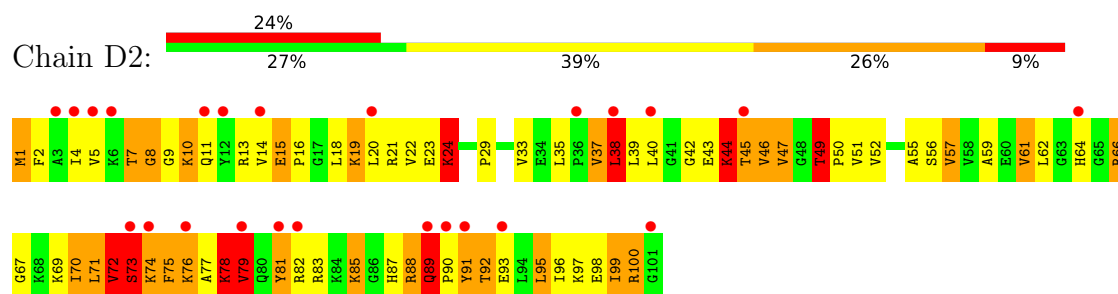
• Molecule 16: 50S ribosomal protein L20



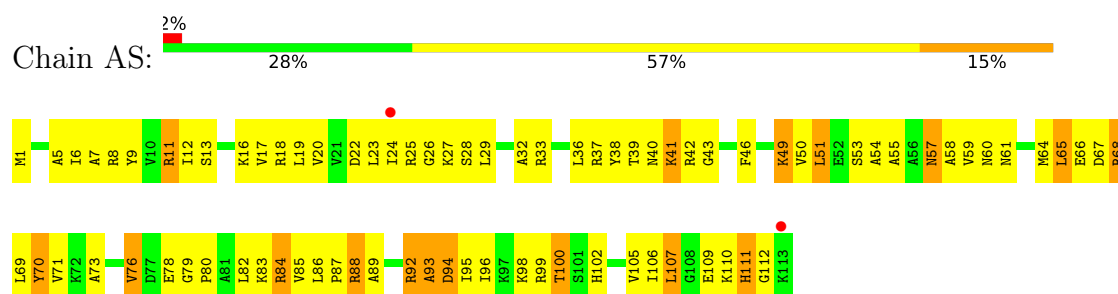
• Molecule 17: 50S ribosomal protein L21



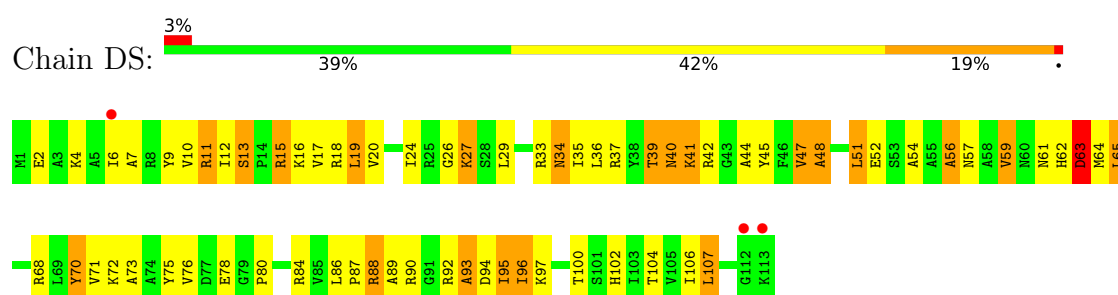
- Molecule 17: 50S ribosomal protein L21



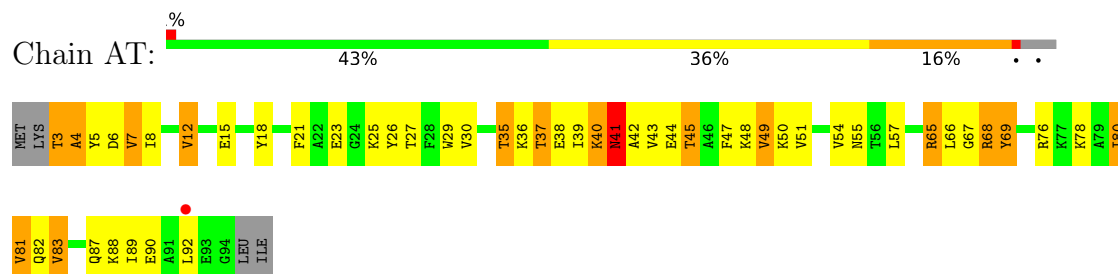
- Molecule 18: 50S ribosomal protein L22



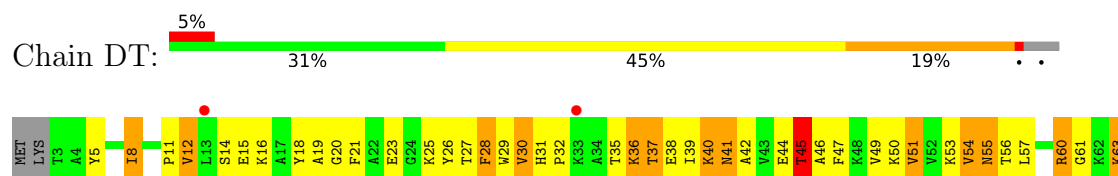
- Molecule 18: 50S ribosomal protein L22

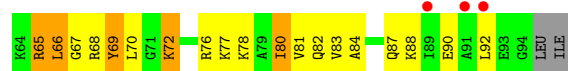


- Molecule 19: 50S ribosomal protein L23

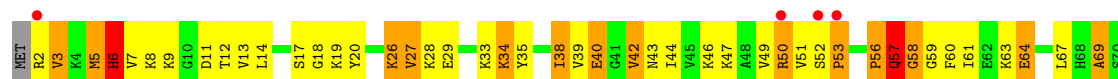


- Molecule 19: 50S ribosomal protein L23

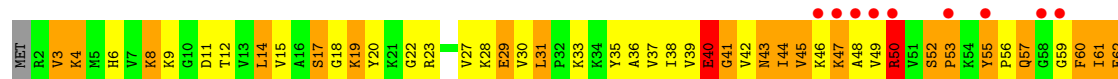
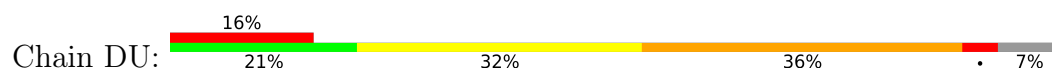




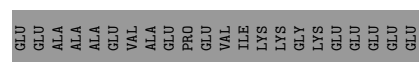
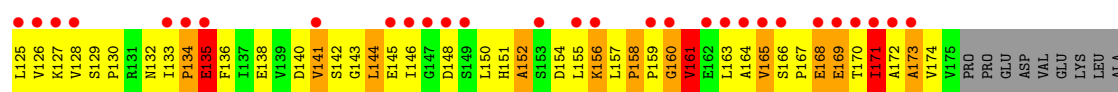
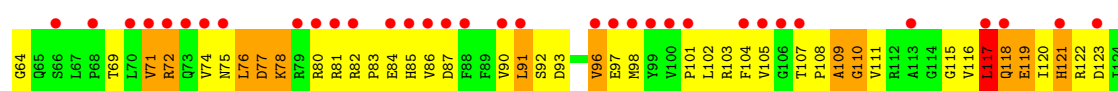
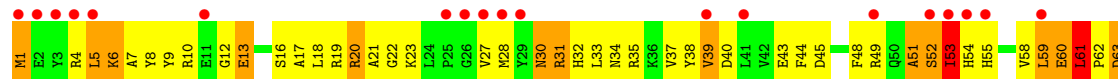
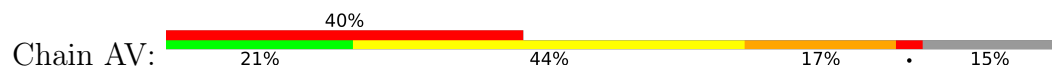
• Molecule 20: 50S ribosomal protein L24



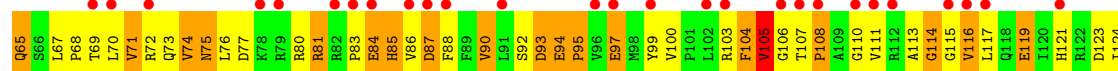
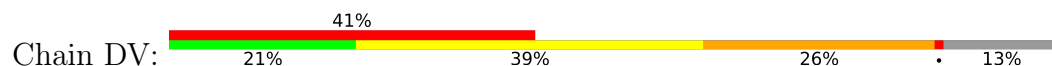
• Molecule 20: 50S ribosomal protein L24



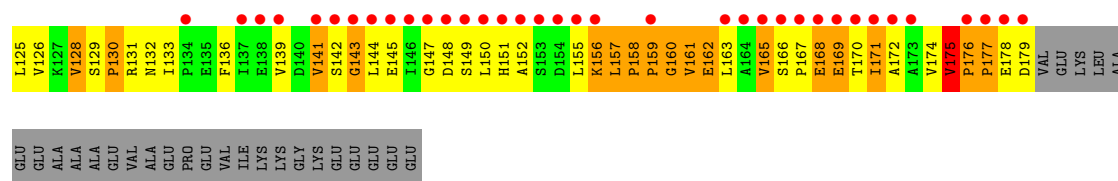
• Molecule 21: 50S ribosomal protein L25



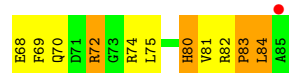
• Molecule 21: 50S ribosomal protein L25



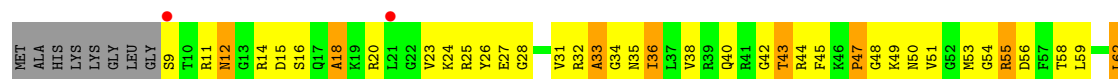




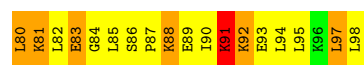
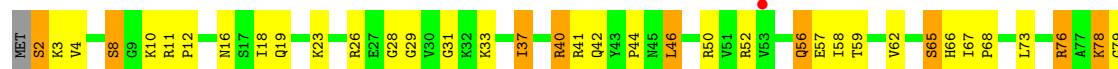
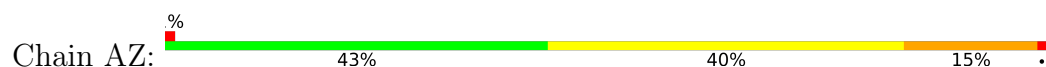
• Molecule 22: 50S ribosomal protein L27



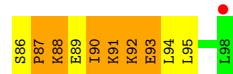
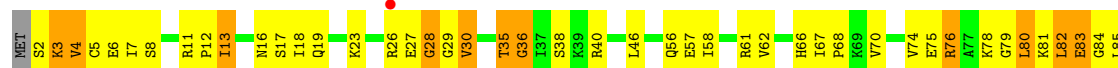
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

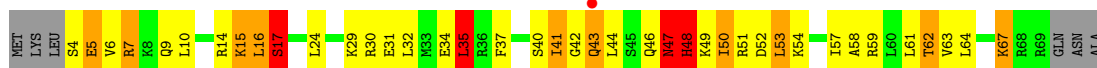


• Molecule 23: 50S ribosomal protein L28

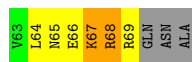
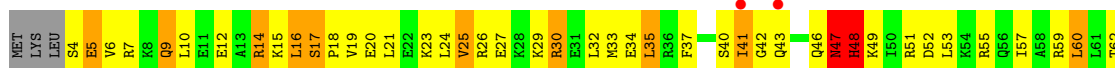


• Molecule 24: 50S ribosomal protein L29

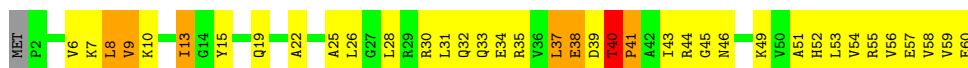




• Molecule 24: 50S ribosomal protein L29



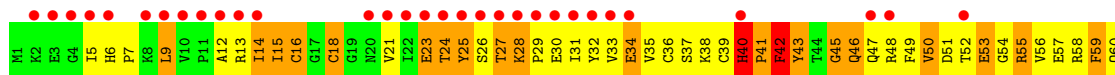
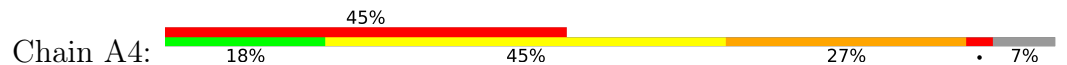
• Molecule 25: 50S ribosomal protein L30



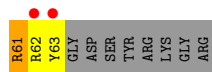
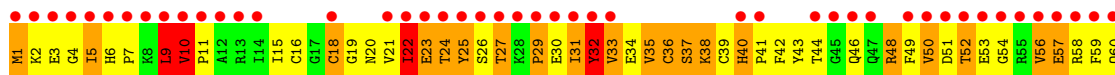
• Molecule 25: 50S ribosomal protein L30



• Molecule 26: 50S ribosomal protein L31

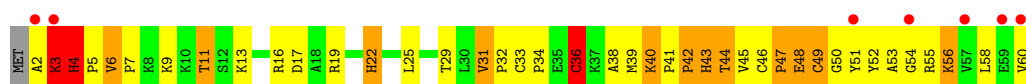


• Molecule 26: 50S ribosomal protein L31



• Molecule 27: 50S ribosomal protein L32

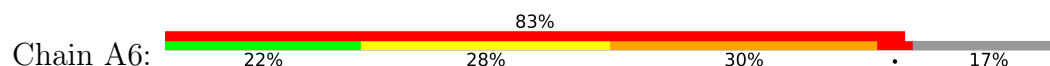




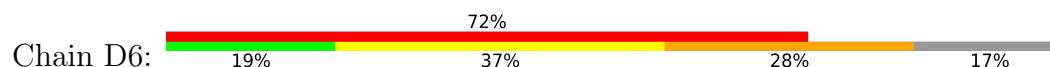
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



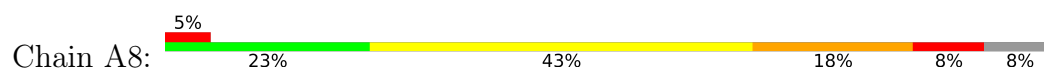
- Molecule 29: 50S ribosomal protein L34



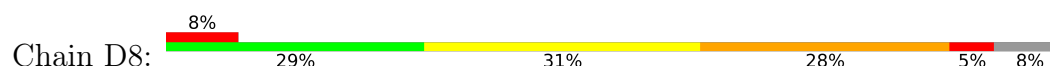
- Molecule 29: 50S ribosomal protein L34

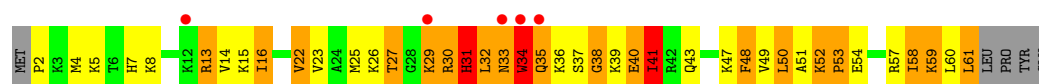


- Molecule 30: 50S ribosomal protein L35



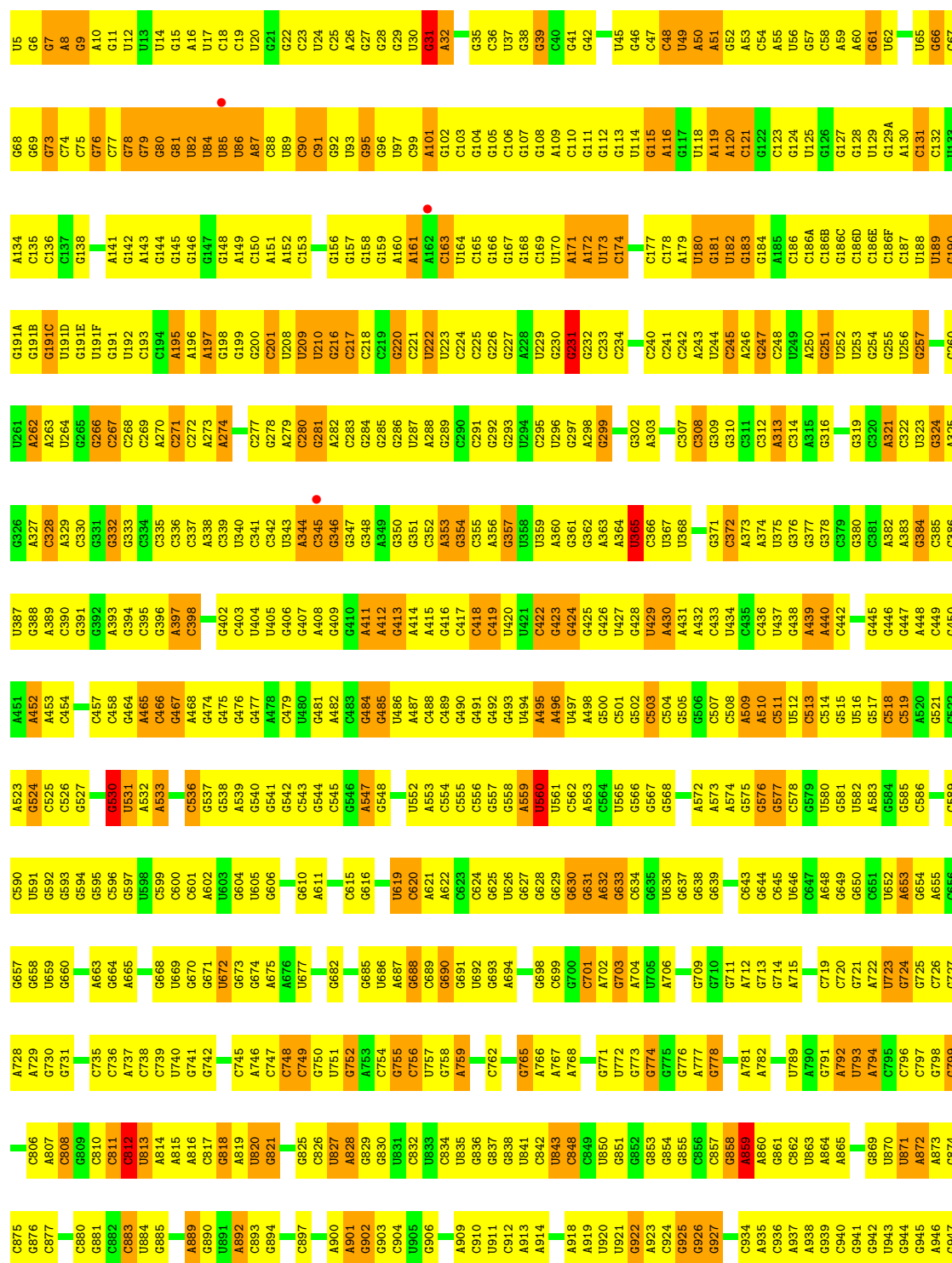
- Molecule 30: 50S ribosomal protein L35





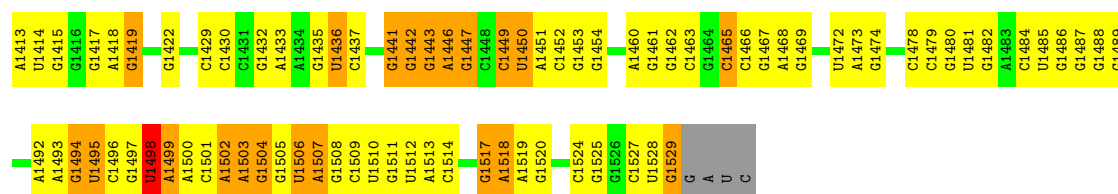
• Molecule 31: 16S ribosomal RNA

Chain BA: 20% 58% 21%

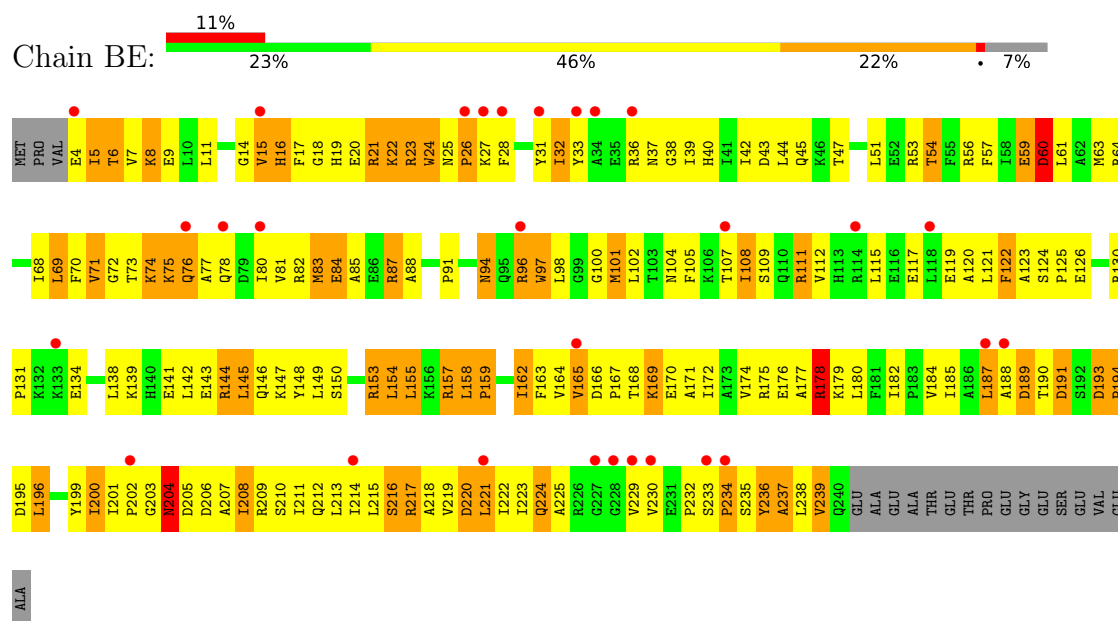




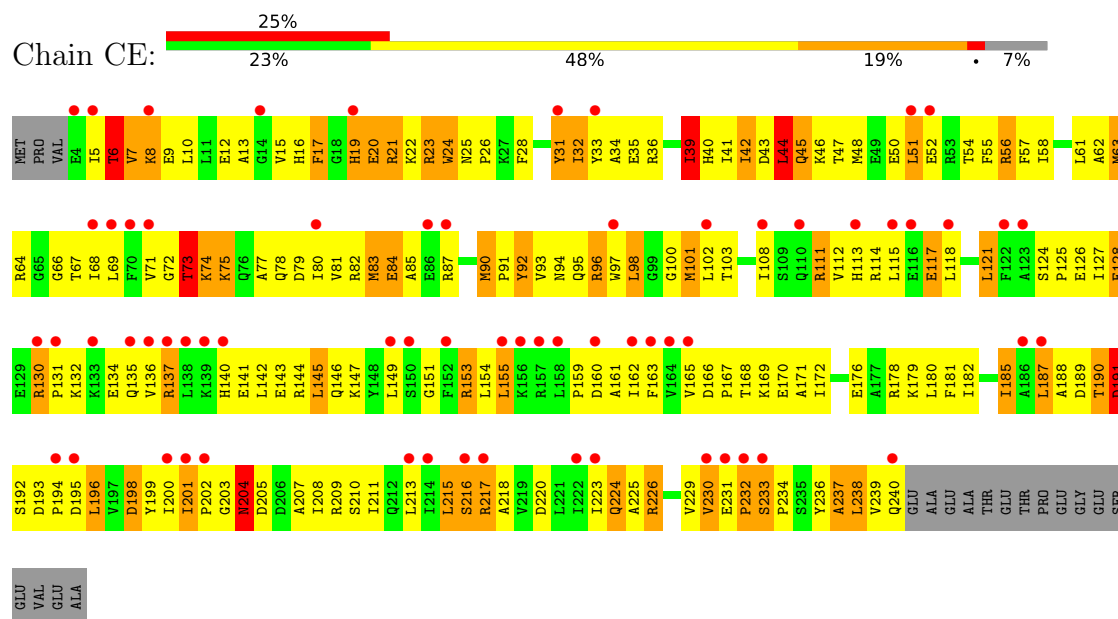
G1347	G1348	A1349	A1350	U1351	C1352	G1353	G1354	G1355	G1356	G1357	U1358	G1359	A1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	A1374	A1375	U1376	A1377	G1378	G1379	G1380	A1381	G1382	C1383	G1384	G1385	G1386	G1387	G1388	G1389	U1390	U1391	G1392	A1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	A1402	C1403	G1404	G1405	U1406																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	G1296	G1297	G1298	A1299	G1300	G1301	G1302	C1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	G1317	G1318	A1319	C1320	C1321	G1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	G1336	G1337	G1338	G1339	G1400	G1401	G1402	C1403	G1404	G1405	U1406																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1224	A1225	C1226	A1227	G1228	A1229	G1230	G1231	U1232	G1233	G1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1242	C1243		C1246	U1247		A1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	C1262	C1263	G1264	G1265	G1266	C1267	A1268	A1269	C1270	G1271	G1272	A1273	G1274	A1275	G1276	C1277	U1278	A1279	G1280	U1281	G1282	G1283	C1284	A1285																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C1163	G1164	G1165	G1166	A1167	A1169	A1170	G1171	G1172	G1173	G1174	G1175	A1176	G1177	G1178	A1179	G1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	G1195	U1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	G1214	G1215	G1216	C1217	A1218	A1280	U1281	G1282	G1283	C1284	A1285																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A1102	G1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113		G1116	G1117	U1118	C1119	G1120	U1121	U1122	A1123	G1124	G1125	U1126	G1127	C1128	C1129	A1130	G1131	G1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	G1145	C1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	U1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A1041	G1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	G1059	C1060	A1061	C1062	G1063	U1064	U1065	C1066	A1067	U1068	U1069	C1070	G1071	U1072	U1073	G1074	C1075	G1076	G1077	U1078	G1079	A1080	G1081	G1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	G1093	U1094	U1095	G1096	U1097	G1098	U1099	C1100	A1101																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A983	C984	C985	A986	C987	G988		U991	U992	G993	A994	C995	A996	U997	A1000	A938	G939	C940	G941	U942	A1004	A1005	C943	U944	G945	C946	A947	C948	A949	U950	G951	U952	G953	A954	A1016	G1017	C1018	U1019	U1020	G1021	G1022	G1023	G1024	U1025	C962	A964	A965	C966	C967	A968	C969	C970	G971	C972	G973	A974	A975	G976	A977	A978	C979	C980	U981	U982																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A1041	G1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	G1059	C1060	A1061	C1062	G1063	U1064	U1065	C1066	A1067	U1068	U1069	C1070	G1071	U1072	U1073	G1074	C1075	G1076	G1077	U1078	G1079	A1080	G1081	G1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	G1093	U1094	U1095	G1096	U1097	G1098	U1099	C1100	A1101																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
A1102	G1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113		G1116	G1117	U1118	C1119	G1120	U1121	U1122	A1123	G1124	G1125	U1126	G1127	C1128	C1129	A1130	G1131	G1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	G1145	C1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	U1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C1163	G1164	G1165	G1166	A1167	A1169	A1170	G1171	G1172	G1173	G1174	G1175	A1176	G1177	G1178	A1179	G1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	G1195	U1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	G1214	G1215	G1216	C1217	A1218	A1280	U1281	G1282	G1283	C1284	A1285																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	G1294	G1295	G1296	G1297	G1298	A1299	G1300	G1301	G1302	C1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	G1317	G1318	A1319	C1320	C1321	G1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	G1336	G1337	G1338	G1339	G1400	G1401	G1402	C1403	G1404	G1405	U1406																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G426	U427	A428	U429	U430	A431	A432	C433	U434	C435	C436	U437	C438	A439	A440	C441	C442	C443	C444	C445	C446	C447	C448	A449	C450	A451	A452	A453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	A468	C469	C470	A471	C472	C473	C474	C475	C476	C477	A478	C479	A480	C481	C482	C483	C484	C485	U486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	U497	A498	C500	C501	C502																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C503	C504	C505		A509	A510	C511	U512	U516	C517	C518	C519	C520	A521	C522	C523	C524	C525	C526	C527	C528	C529	C530	U531	A532	A533	A534	A535	C536	C537	C538	C539	A540	C541	C542	C543	C544	C545	C546	A547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	A559	U560	C561	C562	A563	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	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592



• Molecule 32: 30S RIBOSOMAL PROTEIN S2

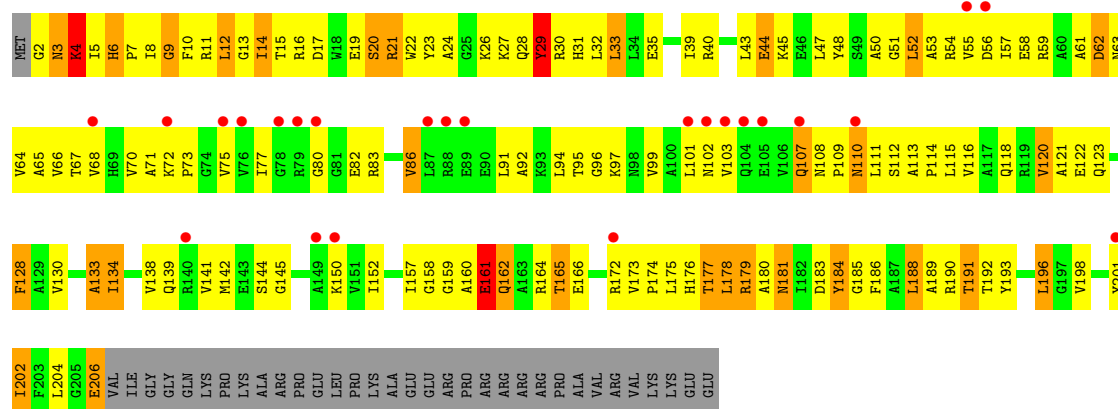


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

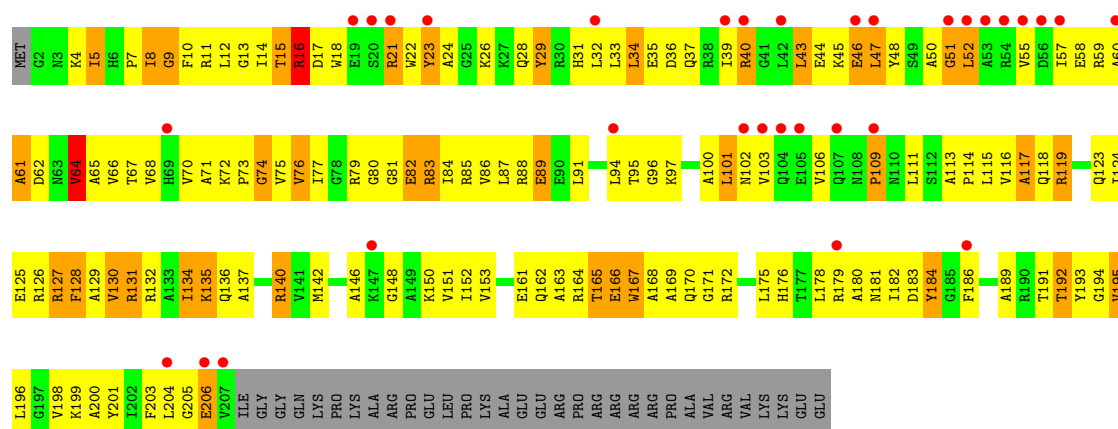


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

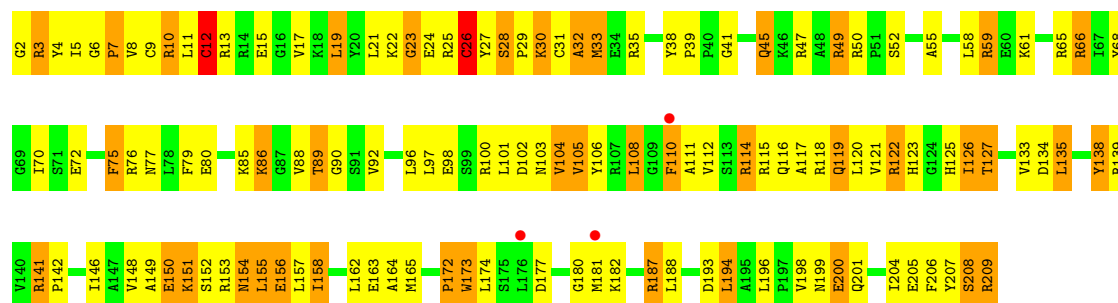




• Molecule 33: 30S RIBOSOMAL PROTEIN S3



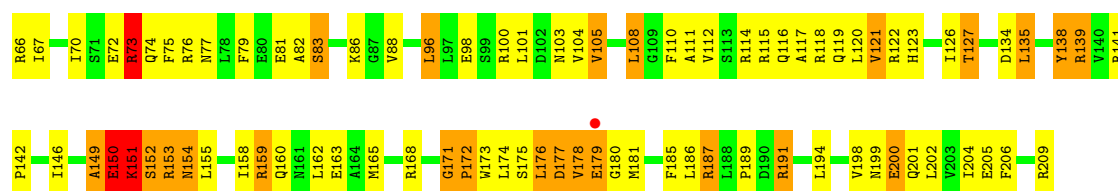
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



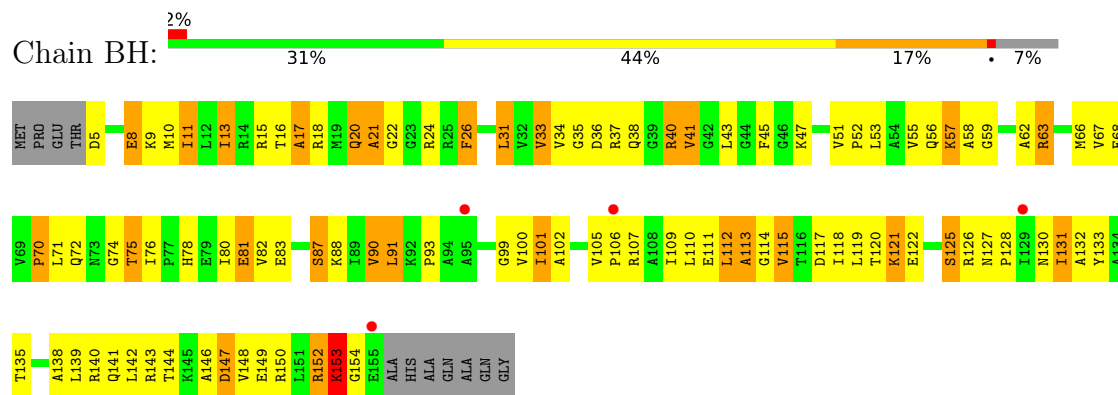
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



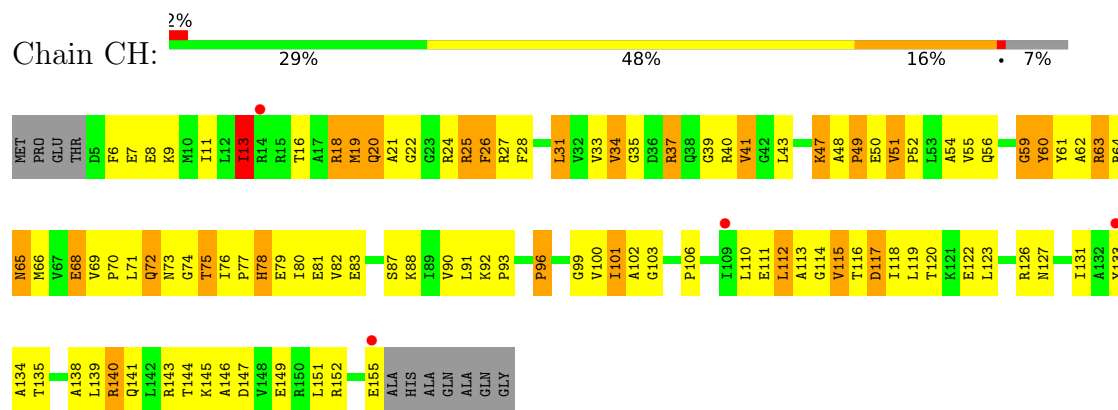




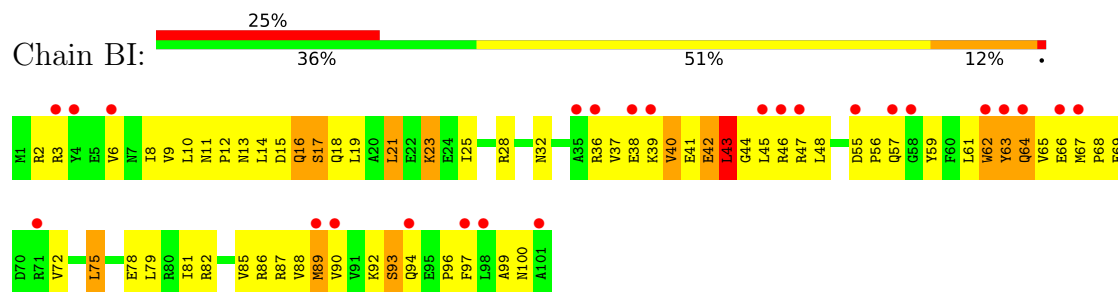
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



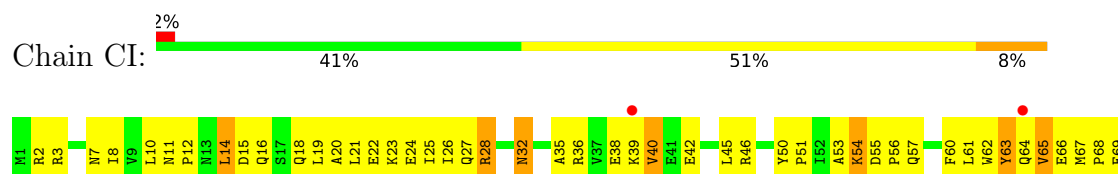
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

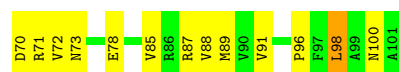


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

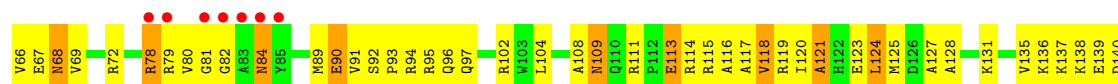
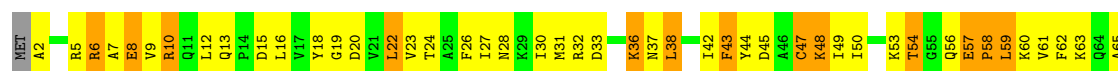


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

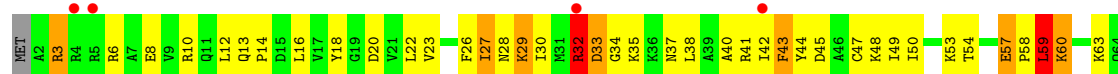




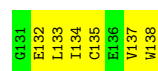
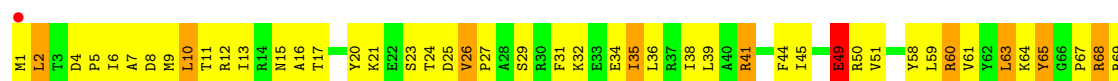
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



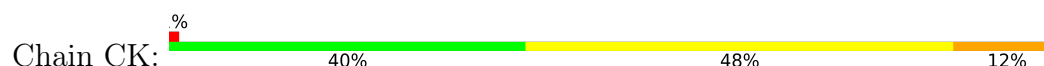
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 38: 30S RIBOSOMAL PROTEIN S8



• Molecule 38: 30S RIBOSOMAL PROTEIN S8





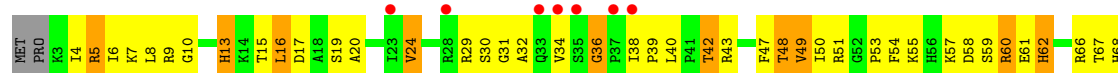
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



• Molecule 39: 30S RIBOSOMAL PROTEIN S9



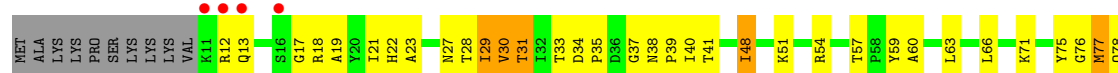
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



• Molecule 40: 30S RIBOSOMAL PROTEIN S10

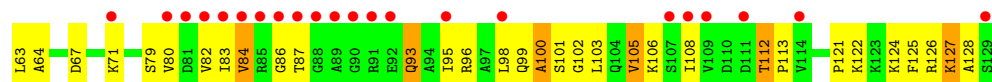
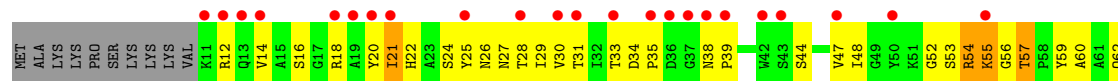
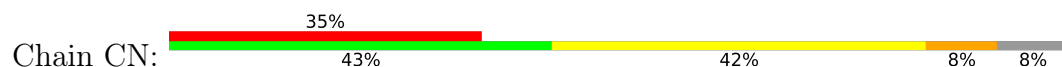


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

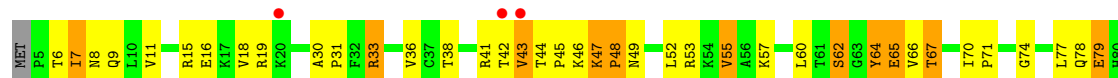




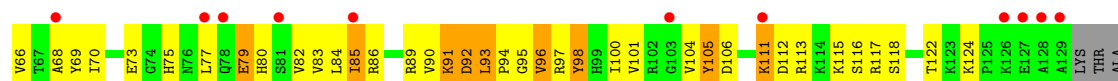
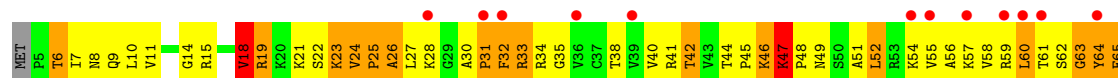
• Molecule 41: 30S RIBOSOMAL PROTEIN S11



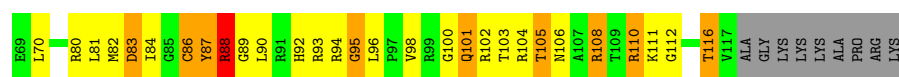
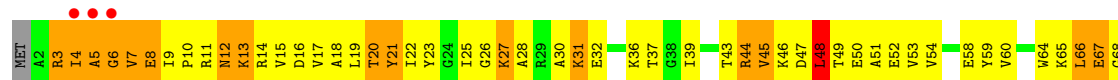
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



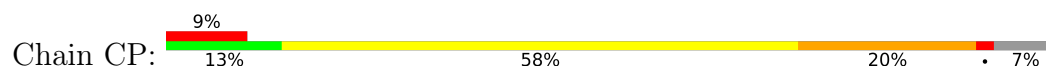
• Molecule 42: 30S RIBOSOMAL PROTEIN S12

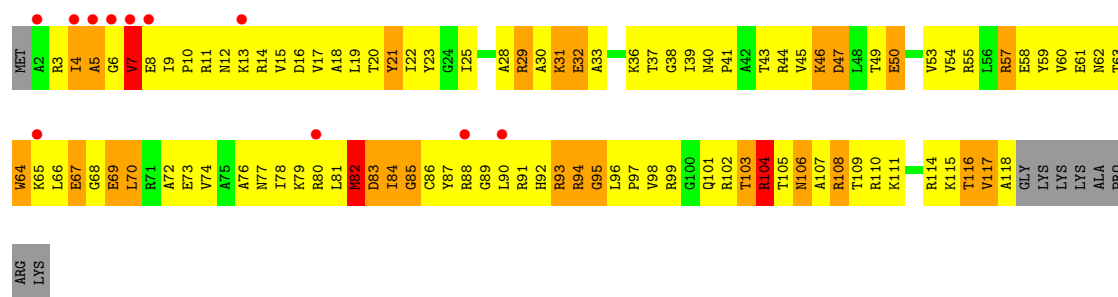


• Molecule 43: 30S RIBOSOMAL PROTEIN S13



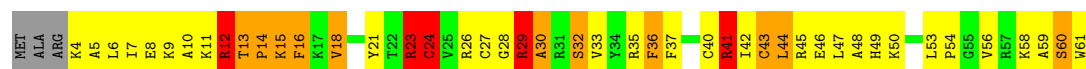
• Molecule 43: 30S RIBOSOMAL PROTEIN S13





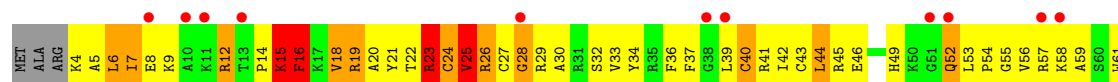
• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain BQ: 21% 48% 18% 8% 5%



• Molecule 44: 30S RIBOSOMAL PROTEIN S14

Chain CQ: 18% 20% 51% 18% 7% 5%



• Molecule 45: 30S RIBOSOMAL PROTEIN S15

Chain BR: 48% 37% 13%



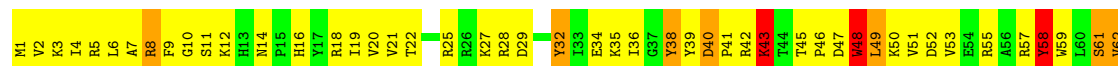
• Molecule 45: 30S RIBOSOMAL PROTEIN S15

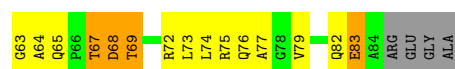
Chain CR: 42% 43% 13%



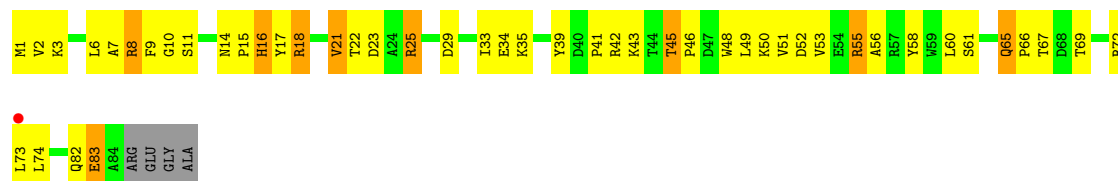
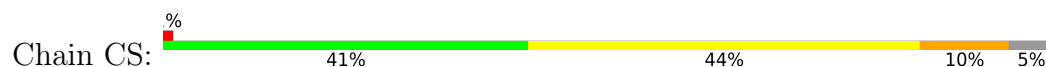
• Molecule 46: 30S RIBOSOMAL PROTEIN S16

Chain BS: 24% 56% 13% 5%

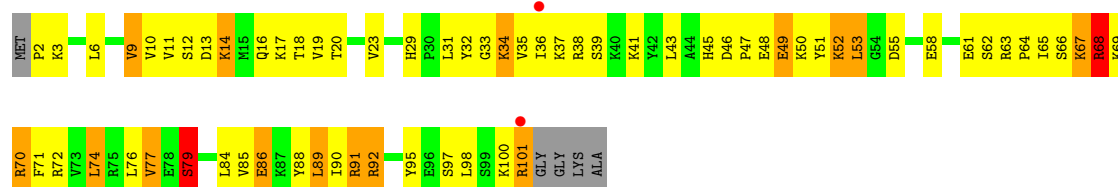




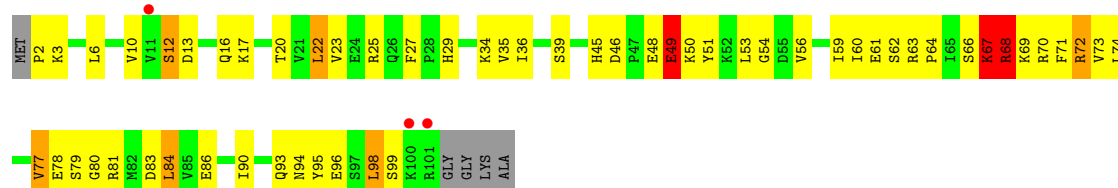
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



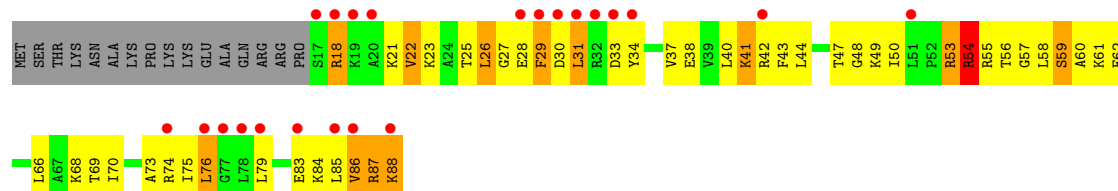
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



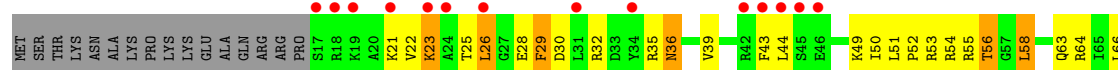
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



• Molecule 48: 30S RIBOSOMAL PROTEIN S18



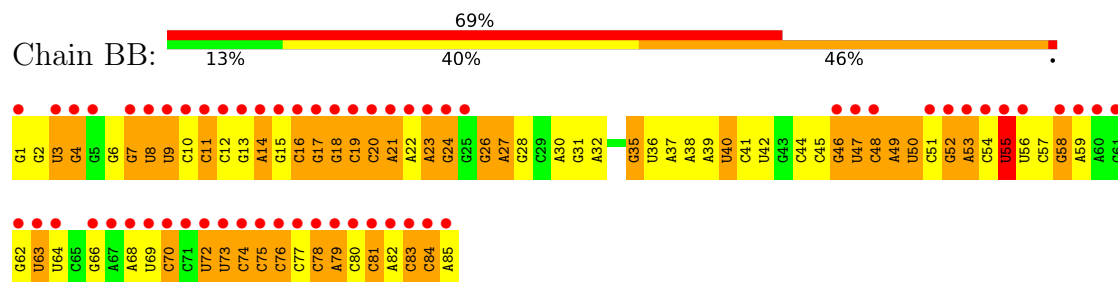
• Molecule 48: 30S RIBOSOMAL PROTEIN S18



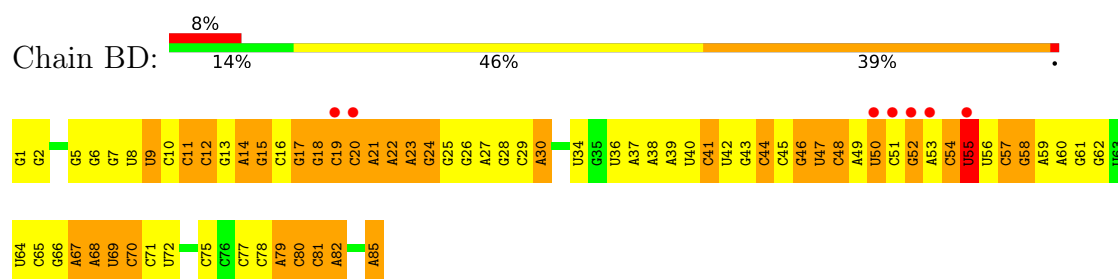




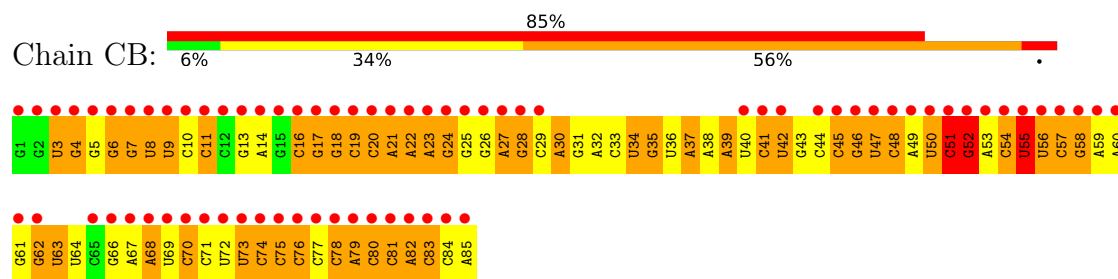
• Molecule 52: TRNA-TYR



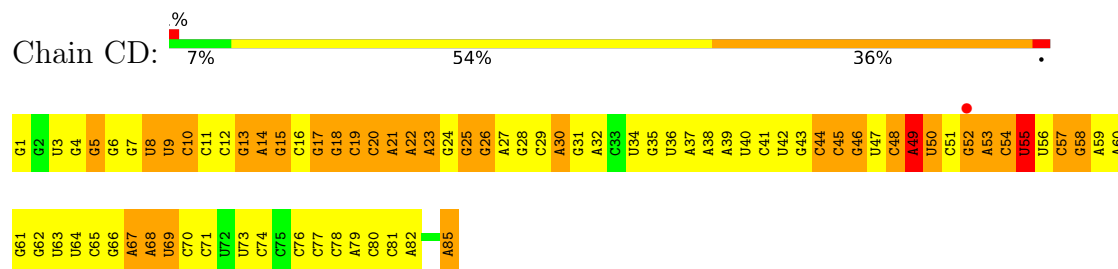
• Molecule 52: TRNA-TYR



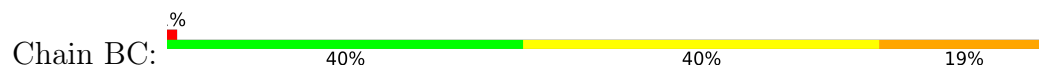
• Molecule 52: TRNA-TYR



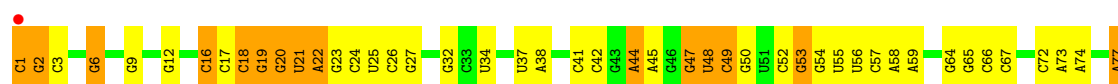
• Molecule 52: TRNA-TYR



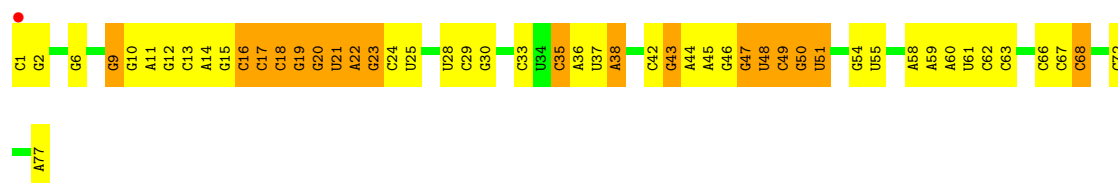
• Molecule 53: TRNA-FMET



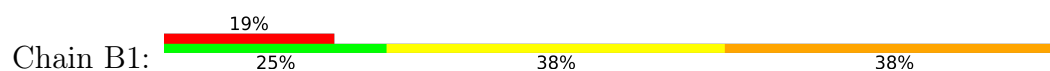




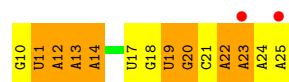
• Molecule 53: TRNA-FMET



• 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, $\alpha$ , $\beta$ , $\gamma$	210.00Å 450.33Å 622.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.64 – 3.30 152.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.64-3.30) 89.2 (152.64-3.00)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, $R_{free}$	0.196 , 0.247 0.197 , 0.244	Depositor DCC
$R_{free}$ test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 80.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	304031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% 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, MG, OHX, PAR

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	0.73	18/70233 (0.0%)	1.21	496/109643 (0.5%)
1	DA	0.64	9/70122 (0.0%)	1.10	332/109469 (0.3%)
2	AB	0.60	0/2928	1.24	32/4568 (0.7%)
2	DB	0.50	0/2928	1.03	7/4568 (0.2%)
3	AD	0.56	0/2165	0.81	1/2919 (0.0%)
3	DD	0.52	0/2165	0.75	0/2919
4	AE	0.47	0/1601	0.72	0/2160
4	DE	0.45	0/1601	0.67	0/2160
5	AF	0.51	0/1620	0.71	0/2194
5	DF	0.38	0/1662	0.65	0/2249
6	AG	0.36	0/1499	0.60	0/2016
6	DG	0.28	0/1499	0.52	0/2016
7	AH	0.43	0/1332	0.66	0/1802
7	DH	0.29	0/1332	0.53	0/1802
8	AK	0.36	0/1151	0.63	0/1558
8	DK	0.36	0/1151	0.63	0/1558
9	AM	0.43	0/1131	0.66	0/1525
9	DM	0.34	0/1131	0.58	0/1525
10	AN	0.46	0/943	0.65	0/1269
10	DN	0.42	0/943	0.63	1/1269 (0.1%)
11	AO	0.44	0/1162	0.81	1/1544 (0.1%)
11	DO	0.32	0/1162	0.57	1/1544 (0.1%)
12	AP	0.45	0/1143	0.63	0/1527
12	DP	0.33	0/1143	0.54	0/1527
13	A0	0.42	0/982	0.67	0/1312
13	D0	0.40	0/974	0.66	0/1302
14	AQ	0.45	0/892	0.72	0/1187
14	DQ	0.33	0/892	0.60	0/1187
15	AR	0.46	0/1155	0.66	0/1542
15	DR	0.41	0/1155	0.61	0/1542
16	A1	0.47	0/982	0.72	0/1306
16	D1	0.37	0/982	0.57	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	A2	0.41	0/790	0.71	1/1057 (0.1%)
17	D2	0.32	0/790	0.60	1/1057 (0.1%)
18	AS	0.46	0/911	0.68	0/1220
18	DS	0.44	0/911	0.62	0/1220
19	AT	0.60	1/739 (0.1%)	0.69	0/993
19	DT	0.48	0/739	0.63	0/993
20	AU	0.50	0/798	0.69	0/1064
20	DU	0.42	0/798	0.65	0/1064
21	AV	0.37	0/1427	0.62	1/1935 (0.1%)
21	DV	0.29	0/1460	0.53	0/1982
22	A3	0.49	0/615	0.72	0/819
22	D3	0.41	0/621	0.66	0/827
23	AZ	0.46	0/770	0.70	0/1022
23	DZ	0.44	0/770	0.69	0/1022
24	AW	0.52	0/560	0.75	1/741 (0.1%)
24	DW	0.40	0/560	0.59	0/741
25	AX	0.41	0/474	0.57	0/635
25	DX	0.33	0/474	0.55	0/635
26	A4	0.39	0/545	0.61	1/733 (0.1%)
26	D4	0.34	0/527	0.62	0/709
27	A5	0.44	0/473	0.65	0/639
27	D5	0.41	0/473	0.65	0/639
28	A6	0.48	0/396	0.64	0/529
28	D6	0.45	0/396	0.67	0/529
29	A7	0.57	0/399	0.76	0/526
29	D7	0.50	0/399	0.69	0/526
30	A8	0.55	0/486	0.81	0/638
30	D8	0.42	0/486	0.65	1/638 (0.2%)
31	BA	0.54	0/36139	1.02	97/56406 (0.2%)
31	CA	0.50	0/36142	0.96	59/56410 (0.1%)
32	BE	0.30	0/1959	0.53	0/2642
32	CE	0.28	0/1959	0.52	0/2642
33	BF	0.34	0/1629	0.53	0/2195
33	CF	0.29	0/1636	0.51	0/2205
34	BG	0.44	2/1733 (0.1%)	0.60	1/2318 (0.0%)
34	CG	0.38	0/1733	0.59	1/2318 (0.0%)
35	BH	0.39	0/1171	0.60	0/1576
35	CH	0.36	0/1171	0.58	0/1576
36	BI	0.37	0/856	0.56	0/1154
36	CI	0.36	0/856	0.56	0/1154
37	BJ	0.33	0/1276	0.52	0/1709
37	CJ	0.30	0/1276	0.50	0/1709
38	BK	0.35	0/1136	0.60	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	CK	0.30	0/1136	0.54	0/1527
39	BL	0.29	0/1029	0.52	0/1379
39	CL	0.30	0/1029	0.53	0/1379
40	BM	0.32	0/814	0.57	0/1095
40	CM	0.30	0/814	0.55	0/1095
41	BN	0.35	0/900	0.58	0/1213
41	CN	0.35	0/900	0.56	0/1213
42	BO	0.46	0/991	0.71	0/1327
42	CO	0.38	0/991	0.65	0/1327
43	BP	0.35	0/938	0.59	0/1258
43	CP	0.28	0/943	0.52	0/1265
44	BQ	0.44	1/485 (0.2%)	0.67	1/643 (0.2%)
44	CQ	0.31	0/485	0.55	0/643
45	BR	0.38	0/745	0.61	0/992
45	CR	0.36	0/745	0.56	1/992 (0.1%)
46	BS	0.31	0/721	0.56	0/970
46	CS	0.34	0/721	0.58	0/970
47	BT	0.38	0/847	0.57	0/1131
47	CT	0.35	0/847	0.53	0/1131
48	BU	0.36	0/596	0.63	0/790
48	CU	0.36	0/596	0.57	0/790
49	BV	0.32	0/638	0.56	0/860
49	CV	0.31	0/638	0.56	0/860
50	BW	0.30	0/765	0.57	0/1007
50	CW	0.33	0/765	0.58	0/1007
51	BX	0.32	0/221	0.52	0/288
51	CX	0.33	0/221	0.53	0/288
52	BB	0.76	0/1992	0.98	2/3099 (0.1%)
52	BD	0.65	0/1992	0.90	3/3099 (0.1%)
52	CB	0.85	0/1992	0.94	6/3099 (0.2%)
52	CD	0.67	0/1992	0.88	6/3099 (0.2%)
53	BC	0.50	0/1835	0.94	6/2859 (0.2%)
53	CC	0.46	0/1835	0.91	1/2859 (0.0%)
54	B1	0.72	0/390	0.91	1/606 (0.2%)
54	C1	0.71	0/390	0.89	0/606
All	All	0.58	31/324159 (0.0%)	0.99	1062/485455 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	3
3	DD	0	1
4	AE	0	1
5	AF	0	1
5	DF	0	1
7	AH	0	1
8	AK	0	1
8	DK	0	1
11	AO	0	1
11	DO	0	1
24	AW	0	1
30	A8	0	1
30	D8	0	1
42	BO	0	1
All	All	0	16

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	774	A	N9-C4	-9.44	1.32	1.37
1	DA	1342	A	N7-C5	-8.92	1.33	1.39
1	DA	783	A	N9-C4	-8.89	1.32	1.37
1	DA	2873	A	N7-C5	-8.61	1.34	1.39
34	BG	12	CYS	CB-SG	7.57	1.95	1.82

The worst 5 of 1062 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	1899	G	N3-C4-N9	-16.88	115.87	126.00
1	AA	1899	G	N3-C4-N9	-14.54	117.28	126.00
1	AA	774	A	C2-N3-C4	-14.31	103.44	110.60
2	AB	81	G	C6-C5-N7	-14.19	121.89	130.40
1	AA	783	A	C5-N7-C8	-13.92	96.94	103.90

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	197	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	47	GLY	Peptide
4	AE	20	ALA	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	AF	47	GLY	Peptide

## 5.2 Too-close contacts

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	31614	2894	0
1	DA	62607	0	31564	2901	0
2	AB	2617	0	1328	138	0
2	DB	2617	0	1328	161	0
3	AD	2115	0	2195	271	0
3	DD	2115	0	2195	239	0
4	AE	1568	0	1634	208	0
4	DE	1568	0	1634	214	0
5	AF	1585	0	1632	178	0
5	DF	1627	0	1680	236	0
6	AG	1474	0	1535	158	0
6	DG	1474	0	1535	164	0
7	AH	1307	0	1382	173	0
7	DH	1307	0	1382	136	1
8	AK	1136	0	1223	123	0
8	DK	1136	0	1223	107	0
9	AM	1104	0	1180	134	0
9	DM	1104	0	1180	145	0
10	AN	933	0	996	64	0
10	DN	933	0	996	75	0
11	AO	1145	0	1228	239	0
11	DO	1145	0	1227	311	0
12	AP	1122	0	1179	189	0
12	DP	1122	0	1179	188	0
13	A0	968	0	1033	129	0
13	D0	960	0	1021	94	0
14	AQ	882	0	943	123	0
14	DQ	882	0	943	137	0
15	AR	1141	0	1202	115	0
15	DR	1141	0	1202	128	0
16	A1	964	0	1022	120	0
16	D1	964	0	1019	158	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	A2	779	0	852	101	0
17	D2	779	0	852	135	0
18	AS	900	0	964	95	0
18	DS	900	0	964	72	0
19	AT	725	0	778	65	0
19	DT	725	0	778	99	0
20	AU	785	0	878	101	0
20	DU	785	0	878	133	0
21	AV	1397	0	1430	168	0
21	DV	1428	0	1454	184	0
22	A3	607	0	628	63	0
22	D3	613	0	633	68	0
23	AZ	763	0	848	71	0
23	DZ	763	0	848	53	0
24	AW	558	0	610	39	0
24	DW	558	0	610	55	0
25	AX	469	0	518	37	0
25	DX	469	0	518	39	0
26	A4	533	0	522	88	0
26	D4	515	0	510	90	0
27	A5	459	0	480	87	0
27	D5	459	0	478	52	0
28	A6	389	0	404	56	0
28	D6	389	0	404	64	0
29	A7	391	0	432	41	0
29	D7	391	0	432	37	0
30	A8	480	0	549	131	0
30	D8	480	0	549	130	0
31	BA	32284	0	16296	1832	1
31	CA	32287	0	16295	1769	0
32	BE	1924	0	1975	195	0
32	CE	1924	0	1975	225	0
33	BF	1605	0	1668	134	0
33	CF	1612	0	1677	179	0
34	BG	1703	0	1763	175	0
34	CG	1703	0	1763	186	0
35	BH	1155	0	1213	115	0
35	CH	1155	0	1213	116	0
36	BI	843	0	857	70	0
36	CI	843	0	857	53	0
37	BJ	1257	0	1296	107	0
37	CJ	1257	0	1296	106	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BK	1116	0	1177	113	0
38	CK	1116	0	1177	79	0
39	BL	1010	0	1037	110	0
39	CL	1010	0	1037	156	0
40	BM	801	0	849	94	0
40	CM	801	0	849	130	0
41	BN	885	0	904	65	0
41	CN	885	0	904	71	0
42	BO	975	0	1062	65	0
42	CO	975	0	1062	123	0
43	BP	928	0	987	106	0
43	CP	933	0	992	134	0
44	BQ	476	0	511	58	0
44	CQ	476	0	512	79	0
45	BR	734	0	771	47	0
45	CR	734	0	771	51	0
46	BS	705	0	725	77	0
46	CS	705	0	725	52	0
47	BT	834	0	904	84	0
47	CT	834	0	904	58	0
48	BU	591	0	662	61	0
48	CU	591	0	662	38	0
49	BV	624	0	636	72	0
49	CV	624	0	636	83	0
50	BW	763	0	861	97	0
50	CW	763	0	861	82	0
51	BX	217	0	234	16	0
51	CX	217	0	234	22	0
52	BB	1814	0	931	140	0
52	BD	1814	0	932	148	0
52	CB	1814	0	931	149	0
52	CD	1814	0	932	156	0
53	BC	1643	0	837	55	0
53	CC	1643	0	837	79	0
54	B1	347	0	174	20	0
54	C1	347	0	174	48	0
55	A0	1	0	0	0	0
55	A1	2	0	0	0	0
55	A3	1	0	0	0	0
55	A5	1	0	0	0	0
55	A7	1	0	0	0	0
55	AA	332	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	AB	6	0	0	0	0
55	AE	3	0	0	0	0
55	AF	2	0	0	0	0
55	AO	1	0	0	0	0
55	B1	1	0	0	0	0
55	BA	114	0	0	0	0
55	BB	13	0	0	0	0
55	BC	4	0	0	0	0
55	BD	1	0	0	0	0
55	BF	1	0	0	0	0
55	BS	1	0	0	0	0
55	BW	1	0	0	0	0
55	C1	2	0	0	0	0
55	CA	121	0	0	0	0
55	CB	3	0	0	0	0
55	CC	7	0	0	0	0
55	CN	1	0	0	0	0
55	D0	1	0	0	0	0
55	D5	1	0	0	0	0
55	D7	1	0	0	0	0
55	DA	272	0	0	0	0
55	DB	7	0	0	0	0
55	DE	1	0	0	0	0
56	A1	14	0	0	0	0
56	A3	7	0	0	1	0
56	A6	7	0	0	1	0
56	AA	1659	0	0	140	0
56	AB	91	0	0	6	0
56	AE	7	0	0	0	0
56	AF	7	0	0	3	0
56	AO	14	0	0	2	0
56	AW	7	0	0	0	0
56	BA	693	0	0	66	0
56	BB	14	0	0	0	0
56	BC	21	0	0	2	0
56	BD	21	0	0	1	0
56	BG	7	0	0	2	0
56	BL	7	0	0	0	0
56	BR	7	0	0	0	0
56	CA	651	0	0	83	0
56	CB	21	0	0	2	0
56	CC	21	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CD	7	0	0	1	0
56	CK	7	0	0	1	0
56	CR	7	0	0	0	0
56	CV	7	0	0	1	0
56	D1	7	0	0	0	0
56	D3	7	0	0	1	0
56	D5	7	0	0	1	0
56	D8	7	0	0	5	0
56	DA	1533	0	0	128	0
56	DB	91	0	0	6	0
56	DF	7	0	0	1	0
56	DO	7	0	0	0	0
57	BA	42	0	45	3	0
57	CA	42	0	45	1	0
58	BG	1	0	0	0	0
58	BQ	1	0	0	0	0
58	CG	1	0	0	0	0
58	CQ	1	0	0	0	0
All	All	304031	0	201063	19321	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 38.

The worst 5 of 19321 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)
11:DO:71:VAL:CG1	11:DO:72:PRO:HD3	1.34	1.57
30:A8:34:TRP:CB	30:A8:35:GLN:HB2	1.34	1.53
20:DU:89:PHE:CE1	20:DU:90:LEU:HG	1.40	1.50
9:DM:17:ASP:HA	9:DM:55:VAL:CG2	1.36	1.49
27:D5:4:HIS:HB3	27:D5:5:PRO:CD	1.40	1.48

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:DH:100:GLY:O[3_555]	1.86	0.34

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	208 (77%)	45 (17%)	17 (6%)	1	11
3	DD	270/276 (98%)	226 (84%)	31 (12%)	13 (5%)	2	17
4	AE	203/206 (98%)	138 (68%)	33 (16%)	32 (16%)	0	1
4	DE	203/206 (98%)	128 (63%)	34 (17%)	41 (20%)	0	1
5	AF	200/210 (95%)	153 (76%)	28 (14%)	19 (10%)	1	4
5	DF	206/210 (98%)	133 (65%)	46 (22%)	27 (13%)	0	2
6	AG	179/182 (98%)	127 (71%)	36 (20%)	16 (9%)	1	5
6	DG	179/182 (98%)	128 (72%)	30 (17%)	21 (12%)	0	2
7	AH	168/180 (93%)	111 (66%)	25 (15%)	32 (19%)	0	1
7	DH	168/180 (93%)	92 (55%)	52 (31%)	24 (14%)	0	1
8	AK	144/148 (97%)	75 (52%)	44 (31%)	25 (17%)	0	1
8	DK	144/148 (97%)	98 (68%)	27 (19%)	19 (13%)	0	2
9	AM	136/140 (97%)	96 (71%)	21 (15%)	19 (14%)	0	1
9	DM	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	0	2
10	AN	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	4	25
10	DN	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	10
11	AO	148/150 (99%)	91 (62%)	29 (20%)	28 (19%)	0	1
11	DO	148/150 (99%)	83 (56%)	21 (14%)	44 (30%)	0	0
12	AP	139/141 (99%)	93 (67%)	27 (19%)	19 (14%)	0	1
12	DP	139/141 (99%)	88 (63%)	29 (21%)	22 (16%)	0	1
13	A0	116/118 (98%)	86 (74%)	21 (18%)	9 (8%)	1	7
13	D0	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	0	2
14	AQ	109/112 (97%)	74 (68%)	26 (24%)	9 (8%)	1	6
14	DQ	109/112 (97%)	60 (55%)	32 (29%)	17 (16%)	0	1
15	AR	135/146 (92%)	101 (75%)	19 (14%)	15 (11%)	0	3

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	DR	135/146 (92%)	101 (75%)	23 (17%)	11 (8%)	1	7
16	A1	115/118 (98%)	82 (71%)	19 (16%)	14 (12%)	0	2
16	D1	115/118 (98%)	73 (64%)	29 (25%)	13 (11%)	0	3
17	A2	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	7
17	D2	99/101 (98%)	64 (65%)	19 (19%)	16 (16%)	0	1
18	AS	111/113 (98%)	94 (85%)	13 (12%)	4 (4%)	4	23
18	DS	111/113 (98%)	89 (80%)	13 (12%)	9 (8%)	1	7
19	AT	90/96 (94%)	78 (87%)	8 (9%)	4 (4%)	3	18
19	DT	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	1	5
20	AU	100/110 (91%)	65 (65%)	18 (18%)	17 (17%)	0	1
20	DU	100/110 (91%)	56 (56%)	18 (18%)	26 (26%)	0	0
21	AV	173/206 (84%)	105 (61%)	42 (24%)	26 (15%)	0	1
21	DV	177/206 (86%)	100 (56%)	35 (20%)	42 (24%)	0	0
22	A3	74/85 (87%)	58 (78%)	11 (15%)	5 (7%)	1	9
22	D3	75/85 (88%)	54 (72%)	15 (20%)	6 (8%)	1	7
23	AZ	95/98 (97%)	75 (79%)	14 (15%)	6 (6%)	1	11
23	DZ	95/98 (97%)	72 (76%)	12 (13%)	11 (12%)	0	2
24	AW	64/72 (89%)	55 (86%)	3 (5%)	6 (9%)	1	4
24	DW	64/72 (89%)	46 (72%)	11 (17%)	7 (11%)	0	3
25	AX	57/60 (95%)	47 (82%)	8 (14%)	2 (4%)	4	24
25	DX	57/60 (95%)	44 (77%)	9 (16%)	4 (7%)	1	9
26	A4	64/71 (90%)	33 (52%)	14 (22%)	17 (27%)	0	0
26	D4	61/71 (86%)	23 (38%)	12 (20%)	26 (43%)	0	0
27	A5	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
27	D5	57/60 (95%)	44 (77%)	7 (12%)	6 (10%)	0	3
28	A6	43/54 (80%)	21 (49%)	13 (30%)	9 (21%)	0	1
28	D6	43/54 (80%)	23 (54%)	9 (21%)	11 (26%)	0	0
29	A7	43/49 (88%)	41 (95%)	0	2 (5%)	2	17
29	D7	43/49 (88%)	38 (88%)	3 (7%)	2 (5%)	2	17
30	A8	58/65 (89%)	39 (67%)	11 (19%)	8 (14%)	0	1
30	D8	58/65 (89%)	40 (69%)	8 (14%)	10 (17%)	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BE	235/256 (92%)	155 (66%)	44 (19%)	36 (15%)	0	1
32	CE	235/256 (92%)	152 (65%)	49 (21%)	34 (14%)	0	1
33	BF	203/239 (85%)	137 (68%)	47 (23%)	19 (9%)	1	4
33	CF	204/239 (85%)	124 (61%)	55 (27%)	25 (12%)	0	2
34	BG	206/208 (99%)	152 (74%)	34 (16%)	20 (10%)	1	4
34	CG	206/208 (99%)	152 (74%)	31 (15%)	23 (11%)	0	3
35	BH	149/162 (92%)	115 (77%)	26 (17%)	8 (5%)	2	14
35	CH	149/162 (92%)	115 (77%)	25 (17%)	9 (6%)	2	12
36	BI	99/101 (98%)	71 (72%)	23 (23%)	5 (5%)	2	16
36	CI	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	8	37
37	BJ	153/156 (98%)	111 (72%)	32 (21%)	10 (6%)	1	10
37	CJ	153/156 (98%)	118 (77%)	22 (14%)	13 (8%)	1	6
38	BK	136/138 (99%)	105 (77%)	24 (18%)	7 (5%)	2	16
38	CK	136/138 (99%)	100 (74%)	24 (18%)	12 (9%)	1	5
39	BL	125/128 (98%)	89 (71%)	25 (20%)	11 (9%)	1	5
39	CL	125/128 (98%)	80 (64%)	29 (23%)	16 (13%)	0	2
40	BM	97/105 (92%)	76 (78%)	20 (21%)	1 (1%)	17	51
40	CM	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	2	15
41	BN	117/129 (91%)	85 (73%)	24 (20%)	8 (7%)	1	9
41	CN	117/129 (91%)	93 (80%)	19 (16%)	5 (4%)	3	19
42	BO	123/132 (93%)	93 (76%)	18 (15%)	12 (10%)	1	4
42	CO	123/132 (93%)	79 (64%)	27 (22%)	17 (14%)	0	1
43	BP	114/126 (90%)	69 (60%)	27 (24%)	18 (16%)	0	1
43	CP	115/126 (91%)	71 (62%)	24 (21%)	20 (17%)	0	1
44	BQ	56/61 (92%)	38 (68%)	5 (9%)	13 (23%)	0	0
44	CQ	56/61 (92%)	32 (57%)	13 (23%)	11 (20%)	0	1
45	BR	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	2	12
45	CR	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	4	24
46	BS	82/88 (93%)	57 (70%)	15 (18%)	10 (12%)	0	2
46	CS	82/88 (93%)	55 (67%)	21 (26%)	6 (7%)	1	8
47	BT	98/105 (93%)	74 (76%)	17 (17%)	7 (7%)	1	9

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	CT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	12
48	BU	70/88 (80%)	53 (76%)	11 (16%)	6 (9%)	1	6
48	CU	70/88 (80%)	58 (83%)	10 (14%)	2 (3%)	5	28
49	BV	76/93 (82%)	56 (74%)	13 (17%)	7 (9%)	1	5
49	CV	76/93 (82%)	49 (64%)	18 (24%)	9 (12%)	0	2
50	BW	97/106 (92%)	65 (67%)	21 (22%)	11 (11%)	0	3
50	CW	97/106 (92%)	70 (72%)	13 (13%)	14 (14%)	0	1
51	BX	23/27 (85%)	15 (65%)	5 (22%)	3 (13%)	0	2
51	CX	23/27 (85%)	15 (65%)	6 (26%)	2 (9%)	1	6
All	All	11319/12052 (94%)	7969 (70%)	2044 (18%)	1306 (12%)	0	2

5 of 1306 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	3	VAL
3	AD	28	GLU
3	AD	29	PRO
3	AD	33	LEU
3	AD	37	LEU

### 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%)	154 (72%)	60 (28%)	0	1
3	DD	214/218 (98%)	164 (77%)	50 (23%)	1	3
4	AE	165/166 (99%)	131 (79%)	34 (21%)	1	5
4	DE	165/166 (99%)	120 (73%)	45 (27%)	0	2
5	AF	161/166 (97%)	126 (78%)	35 (22%)	1	4
5	DF	165/166 (99%)	130 (79%)	35 (21%)	1	5
6	AG	155/156 (99%)	124 (80%)	31 (20%)	1	6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	DG	155/156 (99%)	128 (83%)	27 (17%)	2	10
7	AH	142/148 (96%)	112 (79%)	30 (21%)	1	5
7	DH	142/148 (96%)	116 (82%)	26 (18%)	2	8
8	AK	122/124 (98%)	97 (80%)	25 (20%)	1	5
8	DK	122/124 (98%)	100 (82%)	22 (18%)	2	9
9	AM	117/119 (98%)	87 (74%)	30 (26%)	0	2
9	DM	117/119 (98%)	82 (70%)	35 (30%)	0	1
10	AN	100/100 (100%)	81 (81%)	19 (19%)	1	7
10	DN	100/100 (100%)	84 (84%)	16 (16%)	2	13
11	AO	116/116 (100%)	81 (70%)	35 (30%)	0	1
11	DO	116/116 (100%)	77 (66%)	39 (34%)	0	1
12	AP	111/111 (100%)	88 (79%)	23 (21%)	1	5
12	DP	111/111 (100%)	79 (71%)	32 (29%)	0	1
13	A0	101/101 (100%)	77 (76%)	24 (24%)	1	3
13	D0	100/101 (99%)	80 (80%)	20 (20%)	1	6
14	AQ	87/88 (99%)	63 (72%)	24 (28%)	0	1
14	DQ	87/88 (99%)	66 (76%)	21 (24%)	1	3
15	AR	120/127 (94%)	97 (81%)	23 (19%)	1	7
15	DR	120/127 (94%)	90 (75%)	30 (25%)	0	2
16	A1	93/94 (99%)	71 (76%)	22 (24%)	1	3
16	D1	93/94 (99%)	77 (83%)	16 (17%)	2	10
17	A2	82/82 (100%)	58 (71%)	24 (29%)	0	1
17	D2	82/82 (100%)	53 (65%)	29 (35%)	0	0
18	AS	92/92 (100%)	69 (75%)	23 (25%)	0	2
18	DS	92/92 (100%)	72 (78%)	20 (22%)	1	4
19	AT	74/78 (95%)	58 (78%)	16 (22%)	1	4
19	DT	74/78 (95%)	56 (76%)	18 (24%)	1	3
20	AU	85/91 (93%)	65 (76%)	20 (24%)	1	3
20	DU	85/91 (93%)	57 (67%)	28 (33%)	0	1
21	AV	154/179 (86%)	126 (82%)	28 (18%)	2	8
21	DV	158/179 (88%)	133 (84%)	25 (16%)	3	13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A3	61/67 (91%)	48 (79%)	13 (21%)	1	5
22	D3	62/67 (92%)	55 (89%)	7 (11%)	6	25
23	AZ	82/83 (99%)	64 (78%)	18 (22%)	1	4
23	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	4
24	AW	62/67 (92%)	44 (71%)	18 (29%)	0	1
24	DW	62/67 (92%)	48 (77%)	14 (23%)	1	3
25	AX	51/52 (98%)	42 (82%)	9 (18%)	2	9
25	DX	51/52 (98%)	41 (80%)	10 (20%)	1	6
26	A4	59/63 (94%)	49 (83%)	10 (17%)	2	11
26	D4	57/63 (90%)	45 (79%)	12 (21%)	1	5
27	A5	51/52 (98%)	39 (76%)	12 (24%)	1	3
27	D5	51/52 (98%)	43 (84%)	8 (16%)	3	14
28	A6	44/52 (85%)	32 (73%)	12 (27%)	0	2
28	D6	44/52 (85%)	38 (86%)	6 (14%)	4	18
29	A7	38/42 (90%)	32 (84%)	6 (16%)	3	13
29	D7	38/42 (90%)	29 (76%)	9 (24%)	1	3
30	A8	50/55 (91%)	36 (72%)	14 (28%)	0	1
30	D8	50/55 (91%)	35 (70%)	15 (30%)	0	1
32	BE	205/220 (93%)	167 (82%)	38 (18%)	2	8
32	CE	205/220 (93%)	168 (82%)	37 (18%)	2	9
33	BF	159/188 (85%)	127 (80%)	32 (20%)	1	6
33	CF	160/188 (85%)	132 (82%)	28 (18%)	2	9
34	BG	180/180 (100%)	149 (83%)	31 (17%)	2	10
34	CG	180/180 (100%)	143 (79%)	37 (21%)	1	5
35	BH	116/123 (94%)	89 (77%)	27 (23%)	1	3
35	CH	116/123 (94%)	89 (77%)	27 (23%)	1	3
36	BI	90/90 (100%)	80 (89%)	10 (11%)	7	26
36	CI	90/90 (100%)	78 (87%)	12 (13%)	4	19
37	BJ	126/127 (99%)	96 (76%)	30 (24%)	1	3
37	CJ	126/127 (99%)	103 (82%)	23 (18%)	2	8
38	BK	119/119 (100%)	95 (80%)	24 (20%)	1	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	CK	119/119 (100%)	101 (85%)	18 (15%)	3	15
39	BL	98/99 (99%)	77 (79%)	21 (21%)	1	4
39	CL	98/99 (99%)	73 (74%)	25 (26%)	0	2
40	BM	89/92 (97%)	73 (82%)	16 (18%)	2	9
40	CM	89/92 (97%)	72 (81%)	17 (19%)	1	7
41	BN	90/99 (91%)	76 (84%)	14 (16%)	3	14
41	CN	90/99 (91%)	79 (88%)	11 (12%)	5	23
42	BO	104/109 (95%)	84 (81%)	20 (19%)	1	7
42	CO	104/109 (95%)	80 (77%)	24 (23%)	1	3
43	BP	94/101 (93%)	77 (82%)	17 (18%)	2	9
43	CP	94/101 (93%)	76 (81%)	18 (19%)	1	7
44	BQ	48/50 (96%)	35 (73%)	13 (27%)	0	2
44	CQ	48/50 (96%)	38 (79%)	10 (21%)	1	5
45	BR	79/80 (99%)	69 (87%)	10 (13%)	5	21
45	CR	79/80 (99%)	65 (82%)	14 (18%)	2	9
46	BS	72/74 (97%)	58 (81%)	14 (19%)	1	7
46	CS	72/74 (97%)	60 (83%)	12 (17%)	2	11
47	BT	95/97 (98%)	78 (82%)	17 (18%)	2	9
47	CT	95/97 (98%)	82 (86%)	13 (14%)	4	18
48	BU	63/77 (82%)	53 (84%)	10 (16%)	3	13
48	CU	63/77 (82%)	53 (84%)	10 (16%)	3	13
49	BV	67/80 (84%)	50 (75%)	17 (25%)	0	2
49	CV	67/80 (84%)	47 (70%)	20 (30%)	0	1
50	BW	76/82 (93%)	64 (84%)	12 (16%)	3	13
50	CW	76/82 (93%)	63 (83%)	13 (17%)	2	11
51	BX	20/22 (91%)	20 (100%)	0	100	100
51	CX	20/22 (91%)	18 (90%)	2 (10%)	8	30
All	All	9565/9996 (96%)	7550 (79%)	2015 (21%)	1	5

5 of 2015 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BP	86	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	CH	65	ASN
19	DT	80	ILE
45	BR	67	LEU
32	CE	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

Mol	Chain	Res	Type
47	BT	16	GLN
38	CK	82	HIS
21	DV	132	ASN
50	BW	26	ASN
34	CG	43	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	694 (23%)	62 (2%)
1	DA	2905/2912 (99%)	731 (25%)	60 (2%)
2	AB	121/122 (99%)	23 (19%)	0
2	DB	121/122 (99%)	28 (23%)	1 (0%)
31	BA	1501/1506 (99%)	351 (23%)	39 (2%)
31	CA	1501/1506 (99%)	351 (23%)	49 (3%)
52	BB	83/85 (97%)	45 (54%)	5 (6%)
52	BD	83/85 (97%)	38 (45%)	5 (6%)
52	CB	83/85 (97%)	49 (59%)	8 (9%)
52	CD	83/85 (97%)	35 (42%)	6 (7%)
53	BC	76/77 (98%)	17 (22%)	3 (3%)
53	CC	76/77 (98%)	20 (26%)	3 (3%)
54	B1	15/16 (93%)	7 (46%)	2 (13%)
54	C1	15/16 (93%)	8 (53%)	3 (20%)
All	All	9574/9606 (99%)	2397 (25%)	246 (2%)

5 of 2397 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	17	G
1	AA	23	G
1	AA	34	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	AA	35	G

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BD	21	A
31	CA	686	U
1	DA	2225	A
54	B1	11	U
31	CA	243	A

## 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	1.51	1 (4%)	26,44,47	2.21	9 (34%)
52	MIA	BD	38	52	22,31,32	1.43	1 (4%)	26,44,47	2.97	10 (38%)
52	MIA	CB	38	52	22,31,32	1.67	3 (13%)	26,44,47	2.61	7 (26%)
52	MIA	CD	38	52	22,31,32	1.45	1 (4%)	26,44,47	2.88	10 (38%)

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	-	2/11/33/34	0/3/3/3
52	MIA	BD	38	52	-	6/11/33/34	0/3/3/3
52	MIA	CB	38	52	-	2/11/33/34	0/3/3/3
52	MIA	CD	38	52	-	7/11/33/34	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	CB	38	MIA	C13-C14	6.44	1.51	1.32
52	BB	38	MIA	C13-C14	6.32	1.50	1.32
52	CD	38	MIA	C13-C14	5.97	1.49	1.32
52	BD	38	MIA	C13-C14	5.91	1.49	1.32
52	CB	38	MIA	C2-S10	2.43	1.77	1.75

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	11.99	111.16	102.29
52	CD	38	MIA	C11-S10-C2	10.78	110.27	102.29
52	CB	38	MIA	C11-S10-C2	10.08	109.75	102.29
52	BB	38	MIA	C11-S10-C2	5.32	106.23	102.29
52	CD	38	MIA	C12-C13-C14	-4.64	117.97	127.10

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	BD	38	MIA	O4'-C4'-C5'-O5'
52	BD	38	MIA	C3'-C4'-C5'-O5'
52	BD	38	MIA	N1-C2-S10-C11
52	BD	38	MIA	N3-C2-S10-C11
52	BD	38	MIA	C12-C13-C14-C15

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	BB	38	MIA	2	0
52	BD	38	MIA	7	0
52	CB	38	MIA	5	0
52	CD	38	MIA	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1619 ligands modelled in this entry, 907 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	203	-	0,6,6	0.00	-	-		
56	OHX	A1	204	-	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	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	3335	-	0,6,6	0.00	-	-		
56	OHX	AA	3336	-	0,6,6	0.00	-	-		
56	OHX	AA	3338	-	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	3344	-	0,6,6	0.00	-	-		
56	OHX	AA	3345	-	0,6,6	0.00	-	-		
56	OHX	AA	3346	-	0,6,6	0.00	-	-		
56	OHX	AA	3347	-	0,6,6	0.00	-	-		
56	OHX	AA	3348	-	0,6,6	0.00	-	-		
56	OHX	AA	3349	-	0,6,6	0.00	-	-		
56	OHX	AA	3350	-	0,6,6	0.00	-	-		
56	OHX	AA	3351	-	0,6,6	0.00	-	-		
56	OHX	AA	3352	-	0,6,6	0.00	-	-		
56	OHX	AA	3353	-	0,6,6	0.00	-	-		
56	OHX	AA	3354	-	0,6,6	0.00	-	-		
56	OHX	AA	3355	-	0,6,6	0.00	-	-		
56	OHX	AA	3358	-	0,6,6	0.00	-	-		
56	OHX	AA	3359	-	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	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	-	-		
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	3373	-	0,6,6	0.00	-	-		
56	OHX	AA	3374	-	0,6,6	0.00	-	-		
56	OHX	AA	3375	-	0,6,6	0.00	-	-		
56	OHX	AA	3376	-	0,6,6	0.00	-	-		
56	OHX	AA	3377	-	0,6,6	0.00	-	-		
56	OHX	AA	3378	-	0,6,6	0.00	-	-		
56	OHX	AA	3379	-	0,6,6	0.00	-	-		
56	OHX	AA	3380	-	0,6,6	0.00	-	-		
56	OHX	AA	3381	-	0,6,6	0.00	-	-		
56	OHX	AA	3382	-	0,6,6	0.00	-	-		
56	OHX	AA	3383	-	0,6,6	0.00	-	-		
56	OHX	AA	3384	-	0,6,6	0.00	-	-		
56	OHX	AA	3385	-	0,6,6	0.00	-	-		
56	OHX	AA	3386	-	0,6,6	0.00	-	-		
56	OHX	AA	3387	-	0,6,6	0.00	-	-		
56	OHX	AA	3388	-	0,6,6	0.00	-	-		
56	OHX	AA	3389	-	0,6,6	0.00	-	-		
56	OHX	AA	3390	-	0,6,6	0.00	-	-		
56	OHX	AA	3391	-	0,6,6	0.00	-	-		
56	OHX	AA	3392	-	0,6,6	0.00	-	-		
56	OHX	AA	3393	-	0,6,6	0.00	-	-		
56	OHX	AA	3394	-	0,6,6	0.00	-	-		
56	OHX	AA	3395	-	0,6,6	0.00	-	-		
56	OHX	AA	3396	-	0,6,6	0.00	-	-		
56	OHX	AA	3397	-	0,6,6	0.00	-	-		
56	OHX	AA	3398	-	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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	3408	-	0,6,6	0.00	-	-		
56	OHX	AA	3409	-	0,6,6	0.00	-	-		
56	OHX	AA	3410	-	0,6,6	0.00	-	-		
56	OHX	AA	3411	-	0,6,6	0.00	-	-		
56	OHX	AA	3412	-	0,6,6	0.00	-	-		
56	OHX	AA	3413	-	0,6,6	0.00	-	-		
56	OHX	AA	3414	-	0,6,6	0.00	-	-		
56	OHX	AA	3415	-	0,6,6	0.00	-	-		
56	OHX	AA	3416	-	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	-	-		
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	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-		
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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-		
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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-	-		
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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	202	-	0,6,6	0.00	-	-		
56	OHX	AO	203	-	0,6,6	0.00	-	-		
56	OHX	AW	101	-	0,6,6	0.00	-	-		
57	PAR	BA	1715	-	45,45,45	0.73	2 (4%)	62,67,67	1.69	12 (19%)
56	OHX	BA	1716	-	0,6,6	0.00	-	-		
56	OHX	BA	1717	-	0,6,6	0.00	-	-		
56	OHX	BA	1718	-	0,6,6	0.00	-	-		
56	OHX	BA	1719	-	0,6,6	0.00	-	-		
56	OHX	BA	1720	-	0,6,6	0.00	-	-		
56	OHX	BA	1721	-	0,6,6	0.00	-	-		
56	OHX	BA	1722	-	0,6,6	0.00	-	-		
56	OHX	BA	1723	-	0,6,6	0.00	-	-		
56	OHX	BA	1724	-	0,6,6	0.00	-	-		
56	OHX	BA	1725	-	0,6,6	0.00	-	-		
56	OHX	BA	1726	-	0,6,6	0.00	-	-		
56	OHX	BA	1727	-	0,6,6	0.00	-	-		
56	OHX	BA	1728	-	0,6,6	0.00	-	-		
56	OHX	BA	1729	-	0,6,6	0.00	-	-		
56	OHX	BA	1730	-	0,6,6	0.00	-	-		
56	OHX	BA	1731	-	0,6,6	0.00	-	-		
56	OHX	BA	1732	-	0,6,6	0.00	-	-		
56	OHX	BA	1733	-	0,6,6	0.00	-	-		
56	OHX	BA	1734	-	0,6,6	0.00	-	-		
56	OHX	BA	1735	-	0,6,6	0.00	-	-		
56	OHX	BA	1736	-	0,6,6	0.00	-	-		
56	OHX	BA	1737	-	0,6,6	0.00	-	-		
56	OHX	BA	1738	-	0,6,6	0.00	-	-		
56	OHX	BA	1739	-	0,6,6	0.00	-	-		
56	OHX	BA	1740	-	0,6,6	0.00	-	-		
56	OHX	BA	1741	-	0,6,6	0.00	-	-		
56	OHX	BA	1742	-	0,6,6	0.00	-	-		
56	OHX	BA	1743	-	0,6,6	0.00	-	-		
56	OHX	BA	1744	-	0,6,6	0.00	-	-		
56	OHX	BA	1745	-	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	1746	-	0,6,6	0.00	-	-		
56	OHX	BA	1747	-	0,6,6	0.00	-	-		
56	OHX	BA	1748	-	0,6,6	0.00	-	-		
56	OHX	BA	1749	-	0,6,6	0.00	-	-		
56	OHX	BA	1750	-	0,6,6	0.00	-	-		
56	OHX	BA	1751	-	0,6,6	0.00	-	-		
56	OHX	BA	1752	-	0,6,6	0.00	-	-		
56	OHX	BA	1753	-	0,6,6	0.00	-	-		
56	OHX	BA	1754	-	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	-	-		
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	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	BB	114	-	0,6,6	0.00	-	-		
56	OHX	BB	115	-	0,6,6	0.00	-	-		
56	OHX	BC	105	-	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	BL	201	-	0,6,6	0.00	-	-		
56	OHX	BR	101	-	0,6,6	0.00	-	-		
57	PAR	CA	1722	-	45,45,45	0.70	0	62,67,67	1.82	14 (22%)
56	OHX	CA	1723	-	0,6,6	0.00	-	-		
56	OHX	CA	1724	-	0,6,6	0.00	-	-		
56	OHX	CA	1725	-	0,6,6	0.00	-	-		
56	OHX	CA	1726	-	0,6,6	0.00	-	-		
56	OHX	CA	1727	-	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	1728	-	0,6,6	0.00	-	-		
56	OHX	CA	1729	-	0,6,6	0.00	-	-		
56	OHX	CA	1730	-	0,6,6	0.00	-	-		
56	OHX	CA	1731	-	0,6,6	0.00	-	-		
56	OHX	CA	1732	-	0,6,6	0.00	-	-		
56	OHX	CA	1733	-	0,6,6	0.00	-	-		
56	OHX	CA	1734	-	0,6,6	0.00	-	-		
56	OHX	CA	1735	-	0,6,6	0.00	-	-		
56	OHX	CA	1736	-	0,6,6	0.00	-	-		
56	OHX	CA	1737	-	0,6,6	0.00	-	-		
56	OHX	CA	1738	-	0,6,6	0.00	-	-		
56	OHX	CA	1739	-	0,6,6	0.00	-	-		
56	OHX	CA	1740	-	0,6,6	0.00	-	-		
56	OHX	CA	1741	-	0,6,6	0.00	-	-		
56	OHX	CA	1742	-	0,6,6	0.00	-	-		
56	OHX	CA	1743	-	0,6,6	0.00	-	-		
56	OHX	CA	1744	-	0,6,6	0.00	-	-		
56	OHX	CA	1745	-	0,6,6	0.00	-	-		
56	OHX	CA	1746	-	0,6,6	0.00	-	-		
56	OHX	CA	1747	-	0,6,6	0.00	-	-		
56	OHX	CA	1748	-	0,6,6	0.00	-	-		
56	OHX	CA	1749	-	0,6,6	0.00	-	-		
56	OHX	CA	1750	-	0,6,6	0.00	-	-		
56	OHX	CA	1751	-	0,6,6	0.00	-	-		
56	OHX	CA	1752	-	0,6,6	0.00	-	-		
56	OHX	CA	1753	-	0,6,6	0.00	-	-		
56	OHX	CA	1754	-	0,6,6	0.00	-	-		
56	OHX	CA	1755	-	0,6,6	0.00	-	-		
56	OHX	CA	1756	-	0,6,6	0.00	-	-		
56	OHX	CA	1757	-	0,6,6	0.00	-	-		
56	OHX	CA	1758	-	0,6,6	0.00	-	-		
56	OHX	CA	1759	-	0,6,6	0.00	-	-		
56	OHX	CA	1760	-	0,6,6	0.00	-	-		
56	OHX	CA	1761	-	0,6,6	0.00	-	-		
56	OHX	CA	1762	-	0,6,6	0.00	-	-		
56	OHX	CA	1763	-	0,6,6	0.00	-	-		
56	OHX	CA	1764	-	0,6,6	0.00	-	-		
56	OHX	CA	1765	-	0,6,6	0.00	-	-		
56	OHX	CA	1766	-	0,6,6	0.00	-	-		
56	OHX	CA	1767	-	0,6,6	0.00	-	-		
56	OHX	CA	1768	-	0,6,6	0.00	-	-		
56	OHX	CA	1769	-	0,6,6	0.00	-	-		
56	OHX	CA	1770	-	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	1771	-	0,6,6	0.00	-	-		
56	OHX	CA	1772	-	0,6,6	0.00	-	-		
56	OHX	CA	1773	-	0,6,6	0.00	-	-		
56	OHX	CA	1774	-	0,6,6	0.00	-	-		
56	OHX	CA	1775	-	0,6,6	0.00	-	-		
56	OHX	CA	1776	-	0,6,6	0.00	-	-		
56	OHX	CA	1777	-	0,6,6	0.00	-	-		
56	OHX	CA	1778	-	0,6,6	0.00	-	-		
56	OHX	CA	1779	-	0,6,6	0.00	-	-		
56	OHX	CA	1780	-	0,6,6	0.00	-	-		
56	OHX	CA	1781	-	0,6,6	0.00	-	-		
56	OHX	CA	1782	-	0,6,6	0.00	-	-		
56	OHX	CA	1783	-	0,6,6	0.00	-	-		
56	OHX	CA	1784	-	0,6,6	0.00	-	-		
56	OHX	CA	1785	-	0,6,6	0.00	-	-		
56	OHX	CA	1786	-	0,6,6	0.00	-	-		
56	OHX	CA	1787	-	0,6,6	0.00	-	-		
56	OHX	CA	1788	-	0,6,6	0.00	-	-		
56	OHX	CA	1789	-	0,6,6	0.00	-	-		
56	OHX	CA	1790	-	0,6,6	0.00	-	-		
56	OHX	CA	1791	-	0,6,6	0.00	-	-		
56	OHX	CA	1792	-	0,6,6	0.00	-	-		
56	OHX	CA	1793	-	0,6,6	0.00	-	-		
56	OHX	CA	1794	-	0,6,6	0.00	-	-		
56	OHX	CA	1795	-	0,6,6	0.00	-	-		
56	OHX	CA	1796	-	0,6,6	0.00	-	-		
56	OHX	CA	1797	-	0,6,6	0.00	-	-		
56	OHX	CA	1798	-	0,6,6	0.00	-	-		
56	OHX	CA	1799	-	0,6,6	0.00	-	-		
56	OHX	CA	1800	-	0,6,6	0.00	-	-		
56	OHX	CA	1801	-	0,6,6	0.00	-	-		
56	OHX	CA	1802	-	0,6,6	0.00	-	-		
56	OHX	CA	1803	-	0,6,6	0.00	-	-		
56	OHX	CA	1804	-	0,6,6	0.00	-	-		
56	OHX	CA	1805	-	0,6,6	0.00	-	-		
56	OHX	CA	1806	-	0,6,6	0.00	-	-		
56	OHX	CA	1807	-	0,6,6	0.00	-	-		
56	OHX	CA	1808	-	0,6,6	0.00	-	-		
56	OHX	CA	1809	-	0,6,6	0.00	-	-		
56	OHX	CA	1810	-	0,6,6	0.00	-	-		
56	OHX	CA	1811	-	0,6,6	0.00	-	-		
56	OHX	CA	1812	-	0,6,6	0.00	-	-		
56	OHX	CA	1813	-	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	1814	-	0,6,6	0.00	-	-		
56	OHX	CA	1815	-	0,6,6	0.00	-	-		
56	OHX	CB	104	-	0,6,6	0.00	-	-		
56	OHX	CB	105	-	0,6,6	0.00	-	-		
56	OHX	CB	106	-	0,6,6	0.00	-	-		
56	OHX	CC	108	-	0,6,6	0.00	-	-		
56	OHX	CC	109	-	0,6,6	0.00	-	-		
56	OHX	CC	110	-	0,6,6	0.00	-	-		
56	OHX	CD	101	-	0,6,6	0.00	-	-		
56	OHX	CK	201	-	0,6,6	0.00	-	-		
56	OHX	CR	101	-	0,6,6	0.00	-	-		
56	OHX	CV	101	-	0,6,6	0.00	-	-		
56	OHX	D1	201	-	0,6,6	0.00	-	-		
56	OHX	D3	101	-	0,6,6	0.00	-	-		
56	OHX	D5	102	-	0,6,6	0.00	-	-		
56	OHX	D8	101	-	0,6,6	0.00	-	-		
56	OHX	DA	3061	-	0,6,6	0.00	-	-		
56	OHX	DA	3062	-	0,6,6	0.00	-	-		
56	OHX	DA	3064	-	0,6,6	0.00	-	-		
56	OHX	DA	3065	-	0,6,6	0.00	-	-		
56	OHX	DA	3068	-	0,6,6	0.00	-	-		
56	OHX	DA	3071	-	0,6,6	0.00	-	-		
56	OHX	DA	3073	-	0,6,6	0.00	-	-		
56	OHX	DA	3075	-	0,6,6	0.00	-	-		
56	OHX	DA	3081	-	0,6,6	0.00	-	-		
56	OHX	DA	3082	-	0,6,6	0.00	-	-		
56	OHX	DA	3083	-	0,6,6	0.00	-	-		
56	OHX	DA	3084	-	0,6,6	0.00	-	-		
56	OHX	DA	3087	-	0,6,6	0.00	-	-		
56	OHX	DA	3091	-	0,6,6	0.00	-	-		
56	OHX	DA	3094	-	0,6,6	0.00	-	-		
56	OHX	DA	3099	-	0,6,6	0.00	-	-		
56	OHX	DA	3103	-	0,6,6	0.00	-	-		
56	OHX	DA	3105	-	0,6,6	0.00	-	-		
56	OHX	DA	3109	-	0,6,6	0.00	-	-		
56	OHX	DA	3111	-	0,6,6	0.00	-	-		
56	OHX	DA	3118	-	0,6,6	0.00	-	-		
56	OHX	DA	3124	-	0,6,6	0.00	-	-		
56	OHX	DA	3127	-	0,6,6	0.00	-	-		
56	OHX	DA	3132	-	0,6,6	0.00	-	-		
56	OHX	DA	3134	-	0,6,6	0.00	-	-		
56	OHX	DA	3136	-	0,6,6	0.00	-	-		
56	OHX	DA	3157	-	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	3159	-	0,6,6	0.00	-	-		
56	OHX	DA	3160	-	0,6,6	0.00	-	-		
56	OHX	DA	3162	-	0,6,6	0.00	-	-		
56	OHX	DA	3163	-	0,6,6	0.00	-	-		
56	OHX	DA	3165	-	0,6,6	0.00	-	-		
56	OHX	DA	3166	-	0,6,6	0.00	-	-		
56	OHX	DA	3168	-	0,6,6	0.00	-	-		
56	OHX	DA	3169	-	0,6,6	0.00	-	-		
56	OHX	DA	3170	-	0,6,6	0.00	-	-		
56	OHX	DA	3171	-	0,6,6	0.00	-	-		
56	OHX	DA	3172	-	0,6,6	0.00	-	-		
56	OHX	DA	3173	-	0,6,6	0.00	-	-		
56	OHX	DA	3174	-	0,6,6	0.00	-	-		
56	OHX	DA	3176	-	0,6,6	0.00	-	-		
56	OHX	DA	3212	-	0,6,6	0.00	-	-		
56	OHX	DA	3214	-	0,6,6	0.00	-	-		
56	OHX	DA	3215	-	0,6,6	0.00	-	-		
56	OHX	DA	3217	-	0,6,6	0.00	-	-		
56	OHX	DA	3218	-	0,6,6	0.00	-	-		
56	OHX	DA	3220	-	0,6,6	0.00	-	-		
56	OHX	DA	3221	-	0,6,6	0.00	-	-		
56	OHX	DA	3223	-	0,6,6	0.00	-	-		
56	OHX	DA	3224	-	0,6,6	0.00	-	-		
56	OHX	DA	3226	-	0,6,6	0.00	-	-		
56	OHX	DA	3243	-	0,6,6	0.00	-	-		
56	OHX	DA	3245	-	0,6,6	0.00	-	-		
56	OHX	DA	3246	-	0,6,6	0.00	-	-		
56	OHX	DA	3248	-	0,6,6	0.00	-	-		
56	OHX	DA	3249	-	0,6,6	0.00	-	-		
56	OHX	DA	3251	-	0,6,6	0.00	-	-		
56	OHX	DA	3253	-	0,6,6	0.00	-	-		
56	OHX	DA	3254	-	0,6,6	0.00	-	-		
56	OHX	DA	3255	-	0,6,6	0.00	-	-		
56	OHX	DA	3257	-	0,6,6	0.00	-	-		
56	OHX	DA	3258	-	0,6,6	0.00	-	-		
56	OHX	DA	3335	-	0,6,6	0.00	-	-		
56	OHX	DA	3336	-	0,6,6	0.00	-	-		
56	OHX	DA	3337	-	0,6,6	0.00	-	-		
56	OHX	DA	3338	-	0,6,6	0.00	-	-		
56	OHX	DA	3339	-	0,6,6	0.00	-	-		
56	OHX	DA	3340	-	0,6,6	0.00	-	-		
56	OHX	DA	3341	-	0,6,6	0.00	-	-		
56	OHX	DA	3342	-	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	3343	-	0,6,6	0.00	-	-		
56	OHX	DA	3344	-	0,6,6	0.00	-	-		
56	OHX	DA	3345	-	0,6,6	0.00	-	-		
56	OHX	DA	3346	-	0,6,6	0.00	-	-		
56	OHX	DA	3347	-	0,6,6	0.00	-	-		
56	OHX	DA	3348	-	0,6,6	0.00	-	-		
56	OHX	DA	3349	-	0,6,6	0.00	-	-		
56	OHX	DA	3350	-	0,6,6	0.00	-	-		
56	OHX	DA	3351	-	0,6,6	0.00	-	-		
56	OHX	DA	3352	-	0,6,6	0.00	-	-		
56	OHX	DA	3353	-	0,6,6	0.00	-	-		
56	OHX	DA	3354	-	0,6,6	0.00	-	-		
56	OHX	DA	3355	-	0,6,6	0.00	-	-		
56	OHX	DA	3356	-	0,6,6	0.00	-	-		
56	OHX	DA	3357	-	0,6,6	0.00	-	-		
56	OHX	DA	3358	-	0,6,6	0.00	-	-		
56	OHX	DA	3359	-	0,6,6	0.00	-	-		
56	OHX	DA	3360	-	0,6,6	0.00	-	-		
56	OHX	DA	3361	-	0,6,6	0.00	-	-		
56	OHX	DA	3362	-	0,6,6	0.00	-	-		
56	OHX	DA	3363	-	0,6,6	0.00	-	-		
56	OHX	DA	3364	-	0,6,6	0.00	-	-		
56	OHX	DA	3365	-	0,6,6	0.00	-	-		
56	OHX	DA	3366	-	0,6,6	0.00	-	-		
56	OHX	DA	3367	-	0,6,6	0.00	-	-		
56	OHX	DA	3368	-	0,6,6	0.00	-	-		
56	OHX	DA	3369	-	0,6,6	0.00	-	-		
56	OHX	DA	3370	-	0,6,6	0.00	-	-		
56	OHX	DA	3371	-	0,6,6	0.00	-	-		
56	OHX	DA	3372	-	0,6,6	0.00	-	-		
56	OHX	DA	3373	-	0,6,6	0.00	-	-		
56	OHX	DA	3374	-	0,6,6	0.00	-	-		
56	OHX	DA	3375	-	0,6,6	0.00	-	-		
56	OHX	DA	3376	-	0,6,6	0.00	-	-		
56	OHX	DA	3377	-	0,6,6	0.00	-	-		
56	OHX	DA	3378	-	0,6,6	0.00	-	-		
56	OHX	DA	3379	-	0,6,6	0.00	-	-		
56	OHX	DA	3380	-	0,6,6	0.00	-	-		
56	OHX	DA	3381	-	0,6,6	0.00	-	-		
56	OHX	DA	3382	-	0,6,6	0.00	-	-		
56	OHX	DA	3383	-	0,6,6	0.00	-	-		
56	OHX	DA	3384	-	0,6,6	0.00	-	-		
56	OHX	DA	3385	-	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	3386	-	0,6,6	0.00	-	-		
56	OHX	DA	3387	-	0,6,6	0.00	-	-		
56	OHX	DA	3388	-	0,6,6	0.00	-	-		
56	OHX	DA	3389	-	0,6,6	0.00	-	-		
56	OHX	DA	3390	-	0,6,6	0.00	-	-		
56	OHX	DA	3391	-	0,6,6	0.00	-	-		
56	OHX	DA	3392	-	0,6,6	0.00	-	-		
56	OHX	DA	3393	-	0,6,6	0.00	-	-		
56	OHX	DA	3394	-	0,6,6	0.00	-	-		
56	OHX	DA	3395	-	0,6,6	0.00	-	-		
56	OHX	DA	3396	-	0,6,6	0.00	-	-		
56	OHX	DA	3397	-	0,6,6	0.00	-	-		
56	OHX	DA	3398	-	0,6,6	0.00	-	-		
56	OHX	DA	3399	-	0,6,6	0.00	-	-		
56	OHX	DA	3400	-	0,6,6	0.00	-	-		
56	OHX	DA	3401	-	0,6,6	0.00	-	-		
56	OHX	DA	3402	-	0,6,6	0.00	-	-		
56	OHX	DA	3403	-	0,6,6	0.00	-	-		
56	OHX	DA	3404	-	0,6,6	0.00	-	-		
56	OHX	DA	3405	-	0,6,6	0.00	-	-		
56	OHX	DA	3406	-	0,6,6	0.00	-	-		
56	OHX	DA	3407	-	0,6,6	0.00	-	-		
56	OHX	DA	3408	-	0,6,6	0.00	-	-		
56	OHX	DA	3409	-	0,6,6	0.00	-	-		
56	OHX	DA	3410	-	0,6,6	0.00	-	-		
56	OHX	DA	3411	-	0,6,6	0.00	-	-		
56	OHX	DA	3412	-	0,6,6	0.00	-	-		
56	OHX	DA	3413	-	0,6,6	0.00	-	-		
56	OHX	DA	3414	-	0,6,6	0.00	-	-		
56	OHX	DA	3415	-	0,6,6	0.00	-	-		
56	OHX	DA	3416	-	0,6,6	0.00	-	-		
56	OHX	DA	3417	-	0,6,6	0.00	-	-		
56	OHX	DA	3418	-	0,6,6	0.00	-	-		
56	OHX	DA	3419	-	0,6,6	0.00	-	-		
56	OHX	DA	3420	-	0,6,6	0.00	-	-		
56	OHX	DA	3421	-	0,6,6	0.00	-	-		
56	OHX	DA	3422	-	0,6,6	0.00	-	-		
56	OHX	DA	3423	-	0,6,6	0.00	-	-		
56	OHX	DA	3424	-	0,6,6	0.00	-	-		
56	OHX	DA	3425	-	0,6,6	0.00	-	-		
56	OHX	DA	3426	-	0,6,6	0.00	-	-		
56	OHX	DA	3427	-	0,6,6	0.00	-	-		
56	OHX	DA	3428	-	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	3429	-	0,6,6	0.00	-	-		
56	OHX	DA	3430	-	0,6,6	0.00	-	-		
56	OHX	DA	3431	-	0,6,6	0.00	-	-		
56	OHX	DA	3432	-	0,6,6	0.00	-	-		
56	OHX	DA	3433	-	0,6,6	0.00	-	-		
56	OHX	DA	3434	-	0,6,6	0.00	-	-		
56	OHX	DA	3435	-	0,6,6	0.00	-	-		
56	OHX	DA	3436	-	0,6,6	0.00	-	-		
56	OHX	DA	3437	-	0,6,6	0.00	-	-		
56	OHX	DA	3438	-	0,6,6	0.00	-	-		
56	OHX	DA	3439	-	0,6,6	0.00	-	-		
56	OHX	DA	3440	-	0,6,6	0.00	-	-		
56	OHX	DA	3441	-	0,6,6	0.00	-	-		
56	OHX	DA	3442	-	0,6,6	0.00	-	-		
56	OHX	DA	3443	-	0,6,6	0.00	-	-		
56	OHX	DA	3444	-	0,6,6	0.00	-	-		
56	OHX	DA	3445	-	0,6,6	0.00	-	-		
56	OHX	DA	3446	-	0,6,6	0.00	-	-		
56	OHX	DA	3447	-	0,6,6	0.00	-	-		
56	OHX	DA	3448	-	0,6,6	0.00	-	-		
56	OHX	DA	3449	-	0,6,6	0.00	-	-		
56	OHX	DA	3450	-	0,6,6	0.00	-	-		
56	OHX	DA	3451	-	0,6,6	0.00	-	-		
56	OHX	DA	3452	-	0,6,6	0.00	-	-		
56	OHX	DA	3453	-	0,6,6	0.00	-	-		
56	OHX	DA	3454	-	0,6,6	0.00	-	-		
56	OHX	DA	3455	-	0,6,6	0.00	-	-		
56	OHX	DA	3456	-	0,6,6	0.00	-	-		
56	OHX	DA	3457	-	0,6,6	0.00	-	-		
56	OHX	DA	3458	-	0,6,6	0.00	-	-		
56	OHX	DA	3459	-	0,6,6	0.00	-	-		
56	OHX	DA	3460	-	0,6,6	0.00	-	-		
56	OHX	DA	3461	-	0,6,6	0.00	-	-		
56	OHX	DA	3462	-	0,6,6	0.00	-	-		
56	OHX	DA	3463	-	0,6,6	0.00	-	-		
56	OHX	DA	3464	-	0,6,6	0.00	-	-		
56	OHX	DA	3465	-	0,6,6	0.00	-	-		
56	OHX	DA	3466	-	0,6,6	0.00	-	-		
56	OHX	DA	3467	-	0,6,6	0.00	-	-		
56	OHX	DA	3468	-	0,6,6	0.00	-	-		
56	OHX	DA	3469	-	0,6,6	0.00	-	-		
56	OHX	DA	3470	-	0,6,6	0.00	-	-		
56	OHX	DA	3471	-	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	3472	-	0,6,6	0.00	-	-		
56	OHX	DA	3473	-	0,6,6	0.00	-	-		
56	OHX	DA	3474	-	0,6,6	0.00	-	-		
56	OHX	DA	3475	-	0,6,6	0.00	-	-		
56	OHX	DA	3476	-	0,6,6	0.00	-	-		
56	OHX	DA	3477	-	0,6,6	0.00	-	-		
56	OHX	DA	3478	-	0,6,6	0.00	-	-		
56	OHX	DA	3479	-	0,6,6	0.00	-	-		
56	OHX	DA	3480	-	0,6,6	0.00	-	-		
56	OHX	DA	3481	-	0,6,6	0.00	-	-		
56	OHX	DA	3482	-	0,6,6	0.00	-	-		
56	OHX	DA	3483	-	0,6,6	0.00	-	-		
56	OHX	DA	3484	-	0,6,6	0.00	-	-		
56	OHX	DA	3485	-	0,6,6	0.00	-	-		
56	OHX	DA	3486	-	0,6,6	0.00	-	-		
56	OHX	DA	3487	-	0,6,6	0.00	-	-		
56	OHX	DA	3488	-	0,6,6	0.00	-	-		
56	OHX	DA	3489	-	0,6,6	0.00	-	-		
56	OHX	DA	3490	-	0,6,6	0.00	-	-		
56	OHX	DA	3491	-	0,6,6	0.00	-	-		
56	OHX	DB	208	-	0,6,6	0.00	-	-		
56	OHX	DB	209	-	0,6,6	0.00	-	-		
56	OHX	DB	210	-	0,6,6	0.00	-	-		
56	OHX	DB	211	-	0,6,6	0.00	-	-		
56	OHX	DB	212	-	0,6,6	0.00	-	-		
56	OHX	DB	213	-	0,6,6	0.00	-	-		
56	OHX	DB	214	-	0,6,6	0.00	-	-		
56	OHX	DB	215	-	0,6,6	0.00	-	-		
56	OHX	DB	216	-	0,6,6	0.00	-	-		
56	OHX	DB	217	-	0,6,6	0.00	-	-		
56	OHX	DB	218	-	0,6,6	0.00	-	-		
56	OHX	DB	219	-	0,6,6	0.00	-	-		
56	OHX	DB	220	-	0,6,6	0.00	-	-		
56	OHX	DF	301	-	0,6,6	0.00	-	-		
56	OHX	DO	201	-	0,6,6	0.00	-	-		

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
57	PAR	BA	1715	-	-	6/18/94/94	0/4/4/4
57	PAR	CA	1722	-	-	5/18/94/94	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	1715	PAR	C21-N21	-2.29	1.43	1.47
57	BA	1715	PAR	C31-C21	-2.16	1.50	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	1722	PAR	C11-O51-C51	5.02	123.58	113.70
57	CA	1722	PAR	C13-O52-C52	-4.41	106.98	117.97
57	BA	1715	PAR	C11-O51-C51	4.26	122.08	113.70
57	BA	1715	PAR	C44-C34-C24	4.26	118.49	111.03
57	CA	1722	PAR	C62-C12-N12	-4.23	102.59	110.97

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CA	1722	PAR	O43-C43-C53-O53
57	CA	1722	PAR	C33-C43-C53-O53
57	CA	1722	PAR	C41-C51-C61-O61
57	BA	1715	PAR	C41-C51-C61-O61
57	BA	1715	PAR	O43-C43-C53-O53

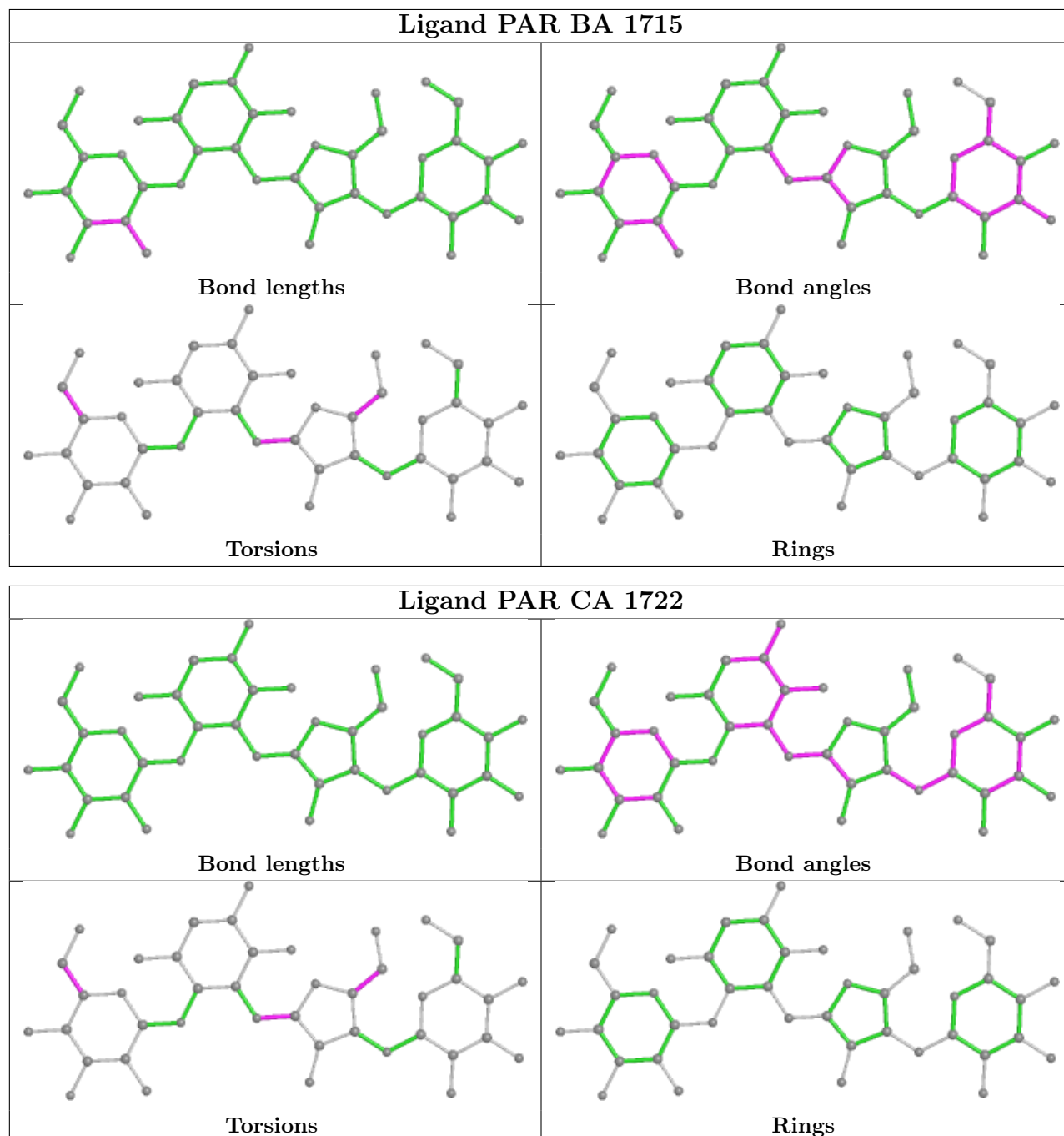
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	1715	PAR	3	0
57	CA	1722	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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%)	-0.31	41 (1%) 75 74	44, 79, 216, 250	0
1	DA	2907/2912 (99%)	-0.24	47 (1%) 72 70	56, 94, 236, 252	0
2	AB	122/122 (100%)	-0.46	1 (0%) 86 86	77, 99, 118, 184	0
2	DB	122/122 (100%)	-0.33	1 (0%) 86 86	98, 129, 153, 204	0
3	AD	272/276 (98%)	0.09	2 (0%) 87 88	42, 67, 88, 106	0
3	DD	272/276 (98%)	0.42	11 (4%) 38 37	52, 78, 98, 130	0
4	AE	205/206 (99%)	0.24	10 (4%) 29 29	54, 90, 135, 147	0
4	DE	205/206 (99%)	0.19	9 (4%) 34 34	61, 102, 153, 167	0
5	AF	202/210 (96%)	-0.16	3 (1%) 73 71	49, 84, 121, 136	0
5	DF	208/210 (99%)	0.35	17 (8%) 11 12	63, 108, 164, 189	0
6	AG	181/182 (99%)	0.79	28 (15%) 2 2	90, 112, 143, 155	0
6	DG	181/182 (99%)	0.99	33 (18%) 1 1	122, 146, 169, 175	0
7	AH	170/180 (94%)	0.08	6 (3%) 44 42	89, 116, 133, 162	0
7	DH	170/180 (94%)	0.57	21 (12%) 4 4	162, 204, 226, 236	0
8	AK	146/148 (98%)	0.21	7 (4%) 30 30	79, 134, 153, 155	0
8	DK	146/148 (98%)	0.17	6 (4%) 37 36	88, 135, 157, 163	0
9	AM	138/140 (98%)	0.16	6 (4%) 35 35	68, 92, 129, 141	0
9	DM	138/140 (98%)	0.18	2 (1%) 75 74	83, 117, 146, 159	0
10	AN	122/122 (100%)	0.25	2 (1%) 72 70	61, 79, 96, 107	0
10	DN	122/122 (100%)	0.37	7 (5%) 24 23	75, 97, 114, 124	0
11	AO	150/150 (100%)	-0.06	7 (4%) 31 31	46, 93, 120, 166	0
11	DO	150/150 (100%)	1.11	39 (26%) 0 0	45, 106, 147, 183	0
12	AP	141/141 (100%)	0.36	13 (9%) 9 10	58, 86, 108, 136	0
12	DP	141/141 (100%)	0.87	25 (17%) 1 1	58, 111, 143, 164	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%)	0.02	1 (0%) 86 86	57, 86, 110, 118	0
13	D0	117/118 (99%)	-0.15	0 100 100	68, 89, 109, 124	0
14	AQ	111/112 (99%)	-0.06	2 (1%) 68 67	67, 97, 120, 133	0
14	DQ	111/112 (99%)	-0.04	3 (2%) 54 53	85, 126, 150, 162	0
15	AR	137/146 (93%)	0.18	3 (2%) 62 61	75, 96, 149, 175	0
15	DR	137/146 (93%)	0.48	11 (8%) 12 13	81, 106, 168, 189	0
16	A1	117/118 (99%)	-0.21	2 (1%) 70 68	58, 81, 110, 142	0
16	D1	117/118 (99%)	0.60	9 (7%) 13 14	71, 109, 145, 167	0
17	A2	101/101 (100%)	0.14	5 (4%) 29 28	51, 104, 126, 143	0
17	D2	101/101 (100%)	1.28	24 (23%) 0 0	65, 134, 147, 155	0
18	AS	113/113 (100%)	0.16	2 (1%) 68 67	61, 77, 108, 161	0
18	DS	113/113 (100%)	0.06	3 (2%) 54 53	66, 82, 116, 162	0
19	AT	92/96 (95%)	-0.02	1 (1%) 80 81	59, 73, 99, 111	0
19	DT	92/96 (95%)	0.15	5 (5%) 26 25	74, 92, 117, 133	0
20	AU	102/110 (92%)	0.36	8 (7%) 13 13	79, 105, 156, 168	0
20	DU	102/110 (92%)	0.76	18 (17%) 1 1	97, 122, 169, 185	0
21	AV	175/206 (84%)	1.95	82 (46%) 0 0	90, 131, 195, 198	0
21	DV	179/206 (86%)	2.70	85 (47%) 0 0	127, 165, 214, 226	0
22	A3	76/85 (89%)	0.04	2 (2%) 56 54	65, 78, 95, 130	0
22	D3	77/85 (90%)	0.14	3 (3%) 39 38	78, 97, 119, 152	0
23	AZ	97/98 (98%)	-0.12	1 (1%) 82 82	59, 79, 131, 161	0
23	DZ	97/98 (98%)	-0.05	2 (2%) 63 62	69, 89, 136, 157	0
24	AW	66/72 (91%)	0.04	1 (1%) 73 71	63, 87, 103, 128	0
24	DW	66/72 (91%)	0.53	2 (3%) 50 50	88, 112, 132, 142	0
25	AX	59/60 (98%)	-0.25	0 100 100	66, 86, 119, 134	0
25	DX	59/60 (98%)	0.97	11 (18%) 1 1	87, 113, 146, 167	0
26	A4	66/71 (92%)	2.25	32 (48%) 0 0	130, 162, 180, 188	0
26	D4	63/71 (88%)	4.06	48 (76%) 0 0	149, 192, 200, 204	0
27	A5	59/60 (98%)	0.59	7 (11%) 4 4	54, 95, 172, 174	0
27	D5	59/60 (98%)	0.43	6 (10%) 7 7	61, 96, 179, 195	0
28	A6	45/54 (83%)	9.35	45 (100%) 0 0	129, 159, 174, 182	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	D6	45/54 (83%)	6.57	39 (86%) 0 0	146, 174, 190, 192	0
29	A7	45/49 (91%)	-0.13	0 100 100	46, 55, 72, 78	0
29	D7	45/49 (91%)	0.06	0 100 100	56, 66, 79, 96	0
30	A8	60/65 (92%)	0.26	3 (5%) 29 28	56, 74, 97, 120	0
30	D8	60/65 (92%)	0.55	5 (8%) 11 12	75, 91, 113, 138	0
31	BA	1502/1506 (99%)	-0.54	4 (0%) 93 94	58, 111, 193, 251	0
31	CA	1502/1506 (99%)	-0.54	3 (0%) 94 96	69, 122, 195, 251	0
32	BE	237/256 (92%)	0.56	29 (12%) 4 4	117, 150, 188, 200	0
32	CE	237/256 (92%)	1.33	65 (27%) 0 0	128, 166, 201, 216	0
33	BF	205/239 (85%)	0.59	24 (11%) 4 4	95, 124, 157, 167	0
33	CF	206/239 (86%)	0.84	32 (15%) 2 2	130, 151, 179, 185	0
34	BG	208/208 (100%)	-0.05	3 (1%) 75 74	95, 119, 141, 152	0
34	CG	208/208 (100%)	0.15	4 (1%) 66 66	94, 114, 136, 151	0
35	BH	151/162 (93%)	0.32	4 (2%) 56 54	81, 109, 130, 166	0
35	CH	151/162 (93%)	0.17	4 (2%) 56 54	106, 124, 148, 171	0
36	BI	101/101 (100%)	1.31	25 (24%) 0 0	86, 111, 127, 152	0
36	CI	101/101 (100%)	0.47	2 (1%) 65 64	83, 108, 131, 149	0
37	BJ	155/156 (99%)	-0.10	8 (5%) 27 26	109, 127, 154, 167	0
37	CJ	155/156 (99%)	-0.08	4 (2%) 56 54	120, 136, 159, 167	0
38	BK	138/138 (100%)	-0.31	1 (0%) 87 88	90, 115, 128, 133	0
38	CK	138/138 (100%)	0.02	2 (1%) 75 74	105, 129, 141, 151	0
39	BL	127/128 (99%)	-0.19	4 (3%) 49 48	98, 148, 166, 173	0
39	CL	127/128 (99%)	-0.36	2 (1%) 72 70	118, 160, 175, 179	0
40	BM	99/105 (94%)	0.46	11 (11%) 5 5	93, 149, 177, 178	0
40	CM	99/105 (94%)	0.26	4 (4%) 38 37	128, 165, 180, 184	0
41	BN	119/129 (92%)	0.68	13 (10%) 5 5	81, 109, 138, 167	0
41	CN	119/129 (92%)	1.67	45 (37%) 0 0	89, 116, 144, 172	0
42	BO	125/132 (94%)	0.33	8 (6%) 19 20	73, 86, 118, 162	0
42	CO	125/132 (94%)	1.02	23 (18%) 1 1	91, 113, 138, 172	0
43	BP	116/126 (92%)	-0.12	3 (2%) 56 54	97, 135, 151, 157	0
43	CP	117/126 (92%)	0.33	11 (9%) 8 9	108, 162, 175, 177	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%)	-0.24	0 100 100	96, 113, 128, 134	0
44	CQ	58/61 (95%)	0.97	11 (18%) 1 1	132, 145, 162, 167	0
45	BR	88/89 (98%)	0.23	0 100 100	81, 103, 125, 130	0
45	CR	88/89 (98%)	0.09	1 (1%) 80 81	88, 116, 138, 145	0
46	BS	84/88 (95%)	-0.10	0 100 100	105, 122, 147, 180	0
46	CS	84/88 (95%)	-0.06	1 (1%) 79 78	96, 108, 131, 164	0
47	BT	100/105 (95%)	-0.11	2 (2%) 65 64	95, 114, 128, 135	0
47	CT	100/105 (95%)	-0.12	3 (3%) 50 50	96, 117, 138, 149	0
48	BU	72/88 (81%)	1.54	22 (30%) 0 0	94, 111, 147, 169	0
48	CU	72/88 (81%)	1.66	18 (25%) 0 0	98, 120, 160, 178	0
49	BV	78/93 (83%)	0.10	5 (6%) 19 20	113, 135, 155, 159	0
49	CV	78/93 (83%)	0.79	17 (21%) 0 1	146, 170, 187, 192	0
50	BW	99/106 (93%)	-0.61	0 100 100	113, 129, 159, 167	0
50	CW	99/106 (93%)	-0.16	1 (1%) 82 82	100, 122, 157, 170	0
51	BX	25/27 (92%)	-0.55	0 100 100	110, 123, 139, 157	0
51	CX	25/27 (92%)	0.04	2 (8%) 12 13	126, 148, 165, 175	0
52	BB	84/85 (98%)	3.42	59 (70%) 0 0	98, 138, 163, 176	0
52	BD	84/85 (98%)	0.27	7 (8%) 11 12	78, 144, 223, 233	0
52	CB	84/85 (98%)	5.75	72 (85%) 0 0	113, 143, 166, 176	0
52	CD	84/85 (98%)	-0.13	1 (1%) 79 78	86, 144, 222, 230	0
53	BC	77/77 (100%)	-0.27	1 (1%) 77 77	82, 117, 146, 159	0
53	CC	77/77 (100%)	-0.19	1 (1%) 77 77	92, 127, 156, 164	0
54	B1	16/16 (100%)	0.78	3 (18%) 1 1	81, 117, 161, 169	0
54	C1	16/16 (100%)	0.88	2 (12%) 4 4	90, 122, 168, 176	0
All	All	21100/21658 (97%)	0.14	1382 (6%) 19 19	42, 108, 188, 252	0

The worst 5 of 1382 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	A6	29	ASN	16.7
52	CB	52	G	16.0
52	CB	16	C	15.1
28	A6	18	ARG	14.8
1	AA	2901	C	14.4

## 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	CB	38	29/30	0.89	0.38	99,111,127,136	0
52	MIA	BD	38	29/30	0.90	0.24	126,140,181,195	0
52	MIA	CD	38	29/30	0.91	0.23	127,140,183,200	0
52	MIA	BB	38	29/30	0.95	0.19	92,99,110,128	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	AA	3291	1/1	0.11	0.43	99,99,99,99	0
55	MG	CA	1685	1/1	0.13	0.48	104,104,104,104	0
55	MG	CA	1672	1/1	0.22	0.76	125,125,125,125	0
55	MG	DA	3320	1/1	0.26	0.44	132,132,132,132	0
55	MG	AA	3222	1/1	0.29	0.42	85,85,85,85	0
55	MG	AA	3078	1/1	0.30	0.27	97,97,97,97	0
55	MG	CA	1629	1/1	0.33	0.50	166,166,166,166	0
55	MG	BB	104	1/1	0.37	0.77	100,100,100,100	0
55	MG	CA	1686	1/1	0.39	0.61	110,110,110,110	0
55	MG	BB	108	1/1	0.40	0.27	80,80,80,80	0
55	MG	DA	3053	1/1	0.41	0.43	116,116,116,116	0
55	MG	AA	3343	1/1	0.42	0.27	92,92,92,92	0
55	MG	DA	3307	1/1	0.42	0.49	119,119,119,119	0
55	MG	AA	3306	1/1	0.42	0.40	100,100,100,100	0
55	MG	BA	1639	1/1	0.45	0.20	101,101,101,101	0
55	MG	DA	3049	1/1	0.45	0.36	104,104,104,104	0
55	MG	BB	113	1/1	0.47	0.25	80,80,80,80	0
55	MG	AA	3089	1/1	0.49	0.23	130,130,130,130	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	1681	1/1	0.50	0.28	111,111,111,111	0
55	MG	CA	1628	1/1	0.51	0.20	137,137,137,137	0
55	MG	BA	1685	1/1	0.53	0.22	93,93,93,93	0
55	MG	BW	201	1/1	0.55	0.19	92,92,92,92	0
55	MG	BA	1695	1/1	0.55	0.23	132,132,132,132	0
55	MG	DA	3322	1/1	0.56	0.18	152,152,152,152	0
55	MG	BA	1602	1/1	0.56	0.23	66,66,66,66	0
55	MG	DA	3203	1/1	0.58	0.59	69,69,69,69	0
55	MG	BB	106	1/1	0.59	0.56	102,102,102,102	0
55	MG	CA	1692	1/1	0.59	0.22	104,104,104,104	0
55	MG	AA	3084	1/1	0.60	0.27	104,104,104,104	0
55	MG	CA	1683	1/1	0.60	0.39	79,79,79,79	0
55	MG	CA	1665	1/1	0.60	0.28	114,114,114,114	0
55	MG	BA	1657	1/1	0.61	0.33	87,87,87,87	0
55	MG	BA	1706	1/1	0.63	0.34	111,111,111,111	0
55	MG	BA	1625	1/1	0.63	0.32	66,66,66,66	0
55	MG	BA	1670	1/1	0.63	0.30	100,100,100,100	0
55	MG	DA	3252	1/1	0.64	0.61	81,81,81,81	0
55	MG	DA	3330	1/1	0.65	0.68	81,81,81,81	0
55	MG	BS	101	1/1	0.65	0.19	81,81,81,81	0
55	MG	CA	1720	1/1	0.65	0.90	110,110,110,110	0
55	MG	AA	3096	1/1	0.66	0.59	76,76,76,76	0
55	MG	BA	1714	1/1	0.66	0.63	83,83,83,83	0
56	OHX	BD	104	7/7	0.66	0.35	94,101,103,107	3
55	MG	AA	3300	1/1	0.66	0.27	81,81,81,81	0
55	MG	AA	3337	1/1	0.66	0.64	73,73,73,73	0
55	MG	BB	105	1/1	0.67	0.17	94,94,94,94	0
55	MG	DA	3311	1/1	0.67	0.41	63,63,63,63	0
55	MG	CA	1699	1/1	0.67	0.44	86,86,86,86	0
55	MG	BA	1704	1/1	0.67	0.09	127,127,127,127	0
55	MG	DA	3048	1/1	0.67	0.49	93,93,93,93	0
55	MG	CA	1641	1/1	0.68	0.48	85,85,85,85	0
55	MG	DA	3303	1/1	0.68	0.20	97,97,97,97	0
55	MG	A3	101	1/1	0.68	0.43	71,71,71,71	0
55	MG	AA	3305	1/1	0.68	0.56	66,66,66,66	0
55	MG	DB	206	1/1	0.68	0.51	81,81,81,81	0
55	MG	CA	1623	1/1	0.68	0.26	96,96,96,96	0
55	MG	CA	1646	1/1	0.68	0.29	79,79,79,79	0
55	MG	DA	3145	1/1	0.69	1.00	82,82,82,82	0
55	MG	CA	1609	1/1	0.69	0.37	112,112,112,112	0
55	MG	BB	102	1/1	0.69	0.29	92,92,92,92	0
55	MG	DA	3100	1/1	0.70	0.31	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	BB	111	1/1	0.70	0.34	80,80,80,80	0
55	MG	BA	1630	1/1	0.70	0.24	109,109,109,109	0
55	MG	CA	1719	1/1	0.70	0.35	94,94,94,94	0
55	MG	DA	3181	1/1	0.70	0.31	98,98,98,98	0
55	MG	CA	1708	1/1	0.70	0.11	95,95,95,95	0
55	MG	DA	3327	1/1	0.70	0.25	73,73,73,73	0
55	MG	BA	1624	1/1	0.71	0.65	79,79,79,79	0
55	MG	AA	3091	1/1	0.71	0.28	85,85,85,85	0
55	MG	CA	1704	1/1	0.71	0.12	135,135,135,135	0
56	OHX	AA	3508	7/7	0.72	0.12	192,206,214,236	1
55	MG	BA	1677	1/1	0.72	0.38	101,101,101,101	0
55	MG	CA	1614	1/1	0.72	0.18	118,118,118,118	0
55	MG	BA	1675	1/1	0.72	0.43	87,87,87,87	0
55	MG	AA	3215	1/1	0.72	0.42	69,69,69,69	0
55	MG	AA	3301	1/1	0.72	0.18	97,97,97,97	0
55	MG	AA	3322	1/1	0.73	0.27	81,81,81,81	0
55	MG	AA	3278	1/1	0.73	0.39	73,73,73,73	0
55	MG	AA	3281	1/1	0.73	0.17	93,93,93,93	0
55	MG	DA	3233	1/1	0.73	0.32	65,65,65,65	0
55	MG	BA	1615	1/1	0.73	0.41	78,78,78,78	0
55	MG	DA	3302	1/1	0.73	0.34	98,98,98,98	0
55	MG	AA	3209	1/1	0.73	0.33	86,86,86,86	0
55	MG	DA	3158	1/1	0.73	0.64	88,88,88,88	0
55	MG	C1	101	1/1	0.73	0.29	102,102,102,102	0
55	MG	BA	1613	1/1	0.73	0.13	116,116,116,116	0
55	MG	CA	1716	1/1	0.73	0.34	79,79,79,79	0
55	MG	AA	3245	1/1	0.73	0.68	70,70,70,70	0
55	MG	CA	1651	1/1	0.74	0.18	73,73,73,73	0
55	MG	AA	3277	1/1	0.74	0.46	94,94,94,94	0
55	MG	BA	1674	1/1	0.74	0.22	67,67,67,67	0
55	MG	CA	1653	1/1	0.74	0.23	75,75,75,75	0
55	MG	DB	201	1/1	0.74	0.12	95,95,95,95	0
55	MG	DA	3259	1/1	0.74	0.34	114,114,114,114	0
55	MG	BA	1703	1/1	0.74	0.22	90,90,90,90	0
55	MG	DA	3201	1/1	0.74	0.46	86,86,86,86	0
55	MG	DA	3112	1/1	0.74	0.55	85,85,85,85	0
55	MG	AA	3269	1/1	0.74	0.36	59,59,59,59	0
55	MG	CA	1718	1/1	0.75	0.28	84,84,84,84	0
55	MG	AA	3323	1/1	0.75	0.26	58,58,58,58	0
55	MG	DA	3328	1/1	0.75	0.21	99,99,99,99	0
55	MG	BA	1621	1/1	0.75	0.27	77,77,77,77	0
55	MG	BA	1683	1/1	0.75	0.33	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	CB	105	7/7	0.75	0.33	139,142,156,183	2
56	OHX	AA	3497	7/7	0.75	0.23	105,127,139,145	1
56	OHX	BA	1804	7/7	0.75	0.17	147,154,164,208	1
55	MG	AA	3141	1/1	0.75	0.34	80,80,80,80	0
55	MG	DA	3264	1/1	0.75	0.15	78,78,78,78	0
55	MG	CC	103	1/1	0.76	0.72	97,97,97,97	0
55	MG	AA	3324	1/1	0.76	0.18	84,84,84,84	0
55	MG	CC	104	1/1	0.76	0.49	89,89,89,89	0
55	MG	DA	3304	1/1	0.76	0.16	89,89,89,89	0
55	MG	DA	3039	1/1	0.77	0.20	102,102,102,102	0
55	MG	BA	1705	1/1	0.77	0.08	109,109,109,109	0
55	MG	BB	110	1/1	0.77	0.27	80,80,80,80	0
55	MG	CA	1617	1/1	0.77	0.13	126,126,126,126	0
55	MG	CA	1662	1/1	0.77	0.40	92,92,92,92	0
55	MG	CA	1668	1/1	0.77	0.43	80,80,80,80	0
55	MG	AA	3154	1/1	0.77	0.23	52,52,52,52	0
55	MG	CB	101	1/1	0.77	0.43	105,105,105,105	0
55	MG	AA	3083	1/1	0.77	0.34	94,94,94,94	0
55	MG	DA	3256	1/1	0.77	0.30	89,89,89,89	0
55	MG	CA	1674	1/1	0.77	0.60	97,97,97,97	0
55	MG	DA	3298	1/1	0.77	0.20	102,102,102,102	0
55	MG	DA	3288	1/1	0.77	0.27	82,82,82,82	0
55	MG	CA	1721	1/1	0.77	0.17	80,80,80,80	0
55	MG	DA	3331	1/1	0.78	0.45	69,69,69,69	0
55	MG	AA	3061	1/1	0.78	0.30	59,59,59,59	0
55	MG	C1	102	1/1	0.78	0.39	104,104,104,104	0
55	MG	DA	3092	1/1	0.78	0.27	74,74,74,74	0
55	MG	CA	1622	1/1	0.78	0.34	89,89,89,89	0
56	OHX	BA	1776	7/7	0.78	0.31	119,138,152,176	2
55	MG	AA	3279	1/1	0.78	0.52	90,90,90,90	0
55	MG	DA	3096	1/1	0.78	0.23	85,85,85,85	0
55	MG	AA	3236	1/1	0.78	0.49	66,66,66,66	0
55	MG	BA	1699	1/1	0.78	0.53	84,84,84,84	0
56	OHX	DB	219	7/7	0.78	0.17	147,161,178,209	1
55	MG	DA	3295	1/1	0.78	0.49	77,77,77,77	0
55	MG	CA	1689	1/1	0.78	0.18	80,80,80,80	0
55	MG	CA	1712	1/1	0.78	0.16	83,83,83,83	0
55	MG	BA	1708	1/1	0.79	0.19	80,80,80,80	0
55	MG	AB	201	1/1	0.79	0.28	85,85,85,85	0
55	MG	AA	3229	1/1	0.79	0.26	65,65,65,65	0
55	MG	AA	3062	1/1	0.79	0.25	97,97,97,97	0
55	MG	AA	3372	1/1	0.79	0.30	80,80,80,80	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	1640	1/1	0.79	0.20	71,71,71,71	0
55	MG	DA	3196	1/1	0.79	0.41	54,54,54,54	0
55	MG	AA	3048	1/1	0.79	0.20	91,91,91,91	0
55	MG	AA	3111	1/1	0.79	0.37	69,69,69,69	0
55	MG	CA	1621	1/1	0.79	0.28	110,110,110,110	0
56	OHX	DA	3124	7/7	0.79	0.15	144,164,170,220	1
56	OHX	CA	1804	7/7	0.79	0.27	145,149,162,192	1
55	MG	CA	1624	1/1	0.79	0.11	114,114,114,114	0
55	MG	DA	3287	1/1	0.80	0.22	102,102,102,102	0
56	OHX	AA	3531	7/7	0.80	0.18	225,229,234,256	1
55	MG	AA	3043	1/1	0.80	0.35	75,75,75,75	0
56	OHX	BA	1813	7/7	0.80	0.19	151,161,170,205	1
55	MG	AA	3156	1/1	0.80	0.31	80,80,80,80	0
55	MG	AA	3235	1/1	0.80	0.11	57,57,57,57	0
55	MG	AA	3142	1/1	0.80	0.46	75,75,75,75	0
55	MG	DA	3325	1/1	0.80	0.31	91,91,91,91	0
55	MG	AA	3092	1/1	0.80	0.12	92,92,92,92	0
55	MG	BA	1612	1/1	0.80	0.33	100,100,100,100	0
55	MG	BA	1680	1/1	0.80	0.22	64,64,64,64	0
55	MG	BA	1687	1/1	0.81	0.24	96,96,96,96	0
55	MG	AA	3284	1/1	0.81	0.31	68,68,68,68	0
55	MG	DA	3042	1/1	0.81	0.23	74,74,74,74	0
55	MG	BA	1650	1/1	0.81	0.23	85,85,85,85	0
55	MG	AA	3076	1/1	0.81	0.24	81,81,81,81	0
55	MG	AA	3257	1/1	0.81	0.32	64,64,64,64	0
55	MG	BC	104	1/1	0.81	0.38	88,88,88,88	0
55	MG	BA	1636	1/1	0.81	0.14	111,111,111,111	0
55	MG	AF	302	1/1	0.81	0.20	83,83,83,83	0
55	MG	D7	101	1/1	0.81	0.49	69,69,69,69	0
55	MG	DA	3313	1/1	0.81	0.34	88,88,88,88	0
55	MG	DA	3242	1/1	0.81	0.57	99,99,99,99	0
55	MG	DA	3318	1/1	0.81	0.19	110,110,110,110	0
55	MG	B1	101	1/1	0.81	0.14	96,96,96,96	0
55	MG	AA	3295	1/1	0.81	0.45	89,89,89,89	0
55	MG	DA	3046	1/1	0.81	0.38	78,78,78,78	0
55	MG	BA	1637	1/1	0.81	0.21	99,99,99,99	0
55	MG	AA	3157	1/1	0.81	0.41	86,86,86,86	0
55	MG	AA	3105	1/1	0.81	0.46	65,65,65,65	0
55	MG	CA	1696	1/1	0.81	0.59	74,74,74,74	0
55	MG	AA	3259	1/1	0.81	0.13	60,60,60,60	0
55	MG	BB	103	1/1	0.81	0.21	105,105,105,105	0
55	MG	AA	3308	1/1	0.81	0.40	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	CA	1797	7/7	0.82	0.36	129,132,139,171	1
55	MG	DA	3333	1/1	0.82	0.31	84,84,84,84	0
55	MG	BA	1709	1/1	0.82	0.15	68,68,68,68	0
55	MG	DA	3069	1/1	0.82	0.13	63,63,63,63	0
55	MG	CA	1687	1/1	0.82	0.29	104,104,104,104	0
55	MG	DA	3310	1/1	0.82	0.22	73,73,73,73	0
55	MG	AA	3316	1/1	0.82	0.18	79,79,79,79	0
55	MG	DA	3054	1/1	0.82	0.15	56,56,56,56	0
55	MG	CA	1657	1/1	0.82	0.21	81,81,81,81	0
55	MG	AA	3193	1/1	0.82	0.39	86,86,86,86	0
55	MG	DA	3296	1/1	0.82	0.35	103,103,103,103	0
55	MG	A1	201	1/1	0.82	0.34	62,62,62,62	0
55	MG	AA	3143	1/1	0.82	0.49	87,87,87,87	0
55	MG	CA	1652	1/1	0.82	0.10	69,69,69,69	0
56	OHX	AA	3538	7/7	0.82	0.17	95,101,128,162	1
55	MG	AA	3334	1/1	0.82	0.15	90,90,90,90	0
55	MG	AA	3122	1/1	0.83	0.25	57,57,57,57	0
55	MG	DA	3270	1/1	0.83	0.68	73,73,73,73	0
55	MG	CA	1715	1/1	0.83	0.38	80,80,80,80	0
55	MG	CB	103	1/1	0.83	0.18	80,80,80,80	0
55	MG	CA	1643	1/1	0.83	0.50	68,68,68,68	0
56	OHX	AA	3520	7/7	0.83	0.25	88,95,98,151	2
55	MG	CA	1620	1/1	0.83	0.27	63,63,63,63	0
55	MG	AA	3120	1/1	0.83	0.50	74,74,74,74	0
56	OHX	AA	3507	7/7	0.83	0.48	120,135,161,172	2
55	MG	AA	3173	1/1	0.83	0.45	65,65,65,65	0
55	MG	CA	1703	1/1	0.83	0.48	84,84,84,84	0
55	MG	BA	1689	1/1	0.83	0.13	80,80,80,80	0
55	MG	DA	3284	1/1	0.83	0.24	89,89,89,89	0
55	MG	CA	1710	1/1	0.83	0.16	78,78,78,78	0
55	MG	CA	1677	1/1	0.83	0.44	73,73,73,73	0
55	MG	DA	3117	1/1	0.83	0.29	82,82,82,82	0
55	MG	DA	3332	1/1	0.83	0.18	78,78,78,78	0
55	MG	DA	3237	1/1	0.83	0.31	85,85,85,85	0
55	MG	AA	3138	1/1	0.83	0.21	78,78,78,78	0
55	MG	BA	1653	1/1	0.83	0.29	64,64,64,64	0
55	MG	CB	102	1/1	0.83	0.34	80,80,80,80	0
56	OHX	DA	3251	7/7	0.83	0.26	102,112,141,176	3
55	MG	CA	1676	1/1	0.84	0.34	78,78,78,78	0
55	MG	BA	1628	1/1	0.84	0.30	95,95,95,95	0
55	MG	AA	3290	1/1	0.84	0.35	66,66,66,66	0
55	MG	DA	3324	1/1	0.84	0.53	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	CA	1774	7/7	0.84	0.18	137,150,161,190	1
55	MG	DA	3244	1/1	0.84	0.29	82,82,82,82	0
55	MG	DA	3278	1/1	0.84	0.38	84,84,84,84	0
55	MG	BA	1696	1/1	0.84	0.27	94,94,94,94	0
56	OHX	BA	1772	7/7	0.84	0.10	165,176,177,219	1
55	MG	CA	1626	1/1	0.84	0.31	124,124,124,124	0
55	MG	CA	1693	1/1	0.84	0.15	55,55,55,55	0
55	MG	AA	3217	1/1	0.84	0.20	66,66,66,66	0
55	MG	DA	3199	1/1	0.84	0.56	77,77,77,77	0
55	MG	CA	1667	1/1	0.84	0.43	78,78,78,78	0
55	MG	DA	3319	1/1	0.84	0.48	69,69,69,69	0
55	MG	CA	1605	1/1	0.84	0.26	75,75,75,75	0
55	MG	DA	3202	1/1	0.84	0.45	65,65,65,65	0
55	MG	BA	1635	1/1	0.84	0.06	86,86,86,86	0
55	MG	CC	107	1/1	0.85	0.27	80,80,80,80	0
55	MG	CA	1627	1/1	0.85	0.27	126,126,126,126	0
55	MG	DA	3306	1/1	0.85	0.51	86,86,86,86	0
55	MG	BA	1643	1/1	0.85	0.21	67,67,67,67	0
55	MG	AA	3060	1/1	0.85	0.24	89,89,89,89	0
56	OHX	AA	3546	7/7	0.85	0.19	101,114,120,164	2
55	MG	AA	3181	1/1	0.85	0.50	71,71,71,71	0
55	MG	A7	101	1/1	0.85	0.41	56,56,56,56	0
55	MG	AA	3107	1/1	0.85	0.42	51,51,51,51	0
55	MG	BA	1622	1/1	0.85	0.18	92,92,92,92	0
56	OHX	AA	3506	7/7	0.85	0.14	104,115,126,178	1
56	OHX	CC	108	7/7	0.85	0.16	130,137,148,169	1
55	MG	DB	207	1/1	0.85	0.18	70,70,70,70	0
55	MG	DA	3183	1/1	0.85	0.25	99,99,99,99	0
55	MG	DA	3110	1/1	0.85	0.53	60,60,60,60	0
55	MG	AA	3038	1/1	0.85	0.48	68,68,68,68	0
55	MG	AA	3311	1/1	0.85	0.31	90,90,90,90	0
55	MG	AA	3189	1/1	0.85	0.34	63,63,63,63	0
55	MG	DA	3300	1/1	0.85	0.33	63,63,63,63	0
55	MG	AA	3088	1/1	0.85	0.31	66,66,66,66	0
55	MG	BA	1666	1/1	0.85	0.44	81,81,81,81	0
55	MG	DA	3294	1/1	0.85	0.16	74,74,74,74	0
55	MG	AA	3247	1/1	0.85	0.51	66,66,66,66	0
55	MG	AA	3270	1/1	0.85	0.64	90,90,90,90	0
56	OHX	BA	1788	7/7	0.85	0.23	123,136,147,176	1
56	OHX	AA	3392	7/7	0.85	0.18	81,92,124,181	2
55	MG	AA	3183	1/1	0.85	0.32	59,59,59,59	0
56	OHX	CA	1815	7/7	0.85	0.11	158,163,177,221	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	DA	3488	7/7	0.85	0.23	87,112,131,159	1
55	MG	DA	3027	1/1	0.85	0.14	78,78,78,78	0
55	MG	BA	1664	1/1	0.85	0.29	54,54,54,54	0
55	MG	AA	3052	1/1	0.86	0.29	71,71,71,71	0
55	MG	BA	1644	1/1	0.86	0.35	62,62,62,62	0
55	MG	BA	1711	1/1	0.86	0.31	90,90,90,90	0
56	OHX	CA	1767	7/7	0.86	0.30	110,139,162,203	1
55	MG	AA	3310	1/1	0.86	0.22	71,71,71,71	0
56	OHX	DB	216	7/7	0.86	0.13	123,138,155,204	1
55	MG	AB	203	1/1	0.86	0.23	58,58,58,58	0
56	OHX	AA	3567	7/7	0.86	0.16	125,135,148,181	2
56	OHX	AA	3455	7/7	0.86	0.15	173,192,201,215	1
55	MG	AA	3282	1/1	0.86	0.10	103,103,103,103	0
55	MG	BA	1608	1/1	0.86	0.13	89,89,89,89	0
56	OHX	AA	3519	7/7	0.86	0.20	103,114,126,154	1
55	MG	DA	3279	1/1	0.86	0.29	68,68,68,68	0
55	MG	DB	205	1/1	0.86	0.18	64,64,64,64	0
55	MG	DA	3289	1/1	0.86	0.17	84,84,84,84	0
55	MG	CA	1671	1/1	0.86	0.28	78,78,78,78	0
55	MG	DA	3180	1/1	0.86	0.43	45,45,45,45	0
55	MG	CA	1618	1/1	0.86	0.09	82,82,82,82	0
56	OHX	DA	3454	7/7	0.86	0.20	136,143,163,191	1
56	OHX	BA	1778	7/7	0.86	0.22	125,131,152,191	1
56	OHX	DA	3474	7/7	0.86	0.21	120,126,143,173	1
56	OHX	DB	220	7/7	0.86	0.20	159,162,171,208	1
55	MG	AA	3289	1/1	0.86	0.47	61,61,61,61	0
55	MG	DA	3200	1/1	0.86	1.13	86,86,86,86	0
55	MG	DA	3090	1/1	0.86	0.34	54,54,54,54	0
55	MG	AA	3161	1/1	0.86	0.24	57,57,57,57	0
56	OHX	DA	3255	7/7	0.86	0.22	93,104,107,143	1
55	MG	AA	3287	1/1	0.86	0.32	66,66,66,66	0
55	MG	AA	3071	1/1	0.86	0.42	84,84,84,84	0
55	MG	BA	1676	1/1	0.86	0.40	78,78,78,78	0
55	MG	DA	3072	1/1	0.87	0.09	93,93,93,93	0
55	MG	AA	3110	1/1	0.87	0.39	76,76,76,76	0
55	MG	AA	3231	1/1	0.87	0.39	57,57,57,57	0
55	MG	AA	3233	1/1	0.87	0.26	82,82,82,82	0
56	OHX	CA	1789	7/7	0.87	0.12	152,164,170,204	1
55	MG	CA	1678	1/1	0.87	0.09	97,97,97,97	0
55	MG	DA	3276	1/1	0.87	0.40	78,78,78,78	0
55	MG	DA	3115	1/1	0.87	0.25	44,44,44,44	0
55	MG	DA	3066	1/1	0.87	0.31	77,77,77,77	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	0.87	0.15	125,128,143,177	1
56	OHX	DA	3462	7/7	0.87	0.12	154,157,165,208	1
55	MG	DA	3102	1/1	0.87	0.25	76,76,76,76	0
55	MG	AA	3082	1/1	0.87	0.29	57,57,57,57	0
55	MG	DA	3020	1/1	0.87	0.60	60,60,60,60	0
55	MG	CA	1691	1/1	0.87	0.19	128,128,128,128	0
55	MG	AA	3174	1/1	0.87	0.15	91,91,91,91	0
55	MG	AA	3307	1/1	0.87	0.30	72,72,72,72	0
55	MG	AA	3203	1/1	0.87	0.45	72,72,72,72	0
55	MG	AA	3170	1/1	0.87	0.62	69,69,69,69	0
55	MG	AA	3160	1/1	0.87	0.38	69,69,69,69	0
55	MG	BA	1686	1/1	0.87	0.15	100,100,100,100	0
55	MG	DA	3238	1/1	0.87	0.42	67,67,67,67	0
56	OHX	DB	218	7/7	0.87	0.37	134,141,153,171	1
55	MG	BA	1697	1/1	0.87	0.48	74,74,74,74	0
56	OHX	AA	3511	7/7	0.87	0.14	133,137,167,178	2
55	MG	BA	1645	1/1	0.87	0.15	76,76,76,76	0
55	MG	AA	3182	1/1	0.87	0.46	66,66,66,66	0
55	MG	DA	3281	1/1	0.87	0.23	65,65,65,65	0
55	MG	DA	3055	1/1	0.87	0.41	54,54,54,54	0
55	MG	AA	3211	1/1	0.87	0.18	58,58,58,58	0
56	OHX	DA	3223	7/7	0.87	0.17	126,133,144,169	1
55	MG	AA	3172	1/1	0.87	0.58	71,71,71,71	0
56	OHX	AA	3528	7/7	0.87	0.27	119,125,142,174	1
55	MG	BB	101	1/1	0.87	0.11	95,95,95,95	0
55	MG	BA	1617	1/1	0.88	0.49	60,60,60,60	0
56	OHX	CR	101	7/7	0.88	0.32	143,150,160,179	1
55	MG	AA	3200	1/1	0.88	0.33	82,82,82,82	0
55	MG	AA	3318	1/1	0.88	0.24	75,75,75,75	0
55	MG	DA	3206	1/1	0.88	0.16	52,52,52,52	0
56	OHX	DA	3448	7/7	0.88	0.13	134,147,163,206	1
55	MG	DA	3022	1/1	0.88	0.70	63,63,63,63	0
55	MG	CC	106	1/1	0.88	0.61	75,75,75,75	0
55	MG	BA	1619	1/1	0.88	0.39	64,64,64,64	0
55	MG	AA	3317	1/1	0.88	0.21	55,55,55,55	0
55	MG	DA	3314	1/1	0.88	0.20	70,70,70,70	0
55	MG	AA	3304	1/1	0.88	0.17	55,55,55,55	0
55	MG	AA	3031	1/1	0.88	0.34	40,40,40,40	0
55	MG	BA	1707	1/1	0.88	0.11	63,63,63,63	0
55	MG	AA	3075	1/1	0.88	0.19	78,78,78,78	0
55	MG	BA	1692	1/1	0.88	0.15	73,73,73,73	0
55	MG	CA	1659	1/1	0.88	0.11	116,116,116,116	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	3151	1/1	0.88	0.32	46,46,46,46	0
56	OHX	CA	1747	7/7	0.88	0.18	129,134,147,212	1
55	MG	DA	3312	1/1	0.88	0.29	81,81,81,81	0
55	MG	BA	1649	1/1	0.88	0.41	92,92,92,92	0
55	MG	AA	3264	1/1	0.88	0.28	51,51,51,51	0
55	MG	CA	1707	1/1	0.88	0.18	97,97,97,97	0
55	MG	BF	301	1/1	0.88	0.24	79,79,79,79	0
55	MG	AA	3251	1/1	0.88	0.61	75,75,75,75	0
56	OHX	D8	101	7/7	0.88	0.20	140,149,164,175	1
55	MG	CA	1615	1/1	0.88	0.20	109,109,109,109	0
55	MG	AA	3125	1/1	0.88	0.21	63,63,63,63	0
55	MG	DA	3308	1/1	0.88	0.23	60,60,60,60	0
55	MG	BA	1648	1/1	0.88	0.40	86,86,86,86	0
56	OHX	DA	3473	7/7	0.88	0.10	138,151,163,196	1
55	MG	BA	1671	1/1	0.88	0.51	68,68,68,68	0
56	OHX	AA	3557	7/7	0.88	0.23	89,102,113,146	1
56	OHX	BA	1803	7/7	0.88	0.08	211,214,221,256	1
55	MG	CA	1714	1/1	0.88	0.42	84,84,84,84	0
56	OHX	CB	104	7/7	0.88	0.64	175,181,183,194	1
55	MG	DA	3155	1/1	0.88	0.30	58,58,58,58	0
55	MG	BA	1681	1/1	0.88	0.32	64,64,64,64	0
55	MG	AA	3254	1/1	0.88	0.35	43,43,43,43	0
56	OHX	BB	115	7/7	0.88	0.25	90,109,116,116	3
55	MG	BA	1690	1/1	0.88	0.11	81,81,81,81	0
56	OHX	DB	217	7/7	0.88	0.19	135,139,157,196	1
56	OHX	BA	1766	7/7	0.88	0.19	108,139,151,181	2
55	MG	DA	3045	1/1	0.88	0.15	61,61,61,61	0
55	MG	BC	102	1/1	0.88	0.40	65,65,65,65	0
56	OHX	AA	3529	7/7	0.88	0.21	114,130,134,179	1
56	OHX	DA	3413	7/7	0.88	0.29	103,122,138,176	1
55	MG	DA	3209	1/1	0.88	0.34	64,64,64,64	0
55	MG	AA	3124	1/1	0.88	0.32	88,88,88,88	0
56	OHX	CA	1785	7/7	0.88	0.18	125,126,143,155	1
55	MG	BB	107	1/1	0.89	0.16	80,80,80,80	0
55	MG	CA	1684	1/1	0.89	0.46	82,82,82,82	0
56	OHX	DA	3405	7/7	0.89	0.18	129,133,151,175	1
56	OHX	DA	3218	7/7	0.89	0.26	96,106,121,133	1
55	MG	AA	3072	1/1	0.89	0.36	73,73,73,73	0
56	OHX	AA	3420	7/7	0.89	0.21	112,125,135,178	2
56	OHX	BA	1765	7/7	0.89	0.26	91,107,120,150	3
55	MG	BA	1634	1/1	0.89	0.14	73,73,73,73	0
56	OHX	AB	216	7/7	0.89	0.19	106,124,147,185	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	1698	1/1	0.89	0.70	86,86,86,86	0
55	MG	AA	3239	1/1	0.89	0.57	52,52,52,52	0
55	MG	CA	1625	1/1	0.89	0.16	87,87,87,87	0
56	OHX	CA	1808	7/7	0.89	0.26	163,164,177,210	1
56	OHX	AA	3530	7/7	0.89	0.29	117,123,125,163	1
55	MG	DA	3114	1/1	0.89	0.39	37,37,37,37	0
56	OHX	CA	1778	7/7	0.89	0.09	148,157,164,202	1
55	MG	DA	3035	1/1	0.89	0.28	95,95,95,95	0
56	OHX	DB	214	7/7	0.89	0.13	145,149,169,184	1
56	OHX	AA	3476	7/7	0.89	0.23	88,98,119,157	1
56	OHX	AB	218	7/7	0.89	0.13	138,141,157,181	1
55	MG	DB	204	1/1	0.89	0.25	76,76,76,76	0
55	MG	DA	3031	1/1	0.89	0.18	77,77,77,77	0
56	OHX	DA	3478	7/7	0.89	0.19	106,110,128,170	1
55	MG	CA	1670	1/1	0.89	0.19	95,95,95,95	0
55	MG	CA	1610	1/1	0.89	0.41	87,87,87,87	0
55	MG	CA	1648	1/1	0.89	0.42	70,70,70,70	0
55	MG	DA	3260	1/1	0.89	0.30	68,68,68,68	0
56	OHX	AA	3512	7/7	0.89	0.18	110,115,138,180	2
56	OHX	DA	3385	7/7	0.89	0.16	78,128,134,201	1
55	MG	BA	1609	1/1	0.89	0.29	65,65,65,65	0
55	MG	DA	3116	1/1	0.89	0.28	62,62,62,62	0
55	MG	AA	3087	1/1	0.89	0.24	82,82,82,82	0
55	MG	DA	3286	1/1	0.89	0.11	77,77,77,77	0
55	MG	CA	1660	1/1	0.89	0.31	97,97,97,97	0
56	OHX	DA	3490	7/7	0.89	0.17	103,106,122,159	3
55	MG	BA	1693	1/1	0.89	0.13	68,68,68,68	0
55	MG	DA	3050	1/1	0.89	0.82	74,74,74,74	0
56	OHX	AA	3554	7/7	0.89	0.24	138,143,153,173	1
55	MG	CA	1701	1/1	0.89	0.23	109,109,109,109	0
56	OHX	DA	3468	7/7	0.89	0.17	143,146,150,189	1
55	MG	DA	3067	1/1	0.89	0.15	82,82,82,82	0
55	MG	DA	3023	1/1	0.89	0.55	70,70,70,70	0
56	OHX	AA	3549	7/7	0.89	0.27	96,102,109,128	2
56	OHX	AA	3515	7/7	0.89	0.24	93,97,116,159	2
56	OHX	AA	3480	7/7	0.89	0.24	111,119,135,158	2
56	OHX	AB	215	7/7	0.89	0.18	110,123,130,165	1
56	OHX	AA	3456	7/7	0.89	0.19	111,115,132,161	3
55	MG	DA	3177	1/1	0.89	0.47	61,61,61,61	0
55	MG	AA	3022	1/1	0.89	0.37	28,28,28,28	0
56	OHX	AA	3513	7/7	0.89	0.20	120,125,139,159	2
55	MG	AA	3058	1/1	0.89	0.12	61,61,61,61	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	3551	7/7	0.89	0.24	97,115,123,153	1
55	MG	AA	3266	1/1	0.89	0.43	62,62,62,62	0
55	MG	DA	3057	1/1	0.89	0.32	58,58,58,58	0
56	OHX	CA	1786	7/7	0.89	0.09	163,163,175,198	1
55	MG	DA	3205	1/1	0.89	0.13	106,106,106,106	0
55	MG	CA	1608	1/1	0.89	0.30	76,76,76,76	0
55	MG	AA	3199	1/1	0.90	0.51	75,75,75,75	0
55	MG	AA	3294	1/1	0.90	0.32	36,36,36,36	0
56	OHX	DA	3447	7/7	0.90	0.12	122,140,155,176	2
55	MG	AA	3325	1/1	0.90	0.42	75,75,75,75	0
55	MG	DA	3030	1/1	0.90	0.20	94,94,94,94	0
55	MG	CA	1647	1/1	0.90	0.46	70,70,70,70	0
56	OHX	AA	3544	7/7	0.90	0.23	118,127,137,169	1
56	OHX	AA	3417	7/7	0.90	0.23	90,102,131,147	3
55	MG	DA	3329	1/1	0.90	0.44	60,60,60,60	0
56	OHX	AB	213	7/7	0.90	0.15	88,108,129,159	3
55	MG	DA	3186	1/1	0.90	0.36	34,34,34,34	0
56	OHX	AA	3451	7/7	0.90	0.19	79,96,106,142	1
56	OHX	DA	3480	7/7	0.90	0.10	125,130,144,190	1
55	MG	DA	3315	1/1	0.90	0.44	78,78,78,78	0
56	OHX	AA	3523	7/7	0.90	0.16	112,123,137,155	1
55	MG	AA	3127	1/1	0.90	0.39	45,45,45,45	0
55	MG	DA	3283	1/1	0.90	0.31	86,86,86,86	0
56	OHX	CA	1811	7/7	0.90	0.18	126,129,137,159	1
55	MG	DA	3037	1/1	0.90	0.43	73,73,73,73	0
55	MG	AA	3099	1/1	0.90	0.34	60,60,60,60	0
55	MG	DA	3140	1/1	0.90	0.42	55,55,55,55	0
55	MG	AA	3176	1/1	0.90	0.43	46,46,46,46	0
55	MG	AA	3028	1/1	0.90	0.39	35,35,35,35	0
55	MG	AA	3165	1/1	0.90	0.68	79,79,79,79	0
56	OHX	AA	3492	7/7	0.90	0.10	139,142,151,196	1
55	MG	BA	1642	1/1	0.90	0.43	69,69,69,69	0
56	OHX	CA	1759	7/7	0.90	0.17	125,133,140,148	1
55	MG	AA	3085	1/1	0.90	0.29	74,74,74,74	0
55	MG	BA	1655	1/1	0.90	0.34	84,84,84,84	0
56	OHX	AA	3505	7/7	0.90	0.15	143,150,161,212	1
55	MG	AA	3240	1/1	0.90	0.50	56,56,56,56	0
56	OHX	AA	3500	7/7	0.90	0.13	118,131,153,193	1
56	OHX	DA	3253	7/7	0.90	0.14	141,144,160,190	1
55	MG	CA	1656	1/1	0.90	0.33	94,94,94,94	0
55	MG	AA	3113	1/1	0.90	0.24	88,88,88,88	0
55	MG	CA	1682	1/1	0.90	0.28	107,107,107,107	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	CA	1783	7/7	0.90	0.20	113,117,137,164	1
56	OHX	AA	3503	7/7	0.90	0.29	99,108,119,150	1
56	OHX	A1	204	7/7	0.90	0.15	107,117,147,182	3
56	OHX	BA	1812	7/7	0.90	0.06	170,174,180,213	1
55	MG	AA	3249	1/1	0.90	0.22	81,81,81,81	0
55	MG	DA	3121	1/1	0.90	0.53	78,78,78,78	0
55	MG	AA	3226	1/1	0.90	0.52	68,68,68,68	0
55	MG	AA	3148	1/1	0.90	0.29	69,69,69,69	0
55	MG	CA	1705	1/1	0.90	0.48	73,73,73,73	0
56	OHX	BA	1790	7/7	0.90	0.09	163,166,178,211	1
55	MG	DA	3151	1/1	0.90	0.28	62,62,62,62	0
56	OHX	BA	1756	7/7	0.90	0.08	153,171,174,206	1
55	MG	BA	1614	1/1	0.90	0.13	73,73,73,73	0
56	OHX	DA	3111	7/7	0.90	0.19	118,129,134,197	1
55	MG	AA	3274	1/1	0.90	0.12	36,36,36,36	0
55	MG	BB	109	1/1	0.90	0.21	80,80,80,80	0
56	OHX	DA	3489	7/7	0.90	0.13	117,121,134,153	1
56	OHX	AA	3522	7/7	0.90	0.20	74,93,104,150	2
55	MG	BA	1607	1/1	0.90	0.11	102,102,102,102	0
55	MG	AA	3117	1/1	0.90	0.21	90,90,90,90	0
55	MG	AA	3126	1/1	0.90	0.32	54,54,54,54	0
55	MG	BA	1688	1/1	0.90	0.18	79,79,79,79	0
55	MG	DA	3033	1/1	0.90	0.24	82,82,82,82	0
55	MG	BC	101	1/1	0.90	0.35	62,62,62,62	0
56	OHX	AA	3498	7/7	0.90	0.34	120,126,136,160	2
56	OHX	BA	1795	7/7	0.90	0.11	152,159,163,204	1
55	MG	AA	3195	1/1	0.91	0.39	58,58,58,58	0
56	OHX	DA	3362	7/7	0.91	0.22	83,98,103,158	1
56	OHX	BA	1791	7/7	0.91	0.13	122,123,136,173	1
56	OHX	AA	3536	7/7	0.91	0.12	99,110,129,173	2
56	OHX	BA	1780	7/7	0.91	0.22	115,123,136,153	1
55	MG	AA	3171	1/1	0.91	0.34	59,59,59,59	0
56	OHX	CB	106	7/7	0.91	0.20	97,107,117,126	6
55	MG	AA	3285	1/1	0.91	0.37	77,77,77,77	0
56	OHX	CA	1787	7/7	0.91	0.16	117,122,135,155	1
56	OHX	AA	3439	7/7	0.91	0.17	114,122,140,194	1
56	OHX	CA	1775	7/7	0.91	0.10	139,154,159,200	1
56	OHX	AA	3502	7/7	0.91	0.10	128,135,148,184	1
56	OHX	DA	3433	7/7	0.91	0.21	104,114,132,147	1
55	MG	BC	103	1/1	0.91	0.51	70,70,70,70	0
56	OHX	BD	102	7/7	0.91	0.10	170,180,207,224	1
56	OHX	AA	3564	7/7	0.91	0.18	94,114,124,148	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	DA	3282	1/1	0.91	0.35	69,69,69,69	0
55	MG	AA	3237	1/1	0.91	0.48	62,62,62,62	0
55	MG	BA	1660	1/1	0.91	0.56	52,52,52,52	0
56	OHX	AA	3482	7/7	0.91	0.19	85,96,105,135	1
55	MG	BA	1710	1/1	0.91	0.33	113,113,113,113	0
55	MG	AA	3090	1/1	0.91	0.39	78,78,78,78	0
55	MG	BA	1632	1/1	0.91	0.21	73,73,73,73	0
56	OHX	CA	1755	7/7	0.91	0.11	119,128,149,178	1
55	MG	BA	1667	1/1	0.91	0.52	73,73,73,73	0
55	MG	AA	3100	1/1	0.91	0.29	58,58,58,58	0
56	OHX	CA	1753	7/7	0.91	0.26	82,120,146,173	3
55	MG	AA	3155	1/1	0.91	0.11	79,79,79,79	0
56	OHX	AA	3526	7/7	0.91	0.25	87,90,101,128	1
55	MG	BA	1661	1/1	0.91	0.49	61,61,61,61	0
56	OHX	AA	3514	7/7	0.91	0.13	126,137,144,183	1
55	MG	AA	3276	1/1	0.91	0.36	76,76,76,76	0
55	MG	DA	3317	1/1	0.91	0.35	85,85,85,85	0
56	OHX	DA	3127	7/7	0.91	0.27	118,132,150,170	2
55	MG	CC	105	1/1	0.91	0.53	66,66,66,66	0
55	MG	DA	3043	1/1	0.91	0.40	73,73,73,73	0
56	OHX	BR	101	7/7	0.91	0.19	132,137,152,164	1
55	MG	DA	3153	1/1	0.91	0.45	69,69,69,69	0
55	MG	DA	3239	1/1	0.91	0.20	79,79,79,79	0
56	OHX	BA	1797	7/7	0.91	0.13	117,130,138,173	1
55	MG	DA	3088	1/1	0.91	0.31	47,47,47,47	0
56	OHX	DA	3476	7/7	0.91	0.11	126,136,143,174	1
56	OHX	D5	102	7/7	0.91	0.28	114,129,141,158	1
56	OHX	DA	3475	7/7	0.91	0.21	126,139,148,175	1
55	MG	DA	3079	1/1	0.91	0.24	49,49,49,49	0
56	OHX	DA	3467	7/7	0.91	0.12	133,139,156,192	1
55	MG	AA	3293	1/1	0.91	0.24	72,72,72,72	0
56	OHX	AA	3527	7/7	0.91	0.10	147,148,161,187	1
55	MG	DA	3213	1/1	0.91	0.39	57,57,57,57	0
56	OHX	BD	103	7/7	0.91	0.15	108,110,116,155	1
55	MG	BA	1610	1/1	0.91	0.15	75,75,75,75	0
55	MG	AA	3167	1/1	0.91	0.16	51,51,51,51	0
55	MG	DA	3235	1/1	0.91	0.47	66,66,66,66	0
55	MG	CA	1713	1/1	0.91	0.18	114,114,114,114	0
55	MG	CA	1654	1/1	0.91	0.23	89,89,89,89	0
55	MG	BA	1691	1/1	0.91	0.19	87,87,87,87	0
56	OHX	DA	3450	7/7	0.91	0.13	133,139,150,199	1
56	OHX	BA	1786	7/7	0.91	0.20	133,136,154,188	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	1654	1/1	0.91	0.35	64,64,64,64	0
56	OHX	BA	1792	7/7	0.91	0.17	118,131,146,181	1
55	MG	BA	1672	1/1	0.91	0.25	82,82,82,82	0
55	MG	AA	3357	1/1	0.91	0.37	69,69,69,69	0
55	MG	DA	3107	1/1	0.91	0.28	42,42,42,42	0
55	MG	AA	3267	1/1	0.91	0.26	37,37,37,37	0
55	MG	BA	1662	1/1	0.91	0.32	56,56,56,56	0
56	OHX	DA	3472	7/7	0.91	0.10	162,171,176,223	1
55	MG	DA	3210	1/1	0.91	0.75	73,73,73,73	0
55	MG	DA	3113	1/1	0.91	0.20	73,73,73,73	0
55	MG	CA	1630	1/1	0.91	0.43	86,86,86,86	0
56	OHX	CA	1799	7/7	0.91	0.30	142,145,160,170	1
56	OHX	DA	3440	7/7	0.91	0.15	142,144,161,189	1
55	MG	CA	1666	1/1	0.91	0.30	75,75,75,75	0
55	MG	DA	3104	1/1	0.91	0.38	64,64,64,64	0
56	OHX	CA	1773	7/7	0.91	0.12	123,130,144,181	1
56	OHX	CA	1754	7/7	0.91	0.17	116,125,134,168	1
56	OHX	DA	3118	7/7	0.91	0.19	99,101,123,146	3
56	OHX	DA	3479	7/7	0.91	0.14	150,159,164,201	1
56	OHX	DA	3484	7/7	0.91	0.16	109,123,139,168	1
56	OHX	DA	3481	7/7	0.91	0.12	136,140,149,177	1
56	OHX	BA	1799	7/7	0.91	0.09	170,176,182,227	1
56	OHX	AB	214	7/7	0.91	0.14	125,133,135,173	1
56	OHX	DA	3220	7/7	0.91	0.12	141,154,156,201	1
55	MG	AA	3230	1/1	0.91	0.48	72,72,72,72	0
56	OHX	CA	1788	7/7	0.91	0.17	138,144,149,176	1
56	OHX	AA	3454	7/7	0.91	0.16	103,116,132,145	1
56	OHX	DB	212	7/7	0.91	0.11	144,152,161,194	1
56	OHX	DA	3172	7/7	0.91	0.32	95,104,112,142	1
55	MG	DA	3323	1/1	0.91	0.54	100,100,100,100	0
55	MG	AA	3238	1/1	0.91	0.46	47,47,47,47	0
56	OHX	BA	1777	7/7	0.92	0.07	176,178,192,246	1
56	OHX	DA	3455	7/7	0.92	0.08	139,144,150,194	1
56	OHX	BL	201	7/7	0.92	0.09	145,153,159,202	1
56	OHX	D3	101	7/7	0.92	0.14	129,139,156,171	2
56	OHX	AA	3495	7/7	0.92	0.19	106,114,133,188	1
56	OHX	DA	3491	7/7	0.92	0.11	104,107,129,176	1
55	MG	DA	3108	1/1	0.92	0.50	56,56,56,56	0
56	OHX	AA	3485	7/7	0.92	0.18	103,114,131,163	1
56	OHX	BC	106	7/7	0.92	0.14	119,120,134,160	1
56	OHX	CA	1780	7/7	0.92	0.09	138,146,156,182	1
55	MG	AA	3114	1/1	0.92	0.39	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
55	MG	CA	1690	1/1	0.92	0.11	93,93,93,93	0
56	OHX	DA	3486	7/7	0.92	0.14	123,132,147,175	1
56	OHX	AA	3539	7/7	0.92	0.10	130,133,143,179	1
55	MG	DA	3025	1/1	0.92	0.17	59,59,59,59	0
55	MG	AA	3055	1/1	0.92	0.30	88,88,88,88	0
55	MG	BA	1627	1/1	0.92	0.21	58,58,58,58	0
55	MG	BA	1712	1/1	0.92	0.05	74,74,74,74	0
56	OHX	BA	1738	7/7	0.92	0.17	112,124,136,189	1
55	MG	AA	3313	1/1	0.92	0.39	82,82,82,82	0
55	MG	BA	1702	1/1	0.92	0.40	84,84,84,84	0
55	MG	DB	203	1/1	0.92	0.11	121,121,121,121	0
56	OHX	DA	3482	7/7	0.92	0.16	128,142,154,190	1
55	MG	AA	3234	1/1	0.92	0.08	68,68,68,68	0
55	MG	DA	3106	1/1	0.92	0.33	80,80,80,80	0
55	MG	AA	3273	1/1	0.92	0.44	60,60,60,60	0
56	OHX	AA	3484	7/7	0.92	0.14	123,137,150,203	1
55	MG	AA	3303	1/1	0.92	0.21	77,77,77,77	0
56	OHX	AA	3555	7/7	0.92	0.19	82,85,105,128	1
55	MG	CA	1688	1/1	0.92	0.17	79,79,79,79	0
56	OHX	DA	3469	7/7	0.92	0.20	116,119,133,163	1
56	OHX	DA	3173	7/7	0.92	0.10	157,163,175,202	1
56	OHX	DA	3415	7/7	0.92	0.16	128,140,160,189	1
55	MG	DA	3028	1/1	0.92	0.45	44,44,44,44	0
56	OHX	CV	101	7/7	0.92	0.09	174,182,196,223	1
56	OHX	BA	1810	7/7	0.92	0.18	138,141,150,186	1
56	OHX	DA	3458	7/7	0.92	0.09	173,175,178,215	1
55	MG	BA	1684	1/1	0.92	0.21	67,67,67,67	0
56	OHX	CA	1809	7/7	0.92	0.07	150,160,169,213	1
56	OHX	DA	3176	7/7	0.92	0.19	162,165,176,192	1
56	OHX	DA	3258	7/7	0.92	0.19	103,111,118,148	1
56	OHX	DA	3442	7/7	0.92	0.15	135,142,161,190	1
56	OHX	DA	3457	7/7	0.92	0.10	149,156,166,200	1
56	OHX	AA	3543	7/7	0.92	0.10	145,150,162,204	1
55	MG	CA	1640	1/1	0.92	0.30	77,77,77,77	0
55	MG	AA	3128	1/1	0.92	0.34	53,53,53,53	0
56	OHX	BA	1750	7/7	0.92	0.16	112,129,139,168	1
55	MG	AA	3162	1/1	0.92	0.23	48,48,48,48	0
56	OHX	BA	1787	7/7	0.92	0.13	124,129,137,172	1
56	OHX	BA	1781	7/7	0.92	0.17	115,133,141,174	1
55	MG	DA	3044	1/1	0.92	0.30	100,100,100,100	0
56	OHX	AA	3501	7/7	0.92	0.12	104,117,124,169	1
56	OHX	DA	3226	7/7	0.92	0.16	120,131,144,175	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	3292	1/1	0.92	0.42	62,62,62,62	0
55	MG	DA	3187	1/1	0.92	0.28	55,55,55,55	0
56	OHX	DA	3171	7/7	0.92	0.20	95,116,127,171	1
55	MG	CA	1680	1/1	0.92	0.35	78,78,78,78	0
55	MG	AA	3081	1/1	0.92	0.21	81,81,81,81	0
56	OHX	BA	1807	7/7	0.92	0.15	133,136,150,177	1
56	OHX	CA	1810	7/7	0.92	0.10	113,132,142,167	1
56	OHX	BA	1757	7/7	0.92	0.20	86,113,131,156	4
55	MG	DA	3271	1/1	0.92	0.41	59,59,59,59	0
55	MG	AB	204	1/1	0.92	0.47	80,80,80,80	0
55	MG	BB	112	1/1	0.92	0.13	80,80,80,80	0
55	MG	AA	3309	1/1	0.92	0.41	77,77,77,77	0
56	OHX	AA	3559	7/7	0.92	0.22	123,137,143,179	1
55	MG	AA	3204	1/1	0.92	0.44	45,45,45,45	0
55	MG	AA	3312	1/1	0.92	0.25	71,71,71,71	0
55	MG	DA	3128	1/1	0.92	0.50	75,75,75,75	0
55	MG	DA	3060	1/1	0.92	0.46	77,77,77,77	0
55	MG	DA	3029	1/1	0.92	0.29	70,70,70,70	0
56	OHX	CA	1757	7/7	0.92	0.14	117,123,150,175	1
56	OHX	BA	1779	7/7	0.92	0.14	129,134,141,170	1
56	OHX	DA	3407	7/7	0.92	0.15	124,134,145,191	1
55	MG	BA	1631	1/1	0.92	0.10	85,85,85,85	0
56	OHX	BA	1737	7/7	0.92	0.13	120,131,149,172	1
55	MG	BA	1647	1/1	0.92	0.39	66,66,66,66	0
55	MG	DA	3179	1/1	0.92	0.42	46,46,46,46	0
55	MG	AA	3033	1/1	0.92	0.33	39,39,39,39	0
55	MG	DA	3017	1/1	0.92	0.41	66,66,66,66	0
55	MG	DA	3219	1/1	0.92	0.22	62,62,62,62	0
55	MG	DA	3326	1/1	0.92	0.42	90,90,90,90	0
56	OHX	CD	101	7/7	0.92	0.10	166,174,199,220	1
56	OHX	DA	3105	7/7	0.92	0.16	134,136,144,206	1
55	MG	AA	3169	1/1	0.92	0.54	47,47,47,47	0
55	MG	BA	1701	1/1	0.92	0.41	68,68,68,68	0
55	MG	BA	1605	1/1	0.92	0.12	81,81,81,81	0
56	OHX	AA	3509	7/7	0.92	0.20	91,109,142,150	3
56	OHX	CA	1769	7/7	0.92	0.11	141,144,170,199	1
55	MG	DA	3154	1/1	0.93	0.30	60,60,60,60	0
55	MG	CA	1602	1/1	0.93	0.42	58,58,58,58	0
56	OHX	AA	3473	7/7	0.93	0.21	104,114,132,167	1
55	MG	DA	3240	1/1	0.93	0.40	64,64,64,64	0
55	MG	AA	3194	1/1	0.93	0.42	56,56,56,56	0
56	OHX	AA	3408	7/7	0.93	0.14	107,111,135,163	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	1682	1/1	0.93	0.08	68,68,68,68	0
55	MG	BA	1700	1/1	0.93	0.05	119,119,119,119	0
55	MG	AA	3103	1/1	0.93	0.41	50,50,50,50	0
55	MG	AA	3094	1/1	0.93	0.51	48,48,48,48	0
56	OHX	BA	1775	7/7	0.93	0.15	113,130,145,176	1
56	OHX	CA	1802	7/7	0.93	0.10	130,138,148,200	1
55	MG	DA	3195	1/1	0.93	0.16	46,46,46,46	0
55	MG	D0	201	1/1	0.93	0.14	51,51,51,51	0
56	OHX	DA	3091	7/7	0.93	0.15	103,121,134,170	1
55	MG	A1	202	1/1	0.93	0.19	75,75,75,75	0
56	OHX	BA	1725	7/7	0.93	0.15	95,114,126,182	1
56	OHX	AA	3448	7/7	0.93	0.10	141,143,155,200	1
56	OHX	AA	3541	7/7	0.93	0.39	131,134,141,173	1
56	OHX	DA	3463	7/7	0.93	0.20	142,149,156,188	1
55	MG	AA	3073	1/1	0.93	0.32	68,68,68,68	0
56	OHX	AA	3524	7/7	0.93	0.13	115,120,140,187	1
56	OHX	CA	1781	7/7	0.93	0.13	153,161,166,239	1
55	MG	AA	3286	1/1	0.93	0.40	83,83,83,83	0
55	MG	DA	3266	1/1	0.93	0.47	88,88,88,88	0
56	OHX	AB	219	7/7	0.93	0.37	112,116,126,139	1
56	OHX	AA	3552	7/7	0.93	0.18	96,106,128,164	1
55	MG	DA	3272	1/1	0.93	0.10	57,57,57,57	0
56	OHX	AA	3540	7/7	0.93	0.15	104,109,137,150	2
56	OHX	BA	1793	7/7	0.93	0.14	129,132,141,164	1
56	OHX	BA	1743	7/7	0.93	0.23	79,96,129,159	2
55	MG	DA	3334	1/1	0.93	0.34	75,75,75,75	0
56	OHX	AA	3560	7/7	0.93	0.16	132,136,153,192	1
55	MG	BA	1618	1/1	0.93	0.33	71,71,71,71	0
56	OHX	BA	1763	7/7	0.93	0.12	123,136,140,184	1
55	MG	BA	1713	1/1	0.93	0.45	81,81,81,81	0
56	OHX	AA	3449	7/7	0.93	0.15	102,118,124,165	1
56	OHX	BA	1808	7/7	0.93	0.20	121,129,141,156	1
55	MG	AA	3004	1/1	0.93	0.36	32,32,32,32	0
55	MG	AA	3029	1/1	0.93	0.29	59,59,59,59	0
55	MG	AA	3297	1/1	0.93	0.07	80,80,80,80	0
55	MG	CA	1645	1/1	0.93	0.50	58,58,58,58	0
56	OHX	AA	3445	7/7	0.93	0.13	118,124,140,177	1
56	OHX	AA	3478	7/7	0.93	0.16	147,161,167,217	1
55	MG	AA	3086	1/1	0.93	0.32	73,73,73,73	0
56	OHX	DA	3485	7/7	0.93	0.17	131,137,152,172	1
56	OHX	DA	3221	7/7	0.93	0.11	120,130,140,174	1
55	MG	DA	3098	1/1	0.93	0.16	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	DA	3452	7/7	0.93	0.17	99,118,125,155	1
56	OHX	DA	3427	7/7	0.93	0.11	134,147,151,184	1
55	MG	DA	3194	1/1	0.93	0.45	48,48,48,48	0
56	OHX	AA	3443	7/7	0.93	0.15	110,114,126,149	2
56	OHX	DA	3159	7/7	0.93	0.19	75,86,105,131	3
56	OHX	AA	3499	7/7	0.93	0.15	107,112,120,152	1
55	MG	CA	1709	1/1	0.93	0.25	76,76,76,76	0
56	OHX	DA	3103	7/7	0.93	0.20	94,102,107,128	2
56	OHX	DA	3434	7/7	0.93	0.13	127,134,154,190	1
55	MG	CA	1673	1/1	0.93	0.33	76,76,76,76	0
56	OHX	DA	3453	7/7	0.93	0.26	145,153,160,191	1
56	OHX	DA	3437	7/7	0.93	0.15	113,120,134,160	1
55	MG	AO	201	1/1	0.93	0.14	66,66,66,66	0
56	OHX	DA	3444	7/7	0.93	0.14	123,132,145,175	1
55	MG	AA	3066	1/1	0.93	0.30	62,62,62,62	0
55	MG	BA	1668	1/1	0.93	0.34	64,64,64,64	0
56	OHX	DA	3438	7/7	0.93	0.13	120,135,146,170	1
55	MG	DA	3189	1/1	0.93	0.62	56,56,56,56	0
55	MG	DA	3032	1/1	0.93	0.11	38,38,38,38	0
56	OHX	BA	1785	7/7	0.93	0.13	117,124,136,144	2
55	MG	AA	3177	1/1	0.93	0.26	46,46,46,46	0
56	OHX	DA	3376	7/7	0.93	0.20	38,106,133,165	3
56	OHX	BA	1769	7/7	0.93	0.09	159,168,172,218	1
56	OHX	CA	1784	7/7	0.93	0.15	127,135,151,190	1
56	OHX	AA	3553	7/7	0.93	0.12	160,165,172,209	1
56	OHX	DB	215	7/7	0.93	0.16	147,149,158,191	1
55	MG	DA	3267	1/1	0.93	0.34	82,82,82,82	0
55	MG	AA	3049	1/1	0.93	0.13	66,66,66,66	0
55	MG	CA	1679	1/1	0.93	0.17	87,87,87,87	0
56	OHX	AA	3367	7/7	0.93	0.25	69,72,90,147	3
55	MG	AA	3079	1/1	0.93	0.38	67,67,67,67	0
55	MG	AA	3118	1/1	0.93	0.23	69,69,69,69	0
55	MG	BA	1611	1/1	0.93	0.37	47,47,47,47	0
55	MG	CA	1694	1/1	0.93	0.37	89,89,89,89	0
55	MG	BA	1663	1/1	0.93	0.74	80,80,80,80	0
55	MG	AA	3135	1/1	0.93	0.35	66,66,66,66	0
56	OHX	AA	3521	7/7	0.93	0.12	103,107,119,167	2
55	MG	CA	1631	1/1	0.93	0.34	74,74,74,74	0
55	MG	BA	1629	1/1	0.93	0.14	79,79,79,79	0
56	OHX	DA	3421	7/7	0.93	0.17	96,112,124,166	1
56	OHX	BA	1742	7/7	0.93	0.11	149,155,172,201	1
55	MG	AA	3319	1/1	0.93	0.09	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	BA	1798	7/7	0.93	0.11	135,136,153,212	1
55	MG	AA	3133	1/1	0.93	0.34	45,45,45,45	0
55	MG	DA	3185	1/1	0.93	0.40	49,49,49,49	0
56	OHX	DA	3459	7/7	0.94	0.16	85,104,120,156	1
55	MG	CA	1675	1/1	0.94	0.40	94,94,94,94	0
55	MG	AA	3283	1/1	0.94	0.10	21,21,21,21	0
56	OHX	DA	3423	7/7	0.94	0.09	127,140,151,201	1
55	MG	DA	3309	1/1	0.94	0.17	68,68,68,68	0
55	MG	CA	1606	1/1	0.94	0.16	70,70,70,70	0
55	MG	AA	3101	1/1	0.94	0.32	47,47,47,47	0
55	MG	DA	3139	1/1	0.94	0.45	54,54,54,54	0
55	MG	AA	3005	1/1	0.94	0.39	48,48,48,48	0
55	MG	AA	3056	1/1	0.94	0.23	55,55,55,55	0
56	OHX	CA	1812	7/7	0.94	0.11	134,141,149,203	1
55	MG	CA	1655	1/1	0.94	0.33	70,70,70,70	0
56	OHX	BA	1754	7/7	0.94	0.08	136,144,152,183	1
55	MG	CA	1661	1/1	0.94	0.52	83,83,83,83	0
56	OHX	DA	3165	7/7	0.94	0.20	123,135,143,168	1
55	MG	DA	3047	1/1	0.94	0.15	79,79,79,79	0
55	MG	AA	3219	1/1	0.94	0.30	65,65,65,65	0
55	MG	AA	3225	1/1	0.94	0.52	52,52,52,52	0
56	OHX	DB	209	7/7	0.94	0.15	130,143,158,186	1
55	MG	AA	3252	1/1	0.94	0.38	52,52,52,52	0
56	OHX	BA	1761	7/7	0.94	0.08	136,147,154,197	1
56	OHX	AO	203	7/7	0.94	0.13	83,92,110,152	1
55	MG	AA	3261	1/1	0.94	0.23	53,53,53,53	0
56	OHX	DA	3477	7/7	0.94	0.07	153,157,164,211	1
56	OHX	DA	3214	7/7	0.94	0.21	82,92,98,133	2
55	MG	BA	1616	1/1	0.94	0.06	101,101,101,101	0
55	MG	DA	3101	1/1	0.94	0.22	59,59,59,59	0
56	OHX	CA	1777	7/7	0.94	0.09	157,162,168,202	1
56	OHX	BA	1748	7/7	0.94	0.14	124,127,141,171	1
55	MG	AA	3268	1/1	0.94	0.16	38,38,38,38	0
56	OHX	DA	3487	7/7	0.94	0.18	106,108,129,150	1
55	MG	DA	3204	1/1	0.94	0.30	58,58,58,58	0
55	MG	CA	1601	1/1	0.94	0.38	75,75,75,75	0
55	MG	BA	1620	1/1	0.94	0.26	73,73,73,73	0
55	MG	AA	3220	1/1	0.94	0.20	38,38,38,38	0
56	OHX	AA	3462	7/7	0.94	0.17	105,108,119,142	2
56	OHX	BA	1783	7/7	0.94	0.10	121,130,148,178	1
55	MG	DB	202	1/1	0.94	0.14	98,98,98,98	0
56	OHX	BA	1782	7/7	0.94	0.11	137,145,154,180	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	BA	1749	7/7	0.94	0.17	112,116,136,168	1
55	MG	AA	3108	1/1	0.94	0.11	54,54,54,54	0
55	MG	DA	3076	1/1	0.94	0.64	54,54,54,54	0
55	MG	AA	3109	1/1	0.94	0.37	38,38,38,38	0
55	MG	DA	3277	1/1	0.94	0.10	89,89,89,89	0
56	OHX	DA	3169	7/7	0.94	0.17	110,124,136,172	1
55	MG	AB	205	1/1	0.94	0.23	68,68,68,68	0
55	MG	CA	1650	1/1	0.94	0.28	66,66,66,66	0
56	OHX	DA	3431	7/7	0.94	0.14	139,144,155,180	1
56	OHX	CA	1798	7/7	0.94	0.17	116,126,129,163	1
56	OHX	A1	203	7/7	0.94	0.16	97,103,123,154	1
56	OHX	BA	1796	7/7	0.94	0.24	119,126,142,152	1
55	MG	DA	3011	1/1	0.94	0.09	84,84,84,84	0
55	MG	AA	3080	1/1	0.94	0.21	63,63,63,63	0
56	OHX	BA	1794	7/7	0.94	0.09	156,163,165,204	1
55	MG	DA	3125	1/1	0.94	0.33	54,54,54,54	0
55	MG	DA	3321	1/1	0.94	0.20	56,56,56,56	0
56	OHX	CA	1792	7/7	0.94	0.11	189,191,192,232	1
56	OHX	CA	1793	7/7	0.94	0.08	142,146,153,194	1
56	OHX	A6	101	7/7	0.94	0.15	112,127,141,158	2
55	MG	AB	202	1/1	0.94	0.18	80,80,80,80	0
56	OHX	DA	3424	7/7	0.94	0.15	124,129,137,157	2
56	OHX	AA	3504	7/7	0.94	0.20	101,103,116,145	2
56	OHX	AA	3569	7/7	0.94	0.13	134,142,144,168	1
55	MG	DA	3077	1/1	0.94	0.56	52,52,52,52	0
55	MG	AA	3131	1/1	0.94	0.55	62,62,62,62	0
56	OHX	DA	3392	7/7	0.94	0.12	115,117,129,183	1
55	MG	BA	1638	1/1	0.94	0.35	104,104,104,104	0
56	OHX	DA	3435	7/7	0.94	0.19	86,99,124,155	1
56	OHX	BA	1747	7/7	0.94	0.20	117,129,140,148	1
56	OHX	CA	1790	7/7	0.94	0.17	99,111,123,147	2
56	OHX	DA	3460	7/7	0.94	0.13	111,124,134,174	1
56	OHX	DA	3394	7/7	0.94	0.12	127,139,150,223	0
56	OHX	DA	3411	7/7	0.94	0.14	104,112,132,163	1
56	OHX	AA	3532	7/7	0.94	0.13	136,144,160,202	1
56	OHX	AA	3425	7/7	0.94	0.10	158,168,177,207	1
55	MG	AA	3159	1/1	0.94	0.43	81,81,81,81	0
56	OHX	DA	3245	7/7	0.94	0.13	95,128,139,165	1
55	MG	AA	3178	1/1	0.94	0.42	76,76,76,76	0
56	OHX	BA	1811	7/7	0.94	0.13	110,118,135,147	1
55	MG	BD	101	1/1	0.94	0.21	103,103,103,103	0
56	OHX	BA	1731	7/7	0.94	0.25	99,107,129,161	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	AF	301	1/1	0.94	0.07	74,74,74,74	0
56	OHX	AA	3568	7/7	0.94	0.16	101,109,114,153	1
55	MG	DA	3014	1/1	0.94	0.35	55,55,55,55	0
55	MG	AA	3263	1/1	0.94	0.32	39,39,39,39	0
56	OHX	DA	3461	7/7	0.94	0.08	171,173,180,211	1
56	OHX	DB	213	7/7	0.94	0.16	125,144,157,169	2
56	OHX	DA	3465	7/7	0.94	0.15	123,136,143,165	1
55	MG	AA	3104	1/1	0.94	0.28	62,62,62,62	0
55	MG	AA	3210	1/1	0.94	0.55	43,43,43,43	0
56	OHX	DA	3087	7/7	0.94	0.16	102,119,134,177	1
55	MG	AA	3243	1/1	0.94	0.40	62,62,62,62	0
55	MG	AA	3321	1/1	0.94	0.35	41,41,41,41	0
57	PAR	CA	1722	42/42	0.94	0.15	72,88,95,97	0
55	MG	A5	101	1/1	0.94	0.33	43,43,43,43	0
55	MG	AA	3314	1/1	0.94	0.15	63,63,63,63	0
56	OHX	BB	114	7/7	0.94	0.29	176,178,180,206	1
55	MG	AA	3132	1/1	0.94	0.54	48,48,48,48	0
56	OHX	BA	1752	7/7	0.94	0.09	168,174,177,207	1
56	OHX	DA	3432	7/7	0.94	0.10	116,131,140,173	1
55	MG	CA	1706	1/1	0.94	0.60	85,85,85,85	0
55	MG	DA	3250	1/1	0.94	0.37	64,64,64,64	0
56	OHX	CA	1800	7/7	0.94	0.08	165,167,172,220	1
56	OHX	A3	102	7/7	0.94	0.19	106,109,134,147	2
55	MG	DA	3229	1/1	0.94	0.44	45,45,45,45	0
56	OHX	CA	1806	7/7	0.94	0.12	138,150,153,181	1
55	MG	DA	3216	1/1	0.94	0.43	71,71,71,71	0
55	MG	BA	1658	1/1	0.94	0.43	47,47,47,47	0
56	OHX	DA	3470	7/7	0.94	0.17	152,169,191,193	1
55	MG	AA	3059	1/1	0.94	0.32	77,77,77,77	0
55	MG	DA	3016	1/1	0.94	0.59	51,51,51,51	0
55	MG	CA	1619	1/1	0.94	0.21	92,92,92,92	0
55	MG	DA	3265	1/1	0.94	0.18	73,73,73,73	0
56	OHX	CA	1801	7/7	0.94	0.10	137,140,148,200	1
56	OHX	CA	1813	7/7	0.94	0.41	138,144,151,179	1
55	MG	DA	3142	1/1	0.94	0.41	76,76,76,76	0
55	MG	AA	3057	1/1	0.94	0.18	56,56,56,56	0
56	OHX	AA	3472	7/7	0.94	0.26	95,115,124,169	1
56	OHX	AA	3481	7/7	0.94	0.15	88,92,119,127	2
56	OHX	DA	3446	7/7	0.94	0.11	118,121,142,162	1
56	OHX	CA	1751	7/7	0.94	0.19	102,126,129,174	1
55	MG	DA	3228	1/1	0.94	0.44	58,58,58,58	0
55	MG	AA	3356	1/1	0.94	0.58	70,70,70,70	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	3464	7/7	0.94	0.25	117,129,143,171	1
56	OHX	CA	1765	7/7	0.94	0.06	169,177,182,233	1
55	MG	AA	3041	1/1	0.94	0.25	59,59,59,59	0
56	OHX	AA	3494	7/7	0.94	0.12	112,122,130,153	1
56	OHX	BA	1745	7/7	0.95	0.13	119,123,132,169	1
55	MG	DA	3137	1/1	0.95	0.42	51,51,51,51	0
56	OHX	AA	3496	7/7	0.95	0.12	107,119,130,176	1
55	MG	AA	3039	1/1	0.95	0.39	50,50,50,50	0
56	OHX	CA	1770	7/7	0.95	0.09	143,153,167,200	1
56	OHX	AA	3488	7/7	0.95	0.14	155,156,163,203	1
55	MG	DA	3038	1/1	0.95	0.23	77,77,77,77	0
55	MG	CA	1702	1/1	0.95	0.48	59,59,59,59	0
56	OHX	DA	3416	7/7	0.95	0.17	112,112,142,167	1
56	OHX	DA	3456	7/7	0.95	0.10	133,142,150,207	1
56	OHX	AA	3374	7/7	0.95	0.20	32,70,109,140	3
56	OHX	DA	3388	7/7	0.95	0.15	108,118,139,160	1
55	MG	DA	3291	1/1	0.95	0.20	66,66,66,66	0
55	MG	DA	3021	1/1	0.95	0.25	62,62,62,62	0
56	OHX	DA	3217	7/7	0.95	0.10	144,149,153,189	1
56	OHX	DA	3425	7/7	0.95	0.09	125,134,139,188	1
55	MG	AA	3074	1/1	0.95	0.11	90,90,90,90	0
55	MG	DA	3184	1/1	0.95	0.54	37,37,37,37	0
55	MG	CA	1642	1/1	0.95	0.57	69,69,69,69	0
55	MG	AA	3130	1/1	0.95	0.38	43,43,43,43	0
56	OHX	AA	3534	7/7	0.95	0.12	103,124,138,161	2
56	OHX	AW	101	7/7	0.95	0.17	112,118,129,149	1
56	OHX	BC	105	7/7	0.95	0.15	129,141,151,159	1
56	OHX	CA	1749	7/7	0.95	0.13	124,137,161,188	2
55	MG	AA	3224	1/1	0.95	0.24	79,79,79,79	0
56	OHX	AB	210	7/7	0.95	0.10	101,108,128,154	1
56	OHX	AA	3459	7/7	0.95	0.15	91,107,133,162	1
56	OHX	BA	1771	7/7	0.95	0.18	101,104,120,152	2
56	OHX	DA	3391	7/7	0.95	0.11	117,125,144,183	1
56	OHX	DA	3243	7/7	0.95	0.22	74,100,112,145	2
56	OHX	CA	1758	7/7	0.95	0.08	150,162,166,191	1
55	MG	BA	1678	1/1	0.95	0.33	44,44,44,44	0
56	OHX	AB	217	7/7	0.95	0.24	100,108,115,151	1
56	OHX	DA	3428	7/7	0.95	0.15	93,108,120,163	1
55	MG	DA	3247	1/1	0.95	0.33	48,48,48,48	0
56	OHX	CA	1807	7/7	0.95	0.27	109,119,124,150	1
56	OHX	CA	1782	7/7	0.95	0.18	134,137,147,160	1
55	MG	AA	3003	1/1	0.95	0.33	39,39,39,39	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	3433	7/7	0.95	0.15	77,91,106,131	2
55	MG	DA	3122	1/1	0.95	0.37	30,30,30,30	0
56	OHX	BA	1764	7/7	0.95	0.14	147,152,158,209	1
56	OHX	DA	3166	7/7	0.95	0.11	159,166,176,197	1
55	MG	DA	3225	1/1	0.95	0.42	55,55,55,55	0
56	OHX	DA	3248	7/7	0.95	0.14	110,118,139,156	1
55	MG	AA	3149	1/1	0.95	0.36	58,58,58,58	0
55	MG	DA	3299	1/1	0.95	0.29	67,67,67,67	0
55	MG	DA	3006	1/1	0.95	0.25	63,63,63,63	0
55	MG	CA	1603	1/1	0.95	0.29	62,62,62,62	0
56	OHX	DA	3449	7/7	0.95	0.10	147,154,162,185	1
56	OHX	DA	3409	7/7	0.95	0.18	103,117,129,162	1
56	OHX	DA	3398	7/7	0.95	0.13	119,127,142,162	1
56	OHX	CA	1794	7/7	0.95	0.16	102,115,122,149	1
55	MG	DA	3152	1/1	0.95	0.39	57,57,57,57	0
56	OHX	AA	3489	7/7	0.95	0.11	136,140,156,178	1
55	MG	DA	3126	1/1	0.95	0.51	63,63,63,63	0
55	MG	AA	3255	1/1	0.95	0.24	47,47,47,47	0
55	MG	DA	3275	1/1	0.95	0.45	53,53,53,53	0
56	OHX	DB	210	7/7	0.95	0.12	119,127,150,173	2
56	OHX	AA	3371	7/7	0.95	0.18	65,79,88,136	2
56	OHX	AA	3464	7/7	0.95	0.13	105,115,140,175	1
56	OHX	DA	3430	7/7	0.95	0.07	176,181,185,214	1
55	MG	DA	3056	1/1	0.95	0.28	48,48,48,48	0
56	OHX	DA	3224	7/7	0.95	0.23	104,110,126,166	1
55	MG	DA	3097	1/1	0.95	0.40	67,67,67,67	0
55	MG	AA	3116	1/1	0.95	0.24	63,63,63,63	0
56	OHX	DA	3163	7/7	0.95	0.20	124,127,154,166	1
55	MG	DA	3191	1/1	0.95	0.35	66,66,66,66	0
55	MG	AA	3260	1/1	0.95	0.38	53,53,53,53	0
55	MG	BA	1669	1/1	0.95	0.31	68,68,68,68	0
56	OHX	DB	211	7/7	0.95	0.13	105,121,145,156	2
56	OHX	AA	3457	7/7	0.95	0.12	86,94,124,185	1
55	MG	BA	1623	1/1	0.95	0.45	39,39,39,39	0
55	MG	DA	3297	1/1	0.95	0.28	70,70,70,70	0
55	MG	AB	206	1/1	0.95	0.45	77,77,77,77	0
56	OHX	DA	3466	7/7	0.95	0.18	116,124,134,165	2
56	OHX	AA	3516	7/7	0.95	0.18	90,98,116,166	1
55	MG	AA	3034	1/1	0.95	0.31	50,50,50,50	0
55	MG	DA	3129	1/1	0.95	0.37	68,68,68,68	0
56	OHX	AA	3517	7/7	0.95	0.08	125,127,137,177	1
55	MG	BA	1606	1/1	0.95	0.23	70,70,70,70	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	3563	7/7	0.95	0.22	128,136,143,179	1
56	OHX	AB	208	7/7	0.95	0.14	95,117,137,155	2
55	MG	DA	3230	1/1	0.95	0.24	51,51,51,51	0
55	MG	DA	3262	1/1	0.95	0.23	59,59,59,59	0
56	OHX	BA	1802	7/7	0.95	0.09	100,117,125,149	1
55	MG	DA	3156	1/1	0.95	0.19	73,73,73,73	0
56	OHX	AB	209	7/7	0.95	0.14	98,103,137,147	3
55	MG	DA	3063	1/1	0.95	0.55	59,59,59,59	0
56	OHX	DA	3390	7/7	0.95	0.13	117,127,135,170	1
56	OHX	DA	3215	7/7	0.95	0.14	97,115,127,150	3
55	MG	DA	3040	1/1	0.95	0.18	66,66,66,66	0
55	MG	AA	3115	1/1	0.95	0.39	57,57,57,57	0
55	MG	DA	3301	1/1	0.95	0.29	60,60,60,60	0
55	MG	CA	1607	1/1	0.95	0.28	86,86,86,86	0
55	MG	CA	1717	1/1	0.95	0.28	64,64,64,64	0
55	MG	CA	1695	1/1	0.95	0.14	94,94,94,94	0
56	OHX	DA	3174	7/7	0.95	0.16	100,112,120,180	1
56	OHX	BA	1744	7/7	0.95	0.13	134,144,157,183	1
56	OHX	AA	3426	7/7	0.95	0.11	104,117,127,168	3
55	MG	CA	1604	1/1	0.95	0.17	72,72,72,72	0
55	MG	AA	3067	1/1	0.95	0.17	50,50,50,50	0
55	MG	AA	3188	1/1	0.95	0.16	29,29,29,29	0
55	MG	AA	3119	1/1	0.95	0.24	86,86,86,86	0
55	MG	AA	3069	1/1	0.95	0.23	54,54,54,54	0
56	OHX	AA	3394	7/7	0.95	0.14	113,123,125,181	1
55	MG	DA	3305	1/1	0.95	0.20	48,48,48,48	0
56	OHX	AA	3561	7/7	0.95	0.14	86,92,112,144	2
55	MG	AA	3064	1/1	0.95	0.25	52,52,52,52	0
55	MG	AA	3244	1/1	0.95	0.34	41,41,41,41	0
55	MG	AA	3053	1/1	0.95	0.21	77,77,77,77	0
56	OHX	AA	3423	7/7	0.95	0.12	100,115,121,157	1
55	MG	CA	1613	1/1	0.95	0.28	73,73,73,73	0
56	OHX	CA	1795	7/7	0.95	0.12	115,125,132,165	1
56	OHX	DA	3414	7/7	0.95	0.12	126,128,140,174	1
56	OHX	AA	3362	7/7	0.95	0.15	104,116,120,168	1
56	OHX	AA	3436	7/7	0.95	0.21	90,93,119,164	1
55	MG	DA	3149	1/1	0.95	0.23	53,53,53,53	0
55	MG	AA	3198	1/1	0.95	0.28	34,34,34,34	0
55	MG	AA	3320	1/1	0.95	0.20	45,45,45,45	0
56	OHX	AA	3447	7/7	0.95	0.10	110,120,136,163	1
55	MG	DA	3086	1/1	0.95	0.44	51,51,51,51	0
55	MG	AA	3137	1/1	0.95	0.31	74,74,74,74	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	OHX	DA	3400	7/7	0.95	0.17	113,116,126,149	1
56	OHX	CK	201	7/7	0.95	0.19	143,148,155,179	1
55	MG	AA	3032	1/1	0.95	0.29	37,37,37,37	0
55	MG	AA	3299	1/1	0.95	0.32	41,41,41,41	0
56	OHX	CA	1761	7/7	0.95	0.09	133,143,154,174	1
56	OHX	AB	211	7/7	0.95	0.11	124,127,142,178	1
55	MG	CA	1700	1/1	0.95	0.31	97,97,97,97	0
56	OHX	CA	1745	7/7	0.95	0.14	117,120,127,165	1
56	OHX	D1	201	7/7	0.95	0.15	110,112,135,162	1
55	MG	BA	1665	1/1	0.95	0.24	53,53,53,53	0
56	OHX	DA	3483	7/7	0.95	0.12	103,116,126,199	1
55	MG	AE	302	1/1	0.95	0.17	74,74,74,74	0
56	OHX	AA	3547	7/7	0.95	0.11	80,87,107,118	1
56	OHX	CA	1731	7/7	0.95	0.19	90,118,129,156	1
55	MG	DA	3178	1/1	0.95	0.65	58,58,58,58	0
55	MG	CA	1644	1/1	0.95	0.35	89,89,89,89	0
56	OHX	AA	3395	7/7	0.95	0.19	100,109,130,162	1
55	MG	AA	3140	1/1	0.95	0.36	70,70,70,70	0
55	MG	CA	1639	1/1	0.95	0.46	69,69,69,69	0
55	MG	DA	3093	1/1	0.95	0.15	46,46,46,46	0
56	OHX	CA	1763	7/7	0.96	0.09	142,143,157,189	1
55	MG	AA	3093	1/1	0.96	0.42	35,35,35,35	0
55	MG	DA	3208	1/1	0.96	0.45	61,61,61,61	0
56	OHX	AA	3474	7/7	0.96	0.12	113,120,132,160	1
56	OHX	AA	3475	7/7	0.96	0.08	132,134,145,192	1
56	OHX	AA	3550	7/7	0.96	0.09	118,128,136,169	1
56	OHX	DA	3168	7/7	0.96	0.17	129,143,154,181	1
55	MG	AA	3023	1/1	0.96	0.30	35,35,35,35	0
55	MG	AA	3298	1/1	0.96	0.26	45,45,45,45	0
56	OHX	AA	3435	7/7	0.96	0.15	83,103,126,156	2
56	OHX	AA	3421	7/7	0.96	0.17	78,84,91,130	1
56	OHX	AB	212	7/7	0.96	0.12	91,105,122,151	3
56	OHX	AA	3405	7/7	0.96	0.12	100,103,111,158	1
56	OHX	AA	3465	7/7	0.96	0.22	82,99,109,148	1
56	OHX	AA	3535	7/7	0.96	0.15	94,101,108,146	1
55	MG	AA	3147	1/1	0.96	0.39	49,49,49,49	0
55	MG	AA	3001	1/1	0.96	0.35	32,32,32,32	0
56	OHX	DA	3445	7/7	0.96	0.10	121,130,142,174	1
56	OHX	CA	1803	7/7	0.96	0.09	137,147,156,198	1
56	OHX	AA	3470	7/7	0.96	0.08	116,126,152,171	1
56	OHX	AA	3416	7/7	0.96	0.18	108,113,125,155	1
56	OHX	CA	1776	7/7	0.96	0.16	112,115,132,151	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	1637	1/1	0.96	0.53	69,69,69,69	0
55	MG	AA	3206	1/1	0.96	0.23	37,37,37,37	0
56	OHX	AA	3404	7/7	0.96	0.09	108,112,133,175	1
56	OHX	BA	1773	7/7	0.96	0.11	135,139,146,167	1
55	MG	AA	3065	1/1	0.96	0.25	46,46,46,46	0
56	OHX	DA	3081	7/7	0.96	0.15	99,102,113,145	1
55	MG	AA	3262	1/1	0.96	0.28	62,62,62,62	0
56	OHX	AA	3463	7/7	0.96	0.14	94,102,127,154	1
55	MG	AA	3050	1/1	0.96	0.39	45,45,45,45	0
55	MG	DA	3133	1/1	0.96	0.26	51,51,51,51	0
56	OHX	CA	1772	7/7	0.96	0.09	142,144,153,197	1
55	MG	AA	3011	1/1	0.96	0.27	44,44,44,44	0
56	OHX	CA	1752	7/7	0.96	0.15	139,147,150,191	1
55	MG	DA	3273	1/1	0.96	0.37	41,41,41,41	0
56	OHX	BA	1751	7/7	0.96	0.18	101,112,132,168	2
55	MG	AA	3275	1/1	0.96	0.59	71,71,71,71	0
55	MG	DA	3285	1/1	0.96	0.40	57,57,57,57	0
56	OHX	DA	3372	7/7	0.96	0.20	90,96,108,138	1
56	OHX	AA	3419	7/7	0.96	0.12	102,113,133,143	3
56	OHX	AA	3442	7/7	0.96	0.12	97,106,127,148	1
55	MG	DA	3274	1/1	0.96	0.39	69,69,69,69	0
55	MG	AA	3205	1/1	0.96	0.13	42,42,42,42	0
56	OHX	AA	3440	7/7	0.96	0.11	83,91,111,141	1
55	MG	AA	3102	1/1	0.96	0.37	52,52,52,52	0
56	OHX	DA	3109	7/7	0.96	0.30	99,116,138,153	1
56	OHX	BA	1774	7/7	0.96	0.12	104,121,130,163	1
55	MG	DA	3058	1/1	0.96	0.41	70,70,70,70	0
56	OHX	AA	3537	7/7	0.96	0.10	164,173,184,214	1
56	OHX	CA	1756	7/7	0.96	0.11	99,109,123,147	2
55	MG	CC	102	1/1	0.96	0.86	69,69,69,69	0
55	MG	AA	3228	1/1	0.96	0.37	53,53,53,53	0
56	OHX	CA	1805	7/7	0.96	0.13	128,130,148,187	1
56	OHX	AA	3491	7/7	0.96	0.17	96,99,117,169	1
55	MG	DA	3147	1/1	0.96	0.31	55,55,55,55	0
55	MG	DA	3263	1/1	0.96	0.26	55,55,55,55	0
55	MG	DA	3131	1/1	0.96	0.35	72,72,72,72	0
55	MG	DA	3211	1/1	0.96	0.40	57,57,57,57	0
55	MG	BA	1601	1/1	0.96	0.34	57,57,57,57	0
55	MG	DA	3024	1/1	0.96	0.28	63,63,63,63	0
55	MG	CA	1638	1/1	0.96	0.37	59,59,59,59	0
55	MG	DA	3292	1/1	0.96	0.25	51,51,51,51	0
56	OHX	AA	3510	7/7	0.96	0.13	98,106,123,159	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	DA	3426	7/7	0.96	0.08	118,125,141,168	1
56	OHX	DA	3443	7/7	0.96	0.17	113,124,137,188	1
56	OHX	DA	3365	7/7	0.96	0.12	100,119,136,159	2
56	OHX	DA	3439	7/7	0.96	0.12	127,146,152,174	1
56	OHX	BA	1759	7/7	0.96	0.08	173,177,187,214	1
56	OHX	BA	1732	7/7	0.96	0.11	128,131,145,175	2
56	OHX	CA	1771	7/7	0.96	0.12	105,107,134,145	1
55	MG	DA	3241	1/1	0.96	0.17	47,47,47,47	0
55	MG	DA	3120	1/1	0.96	0.32	52,52,52,52	0
56	OHX	AA	3441	7/7	0.96	0.14	113,135,152,175	1
55	MG	DA	3269	1/1	0.96	0.42	52,52,52,52	0
56	OHX	BA	1806	7/7	0.96	0.16	110,117,124,159	1
56	OHX	AA	3542	7/7	0.96	0.17	92,98,124,157	1
55	MG	AA	3145	1/1	0.96	0.33	27,27,27,27	0
55	MG	DE	301	1/1	0.96	0.38	52,52,52,52	0
56	OHX	DA	3410	7/7	0.96	0.13	107,112,124,146	1
55	MG	DA	3135	1/1	0.96	0.35	42,42,42,42	0
55	MG	CA	1658	1/1	0.96	0.34	65,65,65,65	0
55	MG	AA	3296	1/1	0.96	0.40	69,69,69,69	0
55	MG	BA	1651	1/1	0.96	0.49	76,76,76,76	0
56	OHX	CA	1762	7/7	0.96	0.08	148,151,154,182	1
56	OHX	AA	3460	7/7	0.96	0.13	131,133,148,193	1
56	OHX	BA	1809	7/7	0.96	0.09	159,162,164,206	1
55	MG	AA	3047	1/1	0.96	0.28	65,65,65,65	0
56	OHX	DA	3099	7/7	0.96	0.27	104,109,114,163	1
56	OHX	BC	107	7/7	0.96	0.14	126,137,143,151	1
55	MG	AA	3250	1/1	0.96	0.36	55,55,55,55	0
55	MG	AA	3339	1/1	0.96	0.52	58,58,58,58	0
56	OHX	CA	1741	7/7	0.96	0.13	101,122,129,156	2
56	OHX	BA	1800	7/7	0.96	0.08	127,133,145,177	1
55	MG	AA	3016	1/1	0.96	0.38	29,29,29,29	0
55	MG	AA	3045	1/1	0.96	0.19	33,33,33,33	0
56	OHX	DA	3367	7/7	0.96	0.21	100,113,133,149	1
57	PAR	BA	1715	42/42	0.96	0.18	61,73,83,89	0
55	MG	AA	3227	1/1	0.96	0.40	61,61,61,61	0
56	OHX	DA	3399	7/7	0.96	0.22	104,107,123,144	2
56	OHX	AA	3386	7/7	0.96	0.17	75,83,104,131	1
55	MG	AA	3232	1/1	0.96	0.10	62,62,62,62	0
56	OHX	DA	3396	7/7	0.96	0.19	96,99,105,140	1
56	OHX	DA	3094	7/7	0.96	0.18	110,121,124,149	1
56	OHX	AA	3479	7/7	0.96	0.17	94,103,125,176	3
56	OHX	AA	3381	7/7	0.96	0.11	127,136,147,180	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	3002	1/1	0.96	0.41	34,34,34,34	0
56	OHX	AA	3565	7/7	0.96	0.12	97,104,114,159	1
55	MG	BA	1673	1/1	0.96	0.42	75,75,75,75	0
56	OHX	AA	3486	7/7	0.96	0.14	95,110,127,153	1
55	MG	AA	3021	1/1	0.96	0.34	35,35,35,35	0
58	ZN	BG	301	1/1	0.96	0.30	84,84,84,84	0
55	MG	CA	1611	1/1	0.96	0.20	81,81,81,81	0
55	MG	AA	3246	1/1	0.96	0.28	44,44,44,44	0
55	MG	DA	3222	1/1	0.96	0.34	83,83,83,83	0
55	MG	AA	3036	1/1	0.96	0.44	48,48,48,48	0
56	OHX	AA	3558	7/7	0.96	0.15	92,100,110,168	1
56	OHX	DA	3441	7/7	0.96	0.10	114,122,135,176	1
55	MG	CA	1616	1/1	0.96	0.41	100,100,100,100	0
56	OHX	DA	3162	7/7	0.96	0.14	128,132,141,207	0
55	MG	AA	3158	1/1	0.96	0.45	49,49,49,49	0
56	OHX	BA	1758	7/7	0.96	0.07	153,155,160,202	1
55	MG	AA	3196	1/1	0.96	0.34	43,43,43,43	0
56	OHX	AA	3483	7/7	0.96	0.17	106,109,118,158	2
55	MG	DA	3261	1/1	0.96	0.38	53,53,53,53	0
56	OHX	CA	1764	7/7	0.96	0.16	113,122,135,168	1
56	OHX	AA	3545	7/7	0.96	0.12	92,105,127,145	2
56	OHX	AA	3467	7/7	0.96	0.12	72,88,95,139	1
56	OHX	DA	3436	7/7	0.96	0.12	121,133,143,171	1
55	MG	DA	3148	1/1	0.96	0.45	50,50,50,50	0
55	MG	AA	3302	1/1	0.96	0.41	72,72,72,72	0
55	MG	DA	3080	1/1	0.96	0.34	43,43,43,43	0
55	MG	DA	3051	1/1	0.96	0.51	39,39,39,39	0
56	OHX	BA	1753	7/7	0.96	0.13	103,110,125,169	1
56	OHX	AA	3525	7/7	0.96	0.10	118,124,140,179	1
55	MG	CN	201	1/1	0.96	0.12	79,79,79,79	0
55	MG	AA	3144	1/1	0.96	0.34	43,43,43,43	0
55	MG	DA	3005	1/1	0.96	0.28	41,41,41,41	0
55	MG	DA	3009	1/1	0.96	0.31	50,50,50,50	0
56	OHX	DA	3408	7/7	0.96	0.14	122,131,146,182	1
56	OHX	AA	3437	7/7	0.96	0.19	76,82,94,136	1
55	MG	AA	3208	1/1	0.96	0.37	62,62,62,62	0
55	MG	AA	3112	1/1	0.96	0.15	87,87,87,87	0
56	OHX	CA	1814	7/7	0.96	0.06	149,152,161,212	1
55	MG	AA	3095	1/1	0.96	0.40	42,42,42,42	0
56	OHX	AA	3398	7/7	0.96	0.15	90,95,125,158	1
56	OHX	CA	1750	7/7	0.96	0.16	110,113,130,151	1
55	MG	DA	3207	1/1	0.97	0.34	37,37,37,37	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	3153	1/1	0.97	0.44	40,40,40,40	0
56	OHX	AA	3562	7/7	0.97	0.14	100,110,119,157	1
55	MG	AA	3123	1/1	0.97	0.18	65,65,65,65	0
55	MG	DA	3182	1/1	0.97	0.26	52,52,52,52	0
56	OHX	DA	3359	7/7	0.97	0.17	99,118,131,143	1
55	MG	DA	3130	1/1	0.97	0.21	48,48,48,48	0
55	MG	AA	3006	1/1	0.97	0.38	40,40,40,40	0
56	OHX	CA	1738	7/7	0.97	0.10	120,123,126,168	1
55	MG	CA	1663	1/1	0.97	0.14	65,65,65,65	0
56	OHX	CA	1760	7/7	0.97	0.08	145,148,151,188	1
55	MG	DA	3167	1/1	0.97	0.28	61,61,61,61	0
56	OHX	BA	1784	7/7	0.97	0.14	94,101,111,137	1
56	OHX	DA	3170	7/7	0.97	0.15	114,125,135,172	1
56	OHX	CA	1728	7/7	0.97	0.15	104,119,138,150	2
55	MG	DA	3089	1/1	0.97	0.45	54,54,54,54	0
55	MG	AA	3253	1/1	0.97	0.38	49,49,49,49	0
56	OHX	AA	3377	7/7	0.97	0.21	77,87,106,151	2
56	OHX	AA	3365	7/7	0.97	0.12	86,102,111,118	3
55	MG	AA	3214	1/1	0.97	0.38	41,41,41,41	0
56	OHX	CA	1796	7/7	0.97	0.09	150,159,170,195	1
55	MG	DA	3316	1/1	0.97	0.25	51,51,51,51	0
56	OHX	BA	1789	7/7	0.97	0.06	132,137,146,191	1
55	MG	CA	1697	1/1	0.97	0.17	66,66,66,66	0
55	MG	DA	3004	1/1	0.97	0.23	32,32,32,32	0
55	MG	AA	3054	1/1	0.97	0.24	83,83,83,83	0
55	MG	BA	1694	1/1	0.97	0.23	60,60,60,60	0
55	MG	AA	3070	1/1	0.97	0.18	56,56,56,56	0
56	OHX	AA	3566	7/7	0.97	0.12	171,177,185,204	1
55	MG	AA	3221	1/1	0.97	0.29	41,41,41,41	0
55	MG	BA	1679	1/1	0.97	0.42	60,60,60,60	0
55	MG	AA	3012	1/1	0.97	0.29	45,45,45,45	0
55	MG	DA	3188	1/1	0.97	0.35	38,38,38,38	0
55	MG	BA	1646	1/1	0.97	0.31	48,48,48,48	0
55	MG	AA	3068	1/1	0.97	0.16	92,92,92,92	0
56	OHX	BA	1762	7/7	0.97	0.14	121,131,144,180	1
56	OHX	AA	3430	7/7	0.97	0.09	119,125,132,176	1
55	MG	CA	1649	1/1	0.97	0.34	92,92,92,92	0
55	MG	CA	1669	1/1	0.97	0.37	48,48,48,48	0
55	MG	AA	3163	1/1	0.97	0.40	34,34,34,34	0
55	MG	DA	3193	1/1	0.97	0.34	43,43,43,43	0
55	MG	DA	3001	1/1	0.97	0.35	39,39,39,39	0
55	MG	AA	3152	1/1	0.97	0.41	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	3150	1/1	0.97	0.23	53,53,53,53	0
55	MG	AA	3258	1/1	0.97	0.31	39,39,39,39	0
56	OHX	AA	3438	7/7	0.97	0.10	113,130,139,188	1
56	OHX	BA	1724	7/7	0.97	0.10	114,121,136,156	0
55	MG	AA	3063	1/1	0.97	0.35	45,45,45,45	0
55	MG	DA	3143	1/1	0.97	0.31	38,38,38,38	0
55	MG	BA	1641	1/1	0.97	0.32	54,54,54,54	0
55	MG	AA	3280	1/1	0.97	0.40	61,61,61,61	0
56	OHX	DA	3406	7/7	0.97	0.13	88,107,111,147	3
56	OHX	AA	3429	7/7	0.97	0.14	84,97,102,156	1
55	MG	AA	3218	1/1	0.97	0.31	35,35,35,35	0
55	MG	DA	3161	1/1	0.97	0.37	41,41,41,41	0
56	OHX	DA	3379	7/7	0.97	0.13	116,134,147,164	1
55	MG	AA	3248	1/1	0.97	0.30	28,28,28,28	0
55	MG	CA	1634	1/1	0.97	0.60	64,64,64,64	0
55	MG	DA	3141	1/1	0.97	0.29	64,64,64,64	0
56	OHX	BA	1801	7/7	0.97	0.11	129,138,143,174	1
56	OHX	CA	1744	7/7	0.97	0.10	128,134,150,164	1
55	MG	AA	3166	1/1	0.97	0.35	41,41,41,41	0
55	MG	CA	1612	1/1	0.97	0.26	95,95,95,95	0
56	OHX	DA	3471	7/7	0.97	0.10	112,124,129,160	1
55	MG	DA	3190	1/1	0.97	0.62	44,44,44,44	0
55	MG	CA	1664	1/1	0.97	0.17	57,57,57,57	0
56	OHX	CA	1743	7/7	0.97	0.10	101,120,132,162	1
55	MG	DA	3010	1/1	0.97	0.36	47,47,47,47	0
55	MG	AA	3186	1/1	0.97	0.17	57,57,57,57	0
56	OHX	AA	3409	7/7	0.97	0.15	99,110,115,152	1
56	OHX	DA	3451	7/7	0.97	0.11	103,107,114,153	1
56	OHX	BA	1767	7/7	0.97	0.09	151,158,165,212	1
55	MG	AA	3015	1/1	0.97	0.30	44,44,44,44	0
55	MG	AA	3027	1/1	0.97	0.28	35,35,35,35	0
56	OHX	AA	3466	7/7	0.97	0.13	98,120,132,157	1
56	OHX	DA	3355	7/7	0.97	0.13	109,111,119,148	2
55	MG	DA	3280	1/1	0.97	0.46	63,63,63,63	0
55	MG	AA	3216	1/1	0.97	0.48	33,33,33,33	0
56	OHX	DA	3366	7/7	0.97	0.16	87,100,130,154	2
56	OHX	DA	3375	7/7	0.97	0.11	129,138,149,173	1
55	MG	AA	3315	1/1	0.97	0.17	50,50,50,50	0
56	OHX	BA	1760	7/7	0.97	0.13	109,109,121,147	1
55	MG	AA	3213	1/1	0.97	0.22	60,60,60,60	0
55	MG	DA	3070	1/1	0.97	0.19	69,69,69,69	0
56	OHX	AA	3446	7/7	0.97	0.16	148,150,154,190	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	DA	3373	7/7	0.97	0.23	93,104,119,171	1
56	OHX	BA	1741	7/7	0.97	0.13	95,110,126,148	1
55	MG	DA	3008	1/1	0.97	0.22	43,43,43,43	0
56	OHX	CA	1766	7/7	0.97	0.08	116,126,135,171	1
55	MG	BA	1656	1/1	0.97	0.40	73,73,73,73	0
56	OHX	CA	1736	7/7	0.97	0.10	163,166,178,209	0
55	MG	AA	3044	1/1	0.97	0.47	42,42,42,42	0
56	OHX	AA	3388	7/7	0.97	0.12	106,112,125,156	1
56	OHX	CA	1742	7/7	0.97	0.11	153,166,169,174	1
56	OHX	CA	1733	7/7	0.97	0.14	109,120,127,147	1
56	OHX	DA	3257	7/7	0.97	0.19	107,112,124,148	1
56	OHX	DA	3254	7/7	0.97	0.27	126,129,138,165	1
55	MG	AA	3014	1/1	0.97	0.36	33,33,33,33	0
56	OHX	BA	1746	7/7	0.97	0.13	95,103,110,146	1
55	MG	BA	1652	1/1	0.97	0.41	68,68,68,68	0
55	MG	DA	3192	1/1	0.97	0.52	60,60,60,60	0
56	OHX	DA	3412	7/7	0.97	0.12	93,110,113,161	1
56	OHX	DO	201	7/7	0.97	0.15	112,117,125,146	1
56	OHX	DA	3083	7/7	0.97	0.13	104,111,120,146	1
55	MG	DA	3293	1/1	0.97	0.48	88,88,88,88	0
56	OHX	AA	3399	7/7	0.97	0.17	97,111,117,147	1
56	OHX	BG	302	7/7	0.97	0.09	138,141,145,177	1
56	OHX	DA	3403	7/7	0.97	0.13	99,105,122,140	1
56	OHX	DA	3132	7/7	0.97	0.10	185,187,192,225	1
55	MG	D5	101	1/1	0.97	0.25	43,43,43,43	0
56	OHX	AA	3412	7/7	0.97	0.10	119,122,141,174	1
55	MG	AA	3025	1/1	0.97	0.36	37,37,37,37	0
56	OHX	CA	1735	7/7	0.97	0.10	146,153,168,212	0
56	OHX	BA	1755	7/7	0.97	0.09	123,128,136,161	1
55	MG	DA	3012	1/1	0.97	0.31	44,44,44,44	0
56	OHX	DA	3393	7/7	0.97	0.11	133,134,150,191	1
55	MG	AA	3097	1/1	0.97	0.24	50,50,50,50	0
56	OHX	AA	3450	7/7	0.97	0.12	97,112,128,161	2
56	OHX	AO	202	7/7	0.97	0.11	93,104,115,140	1
56	OHX	DA	3404	7/7	0.97	0.12	107,121,131,166	1
55	MG	AA	3136	1/1	0.97	0.20	42,42,42,42	0
55	MG	AA	3077	1/1	0.97	0.42	39,39,39,39	0
56	OHX	DA	3402	7/7	0.97	0.10	122,136,148,204	1
55	MG	DA	3018	1/1	0.97	0.31	47,47,47,47	0
55	MG	AA	3241	1/1	0.97	0.34	52,52,52,52	0
55	MG	AA	3265	1/1	0.97	0.25	62,62,62,62	0
56	OHX	CA	1739	7/7	0.97	0.10	140,150,165,188	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	BA	1736	7/7	0.97	0.12	112,121,128,152	1
56	OHX	DA	3383	7/7	0.97	0.13	110,119,138,151	2
56	OHX	CA	1768	7/7	0.97	0.09	123,135,145,174	1
56	OHX	CA	1734	7/7	0.97	0.10	145,147,151,167	1
55	MG	AA	3026	1/1	0.97	0.30	43,43,43,43	0
56	OHX	AA	3428	7/7	0.97	0.08	114,120,124,169	1
56	OHX	BA	1734	7/7	0.97	0.16	92,99,114,146	1
55	MG	CA	1711	1/1	0.97	0.39	57,57,57,57	0
55	MG	AA	3179	1/1	0.97	0.33	39,39,39,39	0
55	MG	BA	1659	1/1	0.97	0.51	43,43,43,43	0
55	MG	DA	3236	1/1	0.97	0.49	62,62,62,62	0
55	MG	BA	1626	1/1	0.97	0.54	47,47,47,47	0
56	OHX	BA	1805	7/7	0.97	0.19	98,103,107,150	1
55	MG	AA	3271	1/1	0.97	0.45	63,63,63,63	0
55	MG	AA	3146	1/1	0.97	0.38	36,36,36,36	0
55	MG	AA	3098	1/1	0.97	0.31	29,29,29,29	0
55	MG	DA	3041	1/1	0.97	0.36	79,79,79,79	0
56	OHX	AA	3556	7/7	0.97	0.16	82,96,111,154	1
55	MG	AA	3256	1/1	0.97	0.43	52,52,52,52	0
55	MG	BA	1698	1/1	0.98	0.42	54,54,54,54	0
56	OHX	DA	3356	7/7	0.98	0.14	85,97,114,129	2
56	OHX	BA	1727	7/7	0.98	0.12	116,137,148,161	1
56	OHX	AA	3453	7/7	0.98	0.13	72,88,95,134	2
55	MG	A0	201	1/1	0.98	0.15	52,52,52,52	0
56	OHX	BA	1733	7/7	0.98	0.09	98,108,118,146	1
56	OHX	AA	3422	7/7	0.98	0.18	63,104,126,147	2
56	OHX	AA	3370	7/7	0.98	0.17	74,85,99,119	1
55	MG	AA	3288	1/1	0.98	0.31	55,55,55,55	0
56	OHX	AA	3385	7/7	0.98	0.17	73,87,109,139	2
55	MG	AA	3018	1/1	0.98	0.28	49,49,49,49	0
56	OHX	CA	1740	7/7	0.98	0.09	125,134,139,166	1
55	MG	AA	3129	1/1	0.98	0.22	43,43,43,43	0
56	OHX	DA	3068	7/7	0.98	0.12	102,127,131,147	0
56	OHX	BA	1768	7/7	0.98	0.15	87,95,105,130	2
56	OHX	BA	1729	7/7	0.98	0.11	110,115,135,137	1
55	MG	DA	3119	1/1	0.98	0.34	38,38,38,38	0
56	OHX	AA	3361	7/7	0.98	0.12	76,81,111,125	3
55	MG	DA	3197	1/1	0.98	0.28	49,49,49,49	0
56	OHX	DA	3084	7/7	0.98	0.14	132,139,149,176	1
56	OHX	AA	3458	7/7	0.98	0.18	96,103,139,158	1
55	MG	DA	3078	1/1	0.98	0.45	42,42,42,42	0
56	OHX	DA	3387	7/7	0.98	0.09	108,115,125,151	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	3223	1/1	0.98	0.30	43,43,43,43	0
56	OHX	AA	3461	7/7	0.98	0.12	102,110,120,148	1
56	OHX	CA	1748	7/7	0.98	0.08	137,145,152,186	1
56	OHX	AA	3369	7/7	0.98	0.11	76,100,116,143	1
56	OHX	BA	1720	7/7	0.98	0.13	95,108,133,161	2
56	OHX	DA	3364	7/7	0.98	0.17	75,93,104,118	1
55	MG	DA	3146	1/1	0.98	0.26	33,33,33,33	0
56	OHX	AA	3360	7/7	0.98	0.14	88,94,111,129	2
55	MG	AA	3017	1/1	0.98	0.39	26,26,26,26	0
56	OHX	BA	1730	7/7	0.98	0.12	106,118,135,150	1
55	MG	AA	3242	1/1	0.98	0.38	43,43,43,43	0
56	OHX	AA	3452	7/7	0.98	0.10	92,103,111,136	1
56	OHX	BA	1728	7/7	0.98	0.08	140,147,157,166	1
55	MG	DA	3175	1/1	0.98	0.44	53,53,53,53	0
56	OHX	AA	3424	7/7	0.98	0.15	84,93,116,147	1
55	MG	AA	3191	1/1	0.98	0.14	39,39,39,39	0
56	OHX	AA	3401	7/7	0.98	0.12	101,105,125,153	1
55	MG	AA	3010	1/1	0.98	0.25	39,39,39,39	0
56	OHX	DA	3363	7/7	0.98	0.12	95,105,122,123	2
55	MG	AA	3201	1/1	0.98	0.43	35,35,35,35	0
55	MG	AA	3139	1/1	0.98	0.24	47,47,47,47	0
56	OHX	CC	110	7/7	0.98	0.16	103,121,132,150	4
55	MG	DA	3026	1/1	0.98	0.28	55,55,55,55	0
55	MG	CA	1635	1/1	0.98	0.34	51,51,51,51	0
56	OHX	DA	3157	7/7	0.98	0.16	76,87,96,121	1
55	MG	DA	3015	1/1	0.98	0.28	56,56,56,56	0
55	MG	DA	3095	1/1	0.98	0.22	58,58,58,58	0
56	OHX	BA	1735	7/7	0.98	0.12	120,129,137,168	1
56	OHX	AA	3378	7/7	0.98	0.14	77,88,108,118	1
56	OHX	AA	3533	7/7	0.98	0.10	79,94,100,134	1
55	MG	DA	3007	1/1	0.98	0.29	43,43,43,43	0
56	OHX	AA	3353	7/7	0.98	0.20	71,99,117,132	1
56	OHX	BA	1723	7/7	0.98	0.17	93,106,124,143	1
56	OHX	DA	3073	7/7	0.98	0.19	89,101,109,132	1
55	MG	DA	3198	1/1	0.98	0.40	44,44,44,44	0
56	OHX	DA	3082	7/7	0.98	0.14	92,102,108,132	1
56	OHX	CA	1732	7/7	0.98	0.13	112,117,126,152	1
56	OHX	AA	3390	7/7	0.98	0.18	48,74,93,125	2
56	OHX	DA	3064	7/7	0.98	0.15	87,100,123,131	3
56	OHX	DA	3354	7/7	0.98	0.15	88,99,121,135	1
56	OHX	DA	3065	7/7	0.98	0.17	55,92,111,137	1
56	OHX	CA	1737	7/7	0.98	0.09	103,118,125,148	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	1729	7/7	0.98	0.15	104,115,126,154	1
56	OHX	AA	3391	7/7	0.98	0.16	69,80,102,109	3
55	MG	DA	3231	1/1	0.98	0.41	50,50,50,50	0
55	MG	DA	3138	1/1	0.98	0.37	43,43,43,43	0
56	OHX	AA	3400	7/7	0.98	0.15	64,77,80,123	1
56	OHX	DA	3420	7/7	0.98	0.10	116,120,125,152	1
56	OHX	AA	3468	7/7	0.98	0.09	110,120,137,165	1
55	MG	DA	3034	1/1	0.98	0.15	69,69,69,69	0
55	MG	AA	3007	1/1	0.98	0.40	43,43,43,43	0
56	OHX	DA	3395	7/7	0.98	0.13	102,109,124,139	1
56	OHX	AA	3375	7/7	0.98	0.12	83,101,103,143	1
55	MG	AA	3187	1/1	0.98	0.26	40,40,40,40	0
55	MG	AA	3190	1/1	0.98	0.23	43,43,43,43	0
55	MG	BA	1604	1/1	0.98	0.20	69,69,69,69	0
56	OHX	DA	3369	7/7	0.98	0.15	89,100,105,125	1
56	OHX	AA	3387	7/7	0.98	0.11	110,123,134,164	1
55	MG	DA	3074	1/1	0.98	0.47	40,40,40,40	0
55	MG	AA	3184	1/1	0.98	0.38	35,35,35,35	0
56	OHX	AA	3366	7/7	0.98	0.17	79,94,104,141	1
55	MG	AA	3272	1/1	0.98	0.42	29,29,29,29	0
55	MG	AA	3134	1/1	0.98	0.44	48,48,48,48	0
56	OHX	AA	3354	7/7	0.98	0.14	96,105,128,164	0
56	OHX	DA	3381	7/7	0.98	0.13	111,118,134,167	1
56	OHX	AA	3380	7/7	0.98	0.15	86,90,110,143	1
56	OHX	DA	3397	7/7	0.98	0.09	104,119,125,149	1
56	OHX	DA	3382	7/7	0.98	0.17	67,85,95,136	2
56	OHX	DA	3246	7/7	0.98	0.14	89,97,107,138	1
56	OHX	AA	3469	7/7	0.98	0.09	103,113,128,153	1
55	MG	AA	3037	1/1	0.98	0.29	55,55,55,55	0
55	MG	AA	3197	1/1	0.98	0.25	57,57,57,57	0
56	OHX	AA	3487	7/7	0.98	0.13	73,82,95,140	2
56	OHX	AA	3427	7/7	0.98	0.12	131,132,136,155	1
56	OHX	DA	3422	7/7	0.98	0.14	92,100,111,154	1
56	OHX	AA	3471	7/7	0.98	0.14	80,105,117,155	1
56	OHX	DA	3429	7/7	0.98	0.09	118,130,143,180	1
56	OHX	DA	3389	7/7	0.98	0.12	82,85,99,113	1
56	OHX	AA	3410	7/7	0.98	0.14	91,99,106,125	1
56	OHX	DA	3348	7/7	0.98	0.13	97,115,128,140	1
56	OHX	DA	3377	7/7	0.98	0.16	91,105,111,146	2
55	MG	DA	3234	1/1	0.98	0.32	41,41,41,41	0
56	OHX	AA	3373	7/7	0.98	0.11	84,96,108,141	1
56	OHX	AA	3518	7/7	0.98	0.10	106,114,121,148	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	3046	1/1	0.98	0.32	50,50,50,50	0
55	MG	AE	303	1/1	0.98	0.24	36,36,36,36	0
55	MG	CA	1633	1/1	0.98	0.53	46,46,46,46	0
55	MG	CC	101	1/1	0.98	0.47	79,79,79,79	0
56	OHX	AA	3364	7/7	0.98	0.15	72,81,97,125	1
56	OHX	BA	1770	7/7	0.98	0.11	114,115,121,163	1
56	OHX	AA	3477	7/7	0.98	0.14	81,92,107,133	2
55	MG	DA	3036	1/1	0.98	0.14	47,47,47,47	0
56	OHX	DA	3384	7/7	0.98	0.13	89,92,105,143	2
56	OHX	AA	3397	7/7	0.98	0.12	96,102,109,143	1
56	OHX	AA	3383	7/7	0.98	0.13	91,96,109,133	1
56	OHX	DA	3358	7/7	0.98	0.11	107,117,135,165	2
56	OHX	AA	3493	7/7	0.98	0.10	102,115,123,140	1
55	MG	DA	3164	1/1	0.98	0.40	63,63,63,63	0
56	OHX	DA	3136	7/7	0.98	0.15	95,108,117,144	1
56	OHX	CA	1746	7/7	0.98	0.09	112,115,128,150	1
55	MG	DA	3085	1/1	0.98	0.41	53,53,53,53	0
56	OHX	AA	3406	7/7	0.98	0.11	93,96,102,133	1
55	MG	AA	3207	1/1	0.98	0.50	44,44,44,44	0
56	OHX	BA	1739	7/7	0.98	0.12	109,119,131,155	1
55	MG	AA	3202	1/1	0.98	0.20	30,30,30,30	0
56	OHX	AA	3414	7/7	0.98	0.15	92,104,120,143	1
55	MG	AA	3009	1/1	0.98	0.24	29,29,29,29	0
56	OHX	DA	3368	7/7	0.98	0.11	86,101,103,132	2
55	MG	DA	3290	1/1	0.98	0.16	37,37,37,37	0
56	OHX	DA	3370	7/7	0.98	0.14	94,102,123,149	1
56	OHX	CC	109	7/7	0.98	0.20	112,114,129,153	3
56	OHX	DA	3418	7/7	0.98	0.11	87,98,117,139	3
56	OHX	AA	3432	7/7	0.98	0.10	129,136,142,160	1
56	OHX	CA	1779	7/7	0.98	0.05	125,132,137,172	1
55	MG	DA	3150	1/1	0.98	0.17	46,46,46,46	0
56	OHX	AA	3431	7/7	0.98	0.13	101,115,120,168	1
56	OHX	DA	3417	7/7	0.98	0.09	145,152,156,188	1
55	MG	AA	3040	1/1	0.98	0.29	59,59,59,59	0
55	MG	DA	3123	1/1	0.98	0.29	38,38,38,38	0
55	MG	DA	3052	1/1	0.98	0.47	42,42,42,42	0
55	MG	CA	1636	1/1	0.98	0.19	82,82,82,82	0
55	MG	AA	3106	1/1	0.98	0.24	72,72,72,72	0
55	MG	BA	1603	1/1	0.98	0.19	40,40,40,40	0
56	OHX	DA	3419	7/7	0.98	0.13	82,93,100,126	2
56	OHX	AA	3346	7/7	0.98	0.17	73,81,101,124	2
55	MG	DA	3232	1/1	0.98	0.62	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	DA	3144	1/1	0.98	0.56	44,44,44,44	0
55	MG	AA	3019	1/1	0.98	0.30	42,42,42,42	0
56	OHX	DA	3071	7/7	0.98	0.14	107,121,146,184	0
55	MG	DA	3227	1/1	0.98	0.31	44,44,44,44	0
56	OHX	AA	3355	7/7	0.98	0.15	88,95,127,131	3
56	OHX	AA	3351	7/7	0.98	0.14	60,68,78,99	3
55	MG	AA	3164	1/1	0.98	0.30	45,45,45,45	0
56	OHX	DA	3062	7/7	0.98	0.18	70,95,103,114	1
55	MG	DA	3002	1/1	0.99	0.47	46,46,46,46	0
56	OHX	DA	3249	7/7	0.99	0.13	93,103,118,149	1
55	MG	AA	3175	1/1	0.99	0.24	46,46,46,46	0
56	OHX	AA	3332	7/7	0.99	0.16	40,73,95,99	2
56	OHX	DA	3342	7/7	0.99	0.15	79,85,102,102	2
55	MG	AA	3051	1/1	0.99	0.37	69,69,69,69	0
56	OHX	AA	3329	7/7	0.99	0.15	73,97,104,113	0
56	OHX	AA	3342	7/7	0.99	0.13	65,86,103,114	1
56	OHX	DA	3360	7/7	0.99	0.13	72,81,91,113	1
56	OHX	DA	3374	7/7	0.99	0.09	127,131,139,156	1
56	OHX	DA	3386	7/7	0.99	0.11	108,110,132,139	1
56	OHX	DA	3345	7/7	0.99	0.14	89,96,107,130	0
56	OHX	AE	304	7/7	0.99	0.11	73,87,113,116	2
56	OHX	DA	3134	7/7	0.99	0.13	114,120,126,150	1
56	OHX	DA	3343	7/7	0.99	0.15	93,113,122,129	0
56	OHX	AF	303	7/7	0.99	0.21	46,54,72,103	0
56	OHX	DB	208	7/7	0.99	0.10	120,124,144,144	2
56	OHX	BA	1722	7/7	0.99	0.08	114,116,123,159	0
56	OHX	AA	3407	7/7	0.99	0.16	53,82,90,103	2
56	OHX	AA	3348	7/7	0.99	0.15	75,81,98,100	3
56	OHX	BA	1726	7/7	0.99	0.09	134,139,145,195	0
56	OHX	DA	3338	7/7	0.99	0.17	72,79,93,112	0
55	MG	DA	3003	1/1	0.99	0.29	43,43,43,43	0
56	OHX	AA	3359	7/7	0.99	0.12	91,110,118,137	1
56	OHX	AA	3368	7/7	0.99	0.09	104,115,121,140	1
56	OHX	DA	3335	7/7	0.99	0.17	87,96,112,126	0
55	MG	AA	3008	1/1	0.99	0.41	32,32,32,32	0
56	OHX	DA	3351	7/7	0.99	0.13	87,96,108,109	1
56	OHX	BA	1740	7/7	0.99	0.13	107,110,122,131	1
56	OHX	AA	3335	7/7	0.99	0.24	62,76,78,127	0
56	OHX	AA	3490	7/7	0.99	0.11	85,93,105,125	1
56	OHX	CA	1727	7/7	0.99	0.09	114,118,131,143	0
58	ZN	BQ	101	1/1	0.99	0.07	135,135,135,135	0
55	MG	DA	3019	1/1	0.99	0.24	41,41,41,41	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	3350	7/7	0.99	0.14	90,99,110,132	1
56	OHX	DA	3160	7/7	0.99	0.18	79,114,122,124	0
55	MG	AA	3185	1/1	0.99	0.41	35,35,35,35	0
56	OHX	AA	3415	7/7	0.99	0.08	90,93,100,146	1
56	OHX	DA	3357	7/7	0.99	0.12	100,118,130,150	1
56	OHX	AA	3376	7/7	0.99	0.11	96,107,117,142	1
55	MG	CA	1632	1/1	0.99	0.50	56,56,56,56	0
56	OHX	AA	3363	7/7	0.99	0.13	89,101,119,137	1
55	MG	DA	3013	1/1	0.99	0.42	40,40,40,40	0
56	OHX	AA	3341	7/7	0.99	0.19	77,80,88,124	1
56	OHX	CA	1791	7/7	0.99	0.11	100,118,129,154	1
55	MG	AA	3035	1/1	0.99	0.18	38,38,38,38	0
58	ZN	CQ	101	1/1	0.99	0.12	120,120,120,120	0
55	MG	AA	3121	1/1	0.99	0.35	65,65,65,65	0
56	OHX	DA	3340	7/7	0.99	0.14	86,102,124,126	1
56	OHX	AA	3402	7/7	0.99	0.13	73,86,98,123	1
56	OHX	CA	1723	7/7	0.99	0.20	84,100,111,141	0
56	OHX	BA	1717	7/7	0.99	0.17	81,90,105,119	0
56	OHX	AA	3396	7/7	0.99	0.10	93,107,119,142	1
56	OHX	AA	3327	7/7	0.99	0.21	38,70,106,113	0
56	OHX	AA	3403	7/7	0.99	0.18	59,89,94,139	1
56	OHX	DA	3378	7/7	0.99	0.09	153,156,169,185	0
56	OHX	DA	3347	7/7	0.99	0.12	89,99,108,134	0
56	OHX	DA	3075	7/7	0.99	0.16	89,91,114,123	1
56	OHX	AA	3350	7/7	0.99	0.13	95,103,113,148	1
58	ZN	CG	301	1/1	0.99	0.27	116,116,116,116	0
56	OHX	AA	3336	7/7	0.99	0.20	67,91,105,145	0
56	OHX	CA	1730	7/7	0.99	0.12	132,134,143,167	0
56	OHX	AA	3345	7/7	0.99	0.09	87,112,122,135	0
55	MG	AA	3013	1/1	0.99	0.37	27,27,27,27	0
55	MG	AA	3212	1/1	0.99	0.41	33,33,33,33	0
56	OHX	DA	3380	7/7	0.99	0.09	108,123,139,150	1
56	OHX	CA	1726	7/7	0.99	0.15	89,98,100,124	1
55	MG	AE	301	1/1	0.99	0.35	51,51,51,51	0
55	MG	AA	3192	1/1	0.99	0.38	34,34,34,34	0
56	OHX	AA	3344	7/7	0.99	0.12	86,92,112,118	1
56	OHX	AA	3330	7/7	0.99	0.18	81,85,101,147	0
56	OHX	BA	1718	7/7	0.99	0.21	68,82,103,130	2
56	OHX	CA	1724	7/7	0.99	0.12	88,111,121,131	0
56	OHX	DA	3401	7/7	0.99	0.12	108,115,120,150	1
56	OHX	DA	3353	7/7	0.99	0.14	102,117,129,132	1
56	OHX	AA	3418	7/7	0.99	0.17	96,110,119,135	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	3180	1/1	0.99	0.47	42,42,42,42	0
56	OHX	AA	3389	7/7	0.99	0.18	80,93,103,143	0
55	MG	AA	3024	1/1	0.99	0.42	45,45,45,45	0
56	OHX	AA	3331	7/7	0.99	0.16	93,94,108,145	0
56	OHX	BA	1721	7/7	0.99	0.10	109,115,141,157	1
56	OHX	DF	301	7/7	0.99	0.12	53,80,83,83	1
56	OHX	AA	3349	7/7	0.99	0.10	94,104,124,143	0
56	OHX	AA	3347	7/7	0.99	0.15	74,77,98,102	2
56	OHX	DA	3337	7/7	0.99	0.24	74,80,86,97	1
56	OHX	BA	1814	7/7	0.99	0.11	88,100,109,173	0
55	MG	AA	3030	1/1	0.99	0.38	36,36,36,36	0
55	MG	BA	1633	1/1	0.99	0.33	77,77,77,77	0
56	OHX	DA	3371	7/7	0.99	0.11	119,121,131,160	1
56	OHX	AA	3328	7/7	0.99	0.16	67,76,86,89	1
56	OHX	DA	3341	7/7	0.99	0.17	87,105,126,140	0
56	OHX	DA	3212	7/7	0.99	0.15	64,77,91,94	1
56	OHX	AA	3434	7/7	0.99	0.17	98,102,107,132	1
56	OHX	AA	3411	7/7	0.99	0.08	107,117,135,154	0
56	OHX	AA	3393	7/7	0.99	0.15	50,81,89,115	2
56	OHX	CA	1725	7/7	0.99	0.11	108,111,122,123	1
56	OHX	AA	3326	7/7	0.99	0.17	75,76,87,119	0
55	MG	DA	3268	1/1	0.99	0.35	44,44,44,44	0
56	OHX	AA	3444	7/7	0.99	0.14	79,89,101,122	2
56	OHX	BA	1716	7/7	0.99	0.17	73,86,99,116	0
55	MG	AA	3168	1/1	0.99	0.44	36,36,36,36	0
55	MG	DA	3059	1/1	0.99	0.28	40,40,40,40	0
56	OHX	AA	3352	7/7	0.99	0.17	80,86,96,122	1
56	OHX	DA	3344	7/7	0.99	0.16	93,104,111,114	1
56	OHX	AB	207	7/7	0.99	0.10	89,93,105,113	1
56	OHX	AA	3358	7/7	0.99	0.12	79,81,92,113	1
56	OHX	DA	3349	7/7	0.99	0.13	103,105,113,143	0
56	OHX	DA	3352	7/7	0.99	0.10	105,120,129,149	0
56	OHX	BA	1719	7/7	0.99	0.15	85,102,114,124	1
56	OHX	DA	3361	7/7	0.99	0.15	68,94,122,134	3
56	OHX	DA	3339	7/7	0.99	0.14	91,96,120,132	0
55	MG	AA	3042	1/1	0.99	0.30	42,42,42,42	0
56	OHX	AA	3413	7/7	0.99	0.14	94,104,121,143	1
56	OHX	DA	3336	7/7	0.99	0.18	86,95,105,106	0
56	OHX	AA	3384	7/7	0.99	0.11	96,100,107,136	1
56	OHX	AA	3340	7/7	0.99	0.15	84,93,95,126	0
55	MG	AA	3020	1/1	0.99	0.43	42,42,42,42	0
56	OHX	AA	3338	7/7	0.99	0.14	66,87,106,113	2

*Continued on next page...*

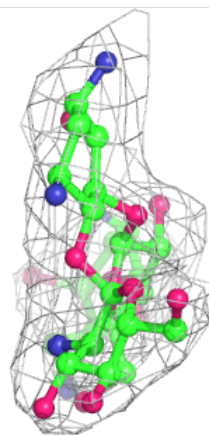
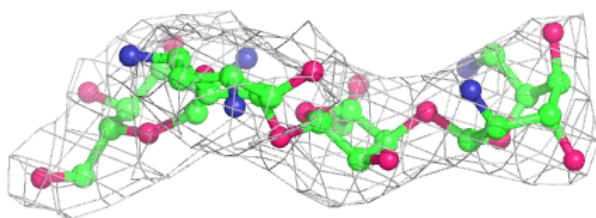
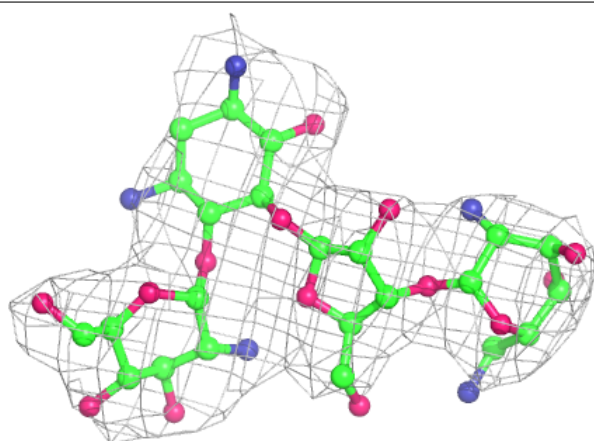
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	OHX	AA	3333	7/7	0.99	0.14	99,103,122,123	0
56	OHX	DA	3061	7/7	1.00	0.13	81,86,92,106	0
56	OHX	AA	3382	7/7	1.00	0.16	65,73,84,93	0
56	OHX	DA	3346	7/7	1.00	0.11	107,113,126,132	0
56	OHX	AA	3379	7/7	1.00	0.23	20,47,62,138	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

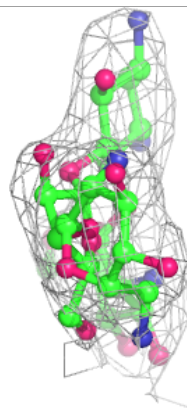
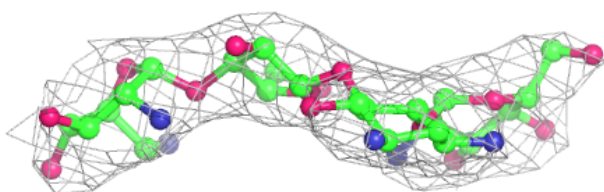
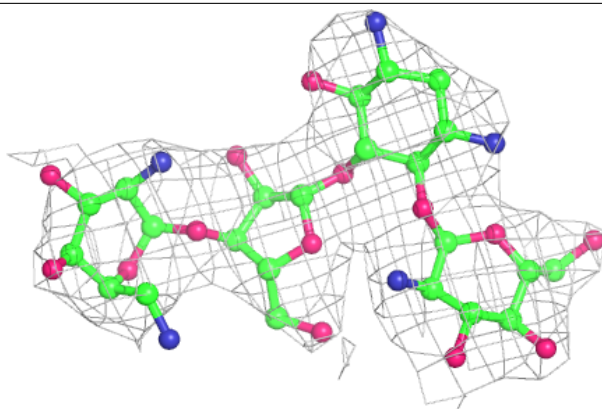
**Electron density around PAR CA 1722:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR BA 1715:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.